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Interim Report on Model Evaluation Methodology and the Evaluation of LEAP

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Engineering Physics Division
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Computer Sciences Division

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Date April 1980

NOTICE This document contains information of a prel m nary nature It is subject to revision or correction and therefore does not represent a f al epo t

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CONTENTS

		Page
Executive Summary		xi
I	Introduction	I-1
II	Approach to Model Evaluation	II-1
III	LEAP and Its Uses	III-1
IV	The Structure of LEAP and Evaluation of Numerical Solution Techniques	IV-1
V	Equations of the Basic Conversion Process	V-1
VI	Economic Evaluation of the Basic Conversion Process (Not included)	VI-1
VII	Verification of the Basic Conversion Process	VII-1
VIII	Sensitivity Analysis by Screening Design	VIII-1
IX	Sensitivity Analysis by Adjoint Methods	IX-1
X	Input Data for Model 22C	X-1
Appendices		
A	ORNL Operating Experience with LEAP	A-1
B	Additional Equations of Basic Conversion Process	B-1

LIST OF TABLES

		Page
III-1	Use of LEAP Subroutines in Model 22C	III-18
III-2	Major Conclusions from LEAP Model 22C Results	III-21
III-3	Important LEAP Responses for Year 2010	III-27
IV-1	Calculate Results[a] Obtained with Model 82	IV-6
IV-2	Best Maximum Error Achieved in Less Than 100 Iterations With Various α Staging Algorithms	IV-17
VII-1	Input Data for the Synthetic Fuel Processes and Oil Refinery Process Necessary for the Basic Conversion Process	VII-5
VII-2	Values for the Aging Multiplier when β_A is varied	VII-13
X-1	Input Data for the Gas Heater in the Residential Sector	X-6
X-2	Input Data for Allocation of the Demand for Space and Water Heat and for Residential End Use Demand	X-7
A-1	DOE/EIA Data Sets Used in the ORNL Model Validation Project	A-2

LIST OF FIGURES

		Page
III-1	Overall network diagram for LEAP Model 22C	III-7
III-2	Network diagram for the residential sector of LEAP Model 22C	III-8
III-3	Network diagram for the industrial sector of LEAP Model 22C	III-9
III-4	Network diagram for the distribution sector of LEAP Model 22C	III-10
III-5	Network diagram for the electricity sector of LEAP Model 22C	III-11
III-6	Network diagrams for the nuclear and imports/exports sectors of LEAP Model 22C	III-12
III-7	Network diagram for the coal sector of LEAP Model 22C	III-13
III-8	Network diagram for the oil/gas sector of LEAP Model 22C	III-14
III-9	Network diagram for the transportation sector of LEAP Model 22C	III-15
III-10	Network diagram for the commercial sector of LEAP Model 22C	III-16
IV-1	Block diagram of Model 82	IV-2
IX-1	Schematic diagram of matrix A and vector ϕ for Model 82 with N = 2	IX-27
IX-2	Schematic diagram of adjoint equations for Model 82 with N = 2 and a particular choice of the response R	IX-30
A-1	ORNL/EIA communication link for model validation program	A-4
A-2	Input deck for batch mode execution of Model 82	A-8
A-3	Sample LEAP commands to change a parameter in Model 82 table 5/3/	A-10

A-4 Model 82 table 5/3/ A-11

A-5 CREST--a code to perturb input parameters to LEAP A-12

A-6 FLOSS--a code used to calculate relative sensitivities A-13

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EXECUTIVE SUMMARY

A Program Objective

This report describes progress made at the Oak Ridge National Laboratory (ORNL) from January through October 1979 toward development and demonstration of a methodology for evaluating energy-economic modeling codes and important results derived from these codes Model projections now or in the near future will never be the sole guide in policy choices however the amount of effort and the quality of scientific talent now dedicated to model development do emphasize the growing role of models in policy analysis Indeed it is the understanding of the limitations and ranges of validity of these computer projections that may ultimately determine their final role The ORNL model evaluation program is attempting to build a "technology" for model evaluation to complement the technology for model construction The basic components of traditional evaluation techniques[1-4] have included review of the model's theoretical basis, data parameters and computational algorithms relative to the intended uses of model results However this entire evaluation sequence has been comprehensively applied in only a few cases

To bolster traditional evaluation methods with more quantitative procedures of interest to the Office of Validation Analysis of the Energy Information Administration (EIA) ORNL is applying sensitivity theory[5-13] as part of a comprehensive effort to quantify the "importance" of various data and model parameters to the key results that are of interest Quantitative estimates for uncertainties associated with some of the primary input variables are also being developed Although sensitivity theory will be used to estimate the propagated effects of uncertainties in data the results of model specification uncertainties (e g , approximation in representation of economic behavior what might have been "left out" of the model) are approached by in-depth evaluation of the model structure itself

In conjunction with EIA's interest in forecasting the long-range impact of new technologies and energy research and development on future energy use the energy-economic modeling code LEAP (Long-Term Energy Analysis Program)[14] was chosen as the initial focus for this research The objectives of this research program are

1 To develop and demonstrate methods (extend and apply traditional procedures) for assessing the scientific basis for the EIA's energy-economy models data and parameters

2 To develop a sensitivity theory for determining the important data used by models in specific applications

3 To quantitatively estimate uncertainties for important data

4 To estimate the confidence limits in the forecasting results and indicate ways in which these limits might be reduced

5 To develop and apply meaningful procedures to improve confidence in forecasts by comparing predictions with observed history

6 To evaluate the range of model applicability by relating the findings in objectives 1 through 5 to the intended model uses

In the following sections our evaluation methodology and the status of the research performed to demonstrate this approach are briefly described In an evaluation of this type it is usually rather easy to find oneself attacking weaknesses and limitations of a given model However it is here recognized that conditions are such that models are often built and used under severe and limiting constraints Our intention is to be honest but constructive, and with the full cognizance of the modeler, to point out those areas requiring improvement

We expect that final reports will discuss all considerations contained in this report, but that those considerations will be discussed more comprehensively

B An Evaluation Procedure

To assure brevity in this summary we have simplified the evaluation procedure described in Section II of this report into four major tasks The approach is described in broad terms and is not intended to be model-specific

1 Describe the Computational Experience

The ORNL evaluation procedure requires "hands-on" experience with the model in question Some of the important elements in this part of the evaluation process are (1) precise specification of the model (what set of computer cards, documentation, etc , are we talking about?), (2) experience acquired in obtaining solutions and in replicating published results (3) determination of whether special purpose models are easily generated (4) reporting of cost computer time and learning investment to use the model effectively and (5) assessment of model transportability

2 Assess the Model Structure and Rationale

This portion of the evaluation has two major components The first is the assessment of the economic foundations of the model The evaluation seeks to specify and verify the model equations, evaluate the basic technological and behavioral assumptions (e g , lags, aggregation), compare results obtained with observed history review performance relative to that of other models and compare and contrast the equations relative

to economic theory The second component deals with the mathematical techniques used Evaluation includes examination of the solution algorithm investigation of convergence and uniqueness properties and assessment of relaxation schemes used to accelerate convergence

3 Develop and Implement a Sensitivity Methodology

The key task in any comprehensive sensitivity analysis is to identify the most important data parameters used to calculate an important result (as determined by the user) of interest Identification here means determination of the sensitivity coefficient $dR/d\xi$, which is the differential rate of change in a result R with respect to a differential change in any parameter of the data base ξ The concept of the importance of such derivatives is not new for example important economic indicators such as supply and price elasticities are themselves sensitivity coefficients Once these derivatives are known for each ξ they can be ranked by absolute magnitude to determine the most important parameters in the problem

4 Assess the Model Input Data

This portion of the evaluation requires review of data definitions (and whether data are "knowable") examination of the nature and structure of the data base review and categorization of data sources (audit trail) and analysis of the quality of selected important data by estimating uncertainties where appropriate

C Computational Experience Preliminary Evaluation for LEAP

Our experience with Model 22C from the reference of a first-time user is described in Appendix A Although several documents[15 16] describing the generic modeling system from which LEAP was developed do exist there remains today no specific document describing the theory embodied in LEAP (itself a modeling system) or Model 22C * the particular specification of LEAP used to determine the results which appear in the 1978 EIA Annual Report to Congress The source program is the only fully reliable guide to detailed model formulation The computer code is not currently transportable To put the model in the public domain the data base management system, which is privately owned needs to be replaced, and core memory requirements (two megabytes for the 1978 Model 22C version) need to be significantly reduced †

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*A draft version of a "LEAP-EMS Users Manual " by Cohen and Pearson is available as well as a draft report by Roger Diedrich et al entitled "LEAP Model Network and Data Documentation ARC-78 " September 1979 It is not clear whether these documents will be formally published

†We understand that work is underway on a new version of LEAP which may require about half of the previous storage (1 megabyte for the new version) This code has not yet been completed

No benchmark problems were available when the Model 22C was actually frozen in June 1979 Section IV of the report describes the structure of LEAP by carrying out the analysis of a specific sample problem (developed at ORNL and designated Model 82) based on a simplified network The work was performed to facilitate the understanding of LEAP and to serve as a testbed for methodology development Although the results of this hypothesized benchmark problem are not intended to be realistic the model itself is representative (i e most generic components of the LEAP Model 22C reference network are retained in the Model 82 sample problem) The rapid computing time associated with this sample model provides an opportunity for cost-effective evaluation methodology development in the area of sensitivity analysis

Little rationale was provided for the choice of Model 22C network structure or specification changes from prior publication of similar models No document related published results in the 1978 Annual Report of EIA to Model 22C output The ARC-78 forecasts were replicated at ORNL but only after some undocumented off-line analysis was understood Finally we estimate that two months are required* for an individual with no prior LEAP experience to gain expertise in running a LEAP problem independently at ORNL

D Model Structure Preliminary Evaluation for LEAP

1 Economics

The specific equations embodied in the ARC-78 (Model 22C) LEAP model are being determined documented and verified as part of the ORNL evaluation effort Section V describes the equations contained in the basic conversion process of LEAP These equations were deduced from available documentation on a generalized modeling system from the code itself and from extremely helpful discussions with the staff of EIA's Long Range Analysis Division Economic evaluation of the model for the basic conversion process was intended to be included in Section VI However this work has not yet been analyzed and will of necessity be delayed in publication until the fall of 1980 As an example of the type of work contained therein it has been found that the particular capacity factor function is not easily related to an underlying production function Thus we cannot ascertain whether the production function displays constant returns to scale consistent with long-run equilibrium solution The practical consequences of this finding have also not yet been ascertained Section VII describes the verification of the basic conversion process that is the equations and parameters reported to be used are discussed, and the explicit programming and data base elements are compared Additional specific details are given in Appendix B It is important to note that the model specification and verification from the evaluation perspective will differ somewhat were it

*This learning period could be reduced if computer access and turnaround time were better, and if access to the authors were more immediate so that questions could be answered more directly

done by the original modeler The evaluation team will specify document and verify what the code represents but not address in a comprehensive fashion the rationale for the various choices made in building the model

Section III of this report introduces the LEAP code and the results to be studied, topics such as available documentation and network design are discussed The genealogy of generalized equilibrium models is reviewed These systems differ significantly, but all systems have more similarities than differences The LEAP Model 22C sector diagram is described The tension between simplicity and fidelity is apparent For example although both oil and gas often come from the same wells, they are treated separately in this model

The important assumptions embodied in Model 22C include the unlimited availability of materials labor and capital the minimum representation of government regulation the lack of energy-economic feedback mechanisms the clairvoyance assumed by investors in making decisions and the lack of constraints on oil imports at the exogenous world price Regional distinctions are also suppressed All model behavior is generalized in a few process subroutines (e g allocation, resources etc) For example, the overall structure assumes that by merely specifying a different set of process parameters the same subroutine can capture an entrepreneur's decision to buy a stove or his decision to build a synfuel plant

Although basically simple in concept the processes are often subject to extensive and detail complications (Some of the complicated features such as learning curves, are actually overridden with the particular choice of model parameters used in ARC-78) Market forces are assumed to dominate subject to behavioral restrictions such as time lags Resource and conversion routines assume that all new plant and production decisions are based on approximate maximization of present value of cash flow with competition End-use demand follows an exogenously set path modified beyond the year 1995 by price elasticity Parameters are included to lessen "bang-bang" effects (i e parameters that indicate the responsiveness of buyers to small differences in the price of some good)

Although these assumptions are listed explicitly herein, the evaluation has not proceeded far enough to identify the consequences of the results of alternative assumptions or approaches

No work has yet started in the areas of comparing LEAP results with observed history* or examining its performance relative to that of comparable models

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*There has been an effort at Lawrence Livermore Laboratory to measure a code similar to LEAP relative to historical performance However we feel that the differences between this code and Model 22C are significant enough to mitigate against drawing conclusions about Model 22C

2 Mathematics

The numerical solution technique used in LEAP is a nonlinear Gauss-Siedel successive overrelaxation (SOR) iteration procedure for most of the code and a Newton-Secant technique for all allocation processes That is all prices and quantities are calculated in each basic process for all time steps and are used immediately after relaxation in the next process module calculation The procedure is generally locally convergent with a linear rate of convergence The method used was developed from experience because no global iterative procedure exists that is guaranteed to solve a general set of coupled nonlinear equations It is even difficult to know a priori whether any solution to a LEAP problem exists and if one exists, whether it would be unique *

The convergence check actually used to generate the 1978 Annual Report to Congress was applied after iteration and included relaxation using current and previous solution estimates This procedure has since been changed, consistent with ORNL recommendations so that convergence is tested before relaxation The apparent convergence using these two approaches differs by a factor of $1/1-\alpha$ where α is the relaxation parameter used for a specific allocation quantity Because α was chosen as $\sim$0 5 for most quantities the reported converged results could have been about twice those assumed (i e 6% instead of 3% for Model 22C) Fortunately however, subsequent comparison indicated that the numerical values obtained for ARC-78 were, in fact within $\sim$1% of a solution correctly converged to within 0 5% Finally, the rationale for the overall scheme of convergence testing in allocation only was unclear from both physical and theoretical viewpoints Global convergence was assumed after checking local quantities on the down-pass in allocation only Here again we performed checks of convergence elsewhere in the Model 22C network and found no cases of important quantities which remained unconverged

Relaxation is used at allocation processes for the market shares (new capacity additions are also relaxed) Again the approach taken does not seem to conform to any known theoretical extrapolation technique (likely as a result of the considerable complexity of the problem including damping effects for behavioral lags) The algorithm used differed from the algorithm in the Decision Focus Inc (DFI) documentation The use of diagonal elements only in the derivative matrix for relaxation must be incorrect because allocation almost always produces cross derivatives (assumed by the algorithm to be zero) Finally the relaxation parameters were numerically constrained to be positive and greater than 0 1, which can clearly lead to situations that will diverge

In summary, a converged solution for Model 22C was obtained which appears, in practical terms to be quite reliable However, the methodology used for both convergence and relaxation requires careful study for future use

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*Further study is now underway at ORNL in this regard

E Sensitivity Analysis Preliminary Evaluation for LEAP

1 Screening

The first technique for sensitivity analysis that was examined dealt with the following approach

a Given M parameters and N runs (N<<M) find the sensitivities approximately and rank them with some quantitative estimate of confidence that is if only a finite number of runs of a large code (and associated large data base) can be made which runs should be performed to learn the most information regarding the relative importance of data?

b Treat the code as a black box sampling input changes randomly, that is, do not bias the choice of runs with unproven "intuition "

The problem as posed is quite general and is therefore relevant to all fields that use large complex computer analysis If such a technique could be developed it would have major advantages of minimal code development, direct consideration of many responses of interest, and capability to handle nonlinearities

After several months of intense study a full analysis has shown that such methods yield no confidence limits on the sensitivities except via addition of significant prior knowledge The analysis is based on a theory of logical inference, which is described in Section VIII The theory is comprehensive in scope and includes "response surface" and "screening" methodologies as particular examples of this more general Bayesian approach Formulas are derived that relate the uncertainty in a model result to uncertainties in the model parameters which express the appropriate values of the sensitivities based on the given information and which include how to determine the best set of runs to make to minimize the variance in a given result

Indeed input variations should <u>not</u> be made randomly, in the sense of arbitrarily! Rather, the appropriate experimental design approach that is developed requires quantitative estimates of uncertainties and correlations for both the data base and the prior estimates of sensitivities (uncertainties bounds signs etc) Such information should be developed in the form of probability distributions based on testable facts rather than on intuition or opinion If the facts regarding the sensitivities lead to a covariance matrix which is diagonal our screening approach results in varying one parameter at a time starting with the one expected to have the greatest impact If the covariance matrix of the sensitivities is not diagonal, particular combinations of data must be varied simultaneously After N such runs are made, the residual uncertainty on the sensitivities for the remaining input data is nothing more than the original prior estimates which were unchanged by this process

Two important conclusions result from this study

a This technique should not be applied (at least for LEAP) by anyone less than an expert and, therefore is probably <u>not</u> appropriate as a third-party evaluation tool

b Problems in assessing sensitivities for large time-consuming computer codes (with large data bases) using reruns about a reference case remain for all statistical sensitivity methods

Thus it would appear that the field would be in considerable difficulty were it not for our preliminary findings in the next section

2 Adjoint Perturbation Theory

Adjoint perturbation theory is discussed in Section IX This is a mathematical technique used to determine exact first derivatives for some model result of interest with respect to <u>all</u> elements of the data input field The theory has recently been extended to include nonlinear coupled sets of equations Implementation of the theory requires no perturbations to the data or prior estimates of importance

The difficulties experienced herein were that significant development was required to derive and solve the adjoint equations for a large and initially unfamiliar (and not completely documented) code The steps in the adjoint technique include determination of many derivatives access and storage of data and solution results from a reference case construction of a new linear matrix system and solution of this adjoint set of equations

Using Model 82 as a test (with the RESOURCE processes temporarily not included) early results using the adjoint method appear very encouraging As soon as the applicability of the method to Model 82 is completely demonstrated it will be applied to Model 22C It is anticipated that results for Model 22C will be available by October 1980

F <u>Model Input Data Preliminary Evaluation for LEAP</u>

Section X presents progress in our effort to evaluate the LEAP input data base with respect to sources and characterization of data types The origin of the Model 22C data base has been examined Data types and definitions were categorized (e g data not used data based on calibration to other models, physical data behavioral data etc) and an audit trail has been initiated The available documents generally describe only one or two of the many "data items" for each activity Procedures used to convert raw data into parameters stored in the data base were not provided and hence many complications of definitions and dimensions were introduced Parts of the data base (Model 22C), such as world oil and gas prices are now (with 20/20 hindsight) clearly obsolete A few specific errors in the Model 22C data base were found and documented and have now been corrected * Calibration and a desire to

*Thus the results from the corrected base case differ slightly from that published in ARC-78

match intuitive results led to substantial revisions of data and incompletely documented constraints on the data base relative to penetration of electric cars and solar energy In almost all cases engineering judgment dominates statistical estimation Detailed evaluation of input data quality did not proceed as far as we had hoped as a result of many obvious complications

1 Estimating uncertainties for behavioral parameters as well as for physical parameters is often difficult

2 The quality of the documentation of the original data base is often poor

3 Many of the root causes of uncertainty are common to various parameters so that important correlations must be assessed

4 Input data to some models are taken as the output predictions from others

5 It is difficult to correlate the input data with "knowable" parameters

6 The input data are sometimes modified in an attempt to model a technological improvement regulatory constraint etc

In spite of the aforementioned difficulties we believe that the inclusion of quantitative uncertainty information is an essential program element if we are to achieve some quantitative measure for uncertainty in output results

G General Remarks

As stated in Section III LEAP and published results from it should ultimately be evaluated as a public information model since citizens need energy data from a source without inherent bias Model results as well as the general conclusions of the modeler, are important Input and output must be available in detail without interminable private communication with the modeler, they must also be available in a time frame commensurate with the release of new projections Many of these ideas can be formalized with reference to the following definitions

An "open" code[17 18] is one which at some stage of development becomes well documented is closely scrutinized in its internals by members of the industry at large is widely used and is frequently modified These are characteristics of most mature and valid technologies We define a code (model) as closed if it is proprietary, not well documented or has not been subjected to critical examination It is likely to be closed if

1 It is not widely used

2 It has never been modified by anyone but its authors

3 It is used only at the site where it was developed

4 If used at other sites it is used only as a "black box"--a converter of input into output

In this light Table 1 presents a subjective impression of whether LEAP (Model 22C) is open closed or somewhere in between It would appear that much work is yet required to bring LEAP to a full "open code package" status a status which would certainly help to enhance the credibility of results derived therefrom

In closing it is important to recall that EIA requires long-term modeling capability Model 22C was a reasonable first attempt to provide complicated information given the incredibly tight time limitations and the existing state-of-the-art It is hoped that future versions (e g that used for projections in ARC-79) will benefit from this initial experience with LEAP development and meet more fully the intent of a public information model

Table 1 Is LEAP "Open," "Closed," or Somewhere in Between?

	The "Open" Code Package		LEAP Status
1	Is generally available	1	Not obvious
2	Is well documented	2	Not yet
3	Does not depend on nonstandard[a] proprietary systems software	3	System 2000
4	Includes benchmarks	4	Not yet
5	Is transportable	5	Not obvious
6	Has mechanism for user feedback	6	Used at one source only
7	Is verified on packaging	7	Verification in progress
8	Is continually critically examined with results in public domain	8	Validation underway

[a]"Standard" proprietary systems software is defined to be that which is routinely distributed by the hardware vendor as essential to operation of the hardware in any computer installation environment

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I INTRODUCTION

A Background

The Office of Energy Information Validation (OEIV) of the Energy Information Administration (EIA) U S Department of Energy (DOE) has begun sponsorship of a program at Oak Ridge National Laboratory (ORNL) to develop and demonstrate a methodology for evaluating energy-economic modeling codes and the important results derived from these codes Such computer programs and associated results provide useful information to decision makers about the potential impact of energy policy and research and development programs on the long-term supply of energy Illustrative issues include allocation of resources among competing technologies on the basis of criteria such as potential market penetration by the end of the century savings in future energy cost or quantity of imported oil

Model projections now, or in the near future will never be the sole guide in policy choices however the amount of effort and the quality of scientific talent now dedicated to model development do emphasize the growing role of models in policy analysis Indeed it is the understanding of the limitations and ranges of validity of these computer projections that may ultimately determine their final role The ORNL model evaluation program is attempting to build a "technology" for model evaluation to complement the technology for model construction The basic components of traditional evaluation techniques[1-4] have included review of the model's theoretical bases, data parameters and computational algorithms relative to the intended uses of the model results However this entire evaluation sequence has been comprehensively applied in only a few cases

B Approach

To bolster traditional evaluation methods[1-4] with more quantitative procedures of interest to the Office of Validation Analysis of the EIA, ORNL is applying sensitivity theory[5-12] as part of a comprehensive effort to quantify the "importance" of various data and model parameters to the key results that are of interest Quantitative estimates for uncertainties associated with some of the primary input variables are also being developed Although sensitivity theory will be used to estimate the propagated effects of uncertainties in data the results of model specification uncertainties (e g , approximation in representation of behavior and what might have been "left out" of the model) are approached by in-depth evaluation of the model structure itself

The inherent complexity of energy-economy models and the nature of their data bases generally make "model evaluation" a difficult task, which is often difficult to quantify The ORNL approach to evaluation

is to attempt to create an operational definition of this task That is for a given scenario only certain results produced by the code are assumed to be "important" (as defined by the users of the code) and a major component of the effort will therefore involve a quantitative determination of the uncertainty that might be placed on these important results (It must be remembered that this conditional uncertainty represents the propagated effect of data uncertainties only, and model specification uncertainties still must be considered) The problem of "range of validity" is likewise defined in terms of a range of important results for which uncertainties can be estimated This approach is extremely pragmatic since this aspect of evaluation can then be reduced to a procedure for uncertainty analysis based on well-established methods derived from sensitivity theory Such an approach is likely to succeed because it has been used to solve the same basic problem in other fields--notably, nuclear reactor physics shielding safety and thermal hydraulics [5-10]

Beyond the considerable effort involved some may feel that propagation of input uncertainties is unnecessary or imprudent, even as a long-range goal One claim is that uncertainties in model parameters representing the future cannot be determined however, if this were true use of these nominal values would be received with much skepticism Another thought has been that, because a model plays out alternative scenarios based only on hypothesized input parameters consideration of uncertainties is not necessary This argument is weak if the model contains so many parameters that the user can be only minimally aware of all the assumptions made Moreover the distinction that a model yields "projections" rather than "forecasts" gives little comfort to the user who must ultimately make decisions based on model outputs "Sensitivity studies " which show the consequences of reasonably altered key input parameters are satisfactory for those parameters that are varied but these few studies do not inform the user of the cumulative consequence of uncertainty in the hundreds of other parameters that are presumably less important

Confining the use of model outputs to ratios or differences, which will be relatively insensitive to some input uncertainties but appropriate for decision making has shown some promise However without some estimate of the propagated uncertainties the user cannot take advantage of this effect objectively In the end the model user must be able to quantitatively estimate the impact of the uncertainties in the model inputs He must know whether the uncertainty is so large that it casts doubt on the resulting conclusion Certainly a few key parameters can be fixed by assumption (to constitute an overall scenario) but even in this case the cumulative uncertainties introduced through the other data and model parameters must be assessed to determine whether these scenarios can really be distinguished, and then the possible ranges in the parameters fixed by assumption must be explicitly considered

The ORNL approach toward quantifying the accuracy and appropriateness of model results as well as the potential utility of the model for

future applications has been described in part in earlier papers [11-12] Use of the approach described herein should (1) enhance traditional validation efforts to assess the logical mathematical and statistical basis of the model structure and (2) supplement studies that compare model projections with observed economic history However it must be clearly understood that although significant progress has been made credible estimates for forecast accuracy will take considerable time to develop

C Focus on LEAP

In conjunction with EIA's interest in forecasting the long-range impact of new technologies and energy research and development on future energy use the energy-economic modeling code LEAP [13] used for the projections (Model 22C) in the 1978 Annual Report to Congress was chosen as the initial focus for this research The purpose of this report is to describe the research conducted between January 1979 when the program was begun and October 1979 * During this period an interdisciplinary team of experts in operations research statistics economics and sensitivity theory worked toward the following overall goals of the program with respect to LEAP evaluation

1 To develop and demonstrate methods (extend and apply traditional procedures) for assessing the scientific basis for the EIA's energy-economy models data and parameters

2 To develop a sensitivity theory for determining the important data used by the models in specific applications

3 To quantitatively estimate uncertainties for important data

4 To estimate uncertainties in the forecasting results and indicate ways in which these might be reduced

5 To develop and apply meaningful procedures to improve confidence in forecasts by comparing predictions against observed history

6 To evaluate the range of applicability of the model by relating the findings in goals 1 to 5 to the intended model uses

Between January and October 1979 the aim was to demonstrate the practicality of important elements of the methodology that were to be used so that the program goals might be demonstrated by the end of FY 80 (October 1980)

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*The LEAP program and data base made available to ORNL was "frozen" in June 1979 (see Appendix A)

However users must still be quite cautious particularly when working with scenarios that reach a generation into the future Modeling current economic behavior is difficult and one can never be sure that our society will continue to follow similar patterns under the altered stimuli of the future

Model output uncertainties can be roughly separated into two categories (1) the propagated effect of uncertainties in the numerical values input by the model user and (2) the result of uncertainties in the model specification The first which can be treated directly by techniques of sensitivity theory is of major importance to model evaluation The second category deals primarily with the techniques used to approximate the interactions and behavior of consumers producers etc , and also with what was "left out" of the model This latter topic is equally important and can only be approached by in-depth evaluation of the model structure itself

D Organization of Report

The present ORNL concept and approach to model evaluation are described in Section II Described in broad terms the approach is not intended to be model-specific Section III introduces the LEAP code and the results to be studied topics such as available documentation and network design are discussed Section IV describes the structure of LEAP and the evaluation of the numerical methods contained therein by carrying out the analysis of a specific sample problem Although the results of this hypothesized benchmark problem are not intended to be realistic the model itself is shown to be sufficiently close to LEAP (i e most important complications in analyzing the LEAP reference results are specifically retained in the Model 82 sample problem) The model is judged appropriate for development and testing of the ORNL methodology

Section V describes the equations contained in the basic conversion process of LEAP At the outset of this study no specific document describing the equations contained in LEAP was available Thus, these equations had to be deduced from available documentation on a generalized modeling system from the code itself and from extremely helpful discussions with the staff of EIA's Long Range Analysis Division Economic evaluation of the model for the basic conversion process was intended to be included in Section VI However this work has not yet been finalized and will of necessity be delayed in publication until the fall of 1980 Section VII then describes the verification of the basic conversion process, that is, the equations and parameters reported to be used are discussed and the explicit programming and data base elements are compared

Section VIII outlines the first of two techniques that can be used to deduce sensitivity coefficients that characterize the relative change in a result of interest for a concomitant relative change in some input data or model parameter The theory presented is comprehensive in scope and includes "response surface" and "screening" methodologies as particular examples of this more general Bayesian approach The advantage of

using this approach is to explicitly indicate assumptions commonly made using other approaches and to avoid overlooking the implications of these assumptions Formulas are derived which relate the uncertainty in a model result to uncertainties in the model parameters which express the approximate values of the sensitivities based on the given information and which indicate how to determine the best set of runs to make to minimize the variance in a given result Some of the major difficulties with this approach deal with (1) how the quality of results changes with degree of knowledge of prior information and (2) how much effort it takes to accumulate a reasonable amount of prior information and to cast it into the proper format Section IX then presents our second approach toward deducing sensitivity coefficients through development of adjoint perturbation technology The limited development requirements probabilistic nature of the results and large computational expense of the Bayesian technology can then be compared with the large programming and development requirements, deterministic nature of the results and limited computational expense of the adjoint technique Section X presents our effort in evaluating the LEAP input data base with respect to sources and characterization of data types Furthermore the work accomplished in developing and documenting a consistent set of definitions and units for the Model 22C data base is described With an effort to establish audit trails for important data (now underway) we hope that we may soon be able to quantify the data quality in terms of uncertainties Finally our operating experience with LEAP from the reference of a first-time user is described in Appendix A, and specific details of equations relevant to the body of the report are given in Appendix B

The purpose of this report is to demonstrate the elements of the ORNL approach to model evaluation and to provide a strong basis for continuing work during the next year

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II APPROACH TO MODEL EVALUATION

The objective of the Office of Energy Information Validation (OEIV) regarding model evaluation, has been described[1] in terms of being able to answer the following questions

1 Considered as a computer device, can the model be understood and used by third parties?

2 What are the model's fundamental mathematical properties?

3 What is the model's logical (e g , physical, statistical economic, engineering) structure? What is the domain of model applications?

4 What is the nature of the data needed to implement to prepare forecasts and to test the model?

5 Are the individual specifications and assumptions supported by data and theory?

6 What can be said about the reliability or uncertainty of the forecasts?

7 How is the model used? For what purposes is it suited?

Toward these ends ORNL has developed a concept of the elements constituting a model evaluation and the necessary procedures required for its implementation (Traditional approaches taken in evaluation methodology are described in Refs 2-5) This approach is described somewhat generally in this chapter, but details specific to LEAP and some related problems can be found in other sections Essential elements of the ORNL concept include (1) identification of user requirements for the model (2) review and development of documentation and computer software associated with use of the model (3) determination of the sensitivity of a result to model input data and parameters (for a specified model structure and data base) (4) evaluation of the model input data and associated uncertainties and (5) study of the code formulation and equation structure, including an assessment of existing model validation conducted by the Office of Applied Analysis To make the evaluation most meaningful and to gain appreciation for the ease of utility and applicability the evaluation includes running the model with its associated data bases

A Identification of User Requirements

At the very heart of any evaluation intended to assess the meaningfulness and accuracy of the model output is the user need--a model cannot be evaluated effectively w thout an intended use The evaluation process is most meaningful when the problem or decision to which the model information is to be directed can be defined accurately and specifically

Thus many schemes may be used to gain insight from actual or potential users These schemes include (1) literature reviews (e g , Administrators Annual Report to Congress,[6] which describes the information gleaned from model projections) (2) direct interviews with people responsible for making or recommending decisions on issues such as resource allocation (3) examination of the Office of Applied Analysis service request forms, which contain brief explanations of intended uses (4) development of a questionnaire directed toward potential users (5) specific input and guidance from the OEIV staff, and (6) an independent assessment of the perceived needs that can be derived for such a model

In many cases the user has only a general idea of what is desired from the model and considerable effort may be required to focus general statements to specific responses that can be directly computed from a combination of model outputs Furthermore the relative accuracy for which certain results are required should be determined if possible This step is necessary for determining whether the present imprecision for specified results of interest is so large that their use is effectively precluded Finally the realization that decisions are never made strictly on the basis of model outputs is vitally important Users often make decisions in an "off-line " undocumented mode If in the long term we are to fully comprehend the role that the energy-economic models can play in influencing policy decisions these additional considerations must be emphasized

In summary our concept of model evaluation begins with a specified result of interest or an apparent perceived need which is provided by the user (possibly in conjunction with the model evaluator) Specific examples for long-range forecasts might deal with the time-dependent change in fractional energy supply or fractional energy consumption (see Table III-3)

B Review and Development of Model Documentation

Although many views exist concerning the elements that constitute model evaluation two items are almost universally accepted

1 Proper documentation is an absolutely essential ingredient for acceptability and utilization of a given computer model

2 As of October 1979 very few models of the energy system have been documented to an extent that would allow (without significant additional effort) independent evaluation by a third party, other than the model developer and intended user

Significant efforts have been made toward describing the documentation required for model assessment [4 7] Several important points can be made

1 The document describing the theory should detail specific information concerning the particular model to be evaluated Quite often complications are introduced when general modeling systems are described while pertinent information relating to the particular model constructed from elements of the general system is overlooked

2 Whereas the particular process equations may be described documentation providing the rationale for selecting a specific input or model parameter is often missing or referred back to ambiguous sources Because major uncertainties can arise from uncertainties in specifying the input data as described below the process for selecting the input must be carefully documented and understood

3 The computer code (and auxiliary software data bases etc) must be frozen at some point in time so that the evaluation can be conducted with respect to a fixed frame of reference Successful modeling tools will be continually improved and upgraded All such changes must be carefully documented and their implications with respect to model evaluation of the reference code must be explicitly noted

4 The model to be evaluated should be accompanied by a relevant but relatively simple sample problem and output listings should be verified as correct by the original modelers Such a sample problem will help assure a new user that he has successfully operated the model on his particular computer It will also enable him to gain significant experience in using the model without performing expensive runs on complicated systems before he has acquired the necessary expertise Furthermore, documentation of computer compatibility of specific models assures a new user that a successful run can be executed using in-house capabilities

In summary, a substantial body of documentation is required before a model evaluation can even begin Much of this documentation, having been provided by the modeler should be available for evaluation at the outset However this may not be true for all models We believe that the evaluator by cooperating with the modeler can perform a necessary service if he tries to help develop at least some of the necessary documentation instead of merely pointing to glaring omissions or the impossibilities of continuing A potential hazard always exists for infringing on the "rights of the modeler" or even creating a situation of "conflict of interest " However, we believe that the evaluator who helps provide the necessary documentation of the condition of the model as he encounters it and who resists the temptation to improve or replace specific features without concurrence of the modeler, makes a contribution that outweighs any potential disadvantages

C Development and Implementation of Sensitivity Methodology

The key task in any sensitivity analysis is to identify the most important data parameters used to calculate a result of interest Identification here means determining the sensitivity coefficient $dR/d\xi$ which is the differential rate of change in a result R with respect to a differential change in any parameter of the data base ξ The concept of the importance of such derivatives is not new for example important economic indicators such as supply and price elasticities are themselves sensitivity coefficients Once these derivatives are known for each ξ they can be ranked by absolute magnitude to determine the most important parameters in the problem This ranking procedure is difficult and costly when the data base and parameter set are large (i e 10^2 to 10^6 data elements) as is usually the case with complex codes

Two complementary sensitivity analysis techniques[8] have been investigated for ranking derivatives The first technique is based on methods for analyzing reruns of the basic code with perturbed data and parameters The major advantage of this technique is that limited code development is required and emphasis is placed mostly on understanding the input data and on the procedures for running the code intelligently Also this method can easily handle multiple results of interest One major disadvantage however is the high cost usually incurred in making many code runs on a one-time basis simply for a sensitivity study Another disadvantage is that the sensitivities are estimated probabilistically rather than deterministically Fewer perturbation runs (N) are made than the number of parameters (M) $N < M$ leads to an undetermined problem Finally, the information requirements for this approach are formidable however these requirements are no different from those used in most procedures to date The difference is that, in many past analyses assumptions were implicit and often overlooked in drawing conclusions In our proposed procedure this information must be provided explicitly

The second technique for analyzing sensitivity is adjoint sensitivity theory [8 9] This approach requires significant development to derive and solve the adjoint equations for a specific code After this task is accomplished however only one solution of the adjoint problem is required to generate all the sensitivity coefficients desired for a given result of interest Furthermore, sensitivity information to some types of methods approximations (e g discretization parameters or integration mesh size) can be obtained directly [9]

The two approaches therefore complement each other well because each is best suited for one of the two kinds of sensitivity studies most requested (1) short-term one-time studies requiring no development work (following the precise specification of the methodology developed in Chapter VIII) and (2) long-term studies based on the repeated use of a single code system

Several items must be clarified at this point First sensitivity analysis is not at all new however, we believe that it has been applied

in the model evaluation field only very selectively That is a priori information about the data perceived to be important is used to make a limited number of reruns to determine whether intuition can be confirmed To our knowledge the adjoint approach taken here to quantitatively determine sensitivities of specific results to all elements of the data base is unique However the sensitivity methodology provides no indication of possibly important parameters that are omitted in the model specification Thus the sensitivity methodology is essential but must be complemented by traditional validation techniques (see Section II F), which examine equation structure and which may test computer forecasts against economic history ("historical validation")

D Evaluation of Model Input Data

One part of the uncertainty in the output of an energy-economy model arises from the uncertainties in and correlations among the model's input parameters Modeler and user confidence in a model and therefore its utility will be increased if one can document the sources of the data and show that the projected impacts of the input uncertainties on the calculated responses of interest are sufficiently small that they will not invalidate the intended uses [10]

For many years the analysis community has assessed the potential impact of such uncertainties by varying key parameters within their estimated ranges of uncertainty As stated earlier "key parameters" have been guided mostly by experience and intuition and should be bolstered considerably by the methodology described in Section II C and in later sections Similarly the concept of "variation within the estimated uncertainty range" needs considerable expansion

Such uncertainty ranges are rarely specified or documented for many reasons

1 Estimating uncertainties for behavioral parameters (e g behavioral lag parameters to avoid the "bang-bang" nature of models) as well as for physical parameters, is often difficult

2 The quality of the documentation of the original data base is often poor

3 Many of the root causes of uncertainty are common to various processes and parameters so that important correlations must be assessed

4 Because input data to some models are taken as the output predictions from others "input" uncertainties become extremely complex to assess

5 It is difficult to correlate the input data with "knowable" parameters

6 The input data are sometimes modified in an attempt to model a technological improvement regulatory constraint etc

Perhaps most important is the fact that no organizational body has ever required them or had the tools to use them even if provided

If we wish to determine the uncertainty of the output we must estimate uncertainties on at least the most important independent inputs The relevant data are not limited to technical coefficients and exogenous variables, they also include any coefficients and variables used to estimate the model parameters As before numerical values for the uncertainties should have arisen as a natural part of the evaluation process from which the data base was originally assessed However in practice such data and documentation are often missing and must be developed as part of the model evaluation process Many of the input data and uncertainties may be common to a large variety of codes thereby giving the uncertainty evaluation a broader applicability

Precise definitions of data elements, the information base from which the data evaluation was deduced and the inclusion of uncertainty information are essential program elements

E Determination of Uncertainty in Output Results Due to Uncertainty in Input Data Parameters (for a Specific Model)

One can estimate the uncertainty in the required model outputs (for a specific model and reference set) that will result from uncertainties in the input data by combining the sensitivity coefficients (partial derivatives) with the uncertainty matrix (variance-covariance matrix) that characterizes the input data The impact of using internally consistent samples drawn from the same range of model data is also easily assessed

F Study of Code Formulation and Equation Structure

As discussed above, the sensitivity and uncertainty methodologies apply to a specific data base and model structure There is no way that one can learn from Sections II C through II E about uncertainties resulting from poor model specification (e g omission of regulatory constraints or important processes) Hence traditional validation techniques which examine the code formulation and equation structure with regard to major assumptions (such as the degree of aggregation) must be examined When validation studies of this type are already available from work sponsored by the Office of Applied Analysis, only an independent review is needed

However, if such studies have not been completed the model evaluation should include some of these more traditional techniques--for example, examination of the theoretical basis behind the equations and model structure, study of basic technological and behavioral assumptions on economic resources, the role and nature of markets, and the dynamics of investment The study of the code formulation should also include assessment of the mathematical implementation, including problems such

as convergence acceleration, and uniqueness and other properties of the solution algorithm It also should contain information related to the ease of using the model

Furthermore, a comparative study of the same problem is a useful tool for gaining perspective on the relative strengths and weaknesses of various codes Thus an assessment of the relationship between the representations employed to those generally used in the professional literature should be included in the model evaluation Finally, examination of model forecasts in light of observed economic history is necessary (but not sufficient) Such historical validation techniques can demonstrate vividly the impact of various constraints and phenomena not present in the model

G Closing Remarks

The use of energy-economic models is becoming increasingly important in providing guidance for making decisions related to national energy policy The goal of this work is to develop and demonstrate the important components of a model evaluation technology that will help determine the appropriate credibility to be associated with these analytical tools and their output forecasts

In an evaluation of this type, it is usually rather easy to find oneself attacking weaknesses and limitations of a given model However, it is here recognized that conditions are such that models are often built and used under severe and limiting constraints Our intention is to be honest, but constructive, and with the full cognizance of the modeler to point to those areas requiring improvement

In addition to traditional validation techniques, which emphasize the equation structure and theoretical basis of the model, a significant sensitivity and uncertainty methodology is being developed and applied This methodology will allow systematic identification of (1) the important parameters dominating the forecast and (2) the propagation of input data uncertainties to output uncertainties

This effort is also intended to generate and document solutions to simplified but relevant benchmark problems, which will serve as a test bed for evaluation methodology development and as an indicator of whether a new user has successfully used the model Significant documentation regarding all aspects of the model and its data base is being generated in the course of this work Such written information is essential for communicating what has been learned about the model and to unambiguously define its status and perceived validity

It is hoped that this sensitivity and uncertainty methodology will add a new dimension of quantitativeness for at least some of the major components of the evaluation Furthermore, our approach strives for an operational endpoint for the evaluation--that is, when a quantitative estimate of uncertainty for important results can be made and defended

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III LEAP AND ITS USES

The Long-Term Energy Analysis Program (LEAP) is an energy-economy model which resides in the Long-Term Energy Analysis Division (LTEAD) of the Integrative Analysis Group in the Office of Applied Analysis Energy Information Administration (EIA) U S Department of Energy LTEAD developed Model 22C of LEAP for two reasons (1) to prepare projections through the year 2020 which were needed for the 1978 EIA Annual Report to Congress[1] and (2) to develop a base for analyses of specific options for federal action In this section we attempt to describe LEAP Model 22C and its uses well enough to provide the background for this interim description of the model evaluation effort at the Oak Ridge National Laboratory (ORNL)

A Historical Setting of the LEAP System

1 Long-Range Energy Modeling

Long-term energy models project scenarios for 20 or more years into the future Long-term models differ from short- and mid-term models because in 20 to 50 years much capital stock will be replaced some resources will suffer major depletion significant population migration may occur to follow altered patterns of economic activity and aggregate demand patterns may be altered through cultural shifts Such cultural shifts have generally not been included endogenously in energy models but capital stock turnover and resource depletion must be considered in any long-term energy model The model complexities required to meet these needs are somewhat compensated for by the typical user's willingness to average over seasonal variations and in some cases to suppress regionality Government policy cannot remain stable for a generation but for present and reasonable policies one must study the possible modes of evolution of the energy system in response to relative price changes induced by resource depletion and technology development

Because scholars government officials and major industries must understand the future implications of what is already known a number of long-term models have been developed This section traces the development of a particular family of "generalized equilibrium" process models in these models energy-related economic activities that are considered central to the modeler's concern are simulated with respect to investment in productive capacity energy flows and money (credit) flows The usefulness of this family of models is not compared here with the usefulness of other families of long-range energy models Brock and Nesbitt[2] have usefully compared several types of large-scale energy system planning models including mid-range models

2 Common Features of the "Generalized Equilibrium" Models

All the models mentioned in this section can actually be classified as modeling systems because the representation of the energy economy can be significantly changed, with less than the original effort to enable

study of a particular interaction of interest The documents referred to below were produced at specific stages of model development and may not reflect this inherent versatility

The models or modeling systems discussed in this section are closely interrelated they differ in important specific aspects, but not in general principle Each is intertemporal solving simultaneously for an entire sequence of time points Each model divides the energy-related part of the economy into convenient sectors and sometimes into geographical regions Regardless of sectorization and regionalization assumptions at least the energy and monetary flows are traced among selected activities which represent aggregated energy-related resource exploitation conversion transportation facilities etc Each model terminates at its "top" with a set of usable energy demands or price-dependent demand functions At its "bottom" each model terminates with a set of resource models which provide an intertemporal analog of supply curves for coal oil and other fuels

For the particular case of a "snapshot" model in which alternative directly competing suppliers of an energy commodity must accept the same price Brock and Nesbitt[2] show how the supply and demand curves can be considered to be propagated through a network of commodity flows so that the elementary ideas of economic equilibrium apply For most specific modeling systems referenced here the allocation of demand among competing suppliers has been handled in a more complex manner which allows some price differences among competing suppliers In any case, the need for intertemporal accounting requires extension of elementary concepts

To provide efficiency for the modeler these systems define categories of economic activities, usually called processes which are modeled in separate subroutines within the system Each process subroutine is capable of representing a range of entities the range is sometimes so broad as to permit use of the same subroutine for the home oil heater and any type of electric utility Model parameters are provided for the subroutine applicable to each network "node" (activity) The parameters may be specific to the portion of overall economy represented by that node The network organization and the process subroutines can be modified in any way consistent with iterative convergence toward a solution and with the techniques used for data base management therefore the modeler is free in principle to mitigate any inappropriateness of model specification that can be addressed by using obtainable data

A common property of the models discussed in this section has been specification of final usable energy demand in a manner that is much less detailed than the models of other activities Levels of economic activity in the various demand sectors largely determine overall energy use and must be obtained exogenously from the output of population and macroeconomic "driver" models The impacts of the energy sector on the remainder of the economy are determined outside the model if at all Impacts of energy cost on other factors that may be substituted for energy effects on the international monetary system of U S oil import

cost and the effect of energy facility construction on investment markets have not been included specifically within any of the published models discussed in the next subsections

To represent the many individual decisions on production level and capacity expansion, the referenced model descriptions assume that decision makers apply the single criterion of (approximate) maximization of the estimated present value of the summed stream of future net cash (credit) flows Real decision makers may include other criteria To enable the chosen approach, each model formulation must embody the technique assumed to be used by the endogenous decision makers to estimate future product prices

3 SRI National Energy Model

The general description of the SRI National Energy Model, discussed in Chapter 4 of Reference 2, applies to all models described in this section The model was originally developed by the Stanford Research Institute (SRI) in cooperation with Gulf Oil Corporation to analyze Gulf Oil investments in alternative synthetic fuels facilities Cazalet[3] has described the SRI model in detail, indicating 1973 as the date of original development Cazalet[4] recently described the use of results from the SRI model in an analysis of President Ford's proposed synthetic fuels program by an interagency Synthetic Fuels Task Force The data base was shared with an ongoing study sponsored by the Council on Environmental Quality [5] The SRI National Energy Model was also used to produce a documented set of fuel and energy price forecasts for EPRI [6]

Only Reference 3 and Volume 2 of Reference 6 delve in any detail into the model specification, therefore, all these reports may have used essentially the same network of commodity flows and the same process equations Some minor differences occurred in the specification of the demand for usable energy, as indicated by the limited application of a price elasticity in Eq (44) of Reference 3 and by the assertion in the Appendix of Volume 1 of Reference 6 that end-use price elasticities were not used in the EPRI study (An extensive discussion of the appropriate choice of price elasticity parameters however is given in the earlier Volume 2 of Reference 6)

4 DFI Energy-Economy Modeling System

In 1978 Decision Focus, Inc delivered a working version of an Energy-Economy Modeling System (EEMS) to the EIA's Office of Applied Analysis An initial demonstration model of the energy portions of the U S economy was documented as an example in Reference 7 The document includes plausibility arguments for the equations used in the subroutines which simulate the portions of the economy that are important to the energy flows The process equations seem similar to those of the SRI National Energy Model, but the software framework may differ greatly because of efforts to enhance flexibility Although the demonstration model was often informally referred to as LEAP one must recognize that

the specific demonstration model was formulated before EIA's own modeling efforts using the DFI system The EEMS delivered to EIA used a general DFI software system [8]

5 LEAP System of the Energy Information Administration

A group led by John Pearson of the EIA's Office of Applied Analysis modified the DFI system[7] in numerous ways For example options were added for on-line modification of parameters used in a particular computer run with this option the parameters can be modified without affecting the master data base which is managed by the EXECUTIVE program of DFI's EEMS Use of this modified system is being documented [9]

The LEAP Energy Modeling System (LEAP-EMS) also differs from the DFI EEMS in that some of the specifications within the process subroutines have been modified These changes some of which are reflected in Section V of this report have not yet been generally documented by the EIA staff

This LEAP-EMS system was used by the Office of Applied Analysis to produce Model 22C which provided the basis for a set of long-term energy projections described in Reference 1 The present report describes the progress made in evaluating Model 22C and the underlying LEAP-EMS modeling system Model 22C is discussed in some detail in Section III B

Since Reference 1 was prepared in early 1979 modification of LEAP-EMS has continued [10] The flexibility of these systems implies that specific valid questions raised in this report may result in improvement of the system or modifications to process specifications to reduce conceptual difficulties

6 Livermore Economic Modeling System

The Livermore Economic Modeling System[11-15] was developed at the Lawrence Livermore Laboratory This system is based primarily on the SRI National Energy Model but a user-oriented modeling language has been developed and documented to facilitate model updates and the associated data handling The inclusion of price and quantity controls in this system facilitated a recent comparative historical simulation [16]

B Model 22C of LEAP

1 Focus of the Modeling Effort

Model 22C of LEAP was developed by EIA's Office of Applied Analysis as a demonstration of the evolving LEAP-EMS system and to provide "in-house" projections of energy flows and prices suitable for inclusion in Reference 1 To meet this need it was desirable that the chosen input assumptions be consistent with concurrent mid-range base-case scenario

output which was also to be described in Reference 1 At the same time advantage might be gained from the LEAP capability to model the changes in patterns of facility construction and energy use expected to be induced by changes in relative price traceable to resource depletion and development of new energy conversion processes Economic activity is treated as exogenous information, and there is no feedback from energy use or cost to the postulated level or pattern of economic activity (except via the "calibration" described below)

Model 22C is defined by the Model Input Tables (identified here as MIT 3 through 22) which are input to LEAP-EMS by the modeler to determine the model network of energy flows identify the computer subroutines chosen to represent the various energy-economy activities and give numerical values for all the input parameters These tables are accessed via the EXECUTIVE program supplied by DFI These MITs and the LEAP-EMS program were transferred to us for this model evaluation study (see Appendix B)

To obtain tractable operation and to focus on the primary requirements, regionality is largely suppressed in Model 22C The United States is treated as one block, and only four international energy flows are recognized Although the DFI demonstration model recognized finance labor and government sectors links involving these sectors are not retained in Model 22C (Since no labor capital or government service balances were ever performed and none of these aggregates fed back to energy demand no immediate loss resulted from abandoning these links Individual process models do consider taxes and the costs of labor and capital and edits summarizing these quantities could be obtained) Prices for all periods are estimated and given in terms of dollars of fixed 1975 "value " To assure general consistency with the mid-range projections, some of the model parameters were adjusted to calibrate output for the year 1995 against results of mid-range projections, which are summarized in Reference 17

Of the general model characteristics indicated above, the ones most contrary to conventional practice are the lack of regionality and the explicit calibration to results of other models of the same part of the economy Problems associated with the lack of regional structure within the (model) nation deserve consideration because traditional regional differences in energy use and fuel choice can be broken only through increments of transportation and environmental control cost that lie outside the present pattern A model that includes a regional substructure is the most direct way to treat this problem endogenously (Model 22C does differentiate some resources by region, such as western coal and Alaskan oil, as well as related postulated synfuel facilities) The political problems that can arise from differential regional economic advantage cannot be handled without a much more comprehensive model that includes feedback from the energy subsystem to each regional economy

One goal in the development of LEAP was to enable analyses of energy technology development options which may be specified by DOE

offices other than EIA or by another government agency [18] Interviews with potential users of this class indicated that the LEAP projections given in Reference 1 were themselves helpful for this purpose, because these LEAP projections provide general published verification of the results of alternative modeling systems [19] and they indicate major fuel flows to permit off-line analysis of the compatibility of development options with the future energy system described by LEAP [20] Criteria in the latter case would include market penetration by the year 2000 and savings in future energy cost or quantity of imported oil There are strong indications that, in practice, most policy studies and even R&D strategy studies require simple models with relatively quick turn-around,[18,21] even though most energy problems develop on the time scale of a professional career and most adopted policy options were contemplated for years before promulgation (It is reasonable, of course, that quick turn-around be required on short-term models, however, short-term crises may not strongly affect energy supply or demand in the long term)

2 Model 22C Network Design

Figure III-1 illustrates the overall sector design of Model 22C, and Figures III-2 through III-10 illustrate the internal design of each sector These figures are edited versions of those supplied by the Office of Applied Analysis [22-23] The accuracy of the representation has been checked against the linkage tables, MITs 3 through 6, which are part of the model input Some activity labels in the figures have been modified, on the basis of the draft network documentation,[23] to better correspond to the portion of the economy included, these labels are marked with an asterisk, and the figure caption cites the activity title that is given in the MITs Each link (line in the figure joining two activity "nodes") represents a commodity (usually energy) flow, the corresponding dollar flow, and the "shadow" dollar flow for each of ten time points 1975 through 2020 The shadow price always corresponds to the free-market "clearing" price, but the transaction price may differ if the market is controlled In Model 22C there is no difference between the two prices In Figure III-1 the heavy lines represent a bundle of links from the same source whereas in Figure III-5, the use of heavier lines represents the three sublinks that may be present for base, intermediate, and peak-load electricity generation

By studying Figs III-1 to III-10, the reader can determine how the energy flows and activities in the economy have been aggregated for Model 22C analysis How well the model represents the energy-related activities indicated by the labels on the activities depends on the process subroutines used and on the parameters input to these subroutines A little information about these routines and parameter sets is included in the paragraphs below Section IV of this report details the structure of LEAP analyses, Section V gives the equations linking the model variables for the basic conversion process used to model each activity represented by a rectangular box in the flowcharts, and Section

ORNL-DWG 80 7672

LEAP MODEL 22 INTERSECTORAL LINKS

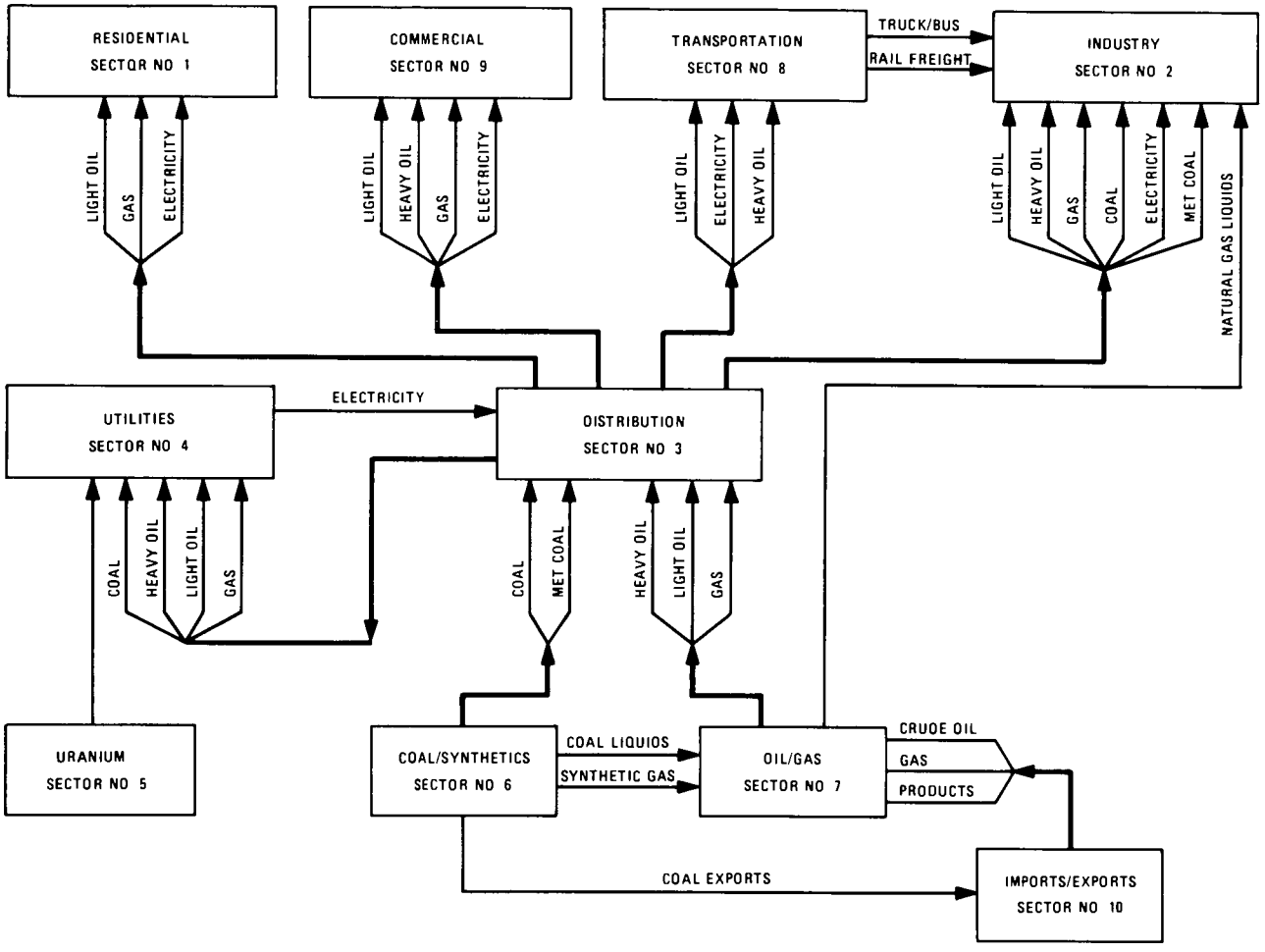


Figure III-1 Overall network diagram for LEAP Model 22C The lines joining the several sectors (see Figures III-2 through III-10) represent intersectoral links along which the model estimates energy commodity and payment flows for each of ten time points, 1975, 1980, , 2020

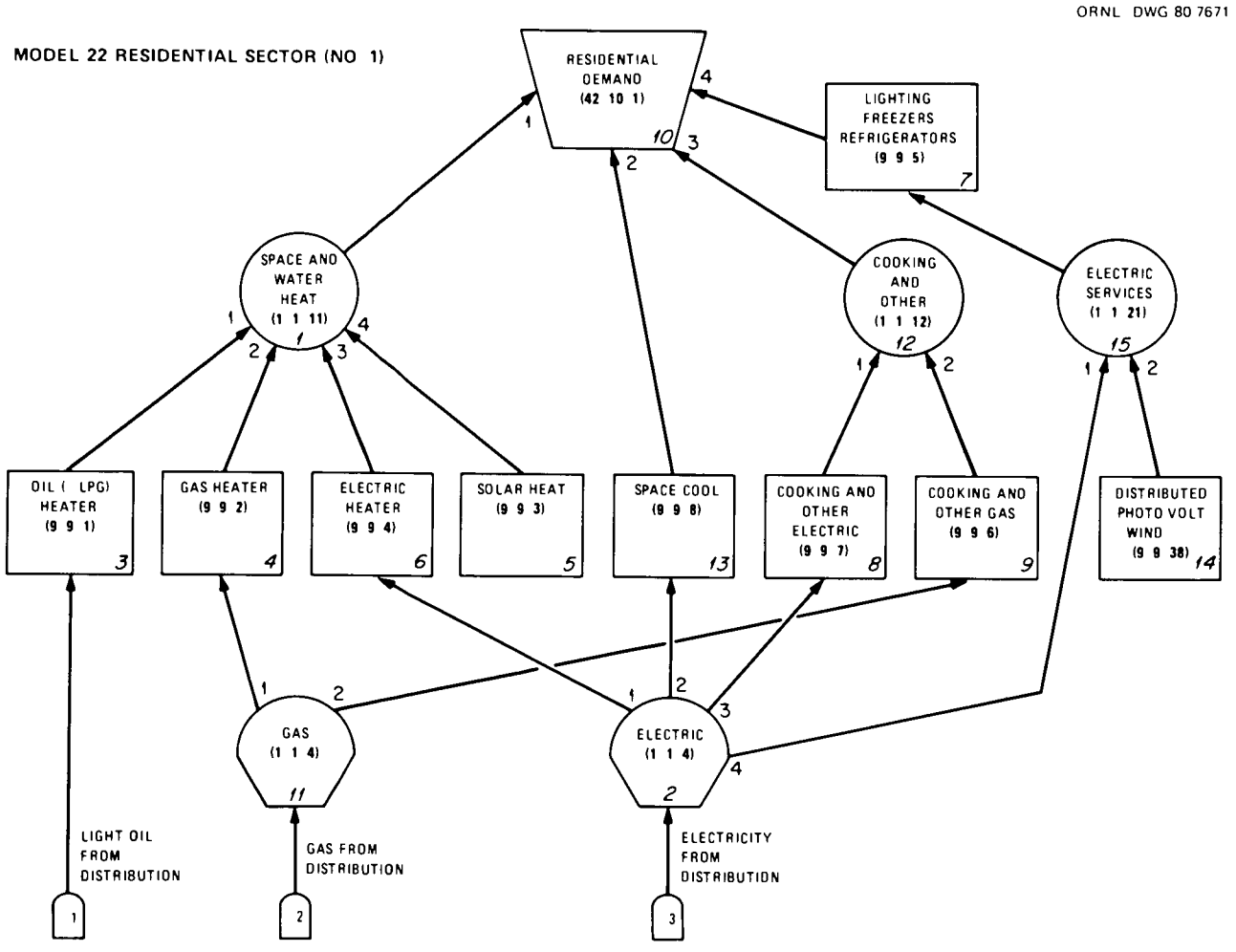


Figure III-2 Network diagram for the residential sector of LEAP Model 22C The numbered rectangular boxes represent aggregate national energy-related economic activities, and the lines represent the links between them along which the model estimates energy commodity and payment flows for time points 1975 through 2020 The links are numbered in accord with model input and output tables The circles represent the process of allocation of demand among two or more competing suppliers The intersectoral links can be traced in Figure III-1 *Activity 7 is labeled "Lighting and Electrical Appliances" in the model input tables

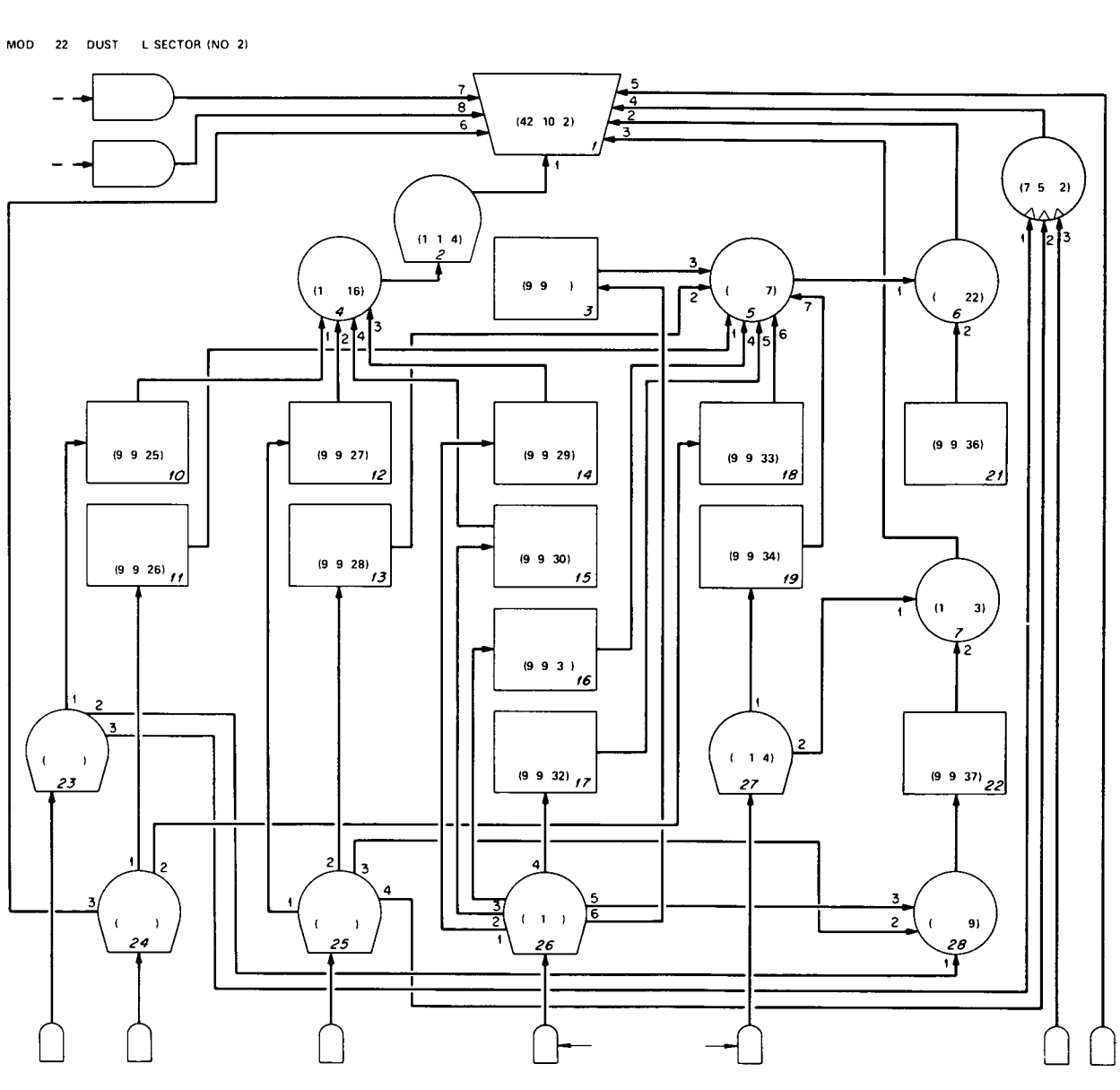


Figure III-3 Network diagram for the industrial sector of LEAP Model 22C (See caption of figure III-2 for basic symbology) Node (activity) 22 represents facilities in the industrial sector to generate electricity at industrial sites or to replace use of utility electricity

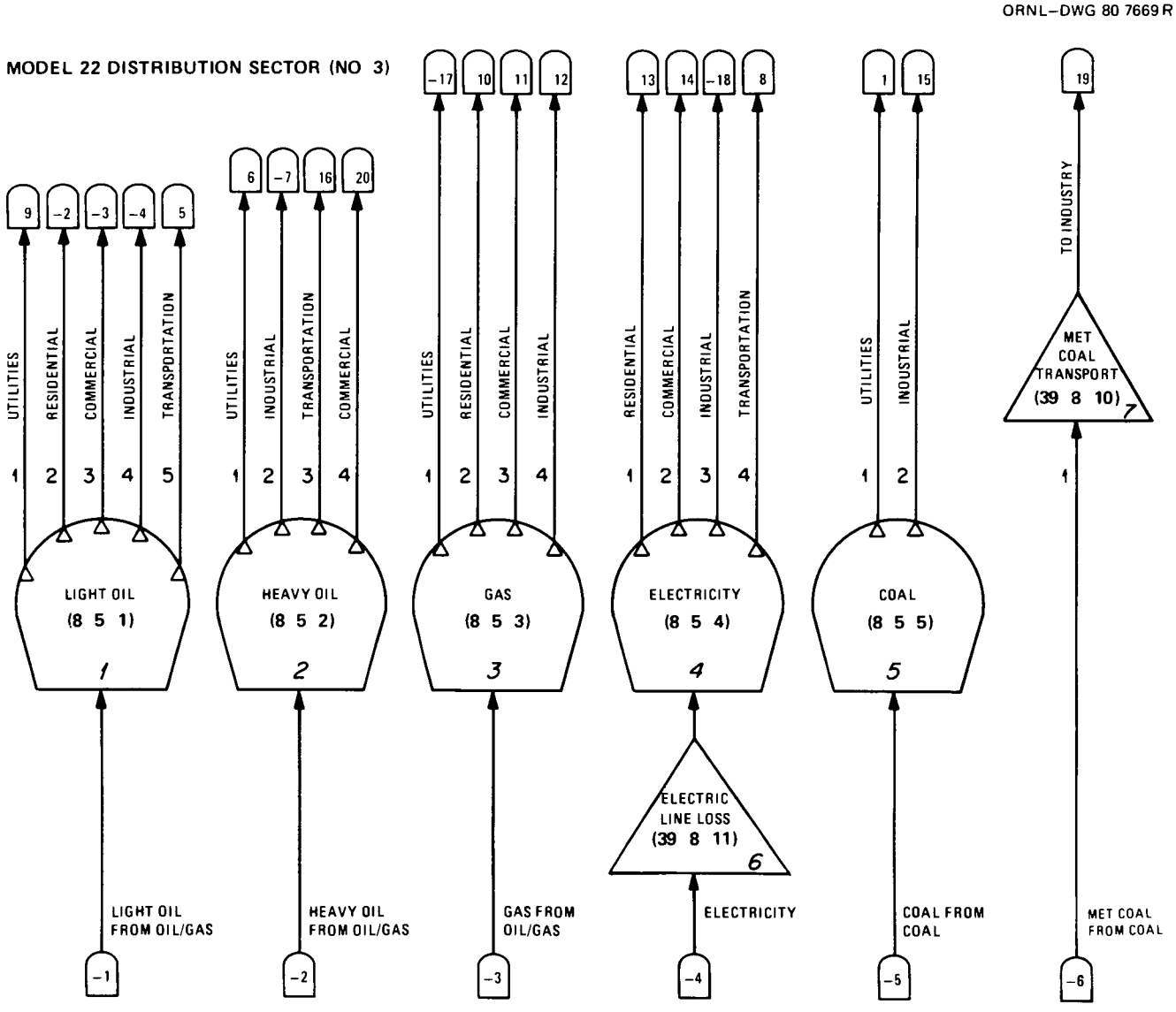


Figure III-4 Network diagram for the distribution sector of LEAP Model 22C (See caption of Figure III-2 for basic symbology) The large circles represent aggregation of demand from different sectors for each major fuel and the differential price incrementation from distribution costs

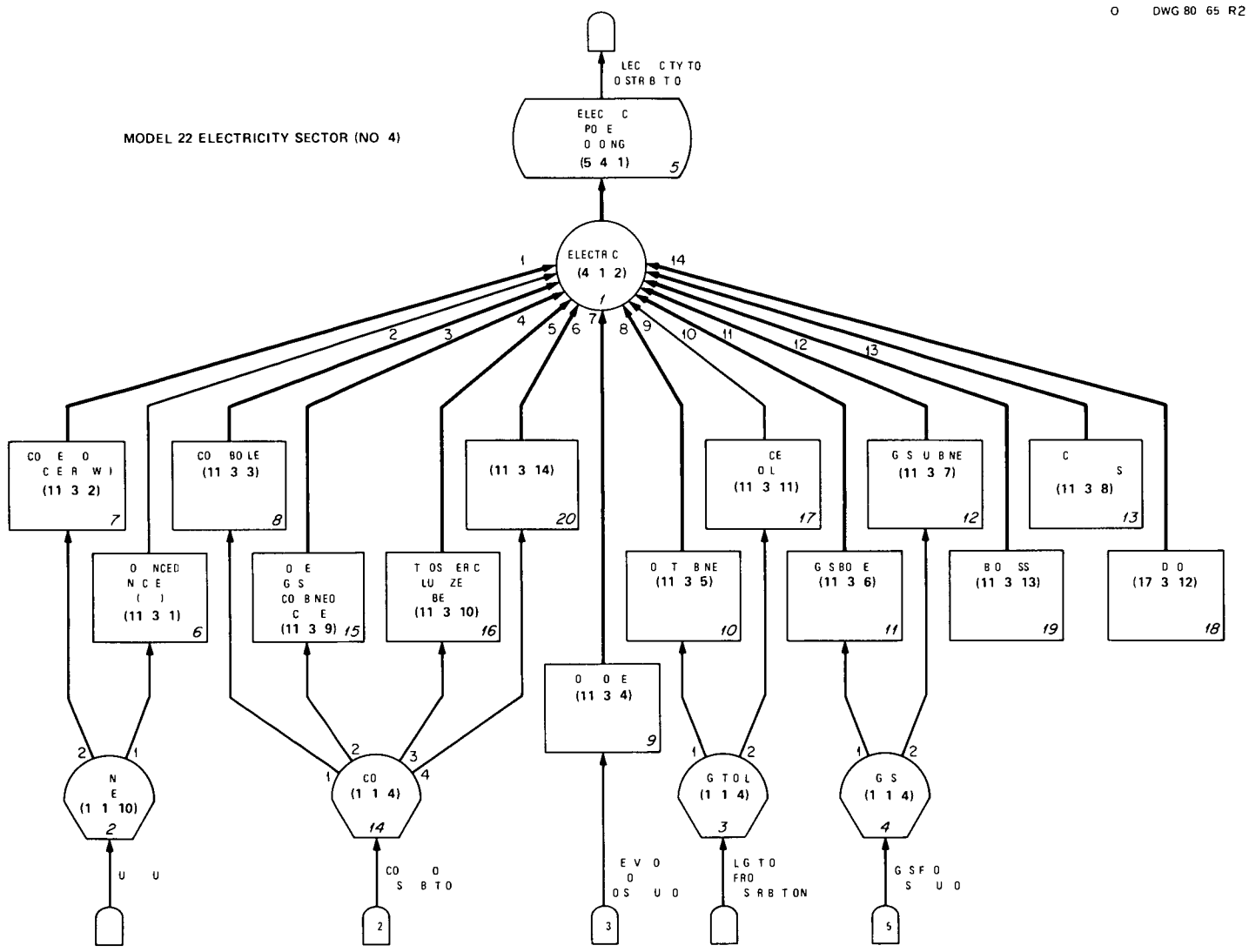
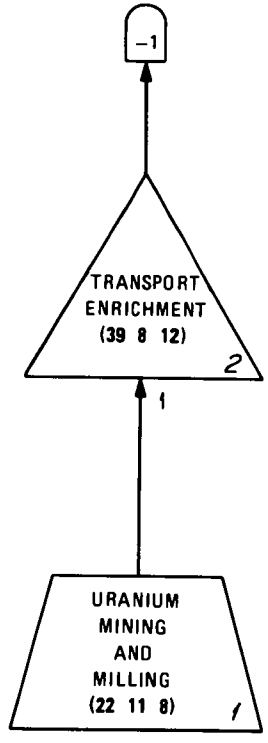


Figure III-5 Network diagram for the electricity sector of LEAP Model 22C (See caption of Figure III-2 for basic symbology) Electric generation by central utilities is represented by three load categories, thus most lines connecting generating activities to the electricity demand allocation node represent three "sublinks" for base, intermediate, and peak loads

ORNL–DWG 80 7677

MODEL 22 NUCLEAR SECTOR (NO 5)



MODEL 22 IMPORTS/EXPORTS SECTOR (NO 10)

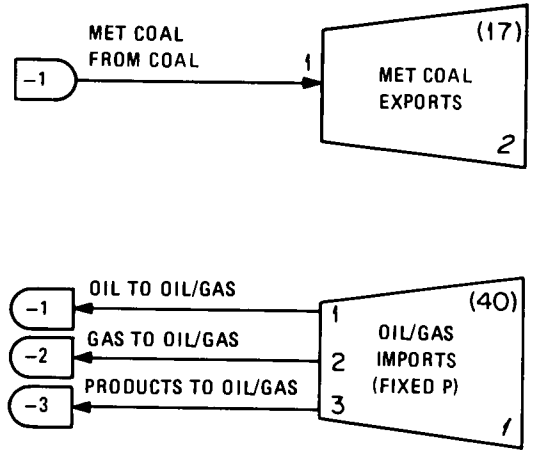


Figure III-6 Network diagrams for the nuclear and imports/exports sectors of LEAP Model 22C (See caption of Figure III-2 for basic symbology)

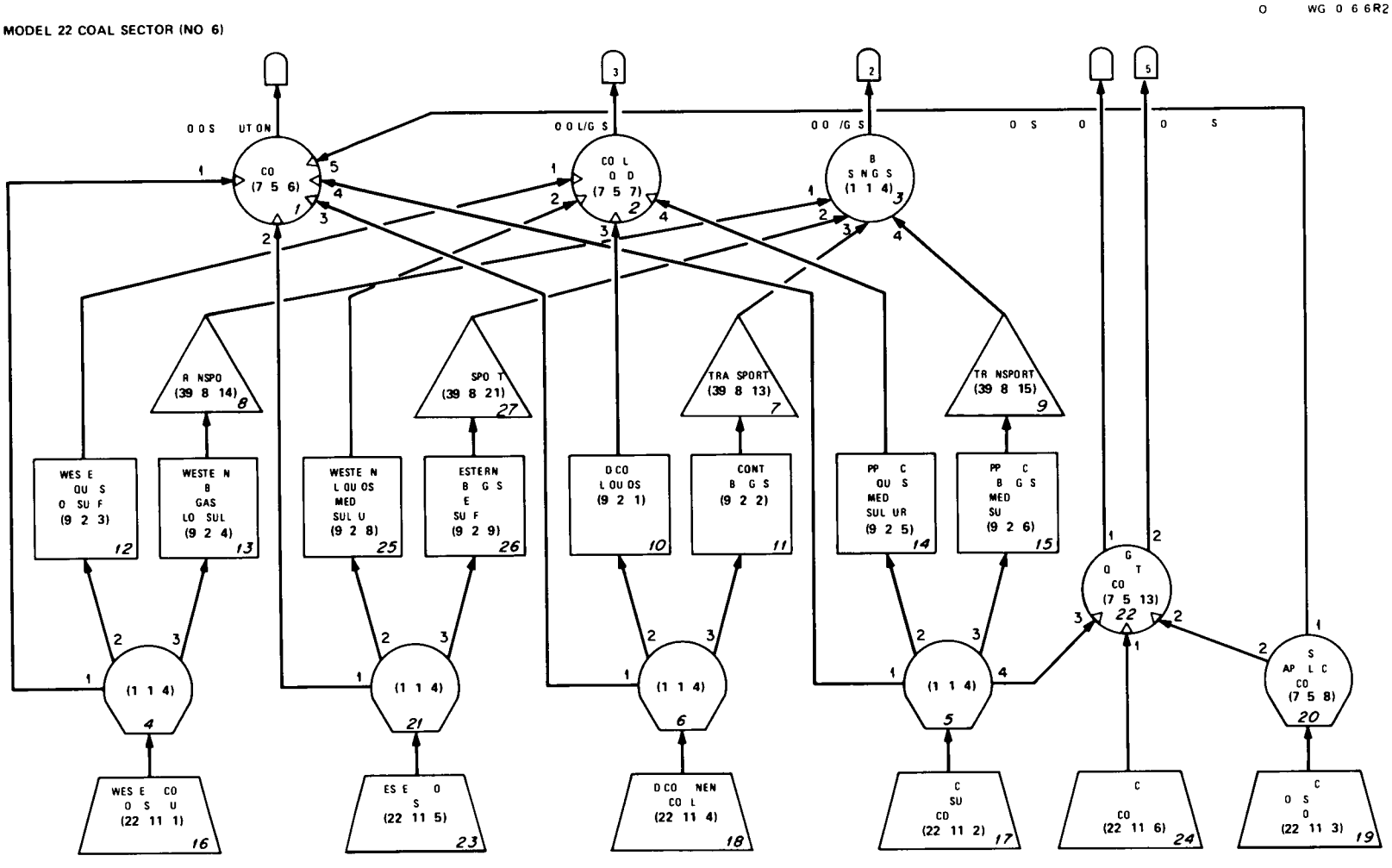


Figure III-7 Network diagram for the coal sector of LEAP Model 22C (See caption of Figure III-2 for the basic symbology)

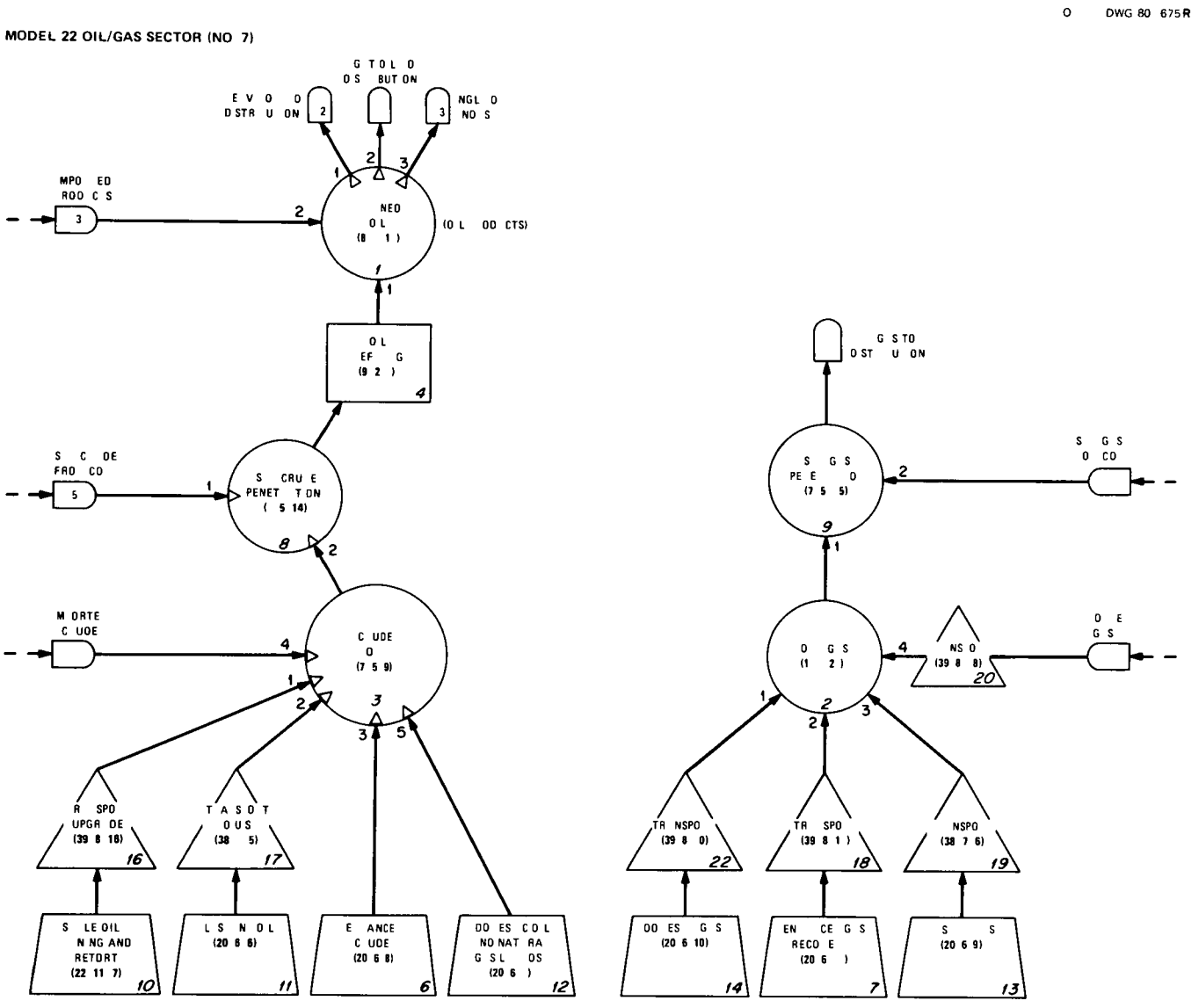


Figure III-8 Network diagram for the oil/gas sector of LEAP Model 22C (See caption of Figure III-2 for basic symbology) *In the model input data tables, node 11 is labeled "North Slope Oil," node 12 is labeled "Domestic Oil and Associated Gas," node 14 is labeled "Non-Associated Gas," and node 13 is labeled "North Slope Gas "

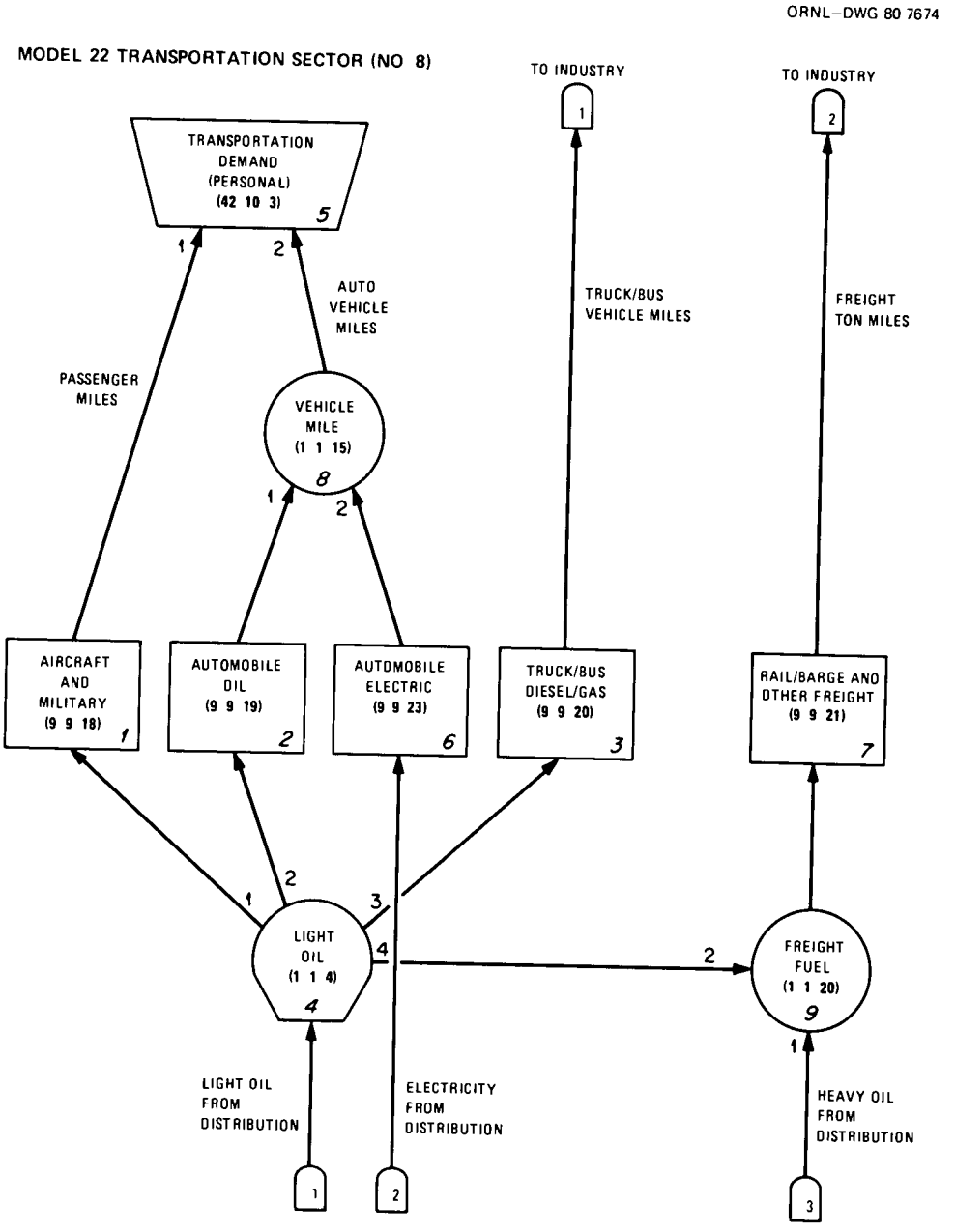


Figure III-9 Network diagram for the transportation sector of LEAP Model 22C (See caption of Figure III-2 for basic symbology)

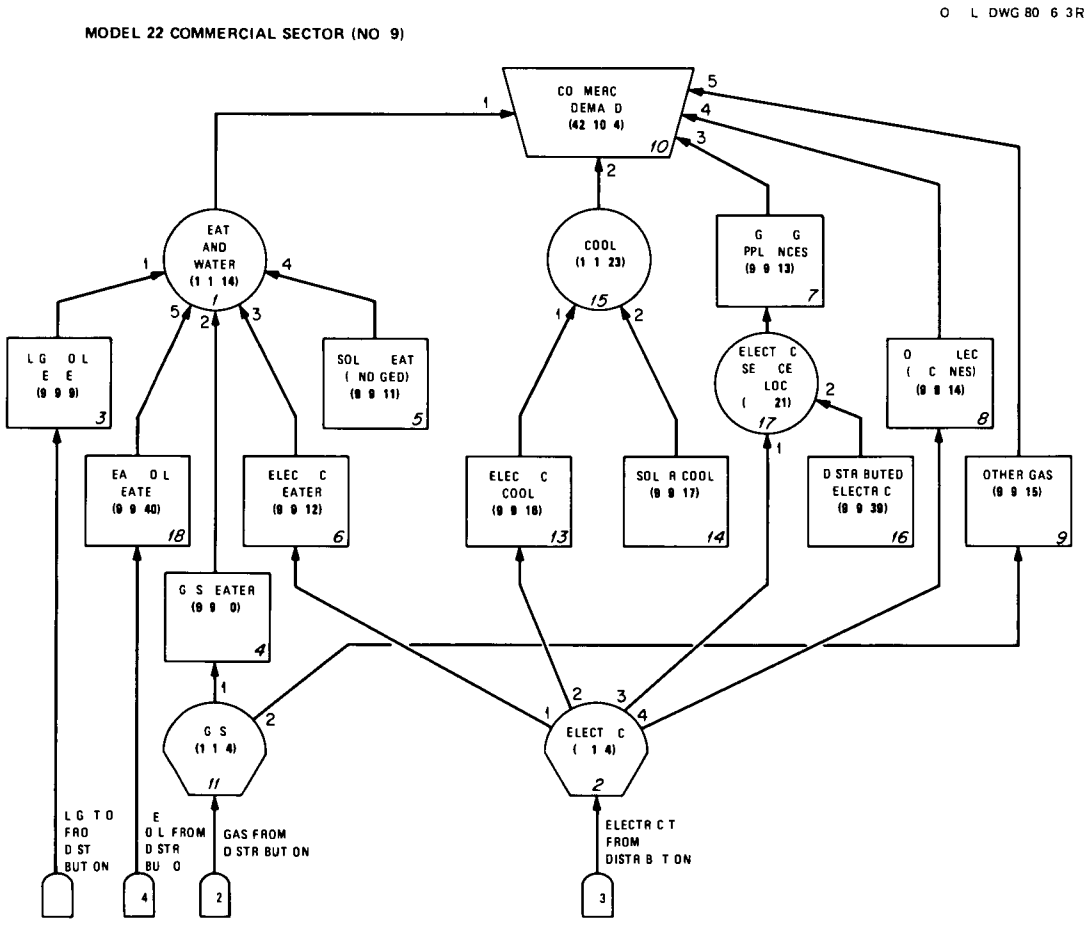


Figure III-10 Network diagram for the commercial sector of LEAP Model 22C (See caption of Figure III-2 for basic symbology)

X introduces the data base used in Model 22C More complete characterization of the implications of the flow charts can be expected in topical reports from this project

Some of the limiting assumptions of Model 22C are apparent from Figures III-2 through III-10 For example in the resource area the subdivision of the oil and gas resource base must be rather arbitrary because (1) natural gas liquids production results from decisions on natural gas rather than decisions on oil, (2) associated gas production is linked to oil drilling investment, (3) the same drilling machinery is used for both oil and gas, and (4) "enhanced recovery" refers to a continuum of options

There were, in Model 22C other examples of limiting assumptions One is the treatment in the "refined oil allocation" of all oil and gas liquids as if they were interchangeable in the marketplace Related to end-use demand are the problems of neglected cross-elasticity (or demand allocation) in cases where competition is possible (e g air vs auto transport) and the lack of representing investments in capital stock modification (retrofit) to effect energy conservation Presumably the impact of some of these network assumptions was investigated and found unimportant although the literature does not contain documentation Nevertheless necessary decisions on network approximations do constrain the ease of obtaining parameters and the class of questions that can be addressed with the resulting model On the other side a simpler network could encompass the major energy flows and one would assume that initial penetration of each new technology could be studied as a perturbation to this system of major flows This conflict--simplicity vs completeness--is ever present in modeling complex systems

3 Process Subroutine Definition

The flowcharts (Figures III-2 through III-10) contain the information keys precisely defining model equations and data Each activity label shows in parentheses (LKN, GP SP) the logical kind number (LKN) generic process (GP) type and specific process (SP) type, as defined in the data input Activity Pointer Table (MIT 7) Functions of these keys are indicated in the next paragraphs

The LKN value designates the subroutine that embodies the model specification for the particular activity and is called within LEAP to generate estimated prices and energy flows at each iteration (At each node subprogram SOLVE reaches a computed GO TO statement through which the LKN specifies the main subroutine sequence to be used at that node)

Table III-1 indicates the LKN values used in Model 22C, the names of the main subroutines thereby called and the extent of use Note that more than one LKN value calls a given subroutine, in this case switches within the subroutine produce relatively minor changes in specification Those uses of the demand allocation subroutine for nodes that have only one energy flow input are counted separately because no allocation of demand among competing suppliers is required These activities just aggregate demand at a single price from two or more

TABLE III 1

Use of LEAP Subroutines in Model 22C

S broutine Name	LKN	Title	Usage by Sector[a] 1	2	3	4	5	6	7	8	9	10
ALCNHO	1	Al ocation of dema d	3	5	0	0	0	1	1	2	3	0
	4	Allocation of demand for electricity	0	0	0	1	0	0	0	0	0	0
	7	Allocation of demand With price increments before[b]	0	1	0	0	0	3	3[e]	0	0	0
	8	Allocation of demand With price increment after[c]	0	0	0	0	0	0	1	0	0	0
	1 7	Common supply[d]	2	5	0	4	0	5	0	1	2	0
	8	Common supply With price increment after[c]	0	0	5	0	0	0	0	0	0	0
ALDUPR	5	Load duration process	0	0	0	1	0	0	0	0	0	0
CNHOLP	9	Homogeneous flat load conversion (basic conversion)	9	13	0	0	0	8	1	5	11	0
	11	Homogeneous load profile conversion	0	0	0	14	0	0	0	0	0	0
DUMMY	17	(No computation[f])	0	0	0	1	0	0	0	0	0	1
RESORC	20	Resource process	0	0	0	0	0	0	6	0	0	0
CESORC[g]	22	Coal resource process	0	0	0	1	1	6	1	0	0	0
TRNSPT	38 39	Transportation	0	0	2	0	1	4	6	0	0	0
IMPORT	40	Oil/gas import	0	0	0	0	0	0	0	0	0	1
DEMAND	42	End use demand[h]	1	1	0	0	0	0	0	1	1	0

[a]Numerical values indicate the number of activities by sector that are modeled with the d cated s bro t ne and logical kind number Sector numbers correspond to numbers in F gu e III 1

[b]For LKN - 7 p ice ncrements a e added to li k prices from the alternative sources of energy flow before the demand is allocated among these sources s for LKN = 1 and before the weighted average price is calculated

[c]For LKN 8 price increments are added to link prices for the various energy flow destinations without affecting the allocation of demand or the prior calculation of a weighted average price

[d]Allocation with only one source of energy flow Energy demands are added to form an aggregate demand all prices are the same

[e]Syngas penetration actually has zero transportation increments

[f]The metallurgical coal export activity has no process subroutine associated with it therefore initial estimates of quantity cannot be altered by the model during iteration toward a solution Hydroelectricity production is also handled with a dummy process e allocation of electricity demand treats this input as a special case

[g]Modified version of RESORC

[h]The end use demand p ocess includes a separate demand function for each link thus there are actually 19 such independent demand functions

higher-level nodes Table III-1 identifies by name the process subroutines called out in the flowcharts and thereby shows that only eight different main subroutines (together with the associated lower-level subprograms) are used to model all the activities in the energy sector of the economy

Generic and specific process indices given on the flowcharts precisely identify many of the input data required by these process subroutines For example, time-independent parameter sets that are held fixed for whole classes of activities are given different GP indices and are tabulated in MIT 11, whereas the parameter sets that are rather unique to one or a few activities are identified by (GP, SP) pairs and are tabulated in the more extensive MIT 12

The process subroutines require detailed evaluation of their appropriateness to represent the various energy-related activities However a few comments can be made here Oil and gas imports are estimated at a stated price, with no constraints on quantity, this assumption seems to be at odds with reality unless projected imports decline The basic conversion process discussed in detail in Sections V and VII, seems more appropriate for modeling major facility construction decisions than for representing equipment procurement in the energy demand areas A much larger number of small decisions commonly occur in equipment procurement, which often includes renovation as well as new construction, than in major facility construction Most of the process subroutines, except the DEMAND and IMPORT subroutines (both relatively simple) have been documented [7]

4 Model 22C Input Data*

For each resource and energy conversion activity Model 22C requires the technical and cost data that are needed to estimate, at each model time point, the present discounted value of the stream of future net dollar flows associated with the model energy flows The real allocation processes require the relative energy flows (market shares) of the various inputs for the initial model year (1975) and the parameters modeling the price- and time-dependent market penetration dynamics for all model time points The demand activities require for each link the indices of activity (taken as projected GNP) sensitivities of each individual end use demand to these activity indices elasticities Energy import prices, hydroelectric production and metallurgical coal export quantity are required for each time point Most parameter values are independent of time because of the assumption of dollars of fixed value for labor materials, and cost of capital

To determine values for all these parameters economic data, previous model descriptions of economic behavior, process cost estimates, and the outputs of other models were used [1,23] These models included

*See Section X for a more detailed discussion of Model 22C input data

macroeconomic projections outputs from the EIA Mid-Term Economic Forecasting System for year 1995 and a variety of more informal models Parameters were taken directly from the macroeconomic model output, but were determined indirectly from the mid-term models through a process of parameter adjustment to cause Model 22C results to give about the same results through 1995 Although the use of intermodel calibration makes evaluation of Model 22C relatively difficult the process can be reasonable if (1) the mid-term models include relevant considerations that are not handled by LEAP and (2) the implied LEAP parameter values are consistent with independent information

C Use of Model 22C for the 1978 Annual Report To Congress

1 Findings That Were Given Emphasis

Highlighting the major findings given in the 1978 EIA Annual Report to Congress should clarify those results that are considered significant and that therefore deserve attention in the model evaluation effort Because the Office of Applied Analysis uses its Mid-Term Economic Forecasting System for projections through 1995 and because some of these projections are used indirectly to calibrate the Model 22C input parameters the Model 22C output values of major interest are for the years 2000 through 2020

Table III-2 lists some qualitative findings emphasized in Reference 1 In the right-hand columns are values taken from tables in Reference 1 that support these conclusions the results depend on the major coordinating assumptions detailed in Table 5 1 of Reference 1 as well as on numerous other data and assumptions The conclusions are roughly ordered with those judged the least secure or significant located toward the bottom Note that in some cases groups of assertions must be taken together to have significance

The qualitative statements in Table III-2 may reflect the most useful model results for a reader or decision maker whereas the numerical values often suggest the amount of output variation that could be tolerated without modifying this qualitative conclusion Our ranking of conclusions does not mean that other more important conclusions have not been obtained by other persons using the results of Reference 1

Some of the qualitative conclusions in Table III-2 such as conclusions 1 4, and 5 seem to concur with the common understanding of energy affairs Other conclusions however, seem to differ markedly from a superficial reading of our past experience For instance,

1 The reduction in residential sector demand (conclusion 3) might seem unlikely in the face of an overall population increase of about 40%

2 The increase in total domestic natural oil production by year 2000 (conclusion 6) differs from recent experience

TABLE III 2

Major Co cl sions f om LEAP Model 22C Res lts[a]

	Qualitative Conclusions	Table Number (In Rerere ce 1)	N erical /alues by Year 1977	2000	2020
1	Coal becomes the dominant primary energy source	5 2	20%[b]	38%[g]	46%
2	Industrial sector increasingly provides the largest sectoral demand	5 2	39%[c]	51%[g]	60%
3	Residential sector demand peaks in the mid term	5 2	11 quad[d]	12 quad	10 quad
4	Relative end use consumption of gas and liquid fuels will decrease through year 2020 to 50%	5 6	83%[e]	65%	50%
5	The relative electrification of our energy end uses will continue to increase through year 2020	5 6	11%[f]	18%	23%
6	Total domestic natural oil production will rise through the mid term but will fall below its present level before vear 2020	5 12	20 quad	23 quad	15 quad
7	Oil imports steadily decline reflecting a dramatic trend toward energy independence	5 12	18 quad	11 quad	7 quad
8	The 1977 total util zation of liquid fuels can be maintained (despite items 6 and 7 above) because of rapid production increases of shale oil and liquids from coal	5 12	38 quad	39 quad	39 quad
9	Total direct and indirect end use of renewable energy sources (including hydroelectricity) is projected to grow slowly includes geothermal efficiencies were approximated to obtain these values from data in Reference 1	5 8 5 9	0 8 quad	2 quad	4 quad
10	By year 2020 most of the coal for electricity generation is expected to be used in the new technologies	5 8	0	38%	59%
11	Primary energy prices will rise more slowly from year 2000 to 2020 (a) crude oil (b) natural gas and (c) coal (prices are in 1978 dollars per million Btu)	5 4 (a) (b) (c)	1 6 0 8 1 0	4 1 3 4 1 2	6 0 4 8 1 6
12	U S primary energy use increases to 169 quads in year 2020	5 2	80 quad	125 quad	169 quad
13	U S total energy end use consumption increases to 104 quads in year 2020	5 2	61 quad	86 quad	104 quad

[a]These conclusions were drawn from the present authors reading of Reference 1 based largely on the empha s wh ch seemed to be given the e

[b]The percentage of the total primary energy supply pro ided by coal

[c]The percentage of total sectoral demand used by the industrial sector

[d]1 quad 10 ^{5} Btu

[e]The percentage of all end use consumption provided by gas and liquid fuels

[f]The percentage of all end use consumption p ovided by electricity

[g]The percentage of all coal sed for electricity generation that is used in new technologies

3 The decline in oil imports (conclusion 7) seems optimistic at the assumed prices

4 The flat consumption of liquid fuels in time (conclusion 8) accompanies an assumed 230% overall increase in real GNP

5 The rate of conversion to new coal-electric technologies (conclusion 10) requires historically rapid introduction

6 Slow projected price increases after year 2000 (conclusion 11) seem too good to be true

However one goal of modeling is to uncover ideas that are less than obvious

The application of LEAP to annual report projections differs somewhat from its potential use for analyzing R&D alternatives or for determining long-range implications of taxes or other incentives that might be used to encourage particular technologies Yet because the nominal projections do show growth and abatement of some major energy technologies one can reasonably assume that some of the model facilities and capabilities necessary for such analyses are present

2 Relationship of Published Results to Raw Model Outputs

An audit was undertaken to determine whether the solution obtained from LEAP Model 22C, when run by the ORNL evaluation group, is the same as that reported in Reference 1 The meaning of some of the tables in Reference 1 was clarified in the course of these comparisons Following these clarifications the ORNL group[24] concluded that the model and data made available to us are the same as those used in preparing Reference 1

Three different sets of Model 22C printout, all compiled from the same underlying solution for prices and energy flows were used in the audit The most useful output was that generated by the RPORT subroutine These data should not be exactly identical to those studied at EIA in the preparation of Reference 1 because one or two additional model iterations were performed to obtain the output therefore values were considered to be in agreement if they differed by less than 0 1 x 10^{15} Btu or 3% of the quoted value, whichever was greater RPORT combines the output from the desired nodes into a labeled tabular form that closely parallels the tables in Reference 1 The other two sets of output were differently organized tabulations of output quantity and price at each node

Because the primary goal was to assure that the correct model was being evaluated in most cases the audit was satisfied whenever the RPORT printout agreed with the corresponding table in Reference 1 (Therefore we cannot at this time report whether or not all published table captions not discussed below unambiguously describe the tabulated

~~RPORT printout agreed with the corresponding table in Reference 1. (Therefore, we cannot at this time report whether or not all published table captions not discussed below unambiguously describe the tabulated~~ combinations of energy flow) When a particular value evoked interest or when the output from the RPORT subroutine did not seem to agree with Reference 1, the raw model outputs were inspected to determine which energy flows were combined to form the published tables

In some cases apparent inconsistencies were quickly resolved In other cases more explicit labeling of the data tables in Reference 1 would have been useful to prevent reader confusion Some examples from Reference 24 are given in the following subsections

a Values for sectoral energy disposition (Table 5 2, Reference 1) were not generally measured at the inputs to the sectoral end-use DEMAND activities, as one might assume (see Figures III-2, III-3 III-9, and III-10) The tabulated results are in fact the sum of all the inputs into each demand sector (as at the bottom of Figure III-2 for the residential sector) plus any energy generated within the sector (i e , solar geothermal, etc) Industrial sector use also includes energy used to refine oil in the oil/gas sector

b The utility conversion losses (Table 5 2, Reference 1) include all the heat energy losses in electricity production from coal oil or other fuels (Figure III-5) plus, for example, the conversion loss that would occur if hydroelectric energy were produced by burning fossil fuel (efficiency = 1/3) The tabulated synthetic fuel conversion loss includes losses in making synthetic gas from coal in the coal sector but not the losses in making low-Btu gas in the industrial sector

c The footnote on Table 5 4 of Reference 1 indicates that the tabulated primary energy prices were determined at a point in the network as close to the resource point as possible and evaluated using a weighted average (based on output quantity) In the case of crude oil prices this note must be understood to imply that prices were taken at the crude oil allocation node in the oil/gas sector and that they include transportation costs Price increments are found in specific process data for generic process 5 Imported oil is excluded from these average prices [25]

d The value of 0 7 quad for solar energy end-use consumption in the residential sector (Table 5 6 of Reference 1) is not found in the Model 22C output for the solar heat activity likewise, the value for electrical energy usage (in Table 5 6) is less than the value given in the model output by a corresponding amount Diedrich et al [23] indicate that the lack of adequate data on solar installations led the Office of Applied Analysis to "drop" that node and correct the electric heater

node to cover the combined input A November 1979 communication from John Pearson[26] clarified that the model node for residential electric heat accounted for a combination of resistance heating, heat pumps, and solar heating Details were given of an off-line analysis, which indicated that the presence and assumed use of the solar option had reduced the required electric input (for the given demand) by about 0 7 quad

e The low-Btu gas flow (Table 5 9 of Reference 1) is not available in any form in the RPORT printout Clarification from Mary Hutzler[25] described the "lo-med Btu with combined cycle" activity in the electrical sector as part of the industrial process Therefore part of the energy output could be counted within the constraints of Table 5 9 An off-line determination was made concerning the share of energy that would be counted as low-Btu gas production

The experience of performing this output audit indicated the need for great care in preparing publications based on energy model results The subdivision of our energy system into any model network is partly arbitrary the inherent ambiguities can be resolved only by precise definition

3 Model 22C as a Public Model

Is Model 22C a public model? Model 22C was used initially to provide the long-term projections in Reference 1 which contains major results and a tabulation of the major assumptions built into the model When Reference 23 is published the network and a first-order explanation of the input data selection will be readily available Most of the process subroutines have been described in Reference 7 which is, however an unnumbered report that documents the routines before any EIA modifications The Office of Applied Analysis staff has been generously helpful to us in resolving many questions that have arisen during our evaluation efforts Presumably the 1979 EIA Annual Report to Congress will contain projections from an updated LEAP model In this environment what standards can be used to judge whether Model 22C is adequately documented? The question actually relates more to any future version than to Model 22C and any answer suggested in this report can serve only to stimulate assessment of the standards that might then be applied (The EIA does have some standards [27] and the Government Accounting Office has prepared a draft report on evaluation guidelines relating to model documentation needs)[28]

All citizens depend on timely and unbiased information, and livelihoods of many depend directly and strongly on an understanding of what is already known about our future energy system Because the EIA is one of few data sources without an inherent motivation toward bias the question of the extent to which Model 22C and its results are effectively public is important

To be public more is required than not to be secret! A concerned person must be able to obtain assumptions and results in whatever detail necessary without imposing with many questions on the time of the group responsible for further development and application of the model Details (possibly partly on magnetic tape) need to be released within a period that is commensurate with the timing of modifications to the model and with the release of new sets of projections Such documentation must include reasoning as well as numbers

Before the consequences of these proposed principles can be worked out the present concept must be clarified that the model as well as the modeler, has objective reality One may accept that a prime function of using a model like LEAP is for the modeler to gain insight about interactions among the facets of the economy However the thesis here is that the public modeler needs to strive to organize the results so that the insight can be transmitted to an interested person on the basis of the model and its results rather than solely on the modeler's assertions

Acceptance of the principles given earlier for related model results exhibited in a sequence of EIA annual reports would imply that detailed network parameter input and solution output must be generally available within a few months of the annual report itself Documentation of any changed portions of the model specification (the process subroutines) and details of the relation between model output data and the results tabulated in the annual report would also be required on this time scale The data base documentation files would need to be arranged so that the exact source of numerical input values could be traced Reference to an organization as a data source would be inadequate Availability of working code packages that can be made to function on an outside user's computer as suggested by Holloway et al[29] might also be needed Careful and thorough publication of the model specification and its justification would be necessary but could proceed over a longer time if the mathematical formulation changes slowly from year to year

Would application of the above standard be impossible in practice even if the required documentation files were prepared in the course of model development? Perhaps some goals must remain unrealized but if considerable commonality among model data bases were established and models were not totally revised in successive years these necessary goals for a public information model could be approached in practice

D Important Responses for LEAP Evaluation

To properly concentrate the detailed evaluation of a model, the "responses" (i e results) of primary interest should be explicitly defined A response is defined as a specific combination of the model output values chosen because it is the quantity that relates a user interest to the model output in a precise manner For LEAP the model outputs are the prices energy flows and perhaps capacity additions when convergence has been achieved A general consideration of important responses is needed to form a basis for even a qualitative evalua-

tion of a model and to focus on the portions of the input data base and model specification of most concern Determination of sensitivity coefficients by the adjoint technique (Section IX) requires precise definition of each response The responses chosen should isolate as clearly as possible the points of concern so that computed values will be minimally influenced by uncertainty in parameters not directly relevant to the issue For this reason important responses will often not be simple sums or averages of the model variables

Table III-3 lists responses believed to be significant for LEAP the list is representative rather than exhaustive but is perhaps still too long for comprehensive numerical coverage Many of the listed responses are related to the major conclusions given in Table III-2, whereas others relate more to the potential use of the model for investigating energy research and development options The listed responses are for the year 2010 but the behavior of similar quantities for the years 2000 through 2020 would be more interesting An effort was made to include several forms of response and to focus on various parts of the model network

To give an indication of how well each response might have to be estimated to avoid forming an incorrect conclusion, an accuracy tolerance for each response projection has been estimated and is listed in Table III-3 For a different conclusion this tolerance may be unnecessarily narrow for example an error in estimating which fuel types or technologies can become important is much more serious than an error of a few years in estimating the timing of the corresponding industrial transition Relative to questions for which resource depletion has a dominant influence "time" could be measured in cumulative GNP or cumulative world oil consumption rather than in years in order to stabilize projections of interfuel competition The purpose for including these first estimates of tolerances into Table III-3 is to introduce the idea that numerical uncertainties in key responses should be estimated even if the model is to be used primarily to gain insight through qualitative conclusions from model results

TABLE III 3

Important LEAP Responses for Year 2010

	Definition of Model Response	22C Numerical Value	± Tolerance[a]
1	Total annual cost of energy to end users per GNP[b c]	0 16	± 0 03
2	Net energy import cost per GNP[c]	0 008	± 0 01
3	Industrial sector annual energy demand as a fraction of total end use demand[d]	0 56	± 0 15
4	Electricity fraction of total end use sector demand[d]	0 21	± 0 07
5	Direct plus indirect annual end use of renewable resources relative to total end use sector demand[e]	0 03	± 0 01
6	Fraction of non renewable domestic primary energy supply provided by coal[f]	0 45	± 0 1
7	Total domestic annual production of natural oil and gas[g]	35×10^{15} Btu	$\pm 5 \times 10^{15}$ Btu
8	Total annual imports of oil oil products and gas	9×10^{15} Btu	$\pm 5 \times 10^{15}$ Btu
9	Total production of domestic shale oil coal liquids and high Btu synthetic gas	12×10^{15} Btu	$\pm 5 \times 10^{15}$ Btu
10	Change in response 1 with a long term tax subsidy equivalent to a 25% capital cost reduction for solar heat capital cost in the residential and commercial sectors	h	30% of change
11	ensitivity of response 1 to the date of commercial availability of all coal liquid conversion technologies	i	30% of sensitivity

[a]Defined so that if there is about a 2/3 probability that the true value lies in the range of ±1 tolerance around the value projected by the model important qualitative conclusions from Model 22C similar to those of Table III 2 remain valid (The values given in this table are estimated tolerances there is no implication that these tolerances are met or not met by output from Model 22C)

[b]Computed from link data to end use demand activities

[c]Based on 1975 GNP of $1 53 x 10^{12} in 1975 ($) Report of the (U S) Council of Economic Advisors U S Govt Printing Office p 183 (January 1979)

[d]Sectoral inputs of electricity are valued at their heat content Coal export is not considered a demand here Total is based on residential industrial commercial and transportation sectors measured at the sector input except for generation within the sector From Table 5 6 of Reference 1

[e]Hydropower and geothermal are included as renewable

[f]Exported coal is not included Renewables and geothermal are also not included LWR nuclear energy is figured as in Table 5 2 of Reference 1

[g]Includes Alaskan sources but excludes shale oil and coal liquids

[h]Model 22C will not support this response but a future LEAP EMS version could do so

[i]Model 22C results are not yet worked out

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IV THE STRUCTURE OF LEAP AND EVALUATION OF NUMERICAL SOLUTION TECHNIQUES

A The Structure of LEAP as Illustrated by a Simple Model

The LEAP system is designed for the study of complex energy systems Model 22C which was used to produce the results in Chapter 5 of Reference 1 is an example of such a complex energy system [2] The modular structure of LEAP also allows construction of very simple energy systems that even though much less complex still contain the main features of the LEAP system A sample model such as the one described in this section is beneficial in understanding LEAP and is essential for developing model validation methodology because it can be executed with a relatively small amount of computing time

A block diagram of Model 82, which contains two sectors, is shown in Figure IV-1 The fact that there are two sectors is not very important in this simple model, but can be of importance in more complex models because various kinds of input data (e g tax rates) may vary with sector The numbers to the left of the boxes called node numbers, merely determine position in a model diagram Each node number corresponds to a series of indices in the LEAP computer code this series of indices in turn determines the calculations that are done at each node The arrows that join the various nodes in Figure IV-1 are called links they represent the direction of energy flow For this discussion arrows entering a node from below (see Figure IV-1) are called input links to a process whereas arrows emerging from a process or node are called output links of that node

Nodes 1 and 3 (in Figure IV-1) are resource processes In LEAP a resource process describes the production of depletable resources (e g crude oil from well drilling) An arrow leads away from but not into, the resource process nodes (Figure IV-1) that is each resource process has an output link but no input link This feature is generic for all resource processes and has an important effect on the calculations that are done at a resource process node In Figure IV-1 nodes 1 and 3 are designated NORTH SLOPE OIL and DOMESTIC OIL, respectively This designation corresponds to that used in Model 22C, which means that in Model 82 all the input data at nodes 1 and 3 are taken from the corresponding nodes in Model 22C [2]

Node 2 represents a transportation process This process is used in LEAP to represent the increase in the cost of energy and any losses that occur as a result of transportation The parameters used in this transportation process in Model 82 are the same as those used in the corresponding node (i e , the node following the NORTH SLOPE OIL resource process) in Model 22C [2]

Imports (node 4 in Model 82) are treated in the same manner and with the use of the same data as in Model 22C [2] The price of imported oil (in units of 1975 dollars per million Btu) is input to LEAP as a

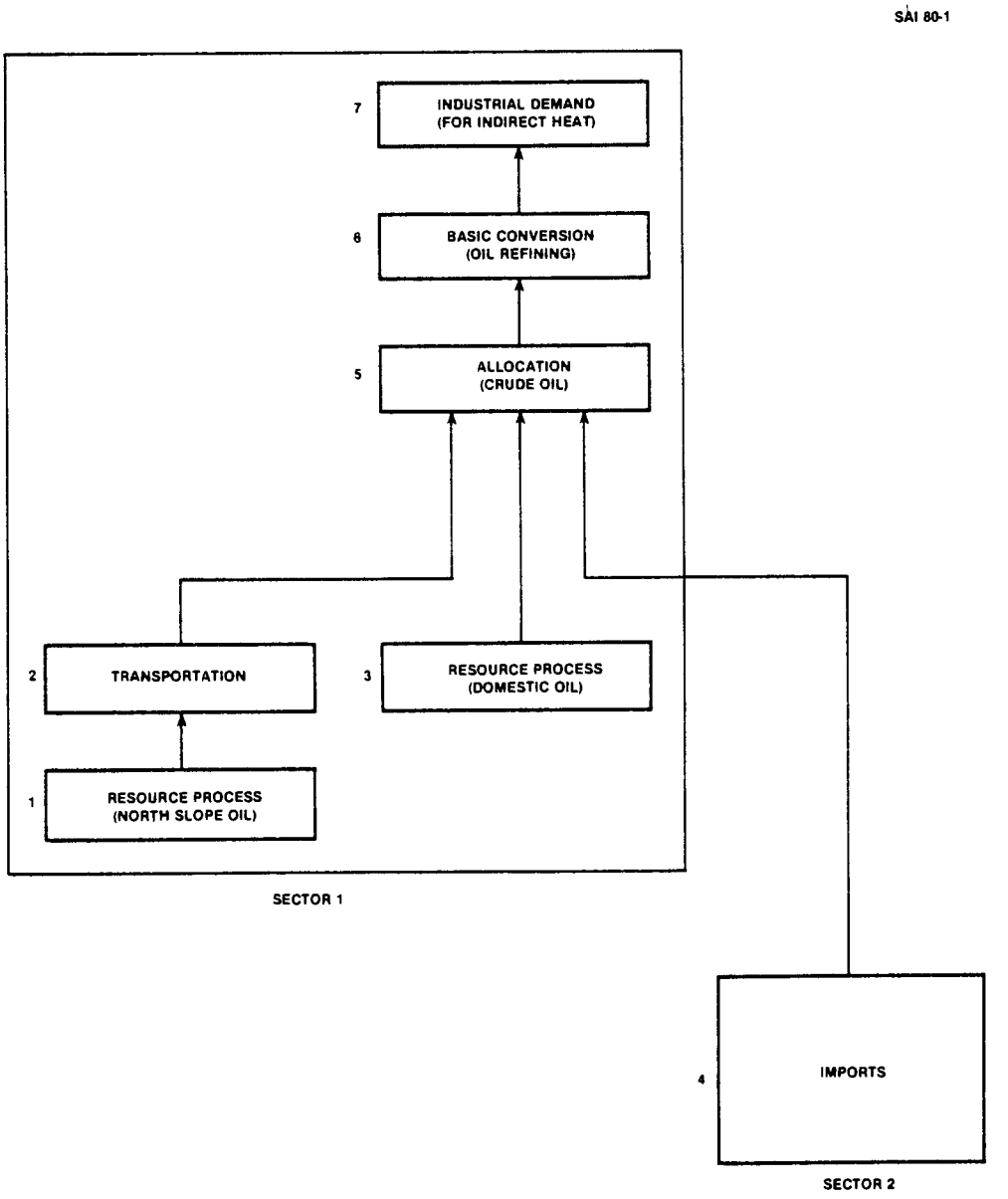

Figure IV-1 Block diagram of Model 82

function of time and it is assumed that at this price any required quantity of oil may be imported

Node 5 in Model 82 is an allocation process A function of an allocation process is to apportion the demand for energy among several competing suppliers As shown in Figure IV-1 an allocation process may have more than one input link The parameters at node 5 in Model 82 correspond to some extent to CRUDE OIL allocation in Model 22C [2] They are not the same as in Model 22C because there are more input links to CRUDE OIL allocation in Model 22C than in Model 82 and because the market share elasticity parameter and the behavioral lag parameter used here are 10 and 5 respectively whereas those used in CRUDE OIL allocation in Model 22C are 5 and 15 respectively The choice of parameters used here emphasizes the response of the allocation process to price differences between competing suppliers and to price changes in time Also the price correction due to transportation that is used in Model 22C CRUDE OIL ALLOCATION has been omitted

Node 6 is a conversion process In LEAP a conversion process is used to describe those technologies that convert energy from one form into another (e g oil refining) Electricity generation is a slight exception to this because the conversion process equations are modified to take into account different load categories that arise because of the fluctuating demand for electric power Formally this difference is not great and in the present computer version of LEAP the electric power generation subroutine with a single load factor is used for all conversion processes other than electric generation In this report the Decision Focus Inc nomenclature of using the term "basic conversion process" to refer to a conversion process that has only one load will be used [3] Thus node 6 in Figure IV-1 is a basic conversion process As indicated by the designation OIL REFINING the conversion data used in Model 82 corresponds to the OIL REFINING node in Model 22C [2]

Finally node 7 in Figure IV-1 is a demand process In LEAP the demand process is used to represent energy end-use consumption The parameters input to the demand process as a function of time determine to a considerable extent the amount of energy that is consumed over time There are in the demand process equations factors that tend to decrease consumption as the price of energy rises nevertheless the actual demand for energy over time is determined primarily by input data The parameters that are used at node 7 in Model 82 are those that are used in Model 22C for the INDUSTRIAL DEMAND (FOR INDIRECT HEAT) [2]

Figure IV-1 with the input data as specified above is a nearly complete specification of Model 82 To be complete initial values (discussed below) must also be specified The model is relatively simple, but the important point is that nearly all the processes that occur in Model 22C also occur in Model 82 In Model 22C the various processes (resource, conversion, etc) occur many more times than in Model 82 but these additional occurrences do not add anything fundamental to Model 22C that is not inherent in Model 82 Processes that are

included in Model 22C but not in Model 82 are a conversion process with several load factors and a distribution process that is similar to a transportation process Also in LEAP in addition to the resource process used here there is an additional somewhat modified resource process (in subroutine CESORC) that is used The fact that much of the data used in Model 82 are taken from Model 22C should prevent the occurrence of extremely spurious results from bad data, but, of course, the results from such a simple model cannot be expected to be realistic What is expected however is that Model 82 is sufficiently similar to Model 22C that theoretical methods that are demonstrated on Model 82 will, with a high degree of probability, be applicable to Model 22C

To further illustrate the LEAP system the variables in Model 82 (i e the quantities that are determined by the LEAP computer code) will be discussed The LEAP system uses discrete time points so that the variables are calculated only at specific points in time An index J that takes values 1 to N will be used to denote time variation In Models 22C and 82, N equals 10 and the time points considered are 1975 to 2020 with 5-year intervals

The variables of primary interest in Model 82 are the price per unit energy and the quantity of energy produced as a function of time on the output link of every process Other quantities are calculated in the code and could be considered variables In fact, in Section V, when the equations of the basic conversion process are considered, it will be convenient to consider plant capacity additions as variables, but for the present discussion the prices and quantities will be considered to be the variables of primary interest

If the variables on the output link of a node are indexed by the node number, the variables on the output link of node 1 in Figure IV-1 may be written

$$P(1\ J) \qquad J = 1\ N$$

$$Q(1\ J) \qquad J = 1\ N$$

where

P(1 J) = price per unit energy on the output link of node 1 at time J,

Q(1 J) = quantity of energy per year on the output link of node 1 at time J

Continuing this counting procedure, one would arrive at a total of 12 N variables--6 output links with 2 N variables on each output link This is incorrect however for two reasons First, the prices on the output link of node 4 IMPORTS, are specified externally and therefore are not to be considered variables Second in Model 82 the quantities Q(6,1) $\frac{1}{S}$ Q(2 1) $\frac{1}{S}$ Q(3,1) and $\frac{1}{S}$ Q(4,1) where S = Q(2,1) + Q(3,1) + Q(4,1)

(i e the quantity of energy per year that goes into the demand process at the first time point of the model as well as the fractional quantities that go into the allocation process at the first time point of the model) must be specified as initial conditions * These quantities must be specified initially because the demand equations and the allocation equations are such that quantities at later times are determined in terms of these initial quantities This then reduces the number of variables to 11 N - 4

The LEAP system is characterized as a generalized equilibrium system An excellent discussion of the meaning of this term and a comparison between general equilibrium models and other types of models have been given by Brock and Nesbitt [4] For purposes of the present discussion the term means simply that in LEAP a general balance exists between supply and demand that is all energy produced is used and conversely any amount of energy that is required can be produced at some price The LEAP system is such that there are enough equations to completely determine all unknowns In Model 82 this means that there are 11 N - 4 independent equations The equations are algebraic and very nonlinear The equations explicitly couple prices and quantities at both future and past times so that the LEAP system is not at all equivalent to a series of "static" models that couple prices and quantities at a specific time The coupled set of nonlinear equations is solved by an iteration scheme that is part of the LEAP computer code This iteration scheme is discussed in Section VII

In Table IV-1 the calculated results are given for Model 82 for the years 1995 and 2020 The results for the other years are also available, but for simplicity are not shown The initial values used in obtaining the results in Table IV-1 were those used for INDUSTRIAL DEMAND (FOR INDIRECT HEAT) and for ALLOCATION (CRUDE OIL) in Model 22C In both Models 22C and 82 inflation is neglected, prices are in 1975 dollars

A few interesting results in Table IV-1 should be noted In both 1995 and 2020 the output price from node 2 is higher than the output price of node 1 but the quantity output from node 2 is the same as the quantity output from node 1 This is because of the manner in which the parameters in the transport process in Model 82 were determined In general the transport process will both increase the price per unit of energy and decrease the quantity of energy available For the years 1995 and 2020 the output prices from nodes 2 and 3 are similar, but the quantity into node 5 from nodes 2 and 3 is quite different The equations of the allocation process with the parameter used here are such that a small increase in price is reflected in a rather large decrease in the quantity allocated In both 1995 and 2020 the price of imported oil (node 4) is so large compared with the price output at nodes 2 and 3 that only a small quantity of oil is imported The output quantity from

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*The quantities Q(2,1), Q(3 1) and Q(4,1) are input to the code, but only the quantities $\frac{1}{S}Q(2,1)$, $\frac{1}{S}Q(3,1)$, and $\frac{1}{S}Q(4,1)$ are used as initial conditions

TABLE IV-1

Calculated Results[a] Obtained With Model 82

Node	Price per Unit Energy on the Output Link of the Indicated Node $\left(\frac{\text{1975 Dollars}}{\text{Million Btu}}\right)$	Quantity of Energy on the Output Link of the Indicated Node (Quadrillion Btu/year)
	YEAR = 1995	
1	1 4	0 93
2	2 1	0 93
3	1 9	7 4
4	3 4[b]	0 62
5	2 0	8 9
6	2 6	8 2
	YEAR = 2020	
1	2 7	5 4
2	3 4	5 4
3	3 3	11 8
4	4 3[b]	0 22
5	3 3	17 4
6	4 0	16 0

[a]A convergence criterion of 5% (STPERR = 0 05) was used in obtaining these results

[b]These values are input to the system and are therefore not calculated They are given here for comparison purposes

node 5 is always the sum of the quantities input to node 5 from nodes 2 3 and 4 The price on the output link of node 5 is an average of the prices on the input links to node 5 which takes into account the quantities on these input links

B Solution of LEAP Equations

1 Introduction

LEAP[3] comprises a coupled set of nonlinear time-dependent equilibrium equations in prices and quantities which in general terms can be written as

$$\bar{N}(\bar{p},\bar{q}) = 0 \qquad \text{(IV 1)}$$

where $\bar{N}$ is a nonlinear algebraic vector function and $\bar{p}$ and $\bar{q}$ are vectors representing prices and quantities respectively in discrete time intervals for all processes in the energy-economy The vector $\bar{N}$ has dimensions equal to two times the number of time intervals (typically 10) times the number of processes for a total dimensionality on the order of several thousand in Model 22C

Because of the nature of the basic conversion process in LEAP the time structure of Eq (IV 1) is such that there are time intervals before and after the time period defining the solution space The prices and quantities in these intervals are specified exogenously and therefore act as boundary values for the problem Equation (IV 1) can also therefore be characterized as a nonlinear boundary value problem

Because of the nonlinear nature of $\bar{N}$ and its large dimension in LEAP (i e many processes are used to construct a typical network) the choice of solution method for such a problem is limited An iterative procedure with some provision for iterate updating was therefore chosen for practical reasons The authors of the code judged that a conventional numerical scheme the Gauss-Siedel/successive overrelaxation (SOR) method[5] was most appropriate Because of other considerations however, the method actually implemented in the code is not strictly a Gauss-Seidel/SOR algorithm but more a combination of several standard iterative procedures

From these comments it is clear that the LEAP algorithm can be classified as a "locally" convergent procedure (i e Gauss-Seidel/SOR is a local scheme[5]) That is it is only designed to find a solution, if one exists near the initial vectors $\bar{p}$ and $\bar{q}$ used to start the iteration procedure The details of this approach are discussed in more detail in later sections It is only important here to recognize that local convergence is being sought and that the local nature of the initial values of $\bar{p}$ and $\bar{q}$ are crucial to the practical success of the algorithm

Without clearly defined answers to existence and uniqueness questions, it is difficult to characterize the solutions that might arise

from the LEAP iteration algorithm For any iterative procedure to be successful under these circumstances it must physically fit the class of problems being solved By this it is meant that the iteration procedure should closely resemble some physical attribute of the problem being modeled As will be seen later the LEAP algorithm is a good attempt at modeling the equilibration of supply and demand driven by consumers and producers in the energy economy

2 Overall Iterative Approach in LEAP

The limited information available in the LEAP documentation indicates that the iterative procedure was chosen after the basic network structure and modular nature of the code were developed Thus, after the analogy to supply and demand equilibrium was incorporated into the model an iterative scheme to fit this problem was then developed As pointed out in the George Washington University report [6] LEAP is not formulated as an optimization problem in economics although documentation associated with LEAP[4] does contain considerable discussion about such an approach The numerical procedures suitable for optimization problems were therefore not used in the code The network and modular structure of LEAP however were the characteristics that lead naturally to implementation of an up-down iterative algorithm This algorithm was only one of many approaches initially tested in the code before its formal release and therefore represents a practical compromise to a difficult theoretical problem

The up-down algorithm is based on the fact that each modular generic process used to construct a LEAP network is a natural supply-demand unit which can be described mathematically by separable supply and demand transformation functions That is

$$\bar{p}_k = \bar{G}_k(\bar{q}_k), \qquad \text{(IV 2)}$$

and

$$\bar{q}_k = \bar{H}_k(\bar{p}_k) \qquad \text{(IV 3)}$$

where $\bar{p}_k$ and $\bar{q}_k$ are the time-interval components of $\bar{p}$ and $\bar{q}$ respectively in the kth generic process, and $\bar{G}_k$ and $\bar{H}_k$ are the process supply and demand transformation functions respectively This separability allows all process prices to be solved for in an up pass given the transformation functions $\bar{G}_k(\bar{q}_k)$ and all process quantities to be solved for in the down pass, given the transformation functions $\bar{H}_k(\bar{p}_k)$

The separability also allows the entire up pass to be written more compactly as

$$\bar{p} = \bar{G}(\bar{q}), \qquad \text{(IV 4)}$$

and the entire down pass to be written as

$$\bar{q} = \bar{H}(\bar{p}), \qquad \text{(IV 5)}$$

where $\bar{G}$ and $\bar{H}$ are the products of all supply and demand process transformation functions respectively These results then allow the equations solved by the entire code to be represented as

$$\bar{q} = \bar{F}(\bar{q}) = \bar{H}[\bar{G}(\bar{q})] \qquad \text{(IV 6)}$$

This symbolic form of the LEAP equations will be useful in analyzing the convergence of the iteration algorithm

The up-down algorithm structure gives rise to the first clear numerical characteristic of LEAP--it is a nonlinear Gauss-Siedel/SOR approach[10] to iteration That is all prices (quantities) are calculated in each basic process module for all time steps and then used immediately in the next adjacent process module calculation This immediate update procedure in the midst of an iteration pass without modification of the calculated value is a nonlinear SOR scheme similar to the Gauss-Siedel iterative approach to linear equations The procedure is locally convergent with a linear rate of convergence and is guaranteed to converge only if the Jacobian of $\bar{F}$ is negative dominant diagonal These characteristics will be discussed later in this section

To complete the general iterative procedure, a visitation sequence is defined for the various processes that make up the network structure so that in any pass (up or down) the algorithm passes through each process only once In principle the visitation sequence can be arbitrary but in practice it is helpful to order this sequence so as to follow the flow of supply to demand on an up pass and the flow of demand to supply on a down pass Thus, the conventional LEAP procedure is to start the iteration process at the bottom (supply side) of the network and proceed to the top (demand side) Because this procedure approximates the supply-demand equilibration process in a Walrusian economic sense, it should lead to a more natural (and hopefully faster) convergence of the Gauss-Siedel iteration scheme in those cases where the algorithm is guaranteed to converge

Note that, in general, the separability of the process transformation functions leads to an upper-triangular matrix for prices on the up pass of the algorithm and a lower-triangular matrix for quantities on the down pass This separability makes the procedure for calculating all prices in a given process dependent only on processes appearing below it in the visitation sequences on the up pass and on processes appearing above it on the down pass The Gauss-Siedel algorithm is well suited for such a decomposed system of equations

3 Convergence Tests

The criteria used to test convergence of this algorithm should be noted at this point In what follows two cases are mentioned (1) the algorithm described in the documentation of the code as it was delivered to ORNL at the outset of this project and (2) the actual algorithm in the code as it is now used at EIA The two algorithms use different

norms for testing convergence The following comments describe the documented version of LEAP Attention will be drawn to the other version of the code only as needed

At some point in any iteration scheme the state of convergence of the solution must be checked, and the approximate solution from one iterate to the next must be updated After much experimentation, the code developers chose to perform these functions only in allocation processes and only on the down pass of the algorithm when quantities are being calculated In each allocation process then, a pointwise convergence check of the components of the quantity vector q_k in the kth allocation process is therefore made These are the only quantities checked for convergence in the whole algorithm The test is of the form

$$\left| \frac{q_{n\,i}^{(0)} - q_{n\,i}^{(I)}}{q_{n\,i}^{(0)}} \right| \leq \varepsilon \quad \text{for all } q_i \in \bar{q}_k, \qquad \text{(IV 7)}$$

where the subscripts n and i refer to the nth iterate of the ith quantity component q_i of the vector $\bar{q}_k$ and the superscripts I and 0 refer to input and output of the nth iteration Note here that in this nomenclature Eq (IV 6) can be rewritten from the vantage point of the kth allocation process as

$$\bar{q}_{n\,k}^{(0)} = \bar{F}_k[\bar{q}_{n\,k}^{(I)}] \qquad \text{(IV 8)}$$

where $\bar{q}_{n\,k}^{(0)}$ is the kth allocation quantity vector calculated on the down pass of the nth iteration $\bar{q}_{n\,k}^{(I)}$ is the kth allocation quantity vector input to the nth iteration and $\bar{F}_k[\bar{q}_{n\,k}^{(I)}]$ is the transformation function representing the rest of the code In practice, the convergence test represented by Eq (IV 7) is only used when the absolute value of $q_{n\,i}^{(0)}$ is greater than 0 001 quad Below this value no check is made of convergence

The rationale for this scheme of testing convergence only in allocation is unclear from both physical and theoretical viewpoints Basically it is a heuristic approach derived from practical experience with the code Most quantities appear to link to some allocation process in any network and these allocation processes appear dispersed in various sectors of the network These quantities are therefore sufficiently decoupled for them to be a good test of overall convergence of all quantities in most models (this is certainly true in the case of Model 22C) This, however, is not the case for any general network that could be constructed with the LEAP system and can lead to complication in more general problems The success of this approach therefore depends on the particular network structure under investigation

Theoretically the choice of allocation quantity convergence leads to the second major characteristics of the iteration algorithm--mixed point and global convergence testing The procedure is a pointwise scheme because it checks the convergence of specific components of the independent variable vector (i e those in each allocation process) It is also a global procedure because the convergence of the components of $\bar{q}$ in allocation imply some global convergence of all other quantities and prices in the code through the transformation functions $\bar{F}$ $\bar{G}$ and $\bar{H}$ What is clear, however is that convergence in allocation quantities in some norm does not imply equal or better convergence of all the other components of the dependent variables in the code

It is necessary here to point out that the specific norm discussed above for checking convergence [i e Eq (IV 7)] is not the one used in the LEAP version that produced the Model 22C results For that problem a convergence check of the form,

$$\left| \frac{q^{(I)}_{n+1,i} - q^{(0)}_{n\ i}}{q^{(0)}_{n,i}} \right| \leq \varepsilon \qquad \text{(IV 9)}$$

was used Results given in subsection 4 will show that the use of Eq (IV 9) leads to convergence of some quantities in Model 22C to within $\varepsilon/(1-\alpha_1)$ where α_1 is the relaxation parameter used for a specific allocation quantity Because α_1 was about 0 5 for these quantities the reported converged results for these quantities actually satisfy an $\sim 2\varepsilon$ convergence criteria (i e about 6% in Model 22C) This test was changed from Eq (IV 9) to Eq (IV 7) in the current EIA version of LEAP and reruns of Model 22C with true convergence to ε show a change of less than a few percent in all major results Only a few quantities with very small magnitudes seem to have converged to only 2ε as predicted by this analysis Therefore in this instance no real problem resulted from using Eq (IV 9) Other problems run with this version of the code however, should be checked because α_1 can potentially be close to unity and differences in convergence of a factor of 10 are possible (i e a 3% convergence criteria could actually be in error by as much as 30% in some quantities)

4 Relaxation and Acceleration

In any iterative procedure a decision must be made at the end of each iteration on how to update the output of the algorithm The documentation for LEAP assumes an update relationship that uses information in each allocation process about input and output quantities on each iteration

$$\bar{q}^{(I)}_{n+1} = \bar{q}^{(I)}_{n} + A^{-1}[\bar{q}^{(0)}_{n} - \bar{q}^{(I)}_{n}] \qquad \text{(IV 10)}$$

where A is in general a matrix of relaxation parameters

This relationship implies that if A = I (the identity matrix) the updated quantity vector $\bar{q}_{n+1}^{(I)}$ is simply $\bar{q}_n^{(0)}$ the output of the code given the input vector $\bar{q}_n^{(I)}$ This update procedure is commonly referred to as "unit relaxation" and is used for all quantities in the code other than those in allocation processes For these later processes a linear combination of $\bar{q}_n^{(I)}$ and $\bar{q}_n^{(0)}$ is used to determine the new input vector $\bar{q}_{n+1}^{(I)}$ Thus the code uses unit relaxation in all non-allocation processes in conjunction with the Gauss-Siedel part of the algorithm and an A matrix in conjunction with another iteration update scheme in allocation processes

Depending on how A is calculated the allocation process portion of the algorithm falls into the class of Newton or Generalized Secant methods[5] for updating The characteristic of these later approaches is again one of local convergence whose rate depends on the particular choice of A (in general linear to quadratic rates are possible) [4] In these schemes initial estimates of the independent variables that are close to the solution are essential for convergence The combination of a Newton's method in allocation and a nonlinear Gauss-Siedel scheme in the rest of the code results in a convergence algorithm of mixed theoretical origin and one which is more complicated than the one described in the LEAP documentation

Looking at this algorithm in more detail one can see that a slightly modified version of this scheme is actually implemented in the LEAP code In particular each allocation process deals with only the fraction of the total quantity demanded (or supplied), and relaxation is applied to these fractions called market shares rather than to the actual quantities themselves This slight difference however complicates the analysis of relaxation considerably because market shares are coupled by behavioral lag coefficients in time These coefficients cause market share changes from one time period to the next to be damped thereby allowing the market to respond incompletely to time changes in demand (or supply) The net effect of such damping is that when relaxation is applied in each time period (i e to each component of the allocation quantity vector) a time lag couples the earlier time period relaxation coefficient to the present time period coefficient This characteristic makes the relaxation parameters a function of the behavioral lag coefficients, complicating the algorithm considerably

In addition to this difference between documentation and code the model developers also sought to relax another variable in the code--new capacity additions in each basic conversion process This choice was based on observations in several practical problems of wide fluctuations in new capacity additions between iterations The modelers chose to damp these oscillations and hopefully improve the convergence of the algo-

rithm The particular relaxation method chosen for this task however is far from being theoretically justified In particular the new capacity addition vector $\bar{N}_w$ in each basic conversion process is relaxed by a constant α That is for each component N_J of the new capacity addition vector $\bar{N}_w$ a relaxed component is computed from

$$N^{(I)}_{n+1\ J} = \alpha N^{(0)}_{n,J} + (1 - \alpha)\ N^{(I)}_{n\ J} \qquad \text{(IV 11)}$$

$$= N^{(I)}_{n\ J} + \alpha\ N^{(0)}_{n,J} - N^{(I)}_{n\ J}$$

where I and 0 again stand for input and output to an iteration In the version of LEAP used for Model 22C $\alpha = 0\ 7$ Such a constant value (i e positive) can generally cause theoretical and practical problems for convergence More will be said about this in subsection 5

At this point the reader should note that the LEAP documentation and the Model 22C code differ significantly in implementing relaxation The LEAP documentation describes a Newton-Secant method for allocation quantities in which the A matrix is evaluated by using derivatives of $\bar{F}$ (i e $\partial\bar{F}/\partial\bar{q}$ the Jacobian of $\bar{F}$) Because the only vectors available in allocation are $\bar{q}^{(I)}$ and $\bar{q}^{(0)}$ for the current and previous iterations a discrete-secant approximation to the partial derivative of $\bar{F}$ is used The Newton approach in its discrete approximation is then

$$A = I - \left(\frac{\partial\bar{F}}{\partial\bar{q}}\right), \qquad \text{(IV 12)}$$

where I is the identity matrix the i jth component of the Jacobian of $\bar{F}$ is given by

$$\left(\frac{\partial\bar{F}}{\partial\bar{q}}\right)_{i\ J} \cong \left(\frac{\Delta\bar{F}_n}{\Delta\bar{q}_n^{(I)}}\right)_{i\ J} = \frac{\Delta q^{(0)}_{n,i}}{\Delta q^{(I)}_{n,J}} \qquad \text{(IV 13)}$$

and $\Delta q_{n\ i} = q_{n\ i} - q_{n-1\ i}$

Since <u>all</u> the input components $q^{(I)}_{n\ J}$ change from iteration to iteration, the partial contribution of the $q^{(I)}_{n\ J}$th element of $\Delta\bar{q}_n^{(I)}$ to $\Delta\bar{q}_n^{(0)}$ cannot be evaluated The modelers therefore assumed that each $q^{(I)}_{n,J}$ component acts independently on only $q^{(0)}_{n\ J}$ This approximation diagonalizes A, giving rise to the following relationship for the relaxation coefficient α_i in terms of the diagonal elements a_{ii} of the A matrix

$$\alpha_1^{-1} \equiv a_{11} \cong \left[1 - \left(\frac{q_{n\,1}^{(0)} - a_{n-1\,1}^{(0)}}{q_{n\,1}^{(I)} - q_{n-1\,1}^{(I)}} \right) \right] \qquad \text{(IV 14)}$$

Generally, this approach has several practical and theoretical limitations leading to nonconvergence of the algorithm in some cases when the off-diagonal elements of the matrix A are non-negligible Because allocation quantities are almost always coupled to one another this diagonalized Newton's method clearly cannot be expected to yield converged results for any general problem If on the other hand, the absolute maximum value of α_1 can be made arbitrarily small (i e this upper limit could be an input parameter to the algorithm) it should be possible from a theoretical point of view[6] to achieve convergence to an accuracy ε which is a function of this upper limit That is, convergence achieved on the nth iteration ε_n, is of the form $\varepsilon_n = \varepsilon_n(\alpha_u)$ where α_u is the imposed upper limit of the α_1's Restricting the upper limits to very small values however, leads to an inordinate number of iterations to achieve convergence to a specific ε This is a result of $\bar{q}_{n+1}^{(I)}$ differing only slightly from $\bar{q}_n^{(I)}$ from iteration to iteration making it possible for example to take several thousand iterations to achieve 1% convergence with $\alpha_u = 0\ 01$ In practice, this approach is not generally acceptable although it might be appealing in some problems

The algorithm above is the one described in the LEAP documentation A different approach however was used in the EIA version of LEAP that was used to generate the results for Model 22C As in the documentation the EIA version uses a diagonal A matrix for updating $\bar{q}_n^{(I)}$ However this similarity ends at this point The EIA algorithm to calculate α_1 appears to be of the form

$$\alpha_1^{-1} \equiv \left[1 - \left(\frac{q_{n-1\,1}^{(I)} - q_{n\,1}^{(0)}}{q_{n-2,1}^{(I)} - q_{n\,1}^{(I)}} \right) \right] \qquad \text{(IV 15)}$$

with a condition that $0\ 1 \leqq \alpha_1 \leqq 0\ 9$ If α_1 is outside this range the upper or lower limit (whichever the case may be) rather than the computed α_1 is used Thus α_1 is always positive and bounded

The theoretical origin of this approach in unknown, and EIA personnel have been unable to give the rationale for its choice The approach appears to be a scheme for finding a sequence of $q_{n\,1}^{(I)}$ values as a function of n that can be used for extrapolation purposes to determine

$q^{(I)}_{n+1\ 1}$ Even if this were the case the form of Eq (IV 15) does not fully conform to any known theoretical extrapolation technique This approach appears to be heuristic and one that happens to work to a limited extent on a limited class of problems

The major drawback of the EIA algorithm appears to be the constraint on α_1 being positive and greater than 0 1 The behavior of the diagonal element partial derivatives of $\bar{F}$ [i e the components $(\partial\bar{F}/\partial\bar{q})_{1\ 1}$] near solution point $\bar{q}_\infty$ will not generally be such that all $(\partial\bar{F}/\partial\bar{q})_{1\ 1} > 0$ When some $(\partial\bar{F}/\partial\bar{q})_{1\ 1} < 0$ the constraints on α_1 can give rise to nonconvergence Also many practical problems have some large partial derivations [i e elements $(\partial\bar{F}/\partial\bar{q})_{1\ 1} > 10$] causing the algorithm to be divergent because of the constraint that $\alpha_1 > 0\ 1$ In particular this latter constraint will likely lead to divergence for all quantities q_1 whose partial derivatives are $(\partial\bar{F}/\partial\bar{q})_{1,1} > 10$ in absolute magnitude

Further analysis here is not warranted because of the lack of any identifiable theory with which to study this algorithm A description of actual experience with this algorithm in some specific LEAP problems is more fruitful

5 Practical Experience with LEAP Algorithms

When the project began little was known about LEAP and its numerical algorithms except that Model 22C results appeared to have converged to within 3%, and the output looked reasonable Since that time the analysis of Model 82 results has produced much experience both practical and theoretical This smaller model has all the essential processes contained in Model 22C but is simple enough to study in some detail through actual runs The following discussion is a direct result of a large body of Model 82 runs These runs can be used indirectly to comment on the expected impact on Model 22C of the algorithms described in subsection 4

Regarding actual degree of convergence the use of the EIA convergence criteria [i e Eq (IV 9)] in Model 22C runs clearly leads to an overstatement of the level of accuracy (i e ε) achieved in the reported results Therefore as a first step in checking Model 22C results the convergence test was changed to that given in Eq (IV 7) and the code was rerun with $\varepsilon = 3\%$ beginning with the "converged" results reported in the EIA 1978 Annual Report to Congress [1] After eight additional iterations the new modified convergence test was satisfied and the results were printed Generally the new results differed by less than 1% from the Annual Report[1] numbers Thus no major discrepancy exists between a solution truly converged to 3% and the results published in the Annual Report [1] The explanation of this result is that

the quantities with the largest magnitudes in Model 22C were already converged to well below 3% in the original EIA run and only quantities with small magnitudes were near the 3% criteria Changing the convergence algorithm simply resulted in these latter quantities converging to the true 3% criteria instead of the effective 6% criteria resulting from the use of Eq (IV 9) with $\alpha_1 \cong 0\ 5$

Note at this point that the common mode in which LEAP runs are ended (i e creating a single extra "data report" iteration after the convergence criteria are satisfied) can sometimes adversely alter the convergence This is possible because of the difference between the algorithm for the first three iterations and all subsequent iterations Because no previous iteration results are available on the first iteration to compute partial derivatives for the Newton scheme the relaxation parameter for all quantities is set to a constant $\alpha_1 = 1\ 0$ This constant however can lead to divergence of the converged results in the single extra iteration used to produce a data report because of the particular behavior of $\bar{F}$ near the solution point Restarting a problem from an already closely converged solution therefore does not continue the iteration process from its termination point Instead it begins the procedure over again using only the solution values themselves as a starting guess (i e all derivative information is lost in a restart) Restarting in this manner is generally a poor procedure and one example of the difficulties encountered in the frozen version of the code

The above comments are the only ones that can be made directly about the LEAP algorithm concerning Model 22C Running Model 82 however, generated a better understanding of this algorithm In Model 82 the runs are usually only a few minutes of CPU time, and changes in the algorithm can readily be explored An attempt to run Model 82 to better than 5% convergence (i e $\varepsilon = 5 \times 10^{-2}$) for screening work provided the first true understanding of the characteristics of the algorithm for this type of problem Many small perturbations had to be made in the model parameters for screening and reruns had to be made to get the perturbed results The algorithm in the code was never able to converge these problems to better than about 5% The characteristic breakdown in convergence was an oscillatory one Convergence to about 5% was achieved after which the convergence moved back up to about 20% before returning to about 5% again

Careful analysis of the relaxation parameters and results of many cases revealed that, in each allocation time period, the A matrix is far from diagonal The diagonality approximation in relaxation, therefore, appears to be the major cause of the observed limited and oscillatory convergence The George Washington University analysis[6] of this algorithm obtained similar results, with the solution asymptotically oscillating between two limit points This double limit point behavior might be the expected long-term pattern of the Model 82 results but it was not worth pursuing because several thousand iterations would be required for confirmation

The oscillatory behavior described above appeared at first to be a possible multiple solution of the Model 82 problem, with solutions about 10% apart in most quantities The George Washington University analysis and additional theoretical work however, led to the conclusion that convergence in the diagonalized Newton scheme is a function of α_1 with the maximum α_1 determining the separation between the limit points To test this theoretical analysis, a diagonalized Newton method was implemented in LEAP with several schemes for reducing the maximum value of α_1 as a function of ε_n (i e the level of convergence achieved in the nth iteration) In each case, the derivatives of $\bar{F}$ needed for the diagonal elements of A were computed from present and previous iteration values and a maximum α_1 value was computed from a formula related to ε_n Results for this species of test runs are summarized in Table IV 2 These results show that the level of convergence can only be minimally improved by staging α_1 and then only at the expense of the number of iterations required Despite these improvements however, the solution in each case still oscillated after the best converged values were achieved and the improved best error values were smaller than the old algorithm by at most only a factor of 2 Again the off-diagonal elements of the A matrix still clearly limit the methodology in this case and prevent realization of the known local convergence characteristics of Newton's method

TABLE IV-2
BEST MAXIMUM ERROR ACHIEVED IN LESS THAN 100 ITERATIONS
WITH VARIOUS α STAGING ALGORITHMS

	α_{max} =	$\sqrt{\varepsilon_n}$	ε_n	$\sqrt{\varepsilon}/4$
Best maximum error	ε_N	0 05	0 05	0 02
Number of iterations	N	48	53	100

A complete analysis of the local partial derivatives for each allocation quantity was made as a last resort The result of this analysis was to hand-choose a constant value of α for all quantities in all time steps to attempt to achieve convergence A value of α = 0 2 yielded convergence to arbitrary accuracy in all perturbed cases of Model 82 Typically, $\varepsilon = 5 \times 10^{-4}$ was achieved in about 50 iterations for all starting guesses, which were small perturbations of the initial base-case quantities These results are surprising and seem to go against the theoretical analysis available for this problem Despite this, a constant α appears to have the net effect of relaxing all quantities at a similar rate so that off-diagonal behavior does not dominate the convergence properties of the algorithm A constant value of α also has

the desirable property of not changing relationships between total quantities (i e the sum of the $q_{n,i}$ s) and their constituents thereby retaining the property that supply equals demand before and after relaxation

Note here that most of the α_i's for the largest quantities in the old algorithm are about 0 5 and this fortuitous result seems to produce most of the convergence down to the level of $\varepsilon \cong 10^{-2}$ observed in the original Model 82 results The use of non-uniform α values seems to result in small quantities being relaxed so as to cause divergence in those quantities with large magnitudes after these latter quantities have by and large converged quickly to $\varepsilon \sim 10^{-2}$

The conclusion that should be drawn from this example is that off-diagonal element behavior is crucial for convergence below a few percent in this sample problem To reach the level of a few percent a diagonalized A matrix seems to be adequate to quickly converge the largest-magnitude quantities The algorithm fails at this point in trying to converge the smaller-magnitude quantities This procedure eventually results in oscillation as the smaller values begin to affect the large well-converged values through off-diagonal mixed partial derivatives The algorithm is reasonable then for answers of a few percent but will not generally converge quantities further even though it is already close to a solution Although staging α_i down as a function of ε_n is a reasonable approach from a theoretical viewpoint it is not entirely adequate to completely converge the solution Only hand-choosing a constant α appears to yield totally converged solutions with this diagonal approach Off-diagonal elements must be estimated to have a generally convergent scheme Several schemes for doing this (i e the Davidon-Fletcher-Powell method[4]) are available in the literature and these need to be explored These conclusions are by no means general ones and careful analysis of the behavior of this algorithm with Model 22C is also in order Indications from DFI are that the convergence of most large models (e g Model 22C) is dominated by the relaxation of new capacity additions in basic conversion processes Here the choice of a constant α may be the fortuitous reason that convergence is achieved in many of these problems despite again off-diagonal dominant behavior of the partial derivative matrix All these conjectures must be tested in some detail before any definitive conclusions can be drawn about LEAP in general and Model 22C results in particular

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V EQUATIONS OF THE BASIC CONVERSION PROCESS

In this section and in Appendix B, the equations of the basic conversion process as used in Models 22C and 82 are presented The fundamental equations are given in this section but a few of the more lengthy equations are given in Appendix B The equations that are presented are the equations that are satisfied at equilibrium no attempt is made to indicate the form of the equations used during the iteration before equilibrium is reached Also some of the generality allowed in the code is not used in Model 22C and is not included in the equations given here There is no documentation of the LEAP equations other than the computer code listing Many of the equations are given in Ref 1 but this reference does not document the LEAP system used in Model 22C Every effort has been made to verify that the equations given here and in Appendix B are those in the computer code but the code is quite complex and the possibility exists that there may be minor differences between the equations and the coding

The interrelations of the various equations are discussed, but no attempt is made to derive the equations or to discuss their validity from an economic point of view A derivation of many of the equations and some discussion of the economic basis of the equations will be found in Ref 1 The equations are given here so that they may be referred to in Section VII and used to obtain the necessary derivatives (Section IX B) for forming the elements of the adjoint matrix (Sections IX A and IX C)

Because the LEAP system uses discrete values of time (i e variables are calculated only at discrete times) the time notation must be established before the equations can be written Two different time functions global and local are used

$$T_G(J) \qquad J = 1 \text{ to } N \tag{V 1}$$

and

$$T_L(J) \qquad J = 1 \text{ to } 2N_p + N \tag{V 2}$$

where

$$N_p = \text{Int}\,[L_c/\Delta] + 1 \tag{V 3}$$

$T_G(J)$ = global time function

$T_L(J)$ = local time function,

N = number of global time points

$2N_p + N$ = number of local time points,

L_c = characteristic plant life

Δ = time interval between global and local time points

Int [ ] means the quantity in square brackets is to be integered

The global time values contain no reference to any process-related parameters and they specify the time values where the model variables are computed The local time values refer specifically to the conversion process through the parameter L_c so that the local time vector varies with node (Section IV) The relation between the two functions is defined by

$$T_G(1) = T_L(N_p + 1) \qquad \text{(V 4)}$$

When working with the equation of a single process such as the basic conversion process it is usually convenient to use local time but in the equations that couple many processes together it is more convenient to introduce global time For future reference note that the value of $T_G(1)$ sets the absolute time scale Unless otherwise stated local time will be used and the notation F(j) means that the function F is to be evaluated at the time $T_L(j)$

All variables and parameters in this section should carry a node index but for simplicity this index will be omitted

A <u>Prices, Quantities, and Capacity Additions</u>

The equations of the basic conversion process must determine the price per unit of energy and the quantity of energy as a function of time on the output link of the process Alternatively if the quantity of energy demanded from the conversion is assumed to be known the equations must determine the quantity of energy (fuel) that is required on the input link to the process The equations must also determine the level of plant capacity additions to be made as a function of time

The variables of the basic conversion process are assumed to be

$$\begin{aligned} &P(j) && j = N_p + 1 \text{ to } N_p + N \\ &Q(j) && j = N_p + 1 \text{ to } N_p + N \\ &N_W(j) && j = N_p + 1 \text{ to } N_p + N \,, \end{aligned} \qquad \text{(V 5)}$$

where

P(j) = price per unit of energy on the output link of the process at local time j,

Q(j) = quantity of energy per year on the output link of the process at local time j,

$N_W(j)$ = capacity additions at local time j (a unit of capacity will produce a unit of energy per year if the capacity factor is unity)

The inclusion of $N_W(j)$ as a variable is somewhat arbitrary For convenience the $N_W(j)$ variable was omitted in Section IV but it will be included in this section and several later sections The $N_W(j)$ will be used as a variable only in resource and conversion processes

Therefore 3 N variables are associated with the basic conversion process and 3 N equations must be specified to determine these variables In Model 82 14 N - 4 variables rather than 11 N - 4 (as in Section IV) will be used Many other quantities must be calculated and could be called variables but for this discussion the quantities in Eq (V 5) are termed the variables of the basic conversion process

The prices on the output link of a conversion process which are determined from the condition that economic profit is zero (Section VII) satisfy the equations

$$-N_C(j) + \sum_{k=j+1}^{2N_p+N-1} [P(k) - \phi(j\ k)]C_f(j\ k)D(j,k) \qquad \text{(V 6)}$$

$$j = N_p + 1 \text{ to } N_p + N$$

$$+ \ [P'(j) - \phi(j,j)]C_{fG}(j\ j)D(j\ j) = 0$$

$$P(j) = P_T(j) \qquad j \geqq N_p + N + 1$$

$$P(j) = \tfrac{1}{2}[P'(j) + P_T(j)] \qquad j = N_p + N$$

$$P(j) = P'(j) \qquad j = 1 \text{ to } N_p + N - 1$$

where

$N_C(j)$ = present value of capital cost of a unit of capacity at time j

$P(j)$ = price per unit energy at time j

$\phi(j\ k)$ = variable operating cost of a plant built at time j and operating at time k (the first subscript will always indicate the time the plant is built and the second subscript will indicate the time the plant is operating)

$C_f(j,k)$ = capacity factor of a plant built at time j and operating at time k

$D(j\ k)$ = discount factor

$C_{fG}(j\ j)$ = approximate capacity factor of a plant built at time j and operating at time j

$P_T(j)$ = price per unit energy at time j as given by the terminal value model

Equations for all these functions are given in the latter parts of this section or in Appendix B

The quantities of energy per year produced by the conversion process (i e , the quantities on the output link of the process) are given by

$$Q(j) = \sum_{k=1}^{j} C_f(k\ j)N_W(k) \qquad j = N_p + 1 \text{ to } N_p + N, \qquad \text{(V 7)}$$

where $Q(j)$ and $N_W(j)$ have been defined in connection with Eq (V 5) Equation (V 7) simply states that the quantity of energy per year produced at time j is obtained by adding the contribution from all plants in place at previous times while taking into account the fact that the capacity factor may differ from unity In Eq (V 7) $N_W(j)$ occurs for values of $j < N_p + 1$ and thus equations must be given to determine these N_W values

Since Eqs (V 6) and (V 7) constitute 2 N equations to determine the 3 N unknowns N equations are still needed These equations arise from the condition that to produce energy the conversion process requires fuel (energy) which must be input to the conversion process The equations expressing this condition may be written

$$Q_I(j) = \sum_{k=1}^{j} Q_F(k\ j)C_f(k\ j)N_W(k) \qquad j = N_p + 1 \text{ to } N_p + N \qquad \text{(V 8)}$$

where

$Q_I(j)$ = quantity of energy per year on the input link of the conversion process at local time j

$Q_F(k\ j)$ = quantity of energy per year required at time j by a plant built at time k to produce one unit of output energy per year at time j

Thus the 3 N equations to determine the 3 N unknowns are available provided that $Q_I(j)$ is known for $j = N_p + 1$ to $N_p + N$ Alternatively if $Q(j)$ for $j = N_p + 1$ to $N_p + N$ is assumed to be known, the equations may be used to determine $Q_I(j)$ for $j = N_p + 1$ to $N_p + N$ in addition to the $P(j)$ and $N_W(j)$ for $j = N_p + 1$ to $N_p + N$

The quantity $N_W(k)$ for $k = N_p + 1$ to $N_p + N$ by its definition must be positive, but the quantity $N_W(k)$ determined by Eqs (V 7) and (V 8) may be negative When this occurs in the DFI code,[1] a plant shutdown algorithm is used to retire plants until $N_W(k)$ is no longer negative In Model 22C this shutdown algorithm is not used, but rather Eqs (V 7) and (V 8) are modified If $N_W(j) < 0$ for a particular $j > N_p + 1$ (say j') then

$$\bar{Q}(j') = \sum_{k=1}^{j'-1} C_f(k\ j')N_W(k) \qquad \text{(V 9)}$$

and Eq (V 7) for this value of j is replaced by

$$N_W(j') = 0 \qquad \text{(V 10)}$$

$$Q(j') = \frac{Q(j')}{\bar{Q}(j')} \sum_{k=1}^{j'} C_f(k\ j')N_W(k) = 0 \qquad \text{(V 11)}$$

and Eq (V 8) for j' is replaced by

$$Q_I(j') = \frac{Q(j')}{\bar{Q}(j')} \sum_{k=1}^{j'} Q_F(k,j')C_f(k,j)N_w(k) = 0 \qquad \text{(V 12)}$$

Note that because of Eqs (V 9) and (V 10) Eq (V 11) reduces to the identity

$$Q(j') = Q(j') \qquad \text{(V 13)}$$

for j' only Thus effectively, one of the equations from Eq (V 7) is replaced by Eq (V 10), and the number of equations is the same as when $N_W(j)$ was non-negative

B <u>Variable Operating Cost</u>

The variable operating cost $\phi(j\ k)$ that occurs in Eq (V 6) is now considered The quantity $Q_I(j)$ that is input to the conversion process and is assumed known was used in Eq (V 8), but as yet the prices on the input link to the conversion process that are also assumed to be known have not been used These prices $P_I(j)$ are used in the variable operating cost since the cost of operation should depend on the cost of energy (fuel) The variable operating cost may be written as

$$\phi(j,k) = \phi_o(j\ k) + Q_F(j\ k)P_I(k) \qquad \begin{array}{l} k \geq j \\ k \geq N_p + 1 \\ k \leq 2N_p + N - 1 \end{array} \qquad \text{(V 14)}$$

where

$\phi(j\ k)$ = variable operating cost per unit energy of a plant built at time j and operating at time k,

$\phi_o(j\ k)$ = portion of the variable operating cost per unit of energy that arises from the cost of labor and materials,

$Q_F(j\ k)$ = quantity used in Eq (V 8),

$$P_I(k) = P_I(N_p + N)(1 + I_f)^{(k-N_p-N)\Delta} \qquad k > N_p + N \qquad \text{(V 15)}$$

where

I_f = rate of inflation for time $k > N_p + N$

Equation (V 15) must be introduced since $P_I(k)$ is not available on the input link to the conversion process if $k > N_p + N$

The quantity $\phi_o(j,k)$ is determined directly from input parameters and may be written

$$\phi_o(j\ k) = \sum_{\ell=1}^{2} V_o f_\ell p_\ell(k) f_A(k - j) f_{c\ell}(j) f_{o\ell}(k) \ , \qquad \text{(V 16)}$$

where

V_o = a constant that is input to determine the variable operating cost per unit of energy due to the cost of labor and materials (also called the variable operating cost in Reference 1),

f_ℓ = fraction of the constant V_o that is due to labor or material cost ($\ell = 1$ for labor $\ell = 2$ for material)

$p_\ell(k)$ = price of labor or material normalized to be unity in 1975 ($\ell = 1$ for labor $\ell = 2$ for material)

$$f_A(k - j) = \exp\left\{\left[\frac{(k-j)\Delta}{L_c}\right]^{\beta_A}\right\} \ , \qquad \text{(V 17)}$$

where

β_A, L_c = constants (the function $f_A(k)$ determines how the variable operating cost increases as the plant ages),

$$
\begin{aligned}
{}_{c\ell}(j) &= g_{\infty\ell} + (1 \quad g_{\infty\ell})(1 \quad \alpha_\ell)^{t_I+(j\ 1)\Delta\ t_A} && t_I+(j\ 1)\Delta > t_A \geq t_I + N_p\ \Delta \\
&= g_{\infty\ell} + (1 - g_{\infty\ell})(1 \quad \alpha_\ell)^{(j\ 1)\Delta\ \ N_p\ \Delta} && t_I+(j\ 1)\Delta \geq t_I + N_p\ \Delta > t_A \\
&= 1 + [t_A \quad t_I \quad (j\ 1)\Delta]\rho && t_A \geq t_I + N_p\ \Delta \\
& && t_A \geq t_I + (j\ 1)\Delta \\
&= 1 + \left[\frac{2T_{EF}\ 2E_{AV}}{0\ 8\ T_{EF}\ L_c}\right][(j\ 1)\Delta \quad N_p\ \Delta] && t_I + N_p\ \Delta > t_I + (j\ 1)\Delta > t_A \\
&= 1 + \left[\frac{2T_{EF}\ 2E_{AV}}{0\ 8\ T_{EF}\ L_c}\right][t_A \quad t_I \quad N_p\ \Delta] \\
&\quad + [t_A \quad t_I \quad (j\ 1)\Delta]\rho && t_I + N_p\ \Delta > t_A \geq t_I + (j\ 1)\Delta
\end{aligned}
\tag{V 18}
$$

where

t_I = time that corresponds to $T_L(1)$

t_A = time when the technology first becomes available,

$g_{\infty\ell}, \gamma_\ell, \rho$ = constants (ℓ = 1 for labor ℓ = 2 for material) *

E_{AV} = average process efficiency that is input to the code,

T_{EF} = Thermal efficiency for the process (before it is modified by time factors)

$$
\begin{aligned}
f_{o\ell}(k) &= f_{\infty\ell} + (1 \quad f_{\infty\ell})(1 \quad \alpha_\ell)^{t_I+(k\ 1)\Delta-t_A} && t_I+(k\ 1)\Delta \quad t_A \geq t_I + N_p\ \Delta \\
&= f_{\infty\ell} + (1 \quad f_{\infty\ell})(1 - \alpha_\ell)^{(k\ 1)\Delta\ \ N_p\ \Delta} && t_I+(k\ 1)\Delta \geq t_I + N_p\ \Delta \quad t_A \\
&= 1 + [t_A \quad t_I \quad (k\ 1)\Delta]\rho && t_A \geq t_I + N_p\ \Delta \\
& && t_A \geq t_I + (k\ 1)\Delta \\
&= 1 + \left[\frac{2T_{EF}\ 2E_{AV}}{0\ 8\ T_{EF}\ L_c}\right][(k\ 1)\Delta \quad N_p\ \Delta] && t_I + N_p\ \Delta \quad t_I + (k\ )\Delta \quad t \\
&= 1 + \left[\frac{2T_{EF}\ 2E_{AV}}{8\ T_{EF}\ L_c}\right][t_A - t_I \quad (N_p)\Delta] \\
&\quad + [t_A \quad t_I \quad (k\ 1)\Delta]\rho && t_I + N_p\ \Delta \quad t_A \geq t_I + (k\ 1)\Delta
\end{aligned}
\tag{V 19}
$$

---

*See footnote next page

where

$f_{\infty\ell}$ α_ℓ, ρ = constants (ℓ = 1 for labor ℓ = 2 for material)

The quantity $Q_F(j,k)$, used in Eq (V 14), may be written

$$Q_F(j\ k) = T_{EF}^{-1}\ f_{c3}(j) f_{o3}(k)\ , \qquad \text{(V 20)}$$

where

$f_{c3}(j), f_{o3}(k)$ = functions as defined in Eqs (V 18) and (V 19) with ℓ = 3 and input constants $g_{\infty 3}$ $f_{\infty 3}$ α_3 and ρ *

C Capacity Factor

The capacity factor that occurs in Eqs (V 6) (V 7) and (V 8) is written

$$C_f(j\ k) = \begin{cases} 0 & k < j \\ \beta & j = 1 \text{ to } N_p,\ k = 1 \text{ to } N_p \\ \dfrac{\beta}{1+\left[\dfrac{\alpha\phi(j,k)}{P(k)}\right]^\gamma} & k \geq N_p + 1,\ k \leq 2N_p + N - 1,\ 1 \leq j \leq N_p + N \end{cases} \qquad \text{(V 21)}$$

where

β = maximum value of the capacity factor

α, γ = constants that determine shape of the capacity factor

Equation (V 21) expresses the fact that the capacity factor is assumed to be a maximum for all time less than $T_L(N_p + 1)$ The lower expression given in Eq (V 21) which is used in most calculations, expresses the important fact that the capacity factor depends explicitly on the variable operating cost Since P(k) occurs in $C_f(j\ k)$, Eq (V 6) contains an implicit dependence on P(k) that is not readily apparent from the form in which Eq (V 6) is written

---

*Equations (V 18) and (V 19) are written somewhat more generally than is allowed in LEAP at present The code requires

$$g_{\infty 1} = g_{\infty 2} = g_{\infty 3}$$
$$f_{\infty 1} = f_{\infty 2}$$
$$\alpha_1 = \alpha_2 = \alpha_3$$

The approximate capacity factor $C_{fG}(J\ J)$ that occurs in Eq (V 6) is given by

$$C_{fG}(J\ J) = \frac{\beta}{1 + \left[\frac{\alpha\phi(J\ J)}{P_G(J)}\right]^{\gamma}} \qquad J = N_p + 1 \text{ to } N_p + N \qquad \text{(V 22)}$$

$$P_G(J) = \phi(J\ J) + \frac{R'(J)}{1+r_e(J)-R'(J)} \left\{ \frac{[1+r_e(J)]N_C(J)}{\beta} - P(J+1) + \phi(J+1\ \ J+1) \right\} \qquad J = N_p + 1 \text{ to } N_p + N \qquad \text{(V 23)}$$

$$R'(J) = \frac{1 - \frac{1}{1+r_e(J)}}{1 - \left\{\frac{1}{[1+r_e(J)]}\right\}^{L_C+1}} \qquad \text{(V 24)}$$

where $r_e(J)$ = the return on equity at time J and the other symbols have previously been defined This approximate capacity factor has the same form as that defined in Eq (V 21) but contains the estimated price $P_G(J)$ rather than the price $P(J)$

D <u>Calculation $N_W(J)$ for $J \leq N_p + 1$</u>

The equations that determine $N_W(J)$ for $J \leq N_p + 1$ must be specified A linear assumption concerning capacity additions for $J \leq N_p + 1$ is used to give

$$N_W(J) = \frac{Q(N_p+1)\ \text{Max}\ \{0,[1-r_s\Delta(N_p+1-J)]\}}{\sum_{k=1}^{N_p+1} \text{Max}\ \{0\ [1-r_s\Delta(N_p+1-k)]\}C_f(k\ N_p+1)} \qquad \text{(V 25)}$$

$$J = 1 \text{ to } N_p + 1$$

with the quantity r_s determined from*

$$E_{AV} = \frac{\sum_{k=1}^{N_p+1} Q_F(k\ N_p+1)C_f(k\ N_p+1)N_W(k)}{Q(N_p+1)} , \qquad (V\ 26)$$

where

E_{AV} = average process efficiency that is input to the code

Note that Eq (V 22) for $j = N_p + 1$ is identical to Eq (V 7) with $j = N_p + 1$

Except for the quantities $N_C(j)$ $D(j\ k)$ and $P(j)$ for $j > N_p + N$ all of the quantities that enter into Eqs (V 6) (V 7), and (V 8) have now been determined Because the equations for these needed quantities are rather lengthy and with one exception do not involve any of the variables, they are given in Appendix B

*In the original DFI system the parameter r_s was input In the version of LEAP that is considered here, Eq (V 26) is used to calculate r_s for the input E_{AV}

REFERENCE FOR SECTION V

1 R J Adler et al , The DFI Energy-Economy Modeling System Final Report Decision Focus Inc Palo Alto California (December 1978)

VI ECONOMIC EVALUATION OF THE BASIC CONVERSION PROCESS

This section was not completed in time to be included in this report

VII VERIFICATION OF THE BASIC CONVERSION PROCESS

A Computer Code for Basic Conversion Process

Attention is now turned to the computer code that operates the basic conversion process and the parameter values that describe the behavioral and technical aspects of the basic conversion process

The computer code that operates the basic conversion process can be separated into three components

1 Routines and logic common to both up and down passes which are executed before execution of either the up or down pass

2 Routines and logic dealing specifically with the up pass, that together calculate the output price vector for the process under consideration

3 Routines and logic dealing specifically with the down pass, that together calculate the demand for factor inputs, including fuels new capacity additions, and operating factors (e g , labor)

Initially, control is passed from the main LEAP program to the basic conversion process sequence through execution of a subroutine named SOLVE SOLVE in turn calls subroutine CNHOLP by telling CNHOLP the specific process (e g petroleum refining) it wishes to reference CNHOLP then assembles the data necessary to execute either the up or down passes, calculates a series of initial quantities, and conducts validity checks on the initial quantities When these operations are completed, final modifications to input parameters are conducted, and control passes to the basic conversion process

The first eleven subroutines to be executed fall into the group common to both the up and down passes The first routine in this series, TIMCHR sets up the local time vector and indices TIMCHR appends NPRIOR time points onto the beginning and the end of the vector NPRIOR is simply the smallest integer multiple of the time period length (DEL) that is greater than or equal to the characteristic plant life

Next a sequence of four subroutines is executed to calculate variable operating costs The first routine in this sequence subroutine AGE, computes the age multipliers used to describe the decline in productivity associated with plant aging These multipliers are multiplied times the base input-output (I/O) coefficients to compute I/O coefficients for each time point An I/O coefficient describes the amount of the input required to generate one unit of output

The subroutine MATLRN is then executed twice MATLRN serves much the same purpose as does subroutine AGE It calculates two learning

multipliers--one for learning as a function of construction time for the ℓth factor and one for learning as a function of operating time for the ℓth factor The learning multipliers are used with the age multipliers to calculate the I/O coefficient

The outputs from these three subroutines are combined in VARCST Its purpose is to compute the variable operating cost $\phi(j\ k)$ of a facility operating at time k which was built at time j Ignoring some subtleties within the program VARCST simply multiplies together for each factor (labor material, and fuel) the base I/O coefficient the operating learning and construction learning coefficients the age multiplier and the price Prices are input for labor and material, whereas the price for fuel is calculated internally

After execution of VARCST the basic conversion process has available a matrix of variable cost elements these elements describe the operating (non-capital) expenses associated with operating a plant built in each time period of the model horizon at each time period after the plant's construction

Next, six additional subroutines are executed these subroutines prepare data and parameters associated with the capital cost calculations that will take place in the up and down passes The first subroutine, INLIZE calculates the capital stock acquisitions that must have occurred before the model's base year in order to meet the output demands of the base year In essence, INLIZE considers the characteristic life of facilities constructed before the model horizon and assumes that capital accumulations occur linearly during this period using a rate such that an average historical efficiency is attained The output from INLIZE is the capital acquisitions in each year before the start of the model horizon, which in effect constitutes a vintage capital series In principle, this same data series could be collected by surveying the capital stock in existence at the start of the model horizon However because few capital stock data are available INLIZE instead provides an estimate of the capital stock by vintage

After INLIZE is completed TCHANG is executed TCHANG is similar in purpose and structure to MATLRN However it computes learning multipliers relevant to the capital input variables whereas the calculations in MATLRN were relevant to the operating factors After TCHANG subroutine DISCNT is executed three times During the first entry to DISCNT interest rates are calculated for periods between the global time points with which the model deals Two points are relevant with regard to this subroutine (1) LEAP allows for variance of discount rates between time periods and (2) some calculations within LEAP are made for time points falling between the global time points for which LEAP calculates its generalized equilibrium solutions This subroutine essentially extrapolates discount factors between global time points to create local discount factors On the second entry to DISCNT, intraperiod discounting factors are calculated for time points before and after the model horizon in the same manner that intraperiod rates were calculated in the previous entry On the final entry, average debt rates are calculated for periods between global time points in the model

horizon The final subroutine in this sequence, VXTDNR simply extends a parameter vector to a point after the final global time point in the model horizon for a period equal to the longest lead time for capital factors

Execution of VXTDNR completes the first set of subroutines The variables specific to either the up or down pass have now been defined Next a test is made to determine whether control should be passed to the up- or down-pass subroutines

Thus in any given call the front end is always executed, and then depending on the mode either the up- or down-pass set of routines is used Recall that on the up pass prices are calculated and on the down pass the new capacity and demand for operating and capital factors are calculated

Assume first that we are on the up pass Subroutine IDC computes the present value of four quantities expressed at the time of initial operation (1) equity financing (2) investment tax credit (3) interest on debt and (4) principal on debt IDC also computes the base capital cost for tax purposes This large and complex subroutine calls subroutine CFSPLT which computes the equity and borrowing split times that preserve the debt financing cost and equity financing cost when the construction lead time is not an integral multiple of the time period length Vectors containing the net present property tax and property tax flow are computed by PTI This routine assumes that the assessed value of the plant is initially equal to the base capital cost of the plant and remains constant in constant dollars, over the life of the plant Subroutine DEPTAX calculates the net present value of depreciation for income tax purposes by using variable-length time periods and time-dependent discount rates

Subroutine NPCST uses the terms calculated above to obtain the net present cost of a plant The terms necessarily represent all capital-related cost factors--equity principal interest, property tax, depreciation and investment tax credit

The next section in the up pass calculates the price corresponding to a plant built in year t, where t occurs after the end of the model horizon The subroutine that is used to do this is TERVAL which calculates the terminal value function beyond the end of the model horizon Several assumptions are made in this routine

1 Cash flows vary linearly across the time period in constant dollars rather than the discount rate remaining constant over the time period after the end of the model horizon

2 The capacity factor function is a step function where the plant operates at maximum capacity for one characteristic life and at zero capacity thereafter

3 Constant dollar prices are constant across the time period after the end of the model horizon, and factor prices are constant, in constant dollars after the end of the horizon

All these assumptions simplify the calculation of net present capital costs of a plant built beyond the model horizon

Several other subroutines available in LEAP but not used in Model 22C will not be discussed Therefore, the TERVAL subroutine essentially ends the up pass

The down pass is concerned with computing the new capacity and demand for operating and capital factors In the first subroutine of the down pass, the program checks the global time For the first global time period, subroutines OFDEM and CFDEM are called and most other down-pass routines are skipped Subroutine OFDEM computes the demand for operating factors whereas CFDEM computes the demand for capital factors If we are past the first model year then the program (1) uses PRICOT(NG) (i e the output price at model year NG) in subroutine PRODCT to compute production from all ages of plants in place and (2) computes the sum over all ages Flow then goes to subroutines OFDEM and CFDEM This step ends the down pass

B Input Parameters for Basic Conversion Process

Two types of data are required to operate the LEAP model (1) parametric values describing economic behavior and technology and (2) initial values for relevant prices and quantities This section considers the parametric values, listed in Table VII-1 of the basic conversion process as it is used, for example for synthetic fuel processes and oil refining The basic conversion process is also used in Model 22C to describe activities other than those considered here Because many parameters can take on values specific to each process each parameter is listed for each process, with processes arranged from left to right

1 Specific Capital Cost

The specific capital cost (SC) used in Eqs (B 7) and (B 8) is the cost of a facility divided by its annual output The product SC C_{LF} or SC (1 - C_{LF}) (C_{LF} defined below) defines capital I/O coefficients for labor and material respectively Model 22C input parameters show a unique SC for oil refineries, an identical SC for synthetic liquids facilities, excluding the west a unique SC for western liquid and gas facilities and an identical SC for high-Btu gas, excluding the west (see Table VII-1)

2 Capital Labor Fraction

The capital labor fraction (C_{LF}) used in Eqs (B 7) and (B 8), is the share of the specific capital cost attributable to direct labor

TABLE VII 1
Input Data for the Synthetic Fuel Processes and Oil Refinery Process
Necessary for the Basic Conversion Process

Data arameter	Specific Process N mber[a]								
	4	10	11	12	13	14	15	25	26
SC	1 5098	10 76	11 68	11 01	10 89	10 6	11 68	10 76	11 68
r_L	0 3998	0 3998	0 3998	0 3998	0 3998	0 3998	0 3998	0 3998	0 3998
$\sqrt{}_o$	0 0999	0 9200	1 2398	1 1798	1 2900	0 920	1 2398	1 1798	1 2900
f_1	0 3998	0 3998	0 998	0 3998	0 3998	0 3998	0 3998	0 3998	0 3998
T_{EF}	0 9200	0 7000	0 7200	0 7000	0 7500	0 7000	0 7200	0 7000	0 7500
IPLTIM	8	8	8	8	8	8	8	8	8
CFLDR	0 1698	0 1698	0 1698	0 1698	0 1698	0 1698	0 1698	0 1698	0 1698
L	1 3584	1 3584	1 3584	1 3584	1 3584	1 3584	1 3584	1 3584	1 3584
t_A	1930	1995	1995	1995	1995	1995	1995	1995	1995
ρ	0 0998	0 0998	0 0998	0 0998	0 0998	0 0998	0 0998	0 0998	0 0998
h_∞	1 000	1 000	1 000	1 000	1 000	1 000	1 000	1 000	1 000
β_c	0 0298	0 0498	0 0498	0 0498	0 0498	0 0498	0 0498	0 0498	0 0498
$g_{\infty\ell}$[b]	1 000	1 000	1 000	1 000	1 000	1 000	1 000	1 000	1 000
$f_{\infty\ell}$[b]	1 000	1 000	1 000	1 000	1 000	1 000	1 000	1 000	1 000
$_\ell$[b]	0 000	0 000	0 000	0 000	0 000	0 000	0 000	0 000	0 000
AVAIL	0 900	0 900	0 900	0 900	0 900	0 900	0 900	0 900	0 900
LOADFC	1 000	1 000	1 000	1 000	1 000	1 000	1 000	1 000	1 000
β	0 90	0 90	0 90	0 90	0 90	0 90	0 90	0 90	0 90
L_c	20	20	20	20	20	20	20	20	20
β_S	3 000	3 000	3 000	3 000	3 000	3 000	3 000	3 000	3 000
EQFR	0 6000	0 6000	0 4500	0 6000	0 4500	0 6000	0 4500	0 6000	0 4500
ROE	0 0998	0 0998	0 0998	0 0998	0 0998	0 0998	0 0998	0 0998	0 0998
RDEBT	0 0398	0 0398	0 0398	0 0398	0 0398	0 0398	0 0398	0 0398	0 0398
EFLIM	1 000	1 000	1 000	1 000	1 000	1 000	1 000	1 000	1 000
AVEFFI	0 905	1 000	1 000	1 000	1 000	1 000	1 000	1 000	1 000
T_L	16	16	16	16	16	16	16	16	16
D	20	20	20	20	20	20	20	20	20
f_T	0 5200	0 5200	0 5200	0 5200	0 5200	0 5200	0 5200	0 5200	0 5200
I_{cr}	0 0998	0 0998	0 0998	0 0998	0 0998	0 0998	0 0998	0 0998	0 0998
p_{rt}	0 0198	0 0198	0 0198	0 0198	0 0198	0 0198	0 0198	0 0198	0 0198
FORPER	1 000	1 000	1 000	1 000	1 000	1 000	1 000	1 000	1 000
I_f	0 00	0 00	0 00	0 00	0 00	0 00	0 00	0 00	0 00
I_f	0 00	0 00	0 00	0 00	0 00	0 00	0 00	0 00	0 00
α	1 000	1 000	1 000	1 000	1 000	1 000	1 000	1 000	1 000
CFSENS	1 3398	1 3398	1 3398	1 3398	1 3398	1 3398	1 3398	1 3398	1 3398
I(J)[c]	1 000	1 000	1 000	1 000	1 000	1 000	1 000	1 000	1 000

[a]Specific process number explanation
- 4 Oil refinery
- 10 Liquids production from mid continent coal
- 11 High BTU gas production from mid continent coal
- 12 Liquids production from western low sulfur coal
- 13 High BTU gas product on from western low sulfur coal
- 14 Liquids production from Appalachian medium high sulfur coal
- 15 High BTU gas production from Appalachian medium high sulfur coal
- 25 Liquids production from western medium high sulfur coal
- 26 High BTU gas production from medium high sulfur coal

[b]Input values identical for ℓ = 1 (labor) and ℓ - 2 (material)

[c]I(J) is defined as unity for all global time points J

charges An identical value of about 40% is entered for each specific process in Table VII-1 By implication materials costs are equal to $(1 - C_{LF})$ or 60%

3 Variable Operating Cost

Variable operating cost (V_o) used in Eq (V 16) is the ratio of the annual non-fuel costs associated with operating a representative facility divided by the annual output of the facility When multiplied by the share of the $\underline{i}$th input in operating costs it yields an I/O coefficient for non-capital non-fuel factors As was true for the SC, values for the V_o are shared by similar conversion processes

4 Operating Labor Fraction

The operating labor fraction (f_1) used in Eq (V 16) is the share of labor costs in variable operating costs An identical value of about 40% is entered for each specific process in Table VII-1 By implication, the material operating fraction is equal to f_2 or 60%

5 Thermal Efficiency

The thermal efficiency (T_{EF}) used in Eq (V 19) is the ratio of the energy content of the output of a process divided by the energy content of the input to the process It is used to calculate the I/O coefficient for fuel inputs The input parameter for the oil refinery process is 92% The conversion processes share T_{EF} parameters ranging from 70 to 75%

6 Planning Lead Time

The planning lead time (IPLTIM) (see parameter 8) is the length of time between which a decision to construct a facility is made and the point at which that facility comes on line These variables enter into the entrepreneur's decision to build a plant because, when calculating his costs and returns he must begin at a point in the future that is equal to the present period plus the planning lead time A value of 8 years is entered for each specific process in Table VII-1

7 Capital Factor Lead Ratio

The capital factor lead ratio (CFLDR) (see parameter 8) is the fraction of the planning lead time that is used to acquire capital factors It is used in calculating the net present revenue of a proposed plant This factor is about 17% By implication, a lead time of about 1 3 years is required to order capital equipment

8 Lead Time

The lead time (L), used in Eq (B 2) is the amount of time necessary to create new capacity This parameter is calculated as the product of IPLTIM and CFLDR

9 Capital Change Rate

The capital initial change rate (β_c) used in Eq (B 6) determines how rapidly the specific capital cost reaches its ultimate limit as defined by h_∞ (see parameter 15) The fact that h_∞ is set to unity renders the effect of β_c null for the activities listed in Table VII-1

10 Construction-Time-Based Operating Technological Change Limit

This parameter ($g_{\infty\ell}$) used in Eq (V 18), acts similarly to the h_∞ variable (B 6) but it is applied to the operating costs This variable is entered as unity and it has no effect on the calculations

11 Production-Time-Based Operating Technological Change Limit

This parameter ($f_{\infty\ell}$) used in Eq (V 19) acts similarly to the $g_{\infty\ell}$ variable It is the ratio of the operating I/O coefficient to the base coefficient assuming that with experience industry will become more efficient This variable is entered into the code as unity for $\ell = 1$ and 2 (i e for labor and material) and it has no effect on the calculations

12 Initial Rate of Change

The initial rate of change (α_ℓ) used in Eqs (V 18) and (V 19) measures the rate of change with which the changes implied by $g_{\infty\ell}$ and $f_{\infty\ell}$ are achieved The calculations are not effected since values of unity are assigned to $g_{\infty\ell}$ and $f_{\infty\ell}$

13 Year Commercially Available

This parameter (t_A) used in Eq (V 18) is the first year that a representative technology can be constructed for commercial use without a cost penalty If a firm attempts to build a facility before this year it must calculate its capital and operating costs using the penalty function discussed under item 14 Except for the oil refining process which became feasible in 1930 all specific processes treated in the basic conversion process will become available in 1995

14 Pre-Commercial Premium Per Year

The pre-commercial premium (ρ) used in Eq (V 18), is the fractional increase in capital and operating costs that must be paid to accelerate the availability date of a facility by 1 year An identical factor of about 10% is entered for each specific process Thus to accelerate a plant by one global time period (5 years) a cost penalty of 50% must be paid

15 Capital Technological Change Limit

The capital change limit (h_∞) used in Eq (B 6) is the ratio of the ultimate capital cost of a facility to its capital cost at the time of first availability This factor permits capital costs of facilities to decrease over time as the industry gains experience with a technology and is used to calculate the specific capital cost A value of unity is entered in each specific process in Table VII-1 and therefore capital factors do not change with time

16 Availability

This parameter (AVAIL) determines the fraction of time that the capacity of a facility can operate taking into account such factors as scheduled maintenance unscheduled downtime and the like A value of 0 90 is entered for each specific process in Table VII-1

17 Load Factor

The load factor (LOADFC) is defined as the percentage of time that a demand is placed on a facility For the basic conversion process in Table VII-1 this factor is set to unity Note that load factor is a characteristic of the demands placed on a facility whereas availability is a plant-related characteristic

18 Maximum Capacity Factor

This value (β) used in Eq (V 21) is obtained as the product of AVAIL•LOADFC (see parameters 16 and 17) It is the maximum value that the capacity factor can take on

19 Characteristic Facility Life

The characteristic facility life (L_c) used in Eq (V 3) is defined as the period of time during which the cost per unit output for a facility doubles For practical purposes this value defines the point at which a facility will close due to obsolescence A value of 20 years is used

20 Facility Aging Rate

The facility aging rate is the fractional increase in operating cost per unit of output per year that occurs when a facility reaches its characteristic life This factor is used to calculate the parameter β_A appearing in Eq (V 17) Like the characteristic life this factor modifies the variable operating cost and seeks to capture the effects of obsolescence A value of 3 0 is entered for each specific process in Model 22C The implications of this parameter and the characteristic life parameter are discussed in detail in Section VII C

21 Tax Depreciation Life

The tax depreciation life (T_L) used in Eq (B 30) is the life of a facility over which the value of the facility is depreciated for income tax purposes This parameter is set to 16 years

22 Debt Life

The debt life (D), used in Eq (B 15), is the period of time used by the entrepreneur to calculate the present value of interest payments plus the present value of principal repayments This value is set to 20

23 Income Tax Rate

The income tax rate (f_T), used in Eq (B 1), is the effective state and federal rate at which corporate income will be taxed It is set at 52% for all specific processes in the basic conversion process

24 Investment Tax Credit Rate

The investment tax credit rate (I_{tcr}), used in Eqs (B 33) and (B 34), is the percentage of new investment that the Internal Revenue Service permits the entrepreneur to credit against income taxes LEAP assumes that this credit is used as soon as it is earned This parameter is set to 0 0998 for all specific processes in the basic conversion process

25 Property Tax Rate

The property tax rate (P_{rt}) used in Eq (B 28), is the percentage of assessed values which must be paid to property taxes This value is set at 0 0198 for all specific processes in the basic conversion process

26 Equity Financing Fraction

The basic conversion process assumes that firms may finance investment by either debt or equity The equity financing fraction (f_E), Eq (B 18) gives the percentage of capital investment that is financed through equity capital The value of f_E ranges from 0 45 to 0 60 for the specific processes in Table VII-1

27 Historical Capacity Additions Change Rate*

This parameter (r_s), used in Eqs (V 25) and (V 26) is the annual change in nameplate capacity characterizing each specific process This variable is used to calculate the implied capital stock, by vintage, associated with each specific process, in lieu of actual data for capital It is also used to calculate capacity commitments at the start of the period In LEAP, this parameter is calculated in subroutine ECALBR which was written by the Long-Term Energy Analysis Division (LTEAD)

28 Forecasting Perfection

The LEAP model makes assumptions as to the entrepreneur's perception of future product prices which may range from a weighted average of past prices to the "true" price values calculated by the model The forecasting perfection parameter (FORPER) is the weighting variable used in this calculation, a value of 1 0 implies perfect perception of future prices, whereas a value of 0 0 implies a historical extrapolation of past price data A value of 1 0 is entered for each specific process in the basic conversion process

29 Historical Inflation Rate

The historical inflation rate (I_f') used in Eq (B 12), is used to describe the rate of inflation at the start of the model period A value of 0 0 is entered to each specific process, implying that all calculations are carried out in base period prices

30 Terminal Inflation Rate

The terminal inflation rate (I_f), used in Eq (V 15), describes the rate of inflation after the last model time period A value of 0 0 is entered to each specific process

31 Capacity Factor Cost Multiplier

The capacity factor cost multiplier (α), used in Eq (V 21), is defined as the ratio of output price to variable operating cost at which the capacity factor is equal to one-half its maximum value This variable serves as a sensitivity coefficient to the capacity factor formula, a value of unity is entered for each specific process in the basic conversion process

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*In LEAP the input parameter RATIN is no longer input for conversion processes Instead RATIN ($=r_s$) is calculated using the input parameter E_{AV}, which has been added as an input parameter [see Eq (V 25)]

32 Capacity Factor Price Sensitivity Parameter

The capacity factor price sensitivity parameter CFSENS is needed to calculate γ which is a second sensitivity parameter in the calculation of the capacity factor CFSENS is defined as the ratio of initial price to final price over which the capacity factor drops from 90% of its maximum to 10% of its maximum A value of 1 3398 is entered for each specific process in the basic conversion process

33 Assessed Value Inflator

The assessed value inflator [I(j)], used in Eq (B 28) is a multiplier used to inflate the assessed values of a facility on which property taxes are paid A value of 1 00 is entered for each specific process in the basic conversion process for each of the ten global time points

34 Return on Equity

The return on equity (ROE) is the required rate of return on equity funds invested and is used to calculate the minimum acceptable price on new facilities

35 Return on Debt

The return on debt (RDEBT) is the interest rate on borrowed funds

36 Thermal Efficiency Limit

The thermal efficiency limit (EFLIM) is the ratio of ultimate thermal efficiency (for fuel) to the initial efficiency at the year of availability

37 Average Efficiency

The average efficiency is obtained by averaging the efficiency of a process from the time of availability to the first model year

C <u>Validity of Basic Conversion Process</u>

Based on the discussions above we now turn to what may be termed the "validity" of the basic conversion process Validity may be interpreted narrowly or it may be extended toward generic consideration of the agreement between the behavior of the model and the real world The present method is to adopt a narrow approach, which considers the effect of the modeling conventions on the model's output, with specific reference to the basic conversion process Moreover, validity is viewed as a continuum rather than a binary classification Ultimately, validity must be viewed as a relationship uniting user needs with model outputs and behavior We have made no attempt to extend the present analysis to that conclusion

In the discussions of basic conversion process validity we will adopt the format followed above by breaking the basic conversion process into (1) front-end components (2) up-pass components, and (3) down-pass components Within each component, individual subroutines that calculate important variables will be considered

1 Front-End Components of the Basic Conversion Process

Recall from above that the front-end of the basic conversion process carries out calculations that are applicable to both the up- and down-pass portions of the solution algorithm On the basis of the previous discussion we can immediately dismiss two subroutines TIMCHR and VXTDNR from further consideration because their function is data management and their specification does not affect model outputs We have limited treatment of these subroutines to verifying that their internal code is consistent with their function Six remaining subroutines affect model outputs in the front-end calculations AGE MATLRN, VARCST INLIZE, TCHANG and DISCNT We shall consider these subroutines individually

a AGE Subroutine AGE reflects the effects of plant and equipment obsolescence in variable operating costs by generating an "aging multiplier " which increases in value over time Because the ratio of variable operating costs to output price is a key determinant of the capacity factor for each vintage capital and by implication the rate at which capital is retired the components of variable costs are highly important to model outputs In principle little doubt exists that obsolescence is a key factor in cost determination The particular method by which LEAP captures this effect however, is somewhat more questionable

The subroutine AGE computes the learning multiplier by assuming that aging follows an exponential pattern The multiplier is given by Eq (V 17)

$$f_A(k - j) = \exp\left\{\left[\frac{(k-j)\Delta}{L_c}\right]^{\beta_A}\right\}$$

where

L_c = characteristic plant life

β_A = steepness parameter

$\Delta(k - j)$ = time in years after the plant is built

Δ = 5 years (the increment between model time points)

The exponential model is versatile in that it can take on several shapes depending on the parameter values The parameter L_c in the aging function is the characteristic plant

life The function implies that when $(k - j)\Delta = L_c$ the aging multiplier takes on the value e = 2 718 After this age the multiplier takes off at a rate dependent on β_A The larger β_A is the faster the aging multiplier increases As a comparison the aging multiplier was computed in 10-year increments until age 50 with a characteristic life of 20 years for β_A = 1 0 3 0 and 20 0 (see Table VII-2) Even a modest increase in β_A can result in a large increase in the aging coefficient In Model 22C the value of β_A is 20 which causes an explosive behavior indicating that when plant age exceeds the plant's characteristic life the plant is economically obsolete

TABLE VII-2

Values for the Aging Multiplier When β_A is Varied

Age $t = (k - j)\Delta$	0	10	20	30	40	50
$f_A(t)$ for $\beta_A = 1$	1 00	1 65	2 72	4 48	7 39	12 18
$f_A(t)$ for $\beta_A = 3$	1 00	1 13	2 72	29 22	2980 96	8848 25
$f_A(t)$ for $\beta_A = 20$	1 00	1 00	2 72	∞	∞	∞

The value of β_A (AGBETA) is determined within the program as a function of the facility aging rate (VOAGRT) and the characteristic facility life (ICLIFE) The variable VOAGRT was estimated by DFI whereas ICLIFE was taken from the Brookhaven National Laboratory data base [1] These references were obtained from a draft documentation paper[2] sent by John Pearson August 2 1979

Several points should be noted about the aging multiplier Although one might generally agree with an exponentially decreasing rate of production in Model 22C the aging multiplier most closely resembles a step function that assumes values of 1 2 7 and infinity This fact places great pressure on the estimation of the characteristic life which LEAP defines as the length of time in which the aging multiplier doubles In fact such a value is likely chosen fairly arbitrarily The principal effect on model output is that little flexibility exists for extending plant lifetimes in response to such factors as increased discount rates Plants simply live out their characteristic lives and are retired

thereafter All this information suggests that the β_A parameter should receive particular attention Whether or not β_A is estimable and it is not clear that it is, the choice of the parameter is a primary determinant of variable operating costs because, as will be shown, the other factors involved in variable operating costs have values close to unity

b MATLRN Subroutine MATLRN produces construction and production learning multiplers which are used to modify the base I/O coefficients for new plants The rationale for this modification is that technological improvements will cause plants of later vintages to be more efficient in operation and less costly to build in terms of input quantities than are plants of earlier vintage A second function of this subroutine is to permit construction of a facility before its "feasible date " but to also impose a penalty for this privilege

The construction and production learning multipliers produced by MATLRN also follow a "geometric" learning curve Specifically, the construction geometric learning curve is defined by Eq (V 18)

$$
\begin{aligned}
c\ell(j) &= g_{\infty\ell} + (1 - g_{\infty\ell})(1 - \alpha_\ell)^{t_I+(j-1)\Delta-t_A} && t_I+(j-1)\Delta > t_A \geq t_I + N_p\Delta \\
&= g_{\infty\ell} + (1 - g_{\infty\ell})(1 - \alpha_\ell)^{(j-1)\Delta - N_p\Delta} && t_I+(j-1)\Delta \geq t_I + N_p\Delta > t_A \\
&= 1 + [t_A - t_I - (j-1)\Delta]\rho && t_A \geq t_I + N_p\Delta \\
& && t_A \geq t_I + (j-1)\Delta \\
&= 1 + \left[\frac{2T_{EF}\ 2E_{AV}}{0.8\ T_{EF}\ L_c}\right][(j-1)\Delta - N_p\Delta] && t_I + N_p\Delta > t_I + (j-1)\Delta > t_A \\
&= 1 + \left[\frac{T_{EF}\ 2E_{AV}}{0.8\ T_{EF}\ L_c}\right][t_A - t_I - N_p\Delta] \\
&\quad + [t_A - t_I - (j-1)\Delta]\rho && t_I + N_p\Delta > t_A \geq t_I + (j-1)\Delta
\end{aligned}
$$

where

ℓ = 1 for labor, 2 for material,

$g_{\infty\ell}$ = technological change limit for factor ℓ

α_ℓ = technological change rate for factor ℓ,

t_I = time that corresponds to the first global time point, $T_L(1)$

t_A = time at which technology first becomes commercially available,

ρ = penalty for early availability

The geometric learning function can assume several shapes depending on the values of the parameters Thus several learning scenarios can be modeled One problem is the number of parameters that are necessary to describe the function Most of these parameters are not estimable in an econometric sense because no data exist but must be hypothesized by experts in the field

In Model 22C the penalty is set at 0 10 which is assigned by the Long-Term Energy Analysis Division (LTEAD) of the EIA [2] The penalty is the same for all eight synthetic fuel sources and for the oil refinery source The time of commercial availability, 1995 is the same for all synthetic fuels, this value was also chosen by LTEAD [2] The technological change limit for production and construction is set equal to 1 for all factors as well as for all synthetic fuel processes and the oil refinery process The effect of this choice of parameters is to drop all learning multipliers except for the penalty function out of the calculation of variable operating costs The present value for this penalty (about 10%) means that a firm that wishes to operate a plant for one period (5 years) before commercial availability would have to pay a penalty of 50% Whether firms would choose to do this in the context of the LEAP model is unknown but unlikely

c <u>VARCST</u> Subroutine VARCST calculates non-capital operating costs by summing the products of input quantities, which are given by I/O coefficients that have been modified by the various multipliers and input prices The calculation to compute variable operating cost at time k for a plant built at time j is defined by Eq (V 9)

$$\phi(j,k) = \phi_0(j,k) \qquad k \geq j \geq N_p + 1$$

$$+ Q_F(j\ k)P_I(k) \qquad k \leq 2N_p + N - 1$$

where

$\phi(j\ k)$ = variable operating cost of a plant per unit of output energy built at time j and operating at time k

$\phi_o(j\ k)$ = portion of the variable operating cost per unit of output energy that arises from the cost of labor and materials

I_f = rate of inflation for times $k > N_p + N$

$Q_F(k\ j)$ = quantity of energy required at time j by plant built at time k and operating with capacity factor unity to produce one unit of output energy at time j

$P_I(j)$ = price on the input link at time j

The quantity $\phi_o(j\ k)$ is given by Eq (V 11)

$$\phi_o(j\ k) = \sum_{\ell=1}^{2} V_o f_\ell p_\ell(k) f_A(k - j) f_{c\ell}(j) f_{o\ell}(k)$$

and $Q_F(j\ k)$ is given by Eq (V 20)

$$Q_F(j\ k) = T_{EF}^{-1}\ f_{c3}(j) f_{o3}(k)$$

Although the calculation in $\phi_o(j\ k)$ appears to summarize a great deal of information the parameter specifications in Model 22C yield a fairly simple relationship Because carrying out calculations of extremely large numbers is pointless VARCST uses a value of 6×10^6 as the largest calculated cost

d <u>INLIZE</u> Subroutine INLIZE calculates the capital stock acquisitions that must have occurred before the model's base year in order to meet the output demands of the base year A linear assumption concerning capacity additions for $j \leq N_p + 1$ is used to give

$$N_W(j) = \frac{Q(N_p+1)\ \mathrm{Max}\ \{0\ [1-r_s\Delta(N_p+1-j)]\}}{\sum_{k=1}^{N_p+1} \mathrm{Max}\ \{0\ [1-r_s\Delta(N_p+1-k)]\} C_f(k\ N_p+1)}$$

$$j = 1 \text{ to } N_p + 1$$

with the quantity r_s determined from

$$E_{AV} = \frac{\sum_{k=1}^{N_p+1} Q_F(k,N_p+1)C_f(k,N_p+1)N_W(k)}{Q(N_p+1)} ,$$

where

E_{AV} = an average process efficiency that is input to the code

r_s = yearly change in capacity additions

The yearly change in capacity additions, r_s, is called RATIN in LEAP This value is calculated within LEAP by subroutine ECALBR, written by LTEAD ECALBR simply calculates the slope of the line by which capacity is added before the first model year to achieve an average process efficiency If the value of r_s is known, then subroutine INLIZE simply sets up the capital stock acquisitions in a linear manner so that the base-year demand is met The manner in which this step is done is appropriate if the linear assumption on capacity additions is acceptable

e TCHANG Subroutine TCHANG is identical to subroutine MATLRN except that it is applied to the capital I/O coefficient to obtain capital costs The same values used to determine a parameter for MATLRN are used for TCHANG

f DISCNT The final subroutine in the front end of the LEAP model DISCNT is used to calculate time-varying discount rates In essence, the purpose of this subroutine is to interpolate unknown, intermediate discount rates from known ones by using a linear method However, initial and terminal discount rates entered into LEAP's present specification are equal As such this subroutine calculates two discount rates, one is the yearly rate, which equals the effect of the equal discount rates over 5 years, and the other is zero

2 Up-Pass Components of the Basic Conversion Process

As defined earlier in this section, the purpose of the up-pass component is to calculate output prices for a conversion process from factor input prices and quantities More specifically, this component must generate sufficient data to solve Eq (V 6)

To calculate the time stream of output prices capital costs and a terminal price value must first be calculated and combined in the appropriate form Variable operating costs have already been calculated in the front end Finally, the capacity factor, which is a function of output price and variable operating cost, must be calculated These calculations are carried out through a sequence of 10 subroutines

a IDC IDC is the first of a series of three subroutines that calculates the component inputs necessary to calculate the present value of capital costs, $N_c(j)$ in Eq (V 6) These components include (1) the cost of equity financing, (2) the cost of debt financing (3) base capital cost for tax purposes, and (4) investment tax credit

DFI documentation[3] describes the IDC subroutine as follows

> Although the financial concepts are not difficult, the implementation is quite complex Most of the complexity, however, arises because we have incorporated the capability to deal with time varying discount rates (i e , return on equity and interest on debt)

This comment aptly describes subroutine IDC, it is a long, difficult-to-follow exercise In Model 22C time-varying discount rates are not used--constant rates are used for all global time points A second element that adds a great deal of complexity to this calculation is the use of different interest rates for debt and equity finance

The final complicating factor involves the use of a series of calculations to adjust for the fact that not all model time spans considered in the model calculations are direct multiples of the model time periods For example the planning lead time for the basic conversion process is 8 years whereas the model operates in 5-year intervals A good deal of computer code is devoted to the necessary approximations for reconciling intraperiod time spans Beyond these calculations the calculations of present value are perfectly straightforward and conventional

b PTI The information provided by subroutine IDC next permits calculation of costs related to property tax, calculations that are basically straightforward and, unlike IDC calculations, uncomplicated First, the assessed value of a facility is calculated

$$\text{assessed value} = B(j,j) \times I(m)/I(j) ,$$

where

$B(j\ j)$ = base facility capital cost [see Eq (B 28)]

$I(j)$ = inflation factors, now set to unity such that j corresponds to the vintage of the capital and m to the present time period

When inflation factors are set to unity, the assessed value and capital cost are assumed to be equal

Next, the amount of taxes to be paid is calculated by multiplying the property tax rate times the assessed value

$$\text{Tax payment} = \text{assessed value} \times p_{rt}$$

An identical rate of 2% is used for all property to be taxed within Model 22C

Finally, the present value of the time stream of property tax payments is calculated in stages by determining the property tax for each global time

$$PT(m) = B(j\ j)p_{rt}\left[\alpha_1(m)\frac{I(m)}{I(j)} + \alpha_2(m)\frac{I(m+1)}{I(j)}\right],$$

where $\alpha_1(m)$ and $\alpha_2(m)$ = intraperiod discount factors

In Model 22C the discount rates are constant across time, which causes $\alpha_2(m)$ to be zero for all time points Thus it vanishes from the above calculation Further, $I(m)$ is unity for all time points so that the seemingly complicated expression above reduces to

$$PT(m) = B(j,j)p_{rt}\alpha_1(m)$$

To calculate the net present value of property tax payments across the life of the facility, simply discount in standard fashion and sum the individual elements This step generally yields

$$V_p(P_t\ j) = B(j,j) \quad p_{rt} \sum_{m=j}^{1+\mathrm{Int}\left[\frac{L_c}{\Delta}\right]} \alpha_1(m)\frac{I(m)}{I(j)} \prod_{k=j}^{m-1} \left[\frac{1}{1+r_e'(k)}\right]^{\Delta}$$

Little can be added regarding the validity of these calculations other than to note that the use of constant parameter values across the processes described leads to essentially identical calculations for each process

c DEPTAX The purpose of this subroutine is to calculate an expression for the present value of depreciation for income tax purposes that occurs over the life of a plant First denote a normalized depreciation schedule $U(m\Delta)$ where U refers to undepreciated value For the mth time period the depreciation that occurs is equal to the difference in undepreciated value at the start and end of the period that is

$$R(m) = \frac{U(m\Delta) - U[(m - 1)\Delta]}{\Delta}$$

which can be converted to a rate per annum by dividing R(m) by the number of years in the mth time period

The present value of depreciation for the mth period is thus

$$PVD(m) = [\alpha_1(m) + \alpha_2(m)]R(m) \quad B(J\ J)$$

or since α_2 is zero

$$PVD(m) = \alpha_1(m)R(m)B(J\ J)$$

To calculate the present value of the stream of depreciated value discount from the end of the period over the life of the facility we proceed as above for net present value of property tax payments that is the present value of depreciation for income tax purposes may be written

$$V_p(D_t\ J) = B(J\ J) \sum_{m=J}^{1+Int\left[\frac{T_L}{\Delta}\right]} \alpha_1(m)R(J + 1 - m) \prod_{k=J}^{m-1} \left[\frac{1}{1+r_e(k)}\right]^{\Delta}$$

Like the discounting applications of the previous subroutines this procedure is a straightforward application of conventional practices

d NPCST This subroutine calculates the net present value of capital costs represented by the variable $N_C(J)$ Because the equation actually calculated is the present value before taxes we can divide by $(1 - f_T)$ and take present values yielding (see Appendix B)

$$N_C(J) = \frac{1}{1-f_T} \quad [V_p(E_q,J)] + V_p(I_{nt}\ J) + V_p\ (P_t,J)$$

$$+ \frac{1}{1-f_T} V_p(P_{rn},J) - \frac{f_T}{1-f_T}[V_p(D_t,J)]$$

$$- \frac{1}{1-f_T}[V_p(I_{tc}\ J)]$$

where V_p is an operator that gives the present value at time J of the first argument in the bracket All of the positively valued expressions are changes borne by the facility, whereas all negatively valued expressions are tax-related adjustments This particular set of calculations raises no questions and is straightforward The income tax rate variable is set at 52%

The next set of subroutines in the up pass is concerned with the pricing calculations The first subroutine TERVAL sets the terminal value of output price from which other prices are calculated Given this price one can calculate the stream of prices which is carried out in subroutine MARCST Finally a series of accounting subroutines, not discussed, completes the up pass

e <u>TERVAL</u> This subroutine calculates the terminal value prices These prices are for a plant built after the end of the model horizon Prices are calculated for one characteristic plant life past the model horizon, backwards to the last year of the model horizon This step is accomplished by writing the present value equation for a new plant constructed in year m beyond the end of the model horizon This present value contains the price at time m, for which the equation may be solved Various simplifying assumptions are necessary to enable the equation to be solved One of these assumptions has been changed for the present code In the previous codes cash flows were assumed to vary linearly across the time period in inflated dollars In this code the cash flows are assumed to vary linearly across the time period in constant dollars [3] DFI believes this simplifies the discounting convention Whether or not this new assumption simplifies the calculations it is identical to that presently specified in the LEAP model for all time periods

Three additional assumptions are made which help to solve the price equation The first of these is to allow the capacity factor function to take on a step function behavior The capacity factor function is defined as

$$C_f(j,m) = \beta \qquad m - j \leq L_c$$
$$= 0 \qquad m - j > L_c$$

where

β = maximum capacity factor of a given plant,

j = time the plant was built

m = time of operation

L_c = characteristic life of the plant

Although in practice this specification has the potential to differ greatly from the continuous form of the capacity factor [see Eq (V 21)] in reality it does not Because of the specification of the aging multipliers capacity is effectively zeroed out after the characteristic life is passed

The second simplification is that the constant dollar prices are roughly constant across the time periods past the end of the model An argument for this is that prices under the concept of constant dollars will change little past the end of the model horizon This assumption implies that the discounting factors can be given as

$$\alpha_1(j) = \frac{1-\left[\frac{1}{1+r_c(j)}\right]^{\Delta}}{1-\left[\frac{1}{1+r_c(j)}\right]}$$

and

$$\alpha_2 = 0$$

where

Δ = DEL = 5 years (the increment between model time points),

$r_c(j)$ = inflated dollar discount rate

Again, since all values in Model 22C are calculated in current dollars, this assumption represents little change

The third major assumption is that the factor prices remain constant in constant dollars, past the end of the horizon This assumption allows substitution of a simplified form for the factor prices into one operating cost of the product

This procedure is comparable with the present Model 22C specification

f MARCST Sufficient information is now available to calculate price as the marginal cost of new plant capacity This calculation is carried out in MARCST by writing an equation for the present value of each flow after taxes and assuming that capital is added until the last unit's addition to cash flow is zero Specifically, the subroutine calculates P(j) for $J = N_p + 1$ to $N_p + N$ from Eq (V 6)

A primary cause for uncertainty in this subroutine concerns the capacity factor

In Model 22C we have

β = maximum value of C_f for the present LEAP specification, which is defined as the product of the availability and the load factor or 0 90 for all specific processes

α = an equivalence factor (i e when α $\phi(j\ k) = P(j)$, the capacity factor is equal to 1/2), for the present LEAP specification α is set to unity, which is defined as CFMULT

γ = a "sensitivity" parameter presently calculated as

$$\frac{2 \ln (9)}{\ln (CFSENS)} = \frac{4\ 394}{\ln (1\ 34)} = 15$$

Using these parameters one can easily evaluate the level of the capacity factor based on alternative ratios of variable cost to price These calculations are shown below

ratio of variable cost to price	0 70	0 80	0 90	1 00	1 10	1 20	1 30
capacity factor	0 89	0 86	0 72	0 45	0 20	0 08	0 03

As the ratio of costs to price moves from 70 to 130%, the capacity factor moves from 89% against a maximum of 90% to a level of 3% Whether these values are "reasonable" is almost impossible to determine except perhaps within the range of proper sign Moreover the parameters of this function have no visible correspondence to parameters that have been estimated in the literature Thus, the capacity factor is a highly descriptive qualitative device, which is based on input from the relatively explosive variable operating cost algorithm

3 Down-Pass Components of the Basic Conversion Process

As defined earlier in the section, the purpose of the down-pass component is to calculate factor inputs for a conversion process from input prices and output prices and quantities More specifically, this component must yield factor demand for both capital and operating inputs Unlike the up pass, in which a series of rather intricate financial calculations had to be performed, the calculations in this section are much simpler and take place through a few subroutines

a PRODCT The purpose of subroutine PRODCT is to create a production schedule from existing capital that is the short-run supply curve This objective is accomplished by solving the equation

$$Q(J) = \sum_{k=1}^{J} C_f(k,J)N_W(k) \qquad J = N_p + 1 \text{ to } N_p + N$$

The prices generated by the up pass imply a distinct capacity factor for each vintage of capital, in contrast this equation evaluates the quantity of output from existing capital stock implied by their prices

After execution of this subroutine, a test is made to determine whether excess or insufficient capital exists--that is whether implied output at prevailing costs and prices is consistent with demand

b ONWPRD If new capacity is needed subroutine ONWPRD is called to calculate the quantity of nameplate capacity needed to meet this demand This function simply divides the output deficit by the capacity factor to obtain the level of new capital needed Because this calculation assumes constant prices no attempt is made to call forth additional output from existing capacity except through the interaction of up and down passes

c OFDEM After the decision as to the quantity of capital in place is made the quantity of operating factors associated with this capital stock must be estimated This step is accomplished by solving the equation

$$Q_I(J) = \sum_{k=1}^{J} Q_F(k,J)C_f(k\ J)N_W(k) \qquad J = N_p + 1 \text{ to } N_p + N$$

No new variables are introduced in this subroutine

D Conclusions

Our review has indicated that the routines within the basic conversion process are consistent with the available documentation This

is not to say, however, that the documentation is complete Given knowledge of the model and its computer code one can determine the accuracy of the documentation but the documentation is insufficient to understand the structure and operation of the LEAP system Moreover, we find no errors in the computer codes or in the basic interpretation of these codes

The model appears to handle a good many of the more important economic interactions quite well In particular, the cost characteristics of financing capital acquisitions are treated in great detail Although, piecewise, the components of the model are congruent with economic theory, it is not clear that the model itself is analogous to a series of general equilibrium solutions Whether or not this is truly important for the model's policy implications is a topic somewhat beyond the scope of this exercise

One suspects that in many cases the model's behavioral parameters have no empirical basis Because of the parameter specifications, much of the complexity allowed in LEAP is not used in Model 22C The capacity factors aging function, penalty functions, and others seem to be wholly heuristic For these variables no parameters have been estimated, or perhaps could have been estimated, by using standard econometric or statistical techniques In most cases the modelers seem to be content to specify the proper sign of the relevant first derivatives A large model with an excess of variables that are difficult to measure, or even estimate, reduces confidence that the model will yield results that reflect reality

Another concern is the similarity of parameter values for the different specific processes For the oil refinery and eight synthetic fuel processes considered in Table VII-1, there is much similarity between the parameters This fact indicates either a great similarity among processes or a great ignorance about the true parameter value for each process No real documentation describing the parameter values exists that is no specific reference to specific pages in a specific journal is given for any parameter

REFERENCES FOR SECTION VII

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VIII SENSITIVITY ANALYSIS BY SCREENING DESIGN

A Introduction

The purpose of sensitivity analysis is to determine the value of the partial derivatives of calculation results with respect to the input data These partial derivatives are called the sensitivity coefficients of the result to the input data Sections VIII and IX are concerned only with linear sensitivity theory, the first-order partial derivatives

Knowledge of the sensitivity coefficients can be useful for several reasons which are all connected with questions related to the uncertainties in the calculation results If one considers the calculation (or rather the model for which the calculation stands) to be exact, then the uncertainty in the calculation results can easily be obtained if the values of the sensitivity coefficients and the uncertainties in the input data are known The sensitivity coefficients can be particularly useful if they are available before the analysis leading to the uncertainties in the input data because they allow the efforts to be concentrated on the subset of input data that gives rise to large sensitivity coefficients

The sensitivity coefficients are also useful in guiding further work related to the calculation itself If the calculation represents an accurate modeling of the process under study availability of the sensitivity coefficients may assist in formulation of more approximate models, where the data having low sensitivity coefficients are handled by means of approximations This may result in great cost savings without adversely affecting the accuracy of the output of the calculation If the calculation is known to be an approximate model of the process under study then sensitivity coefficients may help in pinpointing where improvement in the model is likely to impact the accuracy of the result most heavily

Two main approaches have been developed for determining sensitivity coefficients in the case of complex computer codes with many input parameters the "forward" and "adjoint" techniques The forward approach sometimes referred to as an "experimental design" or "response surface" methodology is based on statistical theory It determines an estimate for the sensitivity coefficients by performing a limited set of "experiments" with the code in which the input parameters are perturbed corresponding changes in the output of the code are then observed and exploited A surface (i e functional form) relating the results from the code for the various input data sets is constructed from which approximate sensitivity coefficients are generated In the adjoint approach (Section IX) a deterministic method is used A new set of equations is developed that is in a sense adjoint to the equations of the model A computer code is written to obtain the solution to the adjoint equations From a single forward and adjoint solution to all the equations the sensitivity coefficients are obtained for all input parameters

In the forward approach one is usually severely restricted in the number of perturbations that one can make in the input parameters because of the costs involved in running the code The number of runs made with the code is much smaller than the number of input parameters The forward method requires development of appropriate estimators for the sensitivity coefficients which use the perturbations made in the input data and the observed outputs of the code A basic assumption underlying all forward approaches is that robust estimators for the large sensitivity coefficients can be found The smaller sensitivity coefficients are inaccessible to estimation procedures as a result of the noise inherent in the procedure The name "screening studies" has been attached to the forward approach because although large sensitivity coefficients could possibly be identified by this method we may not necessarily obtain an accurate value for their absolute magnitude

Much of the initial sensitivity work in the energy model validation effort at ORNL was made in the area of developing a suitable screening methodology Two major considerations were involved in this decision (1) these studies could be started without delay since the input data for them could be generated immediately and (2) if the method proves successful, the presumably higher development cost of an adjoint code could possibly be avoided Our adjoint method experience at ORNL with reactor physics problems had indicated that in some situations, such as in shielding problems the output of the code has large sensitivities to only a small subset of the input data If this situation held for at least some of the outputs of LEAP one of the estimators used in screening for reactor safety codes could conceivably be successful We were particularly interested in approaches for which no prior assumptions (often referred to as engineering judgment and experience in the case of reactor safety codes and to economic judgment in our case) were required to select a subset of the input parameters for the screening phase

The initial screening studies using Model 82 with only 80 input parameters being perturbed for convenience revealed that the "matrix method" of Durston et al [1] appeared to work successfully Some large sensitivity coefficients as determined by direct calculations were identified by the estimator using only 10 or 20 runs of the code when all 80 parameters were perturbed randomly by ±1% for each run A puzzling feature of the estimator was that numerous very small sensitivity coefficients always appeared ranked as having large values as had been found by Durston et al [1] in their safety code study Attempts to understand this feature of the estimator from a theoretical point of view failed, and we became concerned that the estimator may rank high sensitivity coefficients having low values clearly a very undesirable feature if it existed When Durston et al [1] attempted to test this aspect of the estimator by selecting a random sample of sensitivity coefficients that had been ranked as having low values no large sensitivity coefficients were found

Because no theoretical understanding of the problem had been obtained, all 80 sensitivity coefficients were calculated exactly by difference methods (this was feasible in the case of Model 82) The exact sensitivity coefficients were compared with the screening results, and even with 20 random perturbation runs (i e , 25% of the total number of runs required to obtain all the sensitivity coefficients by difference methods) the "efficiency" of the estimator in identifying large sensitivity coefficients was found to be only about 50% This result fell far short of our expectations for a useful estimator and needed an explanation Since screening methods have often been known to be successful in studies in which "engineering judgment" was used to greatly reduce the number of parameters considered in the screening, we suspected that this aspect may be a key element to the success of the method

The use of judgment or opinions in conjunction with statistical formulas in particular Baye's theorem, is not new, but is a controversial and often emotional subject We think that many of the objections that have been raised against such procedures often referred to as Bayesian procedures are largely justified when the two different concepts of probabilities, as plausibilities and as limiting frequencies are intermixed or used interchangeably Probabilities, in the sense of limiting frequencies, as used in most practical applications of statistical theory impose severe limitations in the class of problems that can be successfully treated by statistical methods In the area of "uncertainty analysis " for instance only "statistical uncertainties" (or "statistical" errors) can be dealt with by using statistical theory Within this theory we are powerless to handle the problems of "systematic" errors although these may be perceived to dominate the overall uncertainty A fully axiomatic and rigorous theory of logical inference can be developed from the concept of probabilities as a unique measure of plausibilities

We have investigated the usefulness of such a theory of logical inference, based mostly on the work of Cox[2] and Jaynes,[3] to attack the screening problem rather than the statistical approach initially used This theory, which we will call the LCJ theory of logical inference (after Laplace, Cox, and Jaynes), uses group theoretical methods to assign probabilities conditional upon facts, which are therefore true and does not use any opinions The assignment of probabilities is unique and fully objective if relevant facts that are available for making inferences as to the plausibility for the truth of assertions of interest can be used to generate an invariance group This requirement puts some limitations on the kind of facts that are useful for successfully applying the theory Jaynes calls such facts "testable " Our purpose here is not to develop this theory, but merely to provide an indication of how this theory can be used to investigate the screening problem

In Section VIII B we will explain a few concepts of the LCJ theory and provide the notation In Section VIII C we will study the problem usually referred to as the propagation of uncertainties Section VIII D addresses the problem of screening for various purposes and indicates

how a solution can be found We also show why the matrix method used by Durston et al was not successful Section VIII E draws some conclusions and implications for future work

B LCJ Approach and Notation

The major purpose of Section VIII B is to establish the notation used in the rest of Section VIII However, because the terms used in the LCJ theory of logical inference are similar to the ones used in the more familiar theory of statistics we will explain their meaning in the theory of logical inference This is not an attempt to justify the theory, which we could not do in this report

In this application of the LCJ theory, we need to consider only that we deal with quantities that are constants, but whose true value may or may not be known to us (input data, output data, and sensitivity coefficients) We represent the true value of quantities by Roman letters A lower-case letter will stand for the true value of a single quantity, and a capital letter will stand for the true value of a set of quantities If the symbol s_i stands for the true value of the ith sensitivity coefficient, we will write

$$S \equiv \{s_i\} \ , \ i = 1,2, \quad ,m, \qquad \text{(VIII 1)}$$

to represent the true value of the m components s_i of the generalized vector S Capital letters will also represent matrices--that is the true value of the set of quantities represented by the matrix elements We denote the transpose of a vector or a matrix by a dagger (i e , $S^\dagger$ is the transpose of S)

If we are given some information, written symbolically as J which meets the requirements of the theory to generate unique probabilities for the true value of some constants s_i we write

$$(S|J)\ dS \equiv (\{s_i\}|J) \prod_{i=1}^{m} ds_i \qquad \text{(VIII 2)}$$

Equation (VIII 2) is a "shorthand" notation to represent the probability for the truth of the set of assertions "The values of the m constants s_i are in the interval S and S + dS for fixed dS," conditional upon the truth of the information J We call (S|J) the joint probability density function (joint p d f) for the true value of the s_i's conditional upon the truth of J From the point of view of the LCJ theory, (S|J) represents the only rational statement we can make about the true value of the constant S, given only that J is some true information relevant to the value of S That (S|J) is not a delta function states that, given only J, some uncertainty exists about the true value of S

Presumably an interest in calculating $(S|J)$ implies that we have some use for the true value of S, this means that we care about the true value of S If we did not care an arbitrary value could be used instead of the true value Therefore, some penalty is involved in the intended application for not using the true value If we can specify the nature of the penalty involved in using some value other than the true value for S, and if all we know about the true value is $(S|J)$, we can rationally choose the value to be used and determine the extent of the expected penalty for using this value The penalty involved in the application must be formulated in terms of a function of the difference between the true value S and the value we choose, S_c This function, called the loss function is written $L(S - S_c)$ A rational decision for choosing a value S_c as the true value is based on selecting a value that minimizes the penalties whatever the true value of S This rationale means that we must take the value of S_c that minimizes the integral,

$$\int L(S - S_c)\,(S|J)dS \qquad \text{(VIII 3)}$$

The minimum value of Eq (VIII 3) gives us a measure of expected penalty or "risk " we incur as a result of the uncertainty that exists in the true value of S The function $L(S - S_c)$ must be determined according to the application, and it must be provided by the user before a rational decision can be made in the face of the uncertainties involved In this paper, to be specific, we must make a choice of a loss function, and we shall take it to be quadratic

We will use the conventional notations $\bar{S}$ or $\langle S\rangle$ to denote the expectation value of S over the joint p d f

$$\bar{S} \equiv \langle S\rangle \equiv \{\bar{s}_1\} = \int S(S|J)dS \qquad \text{(VIII 4)}$$

The covariance matrix of the point p d f is given by

$$\langle(\bar{S} - S)(\bar{S} - S)^\dagger\rangle \qquad \text{(VIII 5)}$$

During our derivation we will often use the difference between the true value of a quantity and its expectation value, the special notation for this difference is

$$S - \bar{S} \equiv \delta S \equiv \{\delta S_1\} \equiv \{s_1 - \bar{s}_1\} \qquad \text{(VIII 6)}$$

In this notation the covariance matrix is

$$\langle(S - \bar{S})(S - \bar{S})^\dagger\rangle = \langle\delta S\delta S^\dagger\rangle \qquad \text{(VIII 7)}$$

In LCJ theory, a p d f is used to indicate the extent to which we can logically claim to know the true value of a constant on the basis of certain information The p d f is a measure of what this information J tells us logically about the true value of a constant The LCJ theory is a theory of information

C Propagations of Uncertainties

Section VIII A shows that all uses for sensitivity coefficients are closely related to the uncertainty in the result of the code Section VIII C investigates the problem of the uncertainty in the result of the code and its source The uncertainty in the result of the code comes from two independent sources (1) uncertainties in the input data and (2) uncertainties in the equations that the code represents (i e the modeling uncertainties) These two sources for the uncertainty in the result can be handled with the LCJ theory but for simplicity in this report we consider only the input data uncertainties that is we assume that the model is exact In the LCJ theory we say that our results are conditional upon the truth of the model In subsequent reports we will also consider the model uncertainties that is calculate the overall uncertainty in the result

In Section VIII we assume that there is some uncertainty in the m input parameters We denote by x_i the true value of the input parameters and write $X \equiv \{x_i\}$ We must specify what we know about X and we assume that, conditional upon some information (denoted by G) we are given the joint p d f $(X|G)$ Let us then assume that we are given $(X|G)$ and we write $\bar{X}$ for its expectation value and C for its covariance matrix, that is,

$$C \equiv \{c_{ij}\} = \langle \delta X \delta X^{\dagger} \rangle \qquad \text{(VIII 8)}$$

To simplify the notation, let us also assume that the code has only one output, which we will denote by r to be consistent with the notation introduced in Section VIII B The generalization to several outputs that is $R \equiv \{r_i\}$ is straightforward symbolically the model relationship between the input parameter X and the result r is given by

$$r \equiv r(X) \qquad \text{(VIII 9)}$$

Equation (VIII 10) can be expanded in a Taylor series about the expectation value of X to obtain

$$r \equiv r(X) = r(\bar{X}) + \sum_{i=1}^{m} \frac{\partial r}{\partial x_i} \bigg|_{\bar{X}} (x_i - \bar{x}_i) + O(\delta x_i^2), \qquad \text{(VIII 10)}$$

where $O(\delta x_i^2)$ represents the remainder after the linear term and is of the order of δx_i^2 or higher

Using the notation of Section VIII B, we can rewrite Eq (VIII 10) as

$$r = r(\bar{X}) + S^{\dagger}\delta X + O(\delta x_i^2) \qquad \text{(VIII 11)}$$

where the m elements of the vector S are the first-order derivatives of r(X) evaluated at X -- that is the sensitivity coefficients, or

$$S \equiv \{s_i\} = \left\{ \frac{\partial r}{\partial x_i} \bigg|_{\bar{X}} \right\} \qquad \text{(VIII 12)}$$

We could readily write explicitly the second-order term of Eq (VIII 10) but did not because we are now going to keep only the first two terms of the Taylor expansion, again for the sake of simplicity

Including the quadratic term presents no formal problems, but for our purpose in this report this would only complicate the notation (From a practical point of view inclusion of the quadratic term does complicate matters somewhat) Therefore, our results in this section are also conditional upon the validity of the linear approximation We can then write

$$r \cong r(\bar{X}) + S^{\dagger}\delta X \qquad \text{(VIII 13)}$$

Let us now consider two cases (1) that we know the true value of the sensitivity coefficients (i e , S) and (2) that we do not know exactly the value of S

1 The Value of S is Known Exactly

This condition will be met if all s_i's can be calculated, by using either adjoint sensitivity theory or the forward approach (i e , making small changes in each of the m parameters separately and using the changes in the result of each m run) We consider this case because we need to know the price that must be paid for not knowing the value of S exactly

Equation (VIII 13) shows that if we know S but the true value X is not known, the true value of r is not known to us The relation in Eq (VIII 13) says that we can only have (r|G) If we have a quadratic loss function for whatever application we need r then we must calculate $\bar{r}$ and the variance $\langle \delta r^2 \rangle$

To obtain $\bar{r}$ we take the expectation value of Eq (VIII 13) over the joint p d f (X G)

$$\bar{r} \cong r(\bar{X}) \qquad \text{(VIII 14)}$$

To determine the risk involved in selecting $\bar{r}$ as the true value for r, we first write

$$\delta r \equiv r - \bar{r} \cong r - r(\bar{X}) = S^{\dagger}\delta X \qquad \text{(VIII 15)}$$

then multiply the transpose of Eq (VIII 15) by Eq (VIII 15), and take the expectation value of δr^2 over the joint p d f (X G) The result is

$$\langle \delta r^2 \rangle \cong S^\dagger \langle \delta X \delta X^\dagger \rangle S = S^\dagger C S \qquad \text{(VIII 16)}$$

The results of Eqs (VIII 14) and (VIII 15) are well known since the same formulas are obtained from statistical theory if we consider X to be a multivariate and therefore r to be a variate We have here an example of an economic problem that was encoded into two different mathematical theories, the LCJ theory and the statistical theory, then solved in the two different theories according to their respective rules to yield the same numerical results, but we must translate what these mean in the economic language

2 The Value of S is Not Known Exactly

Very often the value of S cannot be known exactly For instance we do not have adjoint capability and the m + 1 forward runs required by the forward method are not feasible Anticipating the results of the next section, let us assume here that although we do not know the true value of S we have the next best thing namely (S|J) We note first that G is some information, which in the LCJ theory is said to be irrelevant to the true value of S and therefore (S|J) and (X|G) are independent p d f 's This can easily be seen since G is information relevant to the true value of X, for whatever application X is used The information J is relevant only to the functional dependence of r upon X, where X is the true value

Let us use $\bar{S}$ for the expectation value of (S|J) and E for its covariance matrix, that is,

$$E \equiv \langle \delta S \delta S^\dagger \rangle \qquad \text{(VIII 17)}$$

We have the exact relationship

$$S = \bar{S} + S - \bar{S} = \bar{S} + \delta S \qquad \text{(VIII 18)}$$

Equation (VIII 13) is still valid, and we can use Eq (VIII 18) in it This indicates to us that now we only know the p d f (r|GJ) To calculate its expectation value, we must consider the two independent p d f 's, (X|G) and (S|J) The result obtained is therefore still Eq (VIII 14) However, the risks involved in using this value as the true value (i e , the variance of r) is no longer given by Eq (VIII 16), which instead becomes

$$\langle \delta r^2 \rangle_X \cong (\bar{S} + \delta S)^\dagger C(\bar{S} + \delta S) \qquad \text{(VIII 19)}$$

if we only take the expectation value over the joint p d f (X|G), which we have shown by the notation $\langle \delta r^2 \rangle_X$ If we only take $\langle \delta r^2 \rangle_X$, Eq (VIII 19) indicates that $\langle \delta r^2 \rangle_X$ is no longer a constant whose value is known to us since S is not known to us If we write

$$v \equiv v(S) = \langle \delta r^2 \rangle_x \ , \qquad \text{(VIII 20)}$$

it is clear that instead of knowing the true value of v we only have a p d f conditional upon J that is (v|J) We therefore face another decision as to what to use for the true value of v Again assuming a quadratic loss function, we must select $\bar{v}$ as the true value for v, which we do by taking the expectation value of Eq (VIII 19) over the joint p d f (S|J) Noting that C is a known constant, we get

$$\bar{v} \cong \bar{S}^{\dagger} C \bar{S} + \tilde{C}^{\dagger} \tilde{E} = \sum_{i,j=1}^{m} c_{ij} (\bar{s}_i \bar{s}_j + e_{ij}) \qquad \text{(VIII 21)}$$

In Eq (VIII 21) we used the notation,

$$\tilde{C}^{\dagger} \tilde{E} \equiv \sum_{i,j=1}^{m} c_{ij} e_{ij} \qquad \text{(VIII 22)}$$

where $\tilde{C}$ and $\tilde{E}$ are vectors constructed from the covariance matrices C and E through partitioning

Of course, corresponding to this choice of $\bar{v}$ for the true value of v, a risk is involved, which we can determine by calculating the variance of (v J)

$$\langle \delta v^2 \rangle \cong \bar{S}^{\dagger} C E C \bar{S} + \langle \delta S^{\dagger} C \bar{S} \bar{S}^{\dagger} C \delta S \rangle + 2 S^{\dagger} C \langle \delta S \bar{S}^{\dagger} C \delta S \rangle \qquad \text{(VIII 23)}$$

The last two terms of Eq (VIII 23) can be expressed as linear combinations of the elements of the matrix E

Comparing Eqs (VIII 16) and (VIII 21) clearly indicates the penalties incurred for not knowing the sensitivity coefficients S exactly We no longer know exactly the risk in using $\bar{r}$ given by Eq (VIII 14), for the true value of r, and we must use Eq (VIII 21) instead of Eq (VIII 16) Assuming that we have

$$\sum_{i,j=1}^{m} c_{ij} s_i s_j \cong \sum_{i,j=1}^{m} c_{ij} \bar{s}_i \bar{s}_j \ , \qquad \text{(VIII 24)}$$

the risk has increased by $\tilde{E}^{\dagger} \tilde{C}$ There is now a risk in using Eq (VIII 21), and it is given by Eq (VIII 23)

In common language, where risk is equated to a measure of uncertainty, we have an "uncertainty on the uncertainty " We should emphasize that this "uncertainty on the uncertainty" does not arise from any "uncertainty" on the covariance matrix C which is well known, but

from the fact that the sensitivity coefficients s_i are not known exactly

D Screening Analysis

Section VIII D addresses the problem of generating explicitly the joint p d f (S|J) First the class of information that may be included in J is analyzed, and the rationale for optimizing (S|J) is provided

The notation for expressing the fact that n + 1 runs have been performed with the code is set up first The "base case" run is the run performed with all the m parameters x_j set to their expectation value $\bar{x}_j$ the output of the code is then $\bar{r}$ The output of the code for the ith additional run is called r_i Differences obtained from the base-case result $\bar{r}$ are called r'_i, from which the vector R' is formed

$$R' \equiv \left\{r'_i\right\} = \left\{r'_i - \bar{r}\right\} \qquad i = 1 \qquad n \tag{VIII 25}$$

These additional runs are made using ${}_ix_j$ for the value of the jth parameter at the ith run From the $\bar{x}_j$ and the ${}_ix_j$ values we can form an n x m matrix which we call $A \equiv \left[a_{ij}\right]$, where

$$a_{ij} \equiv {}_ix_j - \bar{x}_j \tag{VIII 26}$$

Then, from Eq (VIII 13) we can represent the result of these n + 1 runs by a system of n equations in m unknown constants

$$R' \equiv R'(A) = AS \tag{VIII 27}$$

It is worthwhile to emphasize that S stands for m constants s_i (the first-order derivatives of the result with respect to the parameters) and that a particular matrix A must be selected to obtain R' The vector R' is only a function of the matrix A and the m unknown constants s_i (i e S) This means that the result R' does not depend on the rationale used to select a particular matrix A we indicate this in our notation by writing R'(A) We will investigate later criteria for selecting a particular matrix A to achieve a specific goal because we are free to choose any matrix A In many previous screening studies, a "random procedure" was used to choose the A matrix For us this random procedure only means that an arbitrary A matrix was selected from a subset of all possible A matrices After an A matrix is chosen, the fact that any other A matrix could have been selected is totally immaterial as far as R' is concerned We do not know what value of R' would have been obtained if we had chosen another A matrix Any assumption about what would have been observed for R', if some other matrix had been used is equivalent to an assumption about what the s_i's are

1 $J \equiv R'(A)$ Only

The objective of screening is to obtain approximate values for some or all of the s_i's or approximate rankings based only on the information obtained from performing n + 1 runs with the code We now show that this cannot be done logically that is, it cannot be done with any justifiable degree of confidence, no matter how "degree of confidence" is defined

If we have n independent relations (equations) involving m constants the s_i's and $n < m$ the problem of determining the m constants is ill-posed from a deductive logic point of view because there is no unique solution If the problem is to be well-posed (i e yield a unique solution), m independent equations in the m constants are required The system of m equations in the m constants is then said to define a unique point in the m dimensional space of the constants Each of the m independent equations defines an m - 1 dimensional subspace, in the m dimensional space where the point S must lie Each m + 1 dimensional subspace is unbounded If the m equations are independent the system has a unique solution because only a single point lies at the intersection of these m subspaces From a purely deductive logic point of view, having only n independent equations in the m constants defines an unbounded m-n dimensional subspace, where the point S must lie (i e , every point in this unbounded subspace satisfies the n equations) The only unambiguous statement that can be made about the points of the m-n dimensional subspace defined by R'(A) is that we must have

$$S^{\dagger}S \geq R'^{\dagger}(AA^{\dagger})^{-1}R' \qquad \text{(VIII 28)}$$

for all the points in that subspace This relation can be found in many different ways one of which will be shown later The relation in Eq (VIII 28) is a constraint on the sum of the square of the s_i's, but provides no useful information about the relative magnitude of the individual s_i's required to rank them or about the absolute magnitudes required to estimate them

The LCJ theory of logical inference goes one step further than the above analysis This theory introduces the notion that every point in the m-n dimensional subspace defined by R'(A) is a possible solution and attempts to assign, on a logical basis, a measure for the plausibility that various points of this subspace are the true solution (i e the true value of the m sensitivity coefficients) How this can be done using the "desideratum of consistency" has been shown by Jaynes [3] All we must do is recognize that Eq (VIII 27) defines S as a "position parameter" (i e , a point in an m dimensional space) The only logically consistent measure of plausibility we can then use, if Eq (VIII 27) is the only fact we have to rely on must therefore be translationally invariant This means that we must assign equal plausibility to every point in the m-n dimensional subspace defined by Eq (VIII 27) Any other assignment leads to a contradiction with the

statement that all we know about S is contained in Eq (VIII 27) which cannot differentiate among the points S that lie in the m-n dimensional subspace it defines

Knowing that we must assign equal plausibility to every point of the subspace defined by Eq (VIII 27) to be logically consistent does not, however allow us to assign equal probabilities to every point in that subspace because the subspace is infinite (i e , unbounded), and we cannot normalize the p d f as required by the theory Such p d f 's, which are well-known in the LCJ theory of logical inference, are called "improper" p d f 's To proceed further in the LCJ theory we must have additional independent information of such a nature that, when combined with the underdetermined system of Eq (VIII 27), yields a normalizable p d f

2 $J \equiv R'(A)$ and I

Given only $R'(A)$, we have shown that all points of the m-n dimensional subspace it defines are possible solutions to our problem, and we must assign them equal plausibility for being the true value We have stated that the only logical conclusion we could derive from the knowledge of $R'(A)$ is given by Eq (VIII 28), which gives us a lower limit in the magnitude of the true vector S For our particular application, we are interested in the magnitude of the individual sensitivity coefficients s_1, therefore Eq (VIII 28) is not adequate We want to minimize all elements of the quadratic loss matrix $(S_c - S)(S_c - S)^{\dagger}$, whatever the true value S is With the improper p d f , $[S|R'(A)]$ no value of S_c can minimize our loss In the more conventional language of statistical theory, $R'(A)$ defines a likelihood function, which causes difficulty because it is a constant

To solve our problem we must provide additional information that together with $R'(A)$ will allow a rational choice S_c (i e that will minimize our quadratic loss function and give us an estimate of the risk we take, whatever the true value of S is) Let us call this information I

What type of information must I be in order to make a rational choice? As indicated before, I stands for "testable facts " These facts must be such that, if we propose a p d f corresponding to our state of knowledge at the time we have these facts, we can verify that the p d f agrees with the facts The next stage of the "transformation group argument" is to propose this p d f for all problems for which we are given the same facts If we can establish transformation relations between these problems, the proposed p d f must be invariant under those transformations This is often totally sufficient to establish a unique functional form for the p d f This method of assigning p d f is called a "transformation group argument" and is based on Jaynes' desideratum of consistency "In two different problems, given the same information, we assign the same probability "

In our particular case we seek facts (represented by I) that are relevant to the functional dependence of $r(X)$ about $r(\bar{X})$ One way to obtain these facts is to approximate the behavior of $r(X)$ and estimate the magnitude of the approximations made when $X = \bar{X}$ Such analysis usually yields some relevant testable facts For instance, we may be able to state unequivocably that s_1 is bounded, it must be between two known limits $\bar{s}_1$ and s_1^+, or it must be greater (or less) than some known number The number of testable facts that we can obtain in this way is, of course, a function of the problem our inventiveness, and our resources After we have such facts we can generate a p d f $(S|I)$ with complete objectivity $(S|I)$ may also be an improper p d f but this is not important if, when combined with the information $R'(A)$, the resulting p d f is a proper p d f We can stop gathering information I when this occurs (which presumes that $R'(A)$ is available before we acquire I) We shall see that this is not the best way to proceed This discussion is intended to show that, in general, obtaining completely objective and numerical facts I which are independent of $R'(A)$ and are not therefore mere opinions should be possible The information I represents constraints on the value of S

We will now assume that we have some independent testable facts I and can generate a p d f $(S|I)$ using the LCJ theory of logical inference Next we consider how to generate a p d f $[S|R'(A)\ I]$ that is how to determine a measure of the probability for the true value of S conditional upon both $R'(A)$ and I By applying the conjunction law for plausible assertions,[2] we immediately obtain

$$[S|R'(A)I] \ \alpha \ (S|I)\ [R'(A)|SI] \ , \qquad \text{(VIII 29)}$$

where the constant of proportionality in Eq (VIII 29) can be obtained from the normalization condition on $[S|R'(A)I]$, if $[S|R'(A)I]$ is a proper p d f The relation in Eq (VIII 29) is well known and is often called "Bayes theorem," $(S|I)$ is often called the prior p d f , and $[R'(A)|SI]$ is called the likelihood function We must emphasize that $(S|I)$ is not the representation of an opinion in the LCJ theory but a consequence of the desideratum of consistency based on the facts I

We cannot proceed further at this point without (1) considering a specific problem, taking for I those facts that we could generate, or (2) postulating situations for which a certain class of facts I could be obtained To proceed, we will examine two extreme situations that could be met, resulting in two particular functional forms for (S I)

<u>$(S|I)$ is a uniform p d f</u>

This situation arises if our investigation of the functional dependence of $r(X)$ about $\bar{X}$ yields for each x_1 only an upper and a lower limit for each s_1 These limits (which we will call s_1^- and s_1^+) must also constitute independent facts In practice this requirement of independence of the facts is usually not met We are told by this

information that the true value of S lies inside a "box" bounded by the limits s_i^- and s_i^+ We can form two vectors, S^- and S^+ from these limits, and symbolically write

$$I \equiv S^- S^+ \qquad \text{(VIII 30)}$$

The information will then yield m inequalities which can be written as

$$S^- \leq S \leq S^+ \qquad \text{(VIII 31)}$$

Again because in Eq (VIII 31) S is a position parameter transformation group agreements immediately yield

$$(S|S^- S^+) = \frac{1}{\sum_{i=1}^{m} (s_i^+ - s_i^-)} , \qquad \text{(VIII 32)}$$

since the p d f must be uniform (translationally invariant), and the normalization condition is the volume of the box The likelihood function is then

$$[R'(A)|SI] = [R'(A)|S] = \partial(R' - AS) , \qquad \text{(VIII 33)}$$

where $\partial(R' - AS)$ is the n dimensional delta function in m variables, the s_i's

Applying Eq (VIII 31), we get

$$[S|R'(A)S^- S^+] = \frac{1}{\sum_{i=1}^{m} (s_i^+ - s_i^-)} \partial(R' - AS) \qquad \text{(VIII 34)}$$

Therefore, we can see that here S^- and S^+ (the additional information I) have merely bounded the region in the m-n dimensional subspace defined by R'(A), where the solution must be

In principle at least we can obtain an expectation value $\bar{S}$ and a covariance matrix E for the joint p d f (Eq VIII 34) which are the relevant quantities if we have a quadratic loss function

<u>(S|I) is a normal p d f</u>

This situation arises if we can generate many approximations to r(X) about $\bar{X}$ and if we have many sets of vectors S^- and S^+ to deal with as facts Not all these approximations must be independent of each

other nor must the s_1^+'s and s_1^-'s be independent In this situation however when we combine all these facts and when the conditions for the validity of the central limit theorem hold the resulting p d f (S|I) can be more or less closely approximated by a joint normal p d f , which will have an expectation value (e g , $\bar{S}'$) and a covariance matrix E' Here let I be represented by

$$I \equiv \bar{S}'E' \qquad \text{(VIII 35)}$$

Now we must apply Eq (VIII 29) to incorporate the result of the n runs R'(A) This can be done very easily if we note that the likelihood function [R'(A)|SI], $\partial(R' - AS)$, can be represented as

$$\partial\,(R' - AS) = \lim_{v\to 0} \exp\left[-\frac{1}{2}\,(R' - AS)^{\dagger}\, V^{-1}\,(R' - AS)\right] \qquad \text{(VIII 36)}$$

Here $[S|R'(A)\bar{S}'E']$ must also be a joint normal p d f If we write its expectation value $\bar{S}$ and its covariance matrix E, after some algebra we get

$$\bar{S} - \bar{S}' = E'A^{\dagger}(AE'A^{\dagger})^{-1}(R' - AS') \;, \qquad \text{(VIII 37)}$$

and

$$E' - E = E'A^{\dagger}(AE'A^{\dagger})^{-1}AE' \qquad \text{(VIII 38)}$$

We can easily see that the results of Eqs (VIII 37) and (VIII 38) are closely connected to the "least square" estimation of statistics if we treated S as a variate $\bar{S}$ is in the m-n dimensional space defined by R'(A) and has the minimum distance to $\bar{S}'$ (using the metric E' in the space S)

Equation (VIII 37) allows us to make a connection with an earlier statement about the minimum length of the vector S lying in the space $\underline{R}'(A)$ We can easily obtain the result from Eq (VIII 37) by letting $\bar{S}'$ be the origin and taking an "isotropic metric" in the space of S, that is letting E' be the identity matrix and calling this point Y we get

$$Y = A^{\dagger}(AA^{\dagger})^{-1}R' \qquad \text{(VIII 39)}$$

This point Y is the estimator $\hat{S}$, proposed by Durston et al , that we attempted to use in our early screening studies Eq (VIII 28) can be obtained from Eq (VIII 39) by calculating $Y^{\dagger}Y$

<u>Choice of the A matrix</u>

We now discuss the choice of an A matrix to perform the n additional runs In all previous screening work, the A matrix was chosen in some random fashion (see Durston et al [1]) In the LCJ theory, this

is not a logical way to proceed, and we will now indicate how the A matrix should be chosen

When using the LCJ theory we realize at the outset that we will require some information independent of the n additional runs (referred to as I) Because we cannot predict what I will be, this information should be sought first, and a p d f (S|I) should be generated, from which we calculate $\bar{S}'$ and E' We should now consider the application for the use of the sensitivity coefficients As pointed out in Section VIII A, there are several possible uses for S, in fact we may have several applications in mind The choice of A matrix for one specific application will be illustrated, but the method can be generalized for any situation

Consider that our main purpose is the choice of a value for the output of the code r If our loss function is quadratic, we should take r, and the risk involved is given by

$$v' = \bar{S}'^{\dagger} C \bar{S}' + \tilde{C}^{\dagger} \tilde{E}' \qquad \text{(VIII 40)}$$

If we perform n additional runs of the code, the variance of r will become

$$\bar{v} = \bar{S}^{\dagger} C \bar{S} + \tilde{C}^{\dagger} \tilde{E} \ , \qquad \text{(VIII 41)}$$

because $\bar{S}'$ and E' will be changed to $\bar{S}$ and E These changes will be a function of both (S|I) and R'(A) We must presume that, although $\bar{S}$ will very likely differ from $\bar{S}'$ the major impact of the n additional runs will be on the uncertainties (because R'(A) is information that is independent of I) The net benefit of performing the n additional runs for the application in question can be measured quantitatively

$$\bar{v}' - \bar{v} \approx \tilde{C}^{\dagger} (\tilde{E}' - \tilde{E}) \qquad \text{(VIII 42)}$$

Because we can always express the difference $\tilde{E}' - \tilde{E}$ as a function of R'(A)--for instance Eq (VIII 38) when (S|I) is a normal p d f -- we should choose a matrix A to maximize Eq (VIII 42) Here, the elements of the matrix A will be a function of the elements of the covariance matrices C and E' and, in general, of $\bar{S}'$ also

E Conclusion

From the point of view of the LCJ theory of logical inference, our analysis of the screening problem indicates several serious weaknesses in current statistical approaches, which use only the result of n + 1 runs of the code to perform an estimate of the sensitivity coefficients Using the LCJ theory of logical inference, we have shown that obtaining a generally useful solution (i e , one that is not arbitrary) is not possible New information is needed to estimate a meaningful uncertainty on the estimate of the sensitivity coefficients

The LCJ theory formalism developed in this section is being applied to Model 82 to demonstrate the methodology for generating the information we have called I and the manner in which it is used to solve the screening problem This demonstration exercise should be valuable in assessing the usefulness of the method in more complicated models such as Model 22C

Our analysis makes it quite clear that "screening" for sensitivity coefficients is not a simple "black box approach " as we originally perceived Requiring some objective measure of the uncertainties in the sensitivity coefficients s_1 necessitates much additional work Screening may be useful for "one shot" situations It is unlikely however, to be a substitute for adjoint methods when a code is to be exploited to analyze many problems, over which the time and cost of development of the "adjoint" code may be amortized Screening may still be attractive when one must consider second-order effects, because present second-order adjoint methods have not yet been developed to a very high level of efficiency Whether these adjoint methods can be made much more efficient in general is an open question

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IX SENSITIVITY ANALYSIS BY ADJOINT METHODS

A Adjoint Sensitivity Theory

The major alternative to screening designs in assessing the sensitivity of a result to a large data base is adjoint sensitivity theory In this approach the code can no longer be treated as a black box a substantial amount of development work and a detailed knowledge of the mathematical models involved are needed The advantage of the method, however, is that once this work is done a single adjoint run provides sensitivities to all input parameters exactly In most cases, this is more than enough compensation for the development work invested

To illustrate the theory for the adjoint method it is convenient to treat the energy model under consideration symbolically in terms of a non-linear operator and to carry out the derivation of the sensitivity results abstractly In Section IX B the specific equations for LEAP are introduced explicitly, and the operator results can be used to go directly to the sensitivity results desired To begin, assume that LEAP can be described by a general set of N non-linear equations in N unknowns written symbolically as

$$\bar{f}(\bar{p},\bar{x}) = 0 \qquad \text{(IX 1)}$$

where $\bar{f}$ is an N-vector function of the unknown dependent variable N-vector $\bar{p}$ (e g all quantities and prices in the model) and the independent variable vector $\bar{x}$ (e g all exogenous model parameters) It is assumed for the purposes of this derivation that a unique solution exists for this problem and it is represented by $\bar{p}$

As explained in Section I the adjoint approach focuses on the result of a model calculation to determine the sensitivities of interest for any given problem For this case it is convenient to also generalize the result R of any particular calculation with the model as

$$R = g(\bar{p}\ \bar{x}) \qquad \text{(IX 2)}$$

Here R is the scalar result of a calculation with a particular set of independent parameter values $\bar{x}_0$ also R is in general a non-linear function of the solution vector $\bar{p}$ and possibly also a function of some of the exogenous parameters in $\bar{x}_0$ Using this general form for R, one can easily consider any particular result of interest as simply a redefinition of the function g For instance, if a single price from a calculation were of interest g would simply be defined as $g = p_i$ (the ith component of $\bar{p}$)

With the above definitions the sensitivity problem in differential terms reduces simply to calculating the derivative of R with respect to any element x_i of the parameter vector $\bar{x}$, given the particular set of parameter values $\bar{x}_0$ used to define and solve the model equations If the general element of $\bar{x}$ is defined as simply x (i e dropping the subscript notation) the sensitivity of R to x is given by the derivative dR/dx Differentiating Eq (IX 2) gives

$$\frac{dR}{dx} = \frac{\partial g}{\partial x} + \frac{\partial g}{\partial \bar{p}} \frac{d\bar{p}}{dx} \qquad \text{(IX 3)}$$

Here the first term on the right side of Eq (IX 3) is called the "direct effect" sensitivity, reflecting the explicit dependence of R on x, and the second term is the "indirect effect" sensitivity, reflecting the implicit dependence of R on x through $\bar{p}$ in Eq (IX 1) Note that $\partial g/\partial \bar{p}$ is a row vector, and $d\bar{p}/dx$ is a column vector

The second term in Eq (IX 3) can be evaluated by differentiating Eq (IX 1) with respect to x to give

$$\frac{\partial \bar{f}}{\partial x} + \frac{\partial \bar{f}}{\partial \bar{p}} \frac{d\bar{p}}{dx} = 0 \qquad \text{(IX 4)}$$

Defining two new N-vectors, $\bar{\Phi} \equiv d\bar{p}/dx$ and $\bar{S} \equiv -\partial \bar{f}/\partial x$ and the N x N matrix, $A \equiv \partial \bar{f}/\partial \bar{p}$, Eq (IX 4) can be rewritten as

$$A\bar{\Phi} = \bar{S} \qquad \text{(IX 5)}$$

Here $\bar{\Phi}$ is the differential change in the solution vector $\bar{p}$ with respect to a differential change in x and it solves a linear inhomogeneous equation whose source is the differential change in the vector function $\bar{f}$ with respect to x The fact that A is a linear operator is clear because it is a function only of $\bar{p}$ (albeit non-linear in $\bar{p}$) and not of $\bar{\Phi}$

The expression of dR/dx can now be evaluated by first solving Eq (IX 1) for $\bar{p}$, using this result to evaluate A, and then solving Eq (IX 5) for Φ The resulting solution vector $\bar{\Phi}$ can then be put back into Eq (IX 3) to evaluate dR/dx Two points in this procedure should be noted (1) A is a linear operator, depending only on $\bar{p}$ and $\bar{x}_o$ for its definition, and (2) Eq (IX 5) has to be re-solved for each parameter x whose sensitivity is being investigated because the definition of $\bar{S}$ depends on differentiating $\bar{f}$ with respect to a particular x in $\bar{x}_o$ This last point (i e , the occurrence of operations involving $\partial/\partial x$ in $\bar{S}$) makes it infeasible to study the sensitivity of R to all the elements of a large vector $\bar{x}_o$ of exogenous parameters The first point [i e the linearity of Eq (IX 5)], however, allows the problem to be reformulated in terms of adjoint functions

The set of equations adjoint to Eq (IX 5) is given by

$$A^*\bar{\Phi}^* = \bar{S}^* \qquad \text{(IX 6)}$$

where the adjoint N x N matrix A^* is defined by the classical inner product relationship,

$$\bar{\Phi}^{*T} A\bar{\Phi} = \bar{\Phi}^T A^*\bar{\Phi}^* \qquad \text{(IX 7)}$$

Here the superscript T refers to the transpose of the vector $\bar{\Phi}$ or $\bar{\Phi}^*$

The relationship given in Eq (IX 7) and the fact that A is a matrix operator mean that

$$A^* = A^T \tag{IX 8}$$

Using the inner product relationship defining an adjoint matrix operator [i e , Eq (IX 7)] leads to the most important result of adjoint sensitivity theory--the replacement of the "indirect effect" term in Eq (IX 3) with an equivalent term involving the adjoint function $\bar{\Phi}^*$ This transformation can be established by forming the inner product of $\bar{\Phi}^{*T}$ with Eq (IX 5) and $\bar{\Phi}^T$ with Eq (IX 6) and subtracting one inner product from the other Using the relationship given in Eq (IX 7) then gives

$$\bar{\Phi}^T \quad \bar{S}^* = \bar{\Phi}^{*T} \quad \bar{S} \tag{IX 9}$$

If $\bar{S}^*$ is now suitably defined to be

$$\bar{S}^* = \frac{\partial g}{\partial \bar{p}}^T \tag{IX 10}$$

then the "indirect effect" term in Eq (IX 3) can be evaluated by using the result in Eq (IX 9)

$$\frac{\partial g}{\partial p} \quad \bar{\Phi} = \bar{\Phi}^{*T} \quad \bar{S} \tag{IX 11}$$

This result and the definition of $\bar{S}$ enable Eq (IX 3) to be rewritten finally as

$$\frac{dR}{dx} = \frac{\partial g}{\partial x} - \bar{\Phi}^{*T} \quad \frac{\partial \bar{f}}{\partial x} \tag{IX 12}$$

where ϕ^* is the solution of the adjoint equation,

$$A^*\phi^* = \frac{\partial g}{\partial \bar{p}} \tag{IX 13}$$

Several important observations should be made in regard to the results given in Eqs (IX 12) and (IX 13) The first advantage of this approach is that the adjoint equation is independent of any operation involving differentiation with respect to x This characteristic means that, no matter how large the set of input parameters is only a single adjoint equation needs to be solved to compute dR/dx for all x in $\bar{x}_0$ This is in contrast to any direct method of computing dR/dx by changing each x by a finite amount (i e Δx) and solving Eq (IX 1) to approximately get $dR/dx \cong \Delta R/\Delta x$ or by using Eq (IX 5) directly to solve exactly for $d\bar{p}/dx$ In both of these latter cases, the solution of a large system of equations [i e , either Eq (IX 1) or IX 5)] is needed for each parameter x to be studied The adjoint approach is therefore extremely economical to use, and with a very large set of input parameters, it may be the only approach to obtaining all sensitivity coefficients

The second advantage is that the adjoint equation is a linear equation in Φ^* which is generally much easier to solve than the repeated calculations using Eq (IX 1), which is non-linear The third advantage is that this approach allows the exact sensitivity coefficient dR/dx to be evaluated by using Eq (IX 12) (i e no perturbations in x and no approximations such as $\Delta R/\Delta x \cong dR/dx$ are needed)

On the other hand certain limitations and disadvantages of this method are also apparent The first and foremost disadvantage is that, to construct the adjoint equations [i e Eq (IX 13)] and evaluate dR/dx with Eq (IX 12) various derivatives of f and g must be evaluated analytically This evaluation requires an in-depth knowledge of the functional form of the complete set of equations described by f--no small task for a large code like LEAP Second the structure of the A* matrix, although independent of Φ^* is not independent of p This means that the solution of Eq (IX 1) must be available to construct A* thus tying the adjoint equations to the solution of the forward equations Therefore to evaluate Eq (IX 12) for dR/dx, both solution vectors p and Φ^* must be available in addition to all analytic derivatives of f and g with respect to both p and each x in x_0 The tradeoff between analytic work in the adjoint approach and computational time in the alternative forward approaches is clear and the usefulness of either method will depend on the circumstances of the sensitivity study being contemplated

One additional disadvantage of the adjoint approach is that an adjoint solution is required for each new response whose sensitivity is being studied This is apparent from the source term in Eq (IX 13) which depends on the definition of the response g This highlights the complementary nature of forward and adjoint methods The forward approach gives the sensitivity of <u>all responses</u> to one parameter in one run whereas the adjoint method gives the sensitivities of one response to <u>all parameters</u> in one run The adjoint method is thus clearly more applicable to problems with large numbers of input parameters and few responses of interest from a sensitivity point of view

B Differentiation of the Equations of the Basic Conversion Process to Obtain the Elements of the Forward Sensitivity and Adjoint Sensitivity Matrices*

The discussion in Section IX A indicates that the forward sensitivity equations may be obtained by differentiating the equations of the system In the notation of Eq (IX 4) each equation of the system for a particular global time point is an element of the vector f and by differentiating each of these equations with respect to x where x is any parameter in the system one of the forward sensitivity equations is

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*This section contains considerable mathematical detail Readers who are interested in a general rather than a detailed understanding may find it profitable to read Section IX C before reading Section IX B

generated In this section the equations of the basic conversion process given in Section V and Appendix B are differentiated to obtain the forward sensitivity equations corresponding to the basic conversion process

Let x be any parameter that occurs in any of the equations for any complete model (e g , in Model 82 or 22C) except that x is not a parameter in the basic conversion process being considered This means in the notation of Eq (IX 4) that the elements f_i, of the vector $\bar{f}$ that will be considered are such that $\alpha f_i/\alpha x = 0$ The case for which x is a parameter in the process being considered will be discussed later in this section

$$\sum_{k=j+1}^{2N_p+N-1} \left[\frac{dP(k)}{dx} - \frac{d\phi(j,k)}{dx}\right] C_f(j,k)D(j,k)$$

$$+ \sum_{k=j+1}^{2N_p+N-1} [P(k) - \phi(j,k)] \frac{dC_f(j,k)}{dx} D(j\ k)$$

$$+ \left[\frac{dp'(j)}{dx} - \frac{d\phi(j,j)}{dx}\right] C_{fG}(j,j)D(j,j)$$

$$+ [P'(j) - \phi(j,j)] \frac{dC_{fG}(j\ j)}{dx} D(j,j) = 0 \qquad \text{(IX 14)}$$

$$j = N_p + 1 \text{ to } N_p + N$$

$$\frac{dP(j)}{dx} = \frac{dP_T(j)}{dx} \qquad j \geqq N_p + N + 1 \qquad \text{(IX 15)}$$

$$\frac{dP(j)}{dx} = \tfrac{1}{2}\left[\frac{dP'(j)}{dx} + \frac{dP_T(j)}{dx}\right] \quad j = N_p + N \qquad \text{(IX 16)}$$

$$\frac{dP(j)}{dx} = \frac{dP'(j)}{dx} \qquad j = 1 \text{ to } N_p + N - 1, \qquad \text{(IX 17)}$$

where the fact that $N_C(j)$ and $D(j,k)$ (see Appendix B I and B 2) do not depend on any variables of the basic conversion process or on x has explicitly been used Equation (IX 14) for each value of j is one of the forward sensitivity equations To obtain an equation to eliminate $\frac{d\phi(j,k)}{dx}$, Eq (V 9) is used to give

$$\frac{d\phi(J,k)}{dx} = Q_F(J,k)\,\frac{dP_I(k)}{dx} \qquad \begin{array}{l} k \geq J \\ k \leq N_p + N \\ J \geq N_p + 1 \end{array} \qquad \text{(IX 18)}$$

$$= Q_F(J,k)[1 + I_f]^{(k-N_p-N)\Delta}\,\frac{dP_I(N_p+N)}{dx} \qquad \begin{array}{l} k \geq J \\ k > N_p + N \\ k \leq 2N_p + N - 1 \end{array},$$

where the fact has been used that $\phi_o(J,k)$ (Section V B) does not depend on the variables or on x From Eq (V 21)

$$\frac{dC_f(J,k)}{dx} = 0 \qquad k < N_p + 1$$

$$= -\frac{\beta\left\{\gamma\,\frac{\alpha\phi(J,k)}{P(k)}^{\gamma-1}\right\}}{\left\{1 + \left[\frac{\alpha\phi(J,k)}{P(k)}\right]^{\gamma}\right\}^2} \left\{-\frac{\alpha\phi(J,k)}{P^2(k)}\,\frac{dP(k)}{dx} + \frac{\alpha}{P(k)}\,\frac{d\phi(J,k)}{dx}\right\} \qquad \begin{array}{l} k \geq J \\ k \geq N_p + 1 \\ k \leq 2N_p + N - 1 \end{array} \qquad \text{(IX 19)}$$

and substituting Eq (IX 18) in Eq (IX 19) gives

$$\frac{dC_f(j\ k)}{dx} = 0 \qquad k < N_p + 1$$

$$= -\frac{\beta}{\left\{1 + \left[\frac{\alpha\phi(j,k)}{P(k)}\right]^{\gamma}\right\}^2} \left\{ \gamma \left[\frac{\alpha\phi(j,k)}{P(k)}\right]^{\gamma-1} \right\}$$

$$\left\{ - \frac{\alpha\phi(j,k)}{P^2(k)} \left[\frac{dP(k)}{dx}\right] \right. \qquad k \geq j$$

$$\left. + \frac{\alpha}{P(k)} Q_F(j\ k) \frac{dP_I(k)}{dx} \right\} \qquad k \geq N_p + 1 \qquad k \leq N_p + N \tag{IX 20}$$

$$= -\frac{\beta}{\left\{1 + \left[\frac{\alpha\phi(j,k)}{P(k)}\right]^{\gamma}\right\}^2} \left\{ \gamma \left[\frac{\alpha\phi(j,k)}{P(k)}\right]^{\gamma-1} \right\}$$

$$\left\{ - \frac{\alpha\phi(j,k)}{P^2(k)} \left[\frac{dP(k)}{dx}\right] \right.$$

$$\left. + \frac{\alpha}{P(k)} Q_F(j\ k)[1 + I_f]^{(k-N_p\ N)\Delta} \frac{dP_I(N_p+N)}{dx} \right\}$$

$$k \geq j$$

$$k \geq N_p + N$$

$$k \leq 2N_p + N - 1$$

The derivatives of the quantity $C_{fg}(j,j)$ may be obtained from Eq (V 22) to be

$$\frac{dC_{fG}(j,j)}{} = -\frac{\beta\left[\gamma\left(\frac{\alpha\phi(j,j)}{P_G(j)}\right)^{\gamma-1}\right]}{\left\{1 + \left[\frac{\alpha\phi(j,j)}{P_G(j)}\right]^{\gamma}\right\}^2}$$

$$\left\{ - \frac{\alpha\phi(j,j)}{P_G^{\ 2}(j)} \frac{dP_G(j)}{dx} \right.$$

$$\left. + \frac{\alpha}{P_G(j)} \frac{d\phi(j,j)}{dx} \right\} \qquad j = N_p + 1 \text{ to } N_p + N, \tag{IX 21}$$

and from Eq (V 23)

$$\frac{dP_G(j)}{dx} = \frac{d\phi(j,j)}{dx} + \frac{R'(j)}{1+r_e(j)-R'(j)} \left\{ - \frac{dP(j+1)}{dx} + \frac{d\phi(j+1,j+1)}{dx} \right\} \tag{IX 22}$$

$$j = N_p + 1 \text{ to } N_p + N$$

Using Eq (IX 21) in conjunction with Eqs (IX 18) and (IX 22) one has

$$\frac{dC_{fG}(j\ j)}{dx} = - \frac{\beta\left[\gamma\left(\frac{\alpha\phi(j,j)}{P_G(j)}\right)^{\gamma-1}\right]}{\left\{1 + \left[\frac{\alpha\phi(j,j)}{P_G(j)}\right]^{\gamma}\right\}^2}$$

$$\left\{ \left[- \frac{\alpha\phi(j,j)}{P_G^2(j)} + \frac{\alpha}{P_G(j)} \right] Q_F(j,j) \frac{dP_I(j)}{dx} \right. \tag{IX 23}$$

$$+ \left[- \frac{\alpha\phi(j,j)}{P_G^2(j,j)} \frac{R'(j)}{1+r_e(j)-R'(j)} Q_F(j+1\ \ j+1) \frac{dP_I(j+1)}{dx} \right]$$

$$\left. + \left[- \frac{\alpha\phi(j,j)}{P_G^2(j\ j)} \frac{R'(j)}{1+r_e(j)-R'(j)} \frac{dP(j+1)}{dx} \right] \right\}$$

From Appendix B 3 it may seem that $P_T(j)$ for $j = N_p + N$ to $2N_p + N - 1$ depends on $P_I(N_p + N)$, and thus derivatives $\frac{dP_T(j)}{dx}$ for $j = N_p + N$ to $2N_p + N - 1$ must be eliminated in terms of $\frac{dP_I(N_p + N)}{dx}$ From the equations of Appendix B 3,

$$\frac{dP_T(k)}{dx} = \left[\frac{dV_o'(k)}{dx} - \left(\frac{1}{1+r_c}\right)^{\Delta} \frac{dV_o'(k+1)}{dx}\right] \left\{ \frac{1 - \left(\frac{1}{1+r_c}\right)}{1 - \left(\frac{1}{1+r_c}\right)^{\Delta}} \right\} \tag{IX 24}$$

$$N_p + N \leq k \leq 2N_p + N - 1,$$

and

$$\frac{dV'_o(k)}{dx} = \frac{1 - \left(\frac{1}{1+r_c}\right)^{\Delta}}{1 - \left(\frac{1}{1+r_c}\right)} \left\{ T_{EF}^{-1} \frac{dP_I(N_p+N)}{dx} (1 + I_f)^{[k-(N_p+N]\Delta} \right\}$$

$$\left\{ g_{\infty 3} B_1(3)\psi_\infty[Z_1(3)] + g_{\infty 3} B_2(3)\psi_\infty[Z_2(3)] \right.$$

$$+ \quad [1 - g_{\infty 3}][1 - \alpha_3]^{[t_I+(k-1)\Delta-t_A]} B_1(3)\psi_\infty[Z_3(3)] \qquad \text{(IX 25)}$$

$$\left. + \quad [1 - g_{\infty 3}][1 - \alpha_3]^{[t_I+(k-1)\Delta-t_A]} B_2(3)\psi_\infty[Z_4(3)] \right\},$$

where all symbols are defined in Appendix B 3, and thus

$$\frac{dP_T(k)}{dx} = G(k) \frac{dP_I(N_p+N)}{dx} \qquad k = N_p + N \text{ to } N_p + N - 1 , \qquad \text{(IX 26)}$$

where

$$G(k) = G'(k) - \left[\frac{1}{1+r_c}\right]^{\Delta} G'(k+1)$$

$$G'(k) = \left[T_{EF}^{-1}(1 + I_f)^{[k-(N_p+N)]\Delta}\right] \qquad \text{(IX 27)}$$

$$\left\{ g_{\infty 3} B_1(3)\psi_\infty[Z_1(3)] + g_{\infty 3} B_2(3)\psi_\infty[Z_2(3)] \right.$$

$$+ \quad [1 - g_{\infty 3}][1 - \alpha_3]^{[t_I+(k-1)\Delta-t_A]} B_1(3)\psi_\infty[Z_3(3)]$$

$$\left. + \quad [1 - g_{\infty 3}][1 - \alpha_3]^{[t_I+(k-1)\Delta-t_A]} B_2(3)\psi_\infty[Z_4(3)] \right\}$$

Using Eqs (IX 19) (IX 21), and (IX 22) in Eq (IX 14) gives

$$\sum_{k=j+1}^{2N_p+N-1} \left[H_1(j,k) \frac{dP(k)}{dx} + H_2(j,k) \frac{d\phi(j,k)}{dx} \right]$$

$$+ \left[\frac{dP'(j)}{dx} - \frac{d\phi(j,j)}{dx} \quad C_f(j\ j)D(j,j) \right] \qquad \text{(IX 28)}$$

$$+ \quad [P'(j) - \phi(j\ j)]D(j\ j) \frac{\left\{ -\beta\gamma \left[\frac{\alpha\phi(j,j)}{P_G(j)} \right]^{\gamma-1} \right\}}{\left\{ 1 + \left[\frac{\alpha\phi(j,j)}{P_G(j)} \right]^{\gamma} \right\}^2} \left[\frac{\alpha}{P_G(j)} \quad \frac{d\phi(j,j)}{dx} \right.$$

$$\left. - \frac{\alpha\phi(j,j)}{P_G^{\ 2}(j)} \left\{ \frac{d\phi(j,j)}{dx} + \frac{R'(j)}{1+r_e(j)-R'(j)} \left[- \frac{dP(j+1)}{dx} + \frac{d\phi(j+1\ j+1)}{dx} \right] \right\} \right] = 0$$

$$j = N_p+1 \text{ to } N_p+N$$

where

$$H_1(j,k) = C_f(j\ k)D(j\ k)$$

$$+ [P(k)-\phi(j,k)]D(j\ k) \frac{\left\{ -\beta\gamma \left[\frac{\alpha\phi(j,k)}{P(k)} \right]^{\gamma-1} \right\}}{\left\{ 1 + \left[\frac{\alpha\phi(j,k)}{P(k)} \right]^{\gamma} \right\}^2} \left\{ - \frac{\alpha\phi(j\ k)}{P^2(k)} \right\} \qquad \text{(IX 29)}$$

$$H_2(j,k) = - C_f(j,k)D(j,k)$$

$$+ [P(k)-\phi(j,k)]D(j\ k) \frac{\left\{ -\beta\gamma \left[\frac{\alpha\phi(j,k)}{P(k)} \right]^{\gamma-1} \right\}}{\left\{ 1 + \left[\frac{\alpha\phi(j,k)}{P(k)} \right]^{\gamma} \right\}^2} - \frac{\alpha}{P(k)} \qquad \text{(IX 30)}$$

Now using Eqs (IX 18) and (IX 26) in Eq (IX 28) one obtains

$$\sum_{k=j+1}^{N_p+N} \left[H_1(j\ k) \frac{dP(k)}{dx} \quad H_2(j\ k) Q_F(j\ k) \frac{dP_I(k)}{dx} \right]$$

$$H_3(j) \frac{dP_I(N_p+N)}{dx}$$

$$C_G(j\ j) D(j\ j) \frac{dP\ (j)}{dx} \qquad \text{(IX 31)}$$

$$\left\{ C_{fG}(j\ j) D(j\ j) + [P\ (j) \quad \phi(j\ j)] D(j\ j) \frac{\left\{ \beta\gamma \left[\frac{\alpha\phi(j,j)}{P_G(j)} \right]^{\gamma-1} \right\}}{\left\{ 1 + \left[\frac{\alpha\phi(j,j)}{P_G(j)} \right]^{\gamma} \right\}^2} \left[\frac{\alpha}{P_G(j)} - \frac{\alpha\phi(j,j)}{P_G^2(j)} \right] \right\} Q_F(j\ j) \frac{dP_I(j)}{dx}$$

$$+ [P\ (j) - \phi(j\ j)] D(j\ j) \frac{\left\{ -\beta\gamma \left[\frac{\alpha\phi(j,j)}{P_G(j)} \right]^{\gamma-1} \right\}}{\left\{ 1 + \left[\frac{\alpha\phi(j,j)}{P_G(j)} \right]^{\gamma} \right\}^2} \frac{\alpha\phi(j,j)}{P_G^2(j)} \frac{R\ (j)}{1+r_e(j)-R\ (j)} \frac{dP(j+1)}{dx}$$

$$+ [P\ (j) \quad \phi(j\ j)] D(j\ j) \frac{\left\{ \beta\gamma \left[\frac{\alpha\phi(j,j)}{P_G(j)} \right]^{\gamma-1} \right\}}{\left\{ 1 + \left[\frac{\alpha\phi(j,j)}{P_G(j)} \right]^{\gamma} \right\}^2} \frac{\alpha\phi(j,j)}{P_G^2(j)} \frac{R\ (j)}{1+r_e(j)-R\ (j)} Q_F(j+1\ j+1) \frac{dP_I(j+1)}{dx} = 0$$

$$j = N_p + 1 \text{ to } N_p + N$$

where

$$H_3(j) = \sum_{k=N_p+N+1}^{2N_p+N-1} H_1(j,k) G(k) + H_2(j,k) Q_F(j,k)\ [1 + I_f]^{(k-N_p-N)\Delta} \qquad \text{(IX 32)}$$

Equation (IX 31), together with Eqs (IX 15), (IX 16) and (IX 17) is N of the equations that were discussed in conjunction with the forward sensitivity problem in Section IX A Note for future reference that Eq (IX 31) contains only derivatives of the variables on the output and input links of a process This fact will prove to be significant in Section IX C, when the properties of the A matrix (Section IX A) and its adjoint are considered The coefficients of the derivatives in Eq (IX 31) are individual elements of this A matrix, and these coefficients depend on the values of the variables determined from the original nonlinear set of equations

The next N equations are obtained by differentiating Eq (V 7) to obtain*

$$\frac{dQ(J)}{dx} = \sum_{k=1}^{J} \left[\frac{d}{dx} C_f(k,J)\right] N_W(k) \qquad \text{(IX 33)}$$

$$+ \sum_{k=1}^{J} C_f(k,J) \frac{dN_W(k)}{dx} \qquad J = N_p + 1 \text{ to } N_p + N$$

and from Eq (V 25),

$$\frac{dN_W(k)}{dx} = \frac{dQ(N_p+1)}{dx} \frac{a(k)}{\sum_{J=1}^{N_p+1} a(J)C_f(J,N_p+1)}$$

$$+ \frac{da(k)}{dx} \frac{Q(N_p+1)}{\sum_{J=1}^{N_p+1} a(J)C_f(J,N_p+1)} \qquad \text{(IX 34)}$$

$$- \frac{Q(N_p+1)a(k) \sum_{J=1}^{N_p+1} \left[a(J) \frac{d}{dx} C_f(J\ N_p+1) + C_F(J\ N_p+1) \frac{da(J)}{dx}\right]}{\left[\sum_{J=1}^{N_p+1} a(J)C_f(J,N_p+1)\right]^2} \qquad k < N_p + 1$$

*The modification of Eq (V 7) required when $N_W(k) < 0$ (see discussion at the end of Section V A) is not considered here

where

$$a(k) = \text{Max}\ \{0 \quad 1 - r_s\Delta(N_p + 1 \quad k)]\} \tag{IX 35}$$

$$\frac{da(k)}{dx} = 0 \qquad\qquad 1-r_s\Delta(N_p + 1 - k) < 0$$

$$= \frac{dr_s}{dx}\ [\Delta(N_p + 1 - k)] \qquad 1-r_s\Delta(N_p + 1 - k) > 0 \tag{IX 36}$$

Substituting Eq (V 25) into (V 26) gives

$$E_{AV} = \frac{\sum_{k=1}^{N_p+1} Q_F(k,N_p+1)C_f(k\ N_p+1)a(k)}{\sum_{k=1}^{N_p+1} a(k)C_f(k,N_p+1)} \tag{IX 37}$$

and Eq (IX 37) may be differentiated and solved for $\frac{dr_s}{dx}$ to obtain

$$\frac{dr_s}{dx} = - \frac{\sum_{k=1}^{N_p+1} Q_F(k\ N_p+1)a(k)\ \frac{d}{dx}\ C_f(k,N_p+1)}{H_D\left[\sum_{k=1}^{N_p+1} a(k)C_f(k,N_p+1)\right]}$$

$$+ \frac{\sum_{k=1}^{N_p+1} Q_F(k,N_p+1)C_f(k,N_p+1)a(k) \sum_{\ell=1}^{N_p+1} a(\ell)\ \frac{d}{dx}\ C_f(\ell,N_p+1)}{H_D\left[\sum_{k=1}^{N_p+1} a(k)C_f(k,N_p+1)\right]^2}, \tag{IX 38}$$

where

$$H_D = - \frac{\Delta \sum_{k=k_m}^{N_p+1} Q_F(k,N_p+1)C_f(k,N_p+1)(N_p+1-k)}{\sum_{k=1}^{N_p+1} a(k)C_f(k,N_p+1)} \qquad \text{(IX 39)}$$

$$+ \frac{\sum_{\ell=1}^{N_p+1} Q_F(\ell,N_p+1)C_f(\ell\ N_p+1)a(\ell)\Delta\sum_{k=k_m}^{N_p+1} C_f(k\ N_p+1)(N_p+1-k)}{\left[\sum_{k=1}^{N_p+1} a(k)C_f(k\ N_p+1)\right]^2}$$

$$k_m = 1 + \text{Int}\ [N_p + 1 - \frac{1}{r_s\Delta}\ ] \qquad \text{(IX 40)}$$

and $\frac{d}{dx}\ C_f(k\ N_p+1)$ is given by Eq (IX 20)

Substituting from Eqs (IX 20) and (IX 34)

$$\begin{aligned}
\frac{dQ(J)}{dx} &= H_4(J)\ \frac{dP(J)}{dx} \\
&+ H_5(J)\ \frac{dP_I(J)}{dx} \\
&+ \sum_{k=N_p+1}^{J} C_f(k,J)\ \frac{dN_W(k)}{dx} \qquad \text{(IX 41)} \\
&+ H_6(J)\ \frac{dQ(N_p+1)}{dx} \\
&+ H_7(J)\ \frac{dP(N_p+1)}{dx} \\
&+ H_8(J)\ \frac{dP_I(N_p+1)}{dx} \qquad J = N_p + 1 \text{ to } N_p + N
\end{aligned}$$

where

$$H_4(J) = \sum_{k=1}^{J} N_W(k) \frac{\left\{ - \beta\gamma \left[\frac{\alpha\phi(k,J)}{P(J)} \right]^{\gamma-1} \right\}}{\left\{ 1 + \left[\frac{\alpha\phi(k,J)}{P(J)} \right]^{\gamma} \right\}^2} \left\{ \frac{-\alpha\phi(k,J)}{P^2(J)} \right\}, \qquad \text{(IX 42)}$$

$$H_5(J) = \sum_{k=1}^{J} N_W(k) \frac{\left\{ - \beta\gamma \left[\frac{\alpha\phi(k,J)}{P(J)} \right]^{\gamma-1} \right\}}{\left\{ 1 + \left[\frac{\alpha\phi(k,J)}{P(J)} \right]^{\gamma} \right\}^2} \left\{ \frac{\alpha Q_F(k\ J)}{P(J)} \right\} \qquad \text{(IX 43)}$$

$$H_6(J) = \sum_{k=1}^{N_p} C_f(k\ J) \frac{a(k)}{\sum_{\ell=1}^{N_p+1} a(\ell) C_f(\ell, N_p+1)} \qquad \text{(IX 44)}$$

$$
\begin{aligned}
H_7(J) \sum_{k\ 1}^{N_p} C_f(k\ J) & \frac{[\,Q(N_p+1,a(k)]}{\left\{\sum_{\ell\ 1}^{N_p+1} a(\ell)C_f(\ell\ N_p+1)\right\}^2} \sum_{\ell-1}^{N_p+1} a(\ell) \frac{\left\{\beta\gamma\left[\frac{\alpha\phi(\ell\ N_p+1)}{P(N_p+1)}\right]^{1}\right\}}{\left\{1+\left[\frac{\alpha\phi(\ell\ N_p+1)}{P(N_p+1)}\right]^{\gamma}\right\}^2} \left\{\frac{\alpha\phi(\ell\ N_p+1)}{P^2(N_p+1)}\right\} \\
& + \sum_{k\ k_m}^{N_p} C_f(k\ J) \left[\frac{[\,Q(N_p+1)\Delta(N_p+1\ k)]}{\left\{\sum_{\ell\ 1}^{N_p+1} a(\ell)C_f(\ell\ N_p+1)\right\}^2} + \frac{Q(N_p+1)a(k)\sum_{\ell-\ell_m}^{N_p+1} C_f(\ell\ N_p+1)\Delta(N_p+1\ \ell)}{\left\{\sum_{\ell-1}^{N_p+1} a(\ell)C_f(\ell\ N_p+1)\right\}^3}\right] \\
& \left\{-\frac{1}{H_D}\sum_{\ell\ 1}^{N_p+1} Q_F(\ell\ N_p+1)a(\ell) \frac{(\beta)}{\left\{1+\left[\frac{\alpha\phi(\ell\ N_p+1)}{P(N_p+1)}\right]^{\gamma}\right\}^2} \left\{\gamma\left[\frac{\alpha\phi(\ell\ N_p+1)}{P(N_p+1)}\right]^{\gamma\ 1}\right\}\left[\frac{\alpha\phi(\ell\ N_p+1)}{P^2(N_p+1)}\right]\right. \\
& + \frac{1}{H_D\left\{\sum_{\ell\ 1}^{N_p+1} a(\ell)C_f(\ell\ N_p+1)\right\}} \sum_{\ell\ 1}^{N_p+1} Q_F(\ell\ N_p+1)C_f(\ell\ N_p+1)a(\ell)\sum_{m=1}^{N_p+1} a(m) \frac{(\beta)}{\left\{1+\left[\frac{\alpha\phi(m\ N_p+1)}{P(N_p+1)}\right]^{\gamma}\right\}^2} \\
& \left.\left\{\gamma\left[\frac{\alpha\phi(\ell\ N_p+1)}{P(N_p+1)}\right]^{\gamma\ 1}\right\}\left[\frac{\alpha\phi(m\ N_p+1)}{P^2(N_p+1)}\right]\right\}
\end{aligned}
$$

(IX 45)

$$
\begin{aligned}
H_8(J) \quad & \sum_{1}^{N_p} C_f(k\ J) \frac{[\,Q(N_p+1)a(k)\,]}{\left\{\sum_{\ell=1}^{N_p+1} a(\ell)C_f(\ell\ N_p+1)\right\}^2} \sum_{\ell\ 1}^{N_p+1} a(\ell) \frac{\left\{ \beta\gamma\left[\frac{\alpha\phi(\ell\ N_p+1)}{P(N_p+1)}\right]^{(\ 1)} \right\}}{\left\{1+\left[\frac{\alpha\phi(\ell\ N_p+1)}{P(N_p+1)}\right]^{\gamma}\right\}^2} \left\{\frac{\alpha Q_F(\ell\ N_p+1)}{P(N_p+1)}\right\} \\
& + \sum_{k=k_m}^{N_p} C_f(k\ J) \left[\frac{[\,Q(N_p+1)\Delta(N_p+1\ k)\,]}{\left\{\sum_{\ell\ 1}^{N_p+1} a(\ell)C_f(\ell\ N_p+1)\right\}^2} + \frac{Q(N_p+1)a(k)\sum_{\ell=\ell_m}^{N_p+1} C_f(\ell\ N_p+1)\Delta(N_p+1\ \ell)}{\left\{\sum_{\ell-1}^{N_p+1} a(\ell)C_f(\ell\ N_p+1)\right\}^3} \right] \\
& \left\{ \frac{1}{H_D}\sum_{\ell\ 1}^{N_p+1} Q_F(\ell\ N_p+1)a(\ell) \frac{(\ \beta)}{\left\{1+\left[\frac{\alpha\phi(\ell\ N_p+1)}{P(N_p+1)}\right]^{\gamma}\right\}^2} \left\{\gamma\left[\frac{\alpha\phi(\ell\ N_p+1)}{P(N_p+1)}\right]^{\gamma\ 1}\right\} \left[\frac{\alpha Q_F(\ell\ N_p+1)}{P(N_p+1)}\right] \right. \\
& + \frac{1}{H_D\left\{\sum_{\ell\ 1}^{N_p+1} a(\ell)C_f(\ell\ N_p+1)\right\}} \sum_{\ell-1}^{N_p+1} Q_F(\ell\ N_p+1)C_f(\ell\ N_p+1)a(\ell)\sum_{m=1}^{N_p+1} a(m) \frac{(\ \beta)}{\left\{1+\left[\frac{\alpha\phi(m\ N_p+1)}{P(N_p+1)}\right]^{\gamma}\right\}^2} \\
& \left. \left\{\gamma\left[\frac{\alpha\phi(\ell\ N_p+1)}{P(N_p+1)}\right]^{\gamma\ 1}\right\} \left[\frac{\alpha Q_F(m\ N_p+1)}{P(N_p+1)}\right] \right\}
\end{aligned}
$$

(IX 46)

The final N forward sensitivity equations are obtained by differentiating Eq (V 8) to obtain*

$$\frac{dQ_I(J)}{dx} = \sum_{k=1}^{J} Q_F(k,J) \left[\frac{dC_f(k,J)}{dx}\right] N_W(k) \qquad \text{(IX 47)}$$

$$+ \sum_{k=1}^{J} Q_F(k,J) C_f(k,J) \frac{dN_W(k)}{dx} \qquad J = N_p + 1 \text{ to } N_p + N ,$$

and using Eqs (IX 20) and (IX 41)

$$\frac{dQ_I(J)}{dx} = L_4(J) \frac{dP(J)}{dx}$$

$$+ L_5(J) \frac{dP_I(J)}{dx}$$

$$+ \sum_{k=N_p+1}^{J} Q_F(k\ J)\ C_f(k,J) \frac{dN_W(k)}{dx} \qquad \text{(IX 48)}$$

$$+ L_6(J) \frac{dQ(N_p+1)}{dx}$$

$$+ L_7(J) \frac{dP(N_p+1)}{dx}$$

$$+ L_8(J) \frac{dP_I(N_p+1)}{dx} ,$$

---

*The modification of Eq (V 8) required when $N_W(k) < 0$ (see discussion at the end of Section V A) is not considered here

where

$$L_4(J) = \sum_{k=1}^{J} Q_F(k\ J)N_W(k) \left\{ \frac{-\beta\gamma \left[\frac{\alpha\phi(k,J)}{P(J)}\right]^{\gamma-1}}{\left\{1 + \left[\frac{\alpha\phi(k,J)}{P(J)}\right]^{\gamma}\right\}^2} \right\} \left[\frac{-\alpha\phi(k,J)}{P^2(J)}\right], \quad \text{(IX 49)}$$

$$L_5(J) = \sum_{k=1}^{J} Q_F(k\ J)N_W(k) \left\{ \frac{-\beta\gamma \left[\frac{\alpha\phi(k,J)}{P(J)}\right]^{\gamma-1}}{\left\{1 + \left[\frac{\alpha\phi(k,J)}{P(J)}\right]^{\gamma}\right\}^2} \right\} \left\{\frac{\alpha Q_F(k,J)}{P(J)}\right\} \quad \text{(IX 50)}$$

$$L_6(J) = \sum_{k=1}^{N_p} Q_F(k,J)\ \ C_F(k,J) \quad \frac{a(k)}{\sum_{\ell=1}^{N_p+1} a(\ell)C_f(\ell\ N_p+1)}, \quad \text{(IX 51)}$$

$$
\begin{aligned}
L_7(J) = & -\sum_{k=1}^{N_p} Q_F(k,J)\, C_f(k,J) \frac{[Q(N_p+1)a(k)]}{\left\{\sum_{\ell=1}^{N_p+1} a(\ell)C_f(\ell,N_p+1)\right\}^2} \sum_{\ell=1}^{N_p+1} a(\ell) \frac{\left\{\beta\gamma\left[\frac{\alpha\phi(\ell,N_p+1)}{P(N_p+1)}\right]^{\gamma-1}\right\}}{\left\{1+\left[\frac{\alpha\phi(\ell,N_p+1)}{P(N_p+1)}\right]^{\gamma}\right\}^2} \left\{\frac{\alpha\phi(\ell,N_p+1)}{P^2(N_p+1)}\right\} \\
& + \sum_{k=k_m}^{N_p} Q_c(k,J)\, C_f(k,J) \left[\frac{[Q(N_p+1)\Delta(N_p+1,k)]}{\left\{\sum_{\ell=1}^{N_p+1} a(\ell)C_f(\ell,N_p+1)\right\}^2} + \frac{Q(N_p+1)a(k)\sum_{\ell=\ell_m}^{N_p+1} C_f(\ell,N_p+1)\Delta(N_p+1,\ell)}{\left\{\sum_{\ell=1}^{N_p+1} a(\ell)C_f(\ell,N_p+1)\right\}^3}\right] \\
& \left\{\frac{1}{H_D}\sum_{\ell=1}^{N_p+1} Q_F(\ell,N_p+1)a(\ell) \frac{(\beta)}{\left\{1+\left[\frac{\alpha\phi(\ell,N_p+1)}{P(N_p+1)}\right]^{\gamma}\right\}^2}\left\{\gamma\left[\frac{\alpha\phi(\ell,N_p+1)}{P(N_p+1)}\right]^{\gamma-1}\right\}\left[\frac{\alpha\phi(\ell,N_p+1)}{P^2(N_p+1)}\right]\right. \\
& + \frac{1}{H_D\left\{\sum_{\ell=1}^{N_p+1} a(\ell)C_f(\ell,N_p+1)\right\}} \sum_{\ell=1}^{N_p+1} Q_F(\ell,N_p+1)C_f(\ell,N_p+1)a(\ell)\sum_{m=1}^{N_p+1} a(m) \frac{(\beta)}{\left\{1+\left[\frac{\alpha\phi(m,N_p+1)}{P(N_p+1)}\right]^{\gamma}\right\}^2} \\
& \left.\left\{\gamma\left[\frac{\alpha\phi(\ell,N_p+1)}{P(N_p+1)}\right]^{\gamma-1}\right\}\left[\frac{\alpha\phi(m,N_p+1)}{P^2(N_p+1)}\right]\right\}
\end{aligned}
\tag{IX 52}
$$

$$
\begin{aligned}
L_8(J) \quad & \sum_{k=1}^{N_p} Q_F(k\ J)\ C_f(k\ J)\ \frac{[\ Q(N_p+1)a(k)]}{\left\{\sum_{\ell=1}^{N_p+1} a(\ell)C_f(\ell\ N_p+1)\right\}^2} \sum_{\ell=1}^{N_p+1} a(\ell) \frac{\left\{\beta\gamma\left[\frac{\alpha\phi(\ell\ N_p+1)}{P(N_p+1)}\right]^{\gamma-1}\right\}}{\left\{1+\left[\frac{\alpha\phi(\ell\ N_p+1)}{P(N_p+1)}\right]^{\gamma}\right\}^2} \left\{\frac{\alpha Q_F(\ell\ N_p+1)}{P(N_p+1)}\right\} \\
& + \sum_{k=k_m}^{N_p} Q_F(\ell\ J)\ C_f(k\ J) \left[\frac{[\ Q(N_p+1)\Delta(N_p+1\ k)]}{\left\{\sum_{\ell=1}^{N_p+1} a(\ell)C_f(\ell\ N_p+1)\right\}^2} + \frac{Q(N_p+1)a(k)\sum_{\ell=\ell_m}^{N_p+1} C_f(\ell\ N_p+1)\Delta(N_p+1\ \ell)}{\left\{\sum_{\ell=1}^{N_p+1} a(\ell)C_f(\ell\ N_p+1)\right\}^3}\right] \\
& \left\{\frac{1}{H_D}\sum_{\ell=1}^{N_p+1} Q_F(\ell\ N_p+1)a(\ell)\ \frac{(\beta)}{\left\{1+\left[\frac{\alpha\phi(\ell\ N_p+1)}{P(N_p+1)}\right]^{\gamma}\right\}^2}\left\{\gamma\left[\frac{\alpha\phi(\ell\ N_p+1)}{P(N_p+1)}\right]^{\gamma-1}\right\}\left[\frac{\alpha Q_F(\ell\ N_p+1)}{P(N_p+1)}\right]\right. \\
& + \frac{1}{H_D\left\{\sum_{\ell=1}^{N_p+1} a(\ell)C_f(\ell\ N_p+1)\right\}}\sum_{\ell=1}^{N_p+1} Q_F(\ell\ N_p+1)C_f(\ell\ N_p+1)a(\ell)\sum_{m=1}^{N_p+1} a(m)\ \frac{(\beta)}{\left\{1+\left[\frac{\alpha\phi(m\ N_p+1)}{P(N_p+1)}\right]^{\gamma}\right\}^2} \\
& \left.\left\{\gamma\left[\frac{\alpha\phi(\ell\ N_p+1)}{P(N_p+1)}\right]^{\gamma-1}\right\}\left[\frac{\alpha Q_F(m\ N_p+1)}{P(N_p+1)}\right]\right\}
\end{aligned}
\qquad \text{(IX 53)}
$$

Equations (IX 41) and (IX 48) are 2 N additional equations that were discussed in conjunction with the forward sensitivity problem in Section IX A The elements of the A matrix are the coefficients of the derivatives in Eqs (IX 31), (IX 41), and (IX 48) Note that the algebraic form of these coefficients is independent of the choice of x Note again that these equations contain only derivatives of the variables on the output and input links to the process being considered In Section IX C the structure of the A matrix based on these considerations will be discussed

Before leaving this section, the elements of the vector S (Section IX A) must be considered In the discussion above it was explicitly assumed that x was not a parameter in the basic conversion process being considered, thus the partial derivatives of the equations considered with respect to x were, by assumption, zero To illustrate the types of derivatives that occur let it now be assumed that x is a parameter of the basic conversion process, and to be explicit, let x be the parameter β that occurs in Eq (V 21), (V 22), and (V 23)

If S_A are the elements of S (Section IX A) corresponding to Eq (V 6), then

$$S_A(J) = \left\{ \sum_{k=N_p+1}^{2N_p+N-1} \frac{\partial P_T(k)}{\partial \beta} C_f(J\ k) D(J,k) \right.$$

$$+ \sum_{k=J+1}^{2N_p+N-1} [P(k) - \phi(J,k)] \frac{\partial C_f(J,k)}{\partial \beta} D(J,k)$$

$$+ [P'(J) - \phi(J\ J)] \frac{\partial C_{fG}(J,J)}{\partial \beta} D(J,J) \qquad \text{(IX 54)}$$

$$\left. - \frac{\partial P_T(N_p+N)}{\partial \beta} C_{fG}(J,J) D(J,J) \delta^J_{N_p+N} \right\} \qquad J = N_p + 1 \text{ to } N_p + N,$$

where

$$\delta^J_{N_p+N} = 1 \qquad J = N_p+N$$

$$\delta^J_{N_p+N} = 0 \qquad J \neq N_p+N$$

From Eqs (B 36) and (B 52),

$$\frac{\partial P_T(k)}{\partial \beta} = -\frac{1}{\beta}\left[V_C(k) - \left(\frac{1}{1+r_C}\right)^{\Delta} V_C(k+1)\right] \frac{1-\left(\frac{1}{1+r_c}\right)}{1-\left(\frac{1}{1+r_c}\right)^{\Delta}}$$

$$J = N_p + 1 \text{ to } N_p + N \qquad \text{(IX 55)}$$

and from Eq (V 21)

$$\frac{\partial C_f(J,k)}{\partial \beta} = \frac{1}{1+\left[\frac{\alpha\phi(J,k)}{P(k)}\right]^{\gamma}} \qquad J = N_p + 1 \text{ to } N_p + N \qquad \text{(IX 56)}$$

Also from Eqs (V 22) and (V 23),

$$\frac{\partial C_{fG}(J\ J)}{\partial \beta} = \frac{1}{1+\left[\frac{\alpha\phi(J,J)}{P_G(J)}\right]^{\gamma}} \qquad \text{(IX 56)}$$

$$-\frac{\beta\gamma\left[\frac{\alpha\phi(J,J)}{P_G(J)}\right]^{\gamma-1}}{\left\{1+\left[\frac{\alpha\phi(J,J)}{P_G(J)}\right]^{\gamma}\right\}^2} - \left[\frac{\alpha\phi(J,J)}{P_G^2(J)} \frac{\partial P_G(J)}{\partial \beta}\right] \qquad \text{(IX 57)}$$

$$J = N_p + 1 \text{ to } N_p + N$$

and

$$\frac{\partial P_G(J)}{\partial \beta} = \frac{R'(J)}{1 + r_e(J) - R'(J)} \left\{ -\frac{[1 + r_e(J)]N_C(J)}{\beta^2} - \frac{\partial P_T(J+1)}{\partial \beta} \delta^J_{N_p+N} \right\} \qquad \text{(IX 58)}$$

$$J = N_p + 1 \text{ to } N_p + N$$

Thus from Eqs (IX 55) to (IX 58), all of the derivatives in Eq (IX 54) have been determined, and $S_A(J)$ for $J = N_p + 1$ to $N_p + N$ may be evaluated

Similarly if $S_B(J)$ are the elements of S corresponding to Eq (V 7),

$$
\begin{aligned}
S_B(J) \quad & \frac{\partial}{\partial\beta}\left\{Q(\ ) \sum_{k=1}^{J} C_f(k\ J) N_W(k)\right\} \\
& \sum_{1}^{J}\left[\frac{\partial}{\partial\beta} C_f(k\ J)\right] N_W(k) + \sum_{k=1}^{J} C_f(k\ J)\frac{\partial}{\partial\beta} N_W(k) \\
& - \sum_{k=1}^{J} \frac{N_W(k)}{\left\{1+\left[\frac{\alpha\phi(k\ J)}{P(J)}\right]^{\gamma}\right\}} + \sum_{k=1}^{N_p} C_f(k\ J)\frac{\partial}{\partial\beta}\left[\frac{Q(N_p+1)a(k)}{\left\{\sum_{\ell=1}^{N_p+1} a(\ell)C_f(\ell\ N_p+1)\right\}}\right] \\
& \sum_{k=1}^{J} \frac{N_W(k)}{\left\{1+\left[\frac{\alpha\phi(k\ J)}{P(J)}\right]^{\gamma}\right\}} \\
& \sum_{k=1}^{N_p} \frac{C_f(k\ J)Q(N_p+1)a(k)}{\left\{\sum_{\ell=1}^{N_p+1} a(\ell)C_f(\ell\ N_p+1)\right\}^2}\left\{\sum_{\ell=\ell_m}^{N_p+1}\left[\frac{a(\ell)}{\left\{1+\left[\frac{\alpha\phi(\ell\ N_p+1)}{P(N_p+1)}\right]^{\gamma}\right\}} C_f(\ell\ N_p+1)\Delta(N_p+1\ \ell)\frac{dr_s}{d\beta}\right]\right\} \\
& \sum_{k=k_m}^{N_p}\left[\frac{C_f(k\ J)Q(N_p+1)\Delta(N_p+1-k)\frac{dr_s}{d\beta}}{\sum_{\ell=1}^{N_p+1} a(\ell)C_f(\ell\ N_p+1)}\right] \qquad J = N_p+1 \text{ to } N_p+N
\end{aligned}
\tag{IX 59}
$$

where dr_s/d_β is given by Eq (IX 38) with $x = \beta$

and if $S_C(J)$ are the elements of S corresponding to Eq (V 8),

$$S_C(J) \quad \frac{\partial}{\partial\beta}\left\{Q_I(J) \sum_{k=1}^{J} Q_F(k\ J)C_f(k\ J)N_W(k)\right\} \qquad \text{(IX 60)}$$

$$\sum_{k\ 1}^{J} \frac{Q_F(k\ J)N_W(k)}{1+\left[\frac{\alpha\phi(k\ J)}{P(J)}\right]^{\gamma}}$$

$$\sum_{k-1}^{N_p} \frac{Q_F(k\ J)C_f(k\ J)Q(N_p+1)a(k)}{\left\{\sum_{\ell-1}^{N_p+1} a(\ell)C_f(\ell\ N_p+1)\right\}^2} \left\{\sum_{\ell-\ell_m}^{N_p+1} \left[\frac{a(\ell)}{\left\{1+\left[\frac{\alpha\phi(\ell\ N_p+1)}{P(N_p+1)}\right]^{\gamma}\right\}} C_f(\ell\ N_p+1)\Delta(N_p+1\ \ell)\frac{dr_s}{d\beta}\right]\right\}$$

$$\sum_{k=k_m}^{N_p} \left[\frac{C_f(k\ J)Q(N_p+1)\Delta(N_p+1\ k)\frac{dr_s}{d\beta}}{\sum_{\ell=1}^{N_p+1} a(\ell)C_f(\ell\ N_p+1)}\right] \qquad J = N_p+1 \text{ to } N_p+N\ ,$$

where dr_s/d_β is again given by Eq (IX 38)

Equations (IX 54), (IX 59), and (IX 60) give the 3 N elements of S when x is the β of the basic conversion process being considered The elements of S for other parameters may be obtained in a similar manner There are many parameters, and thus many derivatives such as those in Eqs (IX 54), (IX 59), and (IX 60), if sensitivity coefficients for all parameters in the system are to be obtained However, in large models such as Model 22C, the individual processes are used many times, and the form of the derivatives does not change, thus helping to reduce the labor involved in the analytic differentiation process

Equations (IX 31), (IX 41), and (IX 48), constitute 3 N equations of the set of equations [see Eq (IX 5)], together with Eqs (IX 54), (IX 59), and (IX 60) in the special case when x = β,

$$A\vec{\Phi} = \vec{S} \qquad \text{(IX 52)}$$

It should be clear that the elements of the matrix A are the coefficients of the derivatives of the variables in equations such as (IX 31), (IX 41), and (IX 48)

C Applicability of Adjoint Sensitivity Analysis to LEAP

In this section the forward sensitivity and adjoint sensitivity equations are discussed The discussion is centered about Model 82 (see Section IV) but much of it is also applicable to more complex models such as Model 22C No numerical results are given because they are not yet available, but the discussion will indicate the procedures that will be used to obtain numerical results

The local and global time functions were defined in Section V and the local time index, j, was used throughout Sections V and IX B In this section (as in Section IV), where several processes are considered, it is convenient to use the global time index J The notation is the same as before, but when the global time index J is used, the function is to be evaluated at time $T_G(J)$ [see Eq (V 1)] for example P(J) means that the variable P is to be evaluated at time $T_G(J)$ Capital letters will always be used for global time indices Also in this section (as in Section IV), all variables must be designated by node Thus, as in Section IV P(1 J) will be the price per unit energy on the output link of node 1 at global time $T_G(J)$

Let us first consider the forward sensitivity equation [Eq (IX 52)],

$$A\bar{\Phi} = \bar{S} \ , \qquad \text{(IX 62)}$$

for Model 82 The vector $\bar{\Phi}$ is composed of the derivatives of all variables of the system at all times of interest with respect to x, where x is any parameter that occurs anywhere in Model 82 equations For convenience, the parameter x will be taken to be the β in Eqs (V 21) and (V 22) (i e , $\beta(y)$ is the value of β for node 6) The vector Φ for Model 82, with N (the number of time steps at which the variables are calculated) equaling 2 for convenience, is the column vector shown in Figure IX-1 In Figure IX-1 the notation,

$$Q_\beta(n,J) = \frac{d}{d\beta} Q(n,J) \ , \qquad \text{(IX 63)}$$

has been introduced for simplicity The order in which the variables occur in Φ is arbitrary In Figure IX-1 the highest node number is taken first and with this node number, the Q's from earliest to latest times are followed by the P's from earliest to latest times, which in turn are followed by the N_W's from earliest to latest times As explained in Section IV, Q(6,1) and Q(2,1), Q(3,1), and Q(4,1) are initial conditions, and thus the derivatives of these quantities do not occur in Φ For resource and conversion processes, the plant capacity additions $N_W(n,J)$ have also been used as variables (see Section V) Note that at node 4 only the quantity Q(4,2) is a variable since the prices of imports are inputs to the system As explained in Section V, Model 82 has 14 N - 4 variables, where N is the number of time points at which the variables are calculated, therefore, with N = 2, Φ has 24 components

$$
\begin{bmatrix}
7 & 7 & 7 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
6 & 6 & 6 & 6 & 6 & 6 & 6 & 6 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
6 & 6 & 6 & 6 & 6 & 6 & 6 & 6 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
6 & 6 & 6 & 6 & 6 & 6 & 6 & 6 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
6 & 6 & 6 & 6 & 6 & 6 & 6 & 6 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
6 & 6 & 6 & 6 & 6 & 6 & 6 & 6 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
6 & 6 & 6 & 6 & 6 & 6 & 6 & 6 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 5 & 5 & 5 & 5 & 5 & 5 & 5 & 5 & 0 & 0 & 5 & 5 & 5 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 5 & 5 & 5 & 5 & 5 & 5 & 5 & 5 & 0 & 0 & 5 & 5 & 5 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 5 & 5 & 5 & 5 & 5 & 5 & 5 & 5 & 0 & 0 & 5 & 5 & 5 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 5 & 5 & 5 & 5 & 5 & 5 & 5 & 5 & 0 & 0 & 5 & 5 & 5 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 5 & 5 & 5 & 5 & 5 & 5 & 5 & 5 & 0 & 0 & 5 & 5 & 5 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 3 & 3 & 3 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 3 & 3 & 3 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 3 & 3 & 3 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 3 & 3 & 3 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1
\end{bmatrix}
\begin{bmatrix}
Q_\beta(6,2) \\ P_\beta(6,1) \\ P_\beta(6,2) \\ N_{W\beta}(6,1) \\ N_{W\beta}(6,2) \\ Q_\beta(5,1) \\ Q_\beta(5,2) \\ P_\beta(5,1) \\ P_\beta(5,2) \\ Q_\beta(4,2) \\ Q_\beta(3,2) \\ P_\beta(3\ 1) \\ P_\beta(3,2) \\ N_{W\beta}(3,1) \\ N_{W\beta}(3,2) \\ Q_\beta(2,2) \\ P_\beta(2,1) \\ P_\beta(2,2) \\ Q_\beta(1,1) \\ Q_\beta(1,2) \\ P_\beta(1,1) \\ P_\beta(1,2) \\ N_{W\beta}(1,1) \\ N_{W\beta}(1,2)
\end{bmatrix}
=
\begin{bmatrix}
0 \\ S_A(1) \\ S_A(2) \\ S_B(1) \\ S_B(2) \\ S_C(1) \\ S_C(2) \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0
\end{bmatrix}
$$

$$A\bar{\Phi} = \bar{S}$$

Figure IX-1 Schematic diagram of matrix A and vector $\bar{\phi}$ for Model 82 with N = 2 The parameter β that is considered is that in Eqs (V 21) and (V 22) for node 6, and $Q_\beta(n,J) = \frac{d}{d\beta} Q(n,J)$

A schematic diagram of the A matrix is also shown in Figure IX-1 In this schematic diagram, the elements of the A matrix that can, in principle, be non-zero are indicated by a number that is the elements that are shown as zero are definitely zero whereas the elements that are shown by numerals may or may not be zero The numerals that are used in the schematic diagram are the node numbers from which a given equation arises, that is, the 7's that occur only in the first row indicate that only one equation is obtained from node 7, whereas the 6's in rows 2 to 7 indicate that six equations are obtained from node 6, etc

The structure of the A matrix in the schematic diagram arises from the fact that the equations from a node in LEAP couple only the variables on the input and output links to that node The first row in the A matrix corresponds to an equation from the INDUSTRIAL DEMAND (FOR INDIRECT HEAT) node, which couples the derivative of the quantity Q(6 2) on the node 7 input link to the derivatives of the prices P(6,1) and P(6,2), also on the node input link The equation from the demand node (i e node 7) does not in Model 82 (or 22C) involve the variables N_W(6 1) and N_W(6 2)

The six equations corresponding to rows 2 through 7 in the schematic diagram are from the conversion process, these equations couple the derivatives of variables Q(6 2) P(6,1), P(6,2), N_W(6 1) N_W(6 2) Q(5 1) Q(5 2) P(5 1), and P(5 2) (i e the derivatives of the variables on the input and output links of node 6) There are six equations (i e , 3 N) in this case corresponding to differentiating the equations described in Section V This differentiation is carried out in Section IX B

One should remember that as shown in Section IX B the elements of A are independent of the choice of the parameter x Also in large models such as 22C the basic conversion process is used many times The algebraic form of the elements of the A matrix each time the process is used will be of the form derived in Section IX B That is the rather tedious task of differentiating and programming the equations of a particular process must be carried out only once even if that process is used many times

The allocation process at node 5 provides five equations for the case being considered and couples the derivatives of the variables Q(5,1) Q(5,2), P(5 1), P(5,2), Q(4,2), Q(3,2) P(3,1), P(3,2), Q(2 2), P(2 1) and P(2,2) The actual number of equations supplied by an allocation process is determined by the number of input links The transportation process which is relatively simple, supplies the equations necessary (2 N) to determine the prices and quantities on the output link of the transportation process from the prices and quantities on the input link Resource processes supply (2 N) equations Basically the resource process supplies N fewer equations than a conversion process because a resource process has no input link

In Figure IX-1 the vector on the right-hand side of the schematic diagram is the vector $\bar{S}$ for the particular choice of x [i e , x = β(6)] being considered The non-zero elements of this vector are those given in Eqs (IX 58) (IX 59), and (IX 60)

To consider the adjoint equations, one must specify the response to be considered (Section IX A) The response may be any function of the variables and parameters of the system but as an example the quantity of energy supplied to the INDUSTRIAL DEMAND (FOR INDIRECT HEAT) in the last year of the model will be taken as the response That is, with N = 2 as before

$$R = Q(6,2) \qquad \text{(IX 64)}$$

will be used (see Section IX A) Then, since A* is the transpose of A (i e A^T), the equations adjoint to the forward equation in Figure IX-1 have the schematic form shown in Figure IX-2 and the sensitivity coefficient dR/dβ may be written

$$\frac{dR}{d\beta} = \bar{\phi}^{*T} \quad S \qquad \text{(IX 65)}$$

where the elements of $\bar{\phi}^{*T}$ (i e ϕ_1^* to ϕ_{24}^*) are obtained by solving the equations in Figure IX-2 and the elements of S are shown in Figure IX-1

The important point to note is that A and A^T have many elements that are zero and in the simple example considered here, are of a band form that is, they have non-zero elements near the diagonal, but only zero elements far removed from the diagonal The zero elements in A and A^T and the band form in Figures IX-1 and IX-2 result from the fact that the equations at a node couple only the variables on the input and output links of a node In very large models such as 22C the large number of zeros and, to some extent at least the band form will persist These characteristics are important because it should be possible to exploit them to obtain a solution to the large set of linear equations for a model such as 22C

The present concept of obtaining sensitivity coefficients for Model 22C (i e dR/dx for an arbitrary x) will be to modify the LEAP code so that when equilibrium is reached the elements of the A matrix and the elements of the vector $\bar{S}$ for all x will be evaluated and permanently stored in a form that may be accessed by a computer code (to be written) that will access these data, solve the adjoint equations, and calculate dR/dx for all x By calculating the elements of the adjoint matrix and the elements of $\bar{S}$ in the LEAP code, one will be able to use all the rather complicated data handling that is needed, and already included, in LEAP In particular, the node indexing scheme that is used in LEAP can be used to position the various elements in the A matrix On the other hand, the adjoint equations are linear and can be solved independently of LEAP A relatively straightforward program for solving these equations and calculating the sensitivity coefficients seems desirable at this stage of development

$$
\begin{bmatrix}
7 & 6 & 6 & 6 & 6 & 6 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
7 & 6 & 6 & 6 & 6 & 6 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
7 & 6 & 6 & 6 & 6 & 6 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 6 & 6 & 6 & 6 & 6 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 6 & 6 & 6 & 6 & 6 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 6 & 6 & 6 & 6 & 6 & 6 & 5 & 5 & 5 & 5 & 5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 6 & 6 & 6 & 6 & 6 & 6 & 5 & 5 & 5 & 5 & 5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 6 & 6 & 6 & 6 & 6 & 6 & 5 & 5 & 5 & 5 & 5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 6 & 6 & 6 & 6 & 6 & 6 & 5 & 5 & 5 & 5 & 5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 5 & 5 & 5 & 5 & 5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 5 & 5 & 5 & 5 & 5 & 3 & 3 & 3 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 5 & 5 & 5 & 5 & 5 & 3 & 3 & 3 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 5 & 5 & 5 & 5 & 5 & 3 & 3 & 3 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 3 & 3 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 3 & 3 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 5 & 5 & 5 & 5 & 5 & 0 & 0 & 0 & 0 & 2 & 2 & 2 & 2 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 5 & 5 & 5 & 5 & 5 & 0 & 0 & 0 & 0 & 2 & 2 & 2 & 2 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 5 & 5 & 5 & 5 & 5 & 0 & 0 & 0 & 0 & 2 & 2 & 2 & 2 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 2 & 2 & 2 & 1 & 1 & 1 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 2 & 2 & 2 & 1 & 1 & 1 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 2 & 2 & 2 & 1 & 1 & 1 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 2 & 2 & 2 & 1 & 1 & 1 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1
\end{bmatrix}
\begin{bmatrix}
\phi_2^* \\ \phi_2^* \\ \phi_3^* \\ \phi_4^* \\ \phi_5^* \\ \phi_6^* \\ \phi_7^* \\ \phi_8^* \\ \phi_9^* \\ \phi_{10}^* \\ \phi_{11}^* \\ \phi_{12}^* \\ \phi_{13}^* \\ \phi_{14}^* \\ \phi_{15}^* \\ \phi_{16}^* \\ \phi_{17}^* \\ \phi_{18}^* \\ \phi_{19}^* \\ \phi_{20}^* \\ \phi_{21}^* \\ \phi_{22}^* \\ \phi_{23}^* \\ \phi_{24}^*
\end{bmatrix}
=
\begin{bmatrix}
1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0
\end{bmatrix}
$$

$$A^*\bar{\phi}^* = R_{\bar{\phi}}$$

$$R = Q(6,2)$$

Figure IX-2 Schematic diagram of adjoint equations for Model 82 with N = 2 and a particular choice of the response R

X INPUT DATA FOR MODEL 22C

A Introduction

An effort is underway to study the LEAP input data base in order to determine

1. The definitions and units of the input parameters to enable an audit trail and to aid in interpretation of the output projections

2. The reference sources of the input parameters which are found to be important

3. The categorization of the input parameters into various types,

4. Whether the important parameters are within reasonably established ranges of values

5. Whether the major assumptions made in Model 22C can be tested or assigned reasonable bounds and

6. Whether the particular choice of parameters biased the output projections toward optimism or pessimism

Although this study is not far along it is already obvious that the numerical input data cannot be separated from their usage within the LEAP code for 22C It is therefore useful to categorize these parameters and to isolate those, wherever possible which have no bearing on the output projections * That is many of the input parameters could be labeled "dummy" entries while others are purposely weighted out of the system by some consistent means A few examples will be included in brief outline to show the types of parameters encountered

B Documentation of the Input Data Base for Model 22C

The documentation available for the Model 22C input data exists in various reports "Leap Network and Data Documentation - ARC 78"[1] is now available only in draft form Computerized listings were received by private communication which gave the FORTRAN name the DFI definition (if one exists) the name of the parameter and an indication of the value chosen (see Table X-1) although several input parameters are not included in this list In addition to these computerized listings, this report includes for each of the ten sectors in LEAP (see Figure III-1), one or more pages describing each activity represented in the model network, the function of that particular activity, further information on

*That is, for this particular Model 22C This should not imply that none of these parameters can be varied in later studies

the data sources, and occasional comments which place certain caveats on one or more parameters Unfortunately, however, these descriptions are not complete and most often treat only one or two of the many parameters used to represent that activity in the model The sectors are also shown graphically as network diagrams which are very useful in tracing the input-output flow Immediately preceding the sectoral data several pages have been devoted to descriptions of various parameters which appear as "major assumptions," initial conditions, capital parameters operating parameters, curves for resources, allocation and demand and finally the numerical values of the "global" parameters Some information on the source of the latter occasionally appears

The DFI document[2] includes definitions, units and translation equations for most of the parameters which are input to LEAP A few of the exceptions are described in Reference 1 and/or the associated computer listings but sufficient detail on definitions, units, and translation equations is rarely provided Unfortunately the section on definitions in the DFI document has many inconsistent statements * and the terminology employed is not identical throughout the various sections In addition the DFI definition and/or associated unit may differ for the same parameter which appears in the LEAP input † Rarely do other reference sources employ the same definition, sectors usage and units which are used for LEAP although direct comparison is sometimes possible Nonetheless the increasing importance of the energy-resource projections of long-range models encourages a better understanding of the input data base for LEAP so that it can be more widely disseminated

C Characterization of the Input Data

A very general breakdown of the input data base is attempted by characterizing the parameters as follows

1 Numerical Values (Model 22C)

a Those input data which have no bearing on the output projections

(1) Place holders such as initial product prices which are altered in the iterative process toward a solution,

---

*Although the authors recognize this problem and are interested in making necessary corrections, they have not been able to fit a rewrite into their schedule Of course, some of the errors may be typographical in nature One example is described in the footnote attached to VOAGRT under Table X-1 parameters in Section X D

†See, for example, the footnote attached to ICLIFE under Table X-1 parameters in Section X D

(2) Parameters set equal to zeros or ones which act only as code operating parameters such as Forecasting Perfection (For example, when Forecasting Perfection is set equal to 1 0, as in Model 22C the forecasting perfection block of code is automatically bypassed)

(3) Parameters which are no longer used or not applicable such as Capital Labor Fraction, and

(4) Input data for activities which are no longer implemented * for example solar heating as a separate activity in the residential sector is said in Reference 1 to have been "dropped" from the program, Central Renewables in the utilities sector have been "constrained to predict 0 5 quads in the year 2020," and all explicit conservation activities have been "removed "

b Those input parameters set directly or indirectly on the basis of output from other models

(1) Data chosen so that Model 22C output in the mid term (1995) will track the output of more detailed sectoral models

(2) Data such as GNP growth rate taken from macroeconomic projections and

(3) Resource projections

c Those input parameters taken from historical data on the economy

(1) Data on the energy balance in the initial model year (1975),

(2) Operating and capital costs for facilities of types that already exist and

---

*How this is handled is not always clear since the input/output tables still exist In some cases, the explanation has been found under another activity For example, solar heating has been implemented by raising the efficiency limit on electric heaters from ~ 1 0 to 2 5 to account for heat pump technology and solar penetration in the residential sector

(3) Past trends in financing that are assumed to continue into the future

d Engineering estimates for technologies not yet commercially available

(1) Efficiencies and operating costs expected to be realized in new technologies, and

(2) Capital costs of new facilities based on 1975 costs for labor and materials

e Input parameters which attempt to "capture" economic behavior

(1) Price elasticities of demand, and

(2) Behavioral lags in achieving economic efficiency

Note The prices of imported oil, gas and oil products are input data to LEAP throughout the time frame of the model with no restraints on total quantities This is one of the major assumptions made for Model 22C

2 Sources of the Input Data

Some information on the sources upon which the numerical input data are based can be found in Reference 1 Although published references are rarely available for the behavioral assumptions upon which the long-range projections intimately depend, it is immediately obvious that a great deal of insight, intuitive reasoning, expertise in economic modeling, and knowledge of various technologies were required in order to produce such a complete and intricate input data set for LEAP In fact, few of the parameters are "standalone" choices For this reason, the data base itself is not expected to be frozen for a long time period

D Example of the Input Data for Model 22C

The residential gas heater was chosen as the example to employ because it was commercially available in 1930, thereby making its attributes and operating procedures more familiar to a wider audience An attempt is made here to pull together all the information provided for Model 22C for this example with particular emphasis on the data source documentation, since completion of the work outlined in Section X A intimately depends upon basic knowledge of the origin of each input value

Table X-1 has been taken directly from the computer printout[1] for Sector 1 (Residential) Activity 4 (Gas Heater) (The reference numbers have been added) See Figure III-2, which shows the gas heater as one input to space and water heat which then feeds residential demand The SOURCE AND/OR COMMENT column is further defined in the references but the term GLOBAL perhaps requires further elaboration here GLOBAL parameters are held constant (or nearly constant*) throughout the sectors, the GLOBAL parameters, like others have been generated within the EIA or taken from other reports, sometimes with modifications Therefore the original source for each GLOBAL parameter has been traced and compiled later in this chapter, wherever possible

Note that all inflation rates† and inflators** are assumed to be zero since input and output tables are in constant (1975) dollars (This choice implies at least the assumption that all costs for all activities have the same inflation rate) Gas (aggregated) is supplied to all demand sectors of which residential plays only a small role and gas heaters compete with other water and space heaters (see Figure III-2) which are fueled by oil, electricity and solar In addition gas must be supplied for cooking

To compute the energy flows and prices, allocation and demand parameters are also required in the input tables Those which apply to the production and end use of gas in the Residential Sector are taken from Reference 1 and reproduced in Table X-2 From the input data in Tables X-1 and X-2, it is seen that only the GNP growth rate and demand (or income) elasticities are assumed to vary over the time frame of the model Note the disparity among the parameters representing market shares at equal prices

Although the problems presented by aggregation and disaggregation†† among the data available do not lend themselves to a unique solution

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*The global parameters which are not constant over sectors are the income and property tax rates which are different in the Residential Sector Note that the property tax rate is taken as zero for all activities within the Residential Sector

†RINF1 (Historical Inflation Rate) and RINF2 (Terminal Inflation Rate)

**INFLAT is set equal to 1 0 (a multiplier of the assessed value of a facility which affects property tax)

††This problem is described in detail in Section III and will not be repeated here

TABLE X 1

I p t D t f th G H t i th R d ti I S t

GAS HEATER (HFS)

NODE 102 LOGICAL KIND NO 9 PROCESS 1 1 1

AJOR SSU PTIONS CO VERSIO	I PUT VAL JE(S)	SOURCE AND/OR CO E T
33 FORPER FORECASTING ERFECTION	1 000	GLOBAL[b]
34 RINF1 HISTORICAL INFLATION ATE	0	GLOBAL
35 RINF2 TERMINAL INFLATION RATF	0	GLOBAL
INITIAL CONDITICNS CO VERSION		
30 QUANIY INITIAL PRODJCTIO	010	LTEAC [c]FROM 1975 E ERCY BAL NCE
PRICIY INIT PRLDUCT PRICE	10 00	GLOBAL
31 RATIN HIST CAP ADDITIONS CHANGE RATE	2500E 01	GLOBAL
CAPITAL PA A ETERS CO VE SION		
12 IYR VL YEAR CO ERCI LLY VAIL BLF	1930	DFI[d]
13 EARLY PRE CL KERCI L PRE IUM / YEAR	998 E 01	GLGBAL
5 SCC SPECIFIC CAPITAL CDST	3 35	DERIVED FROM BNL[e]
14 CLI CA ITAL TECH CHANGE I I IT	1 000	IFI
15 CRATE C PITAL I ITIAL Γ E RATE	980E 02	HNL (LT USED)
10 IPLTI PLANNING LEAI TI E	3	DFI
11 CFLDR CAPITAL FACTOR LEAD RATIO	1668	GLOBAL
6 CLFR CA ITAL LABOR FRACTIO	998	GLOB L
29 EQFR EQLITY FI ANCING FRACTIOJ	9980E 01	LTEAL
25 IDLIFE DEBT LIFE	5	LTE C
26 INCTAX INCO E T X RATE	2498	GLOBAL
24 ITXLIF T X DEPRECIATION LIFE	0	B L
28 PTRATE PROPERTY TAX ATE	0	GLOBAL
ROE RETURN CN FCJITY	9980E 01	GLOBAL
RDEBT RETUR CN JE T	980E 01	GLOB L
38 INFLAT ASSESSEL VALUE INFLATOR	1 000	GLOBAL
27 ITCRAT INVESTMENT TA CREDIT RATE	0	GLOBAL
OPERATING ARA ETERS CONVEPSIO		
7 VOC VARIABLE OPERATING COST	6800	DERIVED FRO BNL DATA
9 EFF THERMAL EFFICIENCY	6000	LTEAL ASSU ED SA E AS VERAGE EFFICIENCY
19 EFLI THER AL EFFICIENCY LIMIT	1 380	LTE C DERIVED FRO T E HIRST ODEL[f]
AVEFFI AVEPAGE EFFICIENCY	6000	LTEAC DERIVED FRO T E HIRST ODEL
18 VOCRAT OPERATING INITI L CHANCE TE	7990E 01	LTEAC
16 PRELIM CONSTRUCTION TECH CHA GE LIMIT	1 000	LTE D
17 POSTLM PRODUCTION TECH CH NGE LI IT	1 000	LTEAD
22 ICLIFF CHARALTERISTIC FACILITY LIFE	15	LTEAC
23 VOAGRT FA ILITY AGI G RATE	3 000	GLO L
8 OLFR OPERATING LABOR RACTION	998	CLOBAL
20 AVAIL AVAILABILITY	9000	GLOB L
21 LOADFC LO D FACTOR	1 000	GLOB L
36 CFMULT CAPACITY FACTLR COST ULT	1 000	GLOBAL
37 CFSENS CAP FACTOR PRICE SENSITIVITY	1 340	GLOBAL

Thi t bl p d d itho t dif t f om th p t l t g h h i d
f J h P f th EIA th tl d ft i f R f l i A g t 1979

[b]Th t i ppli d f th p t hi h umed t b t t (ly t t)
ll t iti f ll t th th mod l

L g T E gy A ly i D i Off f I t g ti A ly E gy I f t
Adm i t ti

[d]D i F I (R f 2)

B kh N ti I L b t y (R f 3)

[f]S R f 4

DRAFT

TABLE X 2

I p t D t f All t f th D d f Sp d W t
H t d f R id ti l E d U D d

RESIDENTIAL DEMAND

NODE 145 LOGICAL KIND NO 42 PROCESS 10 1 1 1

DE AND DATA		INPUT VALUE(S)					SOURCE A D/O CO MENT
SENS BEHAVIORAL LAG		8000					(L IH L [b]
ELAS PRICE ELASTICITY		1000					GLOB L
GNP GROWTH RATES	1 THRU 5	0	4 600	3 500	3 000	2 900	
	6 THRU 10	2 400	2 400	2 400	2 400	2 00	
ELASTICITY FOR SERVICE DEMAND 1							LTE D [c]
(SPACE & WATER HEAT)	1 THRU 5	9870	4997	1720	519	2498	
	6 T RU 10	1138	0	0	0	1827	
ELASTICITY FOR SERVICE DEMAND 2							LTEAD
(SPACE COOLING)	1 THRU 5	1 086	1 875	1 517	1 786	1 389	
	6 THRU 10	1 212	0	0	0	1827	
ELASTICITY FOR SERVICE DEMAND 3							LTEAD
(COOKING & OTHER)	1 THRU 5	1 015	1 061	6244	7493	5785	
	6 THRU 10	4304	0	0	0	1827	
ELASTICITY FOR SERVICE DEMAND 4							LTEAD
Q(LIGHTING & APPLIANCES)	1 THRU 5	1 016	1 120	4441	780	6892	
	6 THRU 10	5371	0	0	0	1827	

DEMAND ELASTICITIES ARE SCALED LINEARLY
BETWEEN THE VALUES FOR INDICES 6 AND 10

SPACE & WATER HEAT ALLOCATION (RES)

NODE 143 LOGICAL KIND NO 1 PROCESS 1 1 1 1

ALLOCATION DATA	INPUT VALUE(S)				SOURCE D/OR COM E T
1 SHSENS SHARE PRICE SENSITIVITY	5 000				GLLBAL
2 BELAG BEHAVIORAL LAG	9 000				GLOBAL
3 FREQPR EQUAL PRICE SHARES	365	090	535	010	
FREQPR LABELS	OIL	GAS	ELECTRIC	SOLAR	

COOKING AND OTHER ALLOCATION

NODE 134 LOGICAL KIND NO 1 PROCESS 12 1 1 1

ALLOCATION DATA	INPUT VALUE(S)		SOURCE AND/OR COMMENT
1 SHSENS SHARE PRICE SENSITIVITY	2 500		GLOBAL
2 BELAG BEHAVIORAL LAG	3 000		GLLBAL
3 FREQPR EQUAL PRICE SHARES	9750	2500E 01	LTEAD
FREQPR LABELS	ELECTRIC	GAS	

Th t bl p d d itho t difi ti f th omp t listi gs h h i d
f om J h P f th EIA ith th d ft i f R f 1 i Aug t 1979

[b] Thi t rm i ppli d f th p met hi h med t b t t (e ly t t)
ll ti ti f ll t ithi th mod l

L g T m E gy A ly i D i i Offi f I t g ti A ly i E gy I f t
Admi i t ti

DRAFT

they have been treated by various mechanisms in preparing the input data Some information relating to this important problem has been taken directly from Reference 1

Sector 1 4 GAS HEATER (RESIDENTIAL)

Network I/O Links

The one input link--gas--comes from the gas allocation node (splitting gas between space and water heating and cooking) The output is one of four sources of space and water heat

Function

This node converts gas into space and water heat for the residential sector

Data sources

Operating and capital costs are from BNL Adjustments are made to account for differences in aggregation approaches 1975 average efficiency and efficiency limits were derived from the Hirst residential model 1975 initial quantity was derived from EIA data of total gas demand in the residential sector and Hirst data of shares going to each end-use

Comments [None given]

Model 22C input is described in more detail in the Annual Report to Congress [5] There one finds that the price* elasticity of each end-use demand is assumed to be constant beyond the year 2000 and that this parameter does not affect the solution prior to the year 2000 The population growth rate is one of the major assumptions but is not a direct input to LEAP,[5] it is stated to be used in determining the input demand† elasticities

The sources for the various parameters listed in Tables X-1 and X-2 will now be followed in more detail beginning with the input data of Table X-1 For those parameters with GLOBAL listed as the source, whatever additional comments are provided in Reference 1 for that particular parameter have been added For Table X-2 parameters, comments concerning particular parameters are appended for each activity

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*See ELAS under Table X-2 parameters later in this section

†The demand elasticity is defined in Reference 1 as the rate of change in energy service demand with respect to the rate of change in GNP

1 Table X-1 Parameters

FORPER (Forecasting perfection) Source GLOBAL (Basic assumption 1 0 means perfect forecast)

RINF1 (Historical inflation rate) Source GLOBAL (set equal to 0 0)

RINF2 (Terminal inflation rate) Source GLOBAL (set equal to 0 0)

QUAN1Y (Initial production) Source LTEAD allocation of the amount of gas used for heating in the residential sector based on total energy balance in the year 1975

PRIC1Y (Initial product price) Source GLOBAL, a place holder or dummy entry

RATIN (Capital additions change rate) Source GLOBAL, "this value is calculated within the model "

IYRAVL (Year commercially available) Source DFI

EARLY (Pre-commercial premium/year) Source GLOBAL "assigned by LTEAD "

SCC (Specific capital cost) Source "derived from BNL "

CLIM (Capital Technological Change Limit) Source DFI (set equal to 1 0) From the DFI definition this means that there is no change in ultimate cost compared to the cost when a representative facility became commercially available

CRATE (Capital initial change rate) Source "BNL (not used) " (The numerical value listed with BNL as the source is 0 9800E-02)

IPLTIM (Planning lead time) Source DFI

CFLDR (Capital factor lead ratio) Source GLOBAL (taken from EPRI[6])

CLFR (Capital labor fraction) Source GLOBAL (determined by LTEAD and from the EPRI report[6]) It should be noted, however, that with PLI and PMI set equal to 1 0, this parameter does not affect the output

EQFR (Equity financing fraction) Source LTEAD

IDLIFE (Debt life) Source LTEAD

INCTAX (Income tax rate) Source GLOBAL (taken from EPRI[6])

ITXLIF (Tax depreciation life) Source BNL[3] (set equal to zero)

PTRATE (Property tax rate) Source GLOBAL (set equal to zero without further qualification)

ROE (Return on equity) Source GLOBAL "Set by the Long-Range Division to approximately 7% after tax return with no inflation when combined with RDEBT "

RDEBT (Return on debt) Source See ROE (above)

INFLAT (Assessed value inflator) Source GLOBAL (assumed no inflation since all forecasts are in constant dollars)

ITCRAT (Investment tax credit rate) Source GLOBAL (taken from EPRI[6]), (set equal to 0 0)

VOC (Variable operating cost) Source Derived from BNL data

EFF (Thermal efficiency) Source LTEAD assumed same as average efficiency

EFLIM (Thermal efficiency limit) Source LTEAD derived from HIRST model [4]

AVEFFI (Average efficiency) Source Same as EFLIM (above)

VOCRAT (Operating initial change rate) Source LTEAD

PRELIM (Construction technological change limit) Source LTEAD (set equal to 1 0)

POSTLM (Production technological change rate) Source LTEAD (set equal to 1 0)

ICLIFE (Characteristic facility life)* Source LTEAD

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*This definition is one of many which is confusing in Reference 2, DFI indicates that the characteristic facility age (ACHGAR) is the input parameter and gives different definitions for the two parameters

VOAGRT (Facility aging rate)* Source GLOBAL (with comment that the source is Decision Focus Incorporated in contract model)

OLFR (Operating labor fraction) Source GLOBAL (taken from EPRI[6])

AVAIL (Availability) Source GLOBAL (taken from EPRI[6])

LOADFC (Load factor) Source GLOBAL (Model definition) (set equal to 1 0)

CFMULT (Capacity factor cost multiplier) Source GLOBAL (DFI in contract model) (set equal to 1 0)

CFSENS (Capacity factor price sensitivity) Source GLOBAL (DFI in contract model)

2 Table X-2 Parameters

SENS (Behavioral lag) Source GLOBAL Although this parameter has the same name in allocation and demand it is defined differently and is therefore assigned different FORTRAN names The input was prepared by LTEAD and the Conservation and Renewable Resource Division of the EIA

ELAS (Price elasticity) The source is the same as for SENS (above) It should be noted that the "quoted" price elasticity given in Chapter 5 of the Annual Report To Congress[5] is the long-term price elasticity The input for LEAP is the short-term elasticity and the long-term elasticity (beyond the year 2000) is calculated from

$$ELAS_{long\text{-}term} = ELAS_{short\text{-}term}/(1\text{-}SENS) = -0\ 5$$

for all activities in all sectors As mentioned earlier this parameter has no effect on the output for the years prior to 2000

GNP growth rates Source GLOBAL (this is a major assumption in Model 22C) the numbers 1 thru 5 and 6 thru 10 denote the years in 5-year bins beginning with 1975

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*A rate is usually defined as a fraction with respect to another variable, usually time The DFI definition reads "fractional increase per unit of output per year," but gives the units as dimensionless A 3 0 is somewhat difficult to interpret for the numerical value of a dimensionless fraction

Demand Elasticity Source LTEAD The following comments are taken from Reference 1

> This node computes demand for each of the four residential services based upon an assumed growth rate for each service and upon the price of the services computed by the model Elasticities for service demand for the period 1975 to 2000 were derived from service demand growth rates and GNP growth rates from the Hirst residential model The 2020 value was based on the assumption that the elasticities for residential service demands would approach the ratio of population growth rate to GNP growth rate These values were scaled linearly from 2000 to 2020 interval internally by the model

Note that the demand elasticity is called the income elasticity in the Annual Report To Congress [5] The values in Table X-2 are discussed in more detail in that report than given above

SHSENS (Share price sensitivity) Source GLOBAL This is evidently mislabeled since it is not constant over the residential sector and does not appear in the list of GLOBAL parameters in Reference 1

BELAG (Behavioral lag) See SHSENS (above) and FREQPR (below)

FREQPR (Equal price shares)

Activity 1 (Space and water heat allocation) No source given, but the author assumes it was generated by LTEAD consistent with the following comments in Reference 1

> This node chooses among oil- gas- electric- and solar-generated heat to satisfy total demand for residential space heat and water heat In general it chooses some of each source based on relative prices, previous shares, and source preference at equal prices 1975 shares are derived from the Hirst model of residential fuel use Equal price shares and behavioral lag are adjusted to calibrate 1995 forecasted shares against the Hirst 1995 forecast Penetration of solar heat is not adequately accounted for due to lack of data

Activity 12 (Cooking and other allocation) Source LTEAD with the following comments taken directly from Reference 1 (note that equal price shares differ by a factor of 40 between electric and gas sources)

> 1975 shares are derived from the Hirst model of residential end use Fuel shares at equal prices are adjusted to calibrate 1995 forecasted shares against the Hirst 1995 forecast
> Through the fuel shares at equal prices, this node is heavily biased towards electricity despite the higher cost of electric services This is due to the anticipated growth of services for which gas cannot be used

E Discussion of Input Data from Tables X-1 and X-2

1 Table X-1

Although sensitivity tests have not been completed, the Residential Sector is known to demand only a small fraction of the total energy supply It is interesting however to further elaborate on some of these input parameters due to their overall commonality of usage in Model 22C For example, a major consideration given for the decrease in residential end-use demand by 2020 is the significant increases expected in efficiencies due to technological improvements with time The gas heater thermal efficiency limit of 1 38 was derived using the HIRST model,[4] as was the average efficiency The thermal efficiency was assumed to be equal to the average that is 0 60 Within the LEAP code the gas heater efficiency would be 0 60 in 1975 and would rise to ~0 83* by the year 2020 The BNL[3] and SRI[6] efficiencies for 1975 for gas heating in the Residential/Commercial Space Heating Sector are given as 0 65 and 0 49 respectively

According to a recent survey carried out by D L O'Neal on residential heating systems,[7] it is possible to improve the efficiencies of gas heating systems in various ways although major improvements require significant increases in initial specific capital and operating costs For example a "gas organic fluid absorption heat pump"[†] is projected to save 45% in energy at an 80% specific capital cost increase The 80% cost factor was obtained after a reduction had been applied for the air conditioning option of a heat pump over conventional gas furnaces This 45% in energy savings approximates the LEAP input assumptions [ξ]

According to this report [7] the advanced design Stirling/Rankine heat pump which is expected to come on line by 1985 is the best option on the horizon which would be expected to reach seasonal performance factors** much greater than one [††] Price estimates for the latter system have not yet been located

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*It is interesting to note that 83% is very close to the theoretical upper limit[7] of the steady state efficiency of a conventional gas system

[†]Expected to be marketed in 1981

[ξ]Of course, various modifications in the gas furnace design such as installation of electronic ignition etc , can improve efficiency without complete replacement of the unit, but retrofitting is not an option in the model

**Defined as (Total annual heat energy provided)/(Total annual fuel energy used)

[††]Assuming various energy conservation options described in Reference 7

The important point in this exercise is to note that both capital and operating costs are expected to rise significantly for these advanced systems as they come on line Whether these costs can be reduced with improved technology over time is not clear Although increased efficiency, that is, less energy consumption for the same Btu output is the best option in any case especially for new installations LEAP may not track increased capital and operating costs due to changing technologies (and improved efficiencies) over the time frame of the model While an average efficiency of 0 828 over all gas heaters in the Residential Sector by the year 2020 is not unrealistic it does imply a reduction in energy usage from technological improvements by almost 40% which represents a noteworthy breakthrough

Most of the important parameters in Table X-1 require further documentation than has so far been provided It is notable however that many of the input values for Model 22C presently act as placeholders only and do not affect the output projections

2 Table X-2 Input Data

Except for information on Share Price Sensitivity and Behavioral Lag (SENS and BELAG) the allocation and demand parameters are well described in References 1 and 5 Since the input parameters for Table X-2 are behavioral in character however, they must be associated with the appropriate algorithms for basic understanding This work is now underway and will not be described here

F Summary

Work underway to study the input data base for Model 22C is described A simple example was chosen in order to represent the magnitude of the effort involved in this study due to incomplete documentation available Upon completion of the sensitivity studies the important parameters for the LEAP system will be isolated audited wherever possible, and bounds or limits attached A search for other sources of information which describe the parameters found important in Model 22C will be undertaken

REFERENCES FOR SECTION X

1 Roger Diedrich, Colleen Cornett and John Pearson "LEAP Network and Data Documentation-ARC 78 " draft (September 1979) The August 1979 draft of the same report was accompanied by the computerized tables mentioned herein

2 R J Adler et al The DFI Energy-Economy Modeling System, Final Report, Decision Focus Inc , Palo Alto California (December 1978)

3 N Bhagat et al "Evaluation of Technological Data in the DFI and PIES Models " BNL-50949 Brookhaven National Laboratory (April 1979)

4 Hirst Model -- Structural Residential Energy Use Model, Oak Ridge National Laboratory, Oak Ridge, Tennessee

5 J Pearson et al , "Long-Term Energy Supply and Demand " Chapter 5 of the Annual Report To Congress 1978 DOE/EIA-0173/3 (May 1979) (see also the Appendix to that volume)

6 (SRI International), Fuel and Energy Price Forecasts Vol 1 Quantities and Long Term Marginal Prices, EPRI EA-433, Electric Power Research Institute report, (September 1977) Vol 2 Data Base (February 1977)

7 D L O'Neal, Energy and Cost Analysis of Residential Heating Systems ORNL/CON-25 (July 1978)

APPENDIX A
ORNL OPERATING EXPERIENCE WITH LEAP

To support the Model Validation Project personnel at the Oak Ridge National Laboratory (ORNL) execute LEAP (Long-Term Energy Analysis Program) on the Energy Information Administration's (EIA's) computer facility In this appendix the ORNL operating experiences with remotely executing LEAP on the EIA facility with specific LEAP energy-economy models and with auxiliary codes developed for sensitivity analysis, are described Experiences with LEAP are described from the perspective of a first-time user of the system

1 Getting Started

The Decision Focus, Inc (DFI) energy-economy modeling system and the DFI computer modeling software are described in References 1 and 2 respectively The LEAP system, which consists of the LEAP computer code, a data transfer system a data base storage system and a data editing and display system was developed by DFI and EIA within the context of the DFI energy-economy modeling system The EIA's Long Term Energy Analysis Division (LTEAD) had approximately one year of operating experience with the LEAP system at the time the Model Validation Project began (January 1979) Although the LEAP code and models were still being developed, LTEAD made the LEAP system and the data base for energy-economy Models 22C and 88 available to ORNL on the EIA computer facility in March 1979 The LEAP program and Model 22C were subsequently "frozen" by LTEAD in May 1979 Data sets that comprise the DOE/EIA LEAP system (i e , the LEAP source deck, the LEAP load module, the data base for the various energy-economy models etc) are maintained by LTEAD on on-line disks at the EIA facility The EIA data sets that have been used by ORNL during the course of the project are identified in Table A-1 Note that comments relating to experience with the various data sets are included in the table

The LEAP data base is accessed by the LEAP code via a commercial data base management system--System 2000 (S2K) S2K is leased by DOE/EIA and is provided as a software package on the EIA computer facility

Optimum Systems, Inc operates the EIA computer facility exclusively for EIA Through January 1980 the facility was located at Rockville Maryland The Rockville facility consisted of two IBM 370/168 central processing units (CPUs) connected in multiprocessor mode[3] Verbal authorization for an ORNL-EIA Rockville Computing Facility link for ORNL model validation computing requirements was granted by the Manager of Data Communications, DOE Office of ADP Services, Washington, D C The initial authorization granted in March 1979, was for 1 5 h of interaction time during normal working hours In response to an ORNL request in November 1979, ADP Services authorized an increase in the ORNL-Rockville interaction time to 4+ h/day

TABLE A 1

DOE/EIA Data Sets Used in the ORNL Model Validation Project

Data Set	Date Received	Recommended by	Copied from EIA DSNAME	Experience
88[a]	3/10/79	R Heilbron	CN6424 PRJ LEAP MODEL88 STRING DATA	Would not converge C Cornett indicated the model was out of date
88[a]	4/10/79	S Cohen	CN6132 SC2 CC2 M88 DATA	Would not set up
88[a]	4/16/79	C Cornett	CN6132 CC2 MODSTR M88 SUSAN DATA	Initially would not set up Title changed from 21 to 24 characters converged 4/25/79
22C[a]	5/5/79	S Cohen	Transferred by S Cohen	Converged 6/11/79
22C[a]	5/24/79	C Cornett	CN6132 JP3 STRING DATA	Frozen input tables obtained case converged 6/21/79
LEAP Source	3/10/79 4/11/79	R Heilbron S Cohen	CN6424 PRJ LEAP FORTRAN CN6132 PRJ LEAP FORT	Not complete subroutines missing Pearson informed ORNL that source was out of date 4/18/79
	5/7/79	S Cohen	Transferred by S Cohen	Source complete but did not correspond to 4/11/79 load module
	6/7/79	S Cohen	Transferred by S Cohen	Frozen source and derived load module transferred together
LEAP Load Module	4/11/79	S Cohen	CN6132 PRJ LEAP V2 LOAD	Have been executing from this load module with no problems
	6/7/79	S Cohen	Transferred by S Cohen	Transferred to ORNL with LEAP source (it works!) source corresponds to load module
S2K Utility Package	3/12/79	S Cohen		Have used the following functions LOAD S DELETE LOAD L SHOW UNLOAD RELOAD
LEAP CLIST	3/10/79	R Heilbron		Documented in memo from S Cohen 10/23/78 Document Draft of Pearson memo on executing LEAP interactively 1/24/79 S Cohen is working on updating the documentation (first draft received 6/26/79 second draft received 10/26/79)[b]
EXEC CLIST	3/12/79	S Cohen		Have been able to make changes to the data base display tables etc interactively and in batch mode

[a]Model string file

[b]Refers to Reference 4 of Appendix A

During December 1979, EIA installed two IBM 3033 computers and associated hardware and software in the Forrestal Building in Washington D C The EIA Washington facility is expected to become operational during the first part of February 1980 At that time EIA is expected to move the project data base, programs, etc , from Rockville to Washington

Project personnel adhere to the EIA computer system security and privacy policy as stated in Section 7 of the ODS Standards and Procedures Manual Each user of the EIA computing system has a user ID and a keyword which must be used with each computing job To enhance the security system the DOE Office of ADP Services changes the keywords periodically In addition the EIA utilizes software to provide computer users with enhanced security for their data--the ACF2 Access Control Facility

ORNL's Engineering Physics Division (EPD) has two DATA 100 Model 78 RJE terminals which are used to support the DOE/EIA project and other EPD projects Both DATA 100 terminals have existing software to emulate a HASP work station as required by the EIA computer facility As depicted in Figure A-1 the DATA 100 terminals and ORNL remote "desk" terminals are linked to the EIA facility via commercial or FTS phone lines Using the ORNL-EIA link LEAP is executed in both batch processing and interaction modes (For continuing support of the project a communication controller a medium-speed line printer and additional desk terminals are being acquired)

In anticipation of the relocation of the EIA computer facility approval was requested in November 1979 for use of General Services Administration (GSA) data transmission service (i e Telpak or Tymnet service) between ORNL and the EIA Washington facility The request for the GSA service noted that ORNL project personnel interact with the EIA facility an average of 4 h/day via two remote terminals and 2 5 h/day via an RJE terminal By March 1980 the project computer needs were expected to increase to 5 h/day via remote terminals and 4 h/day via an RJE terminal The computing needs are expected to continue to increase through 1981 (Until the GSA service becomes available the project will continue to use FTS service for data transmission)

An ORNL operational staff to support the model validation project was assembled during January and February 1979 Additional personnel have been added to the staff as computing needs have increased Personnel with extensive experience in computer applications are selected to execute LEAP

LEAP is executed via batch mode or interactively through a combination of IBM Time Sharing Option (TSO) and SUPERWYLBUR--Program Language Interfaces In the early phases of the project selected project personnel attended the "Introduction to SUPERWYLBUR" and "SUPERWYLBUR Text Editing" courses which were taught by Optimum Systems Inc in Washington D C Having extensively used ORNL in-house IBM computing equipment project personnel had no problem with the mechanics of executing on the EIA IBM computers

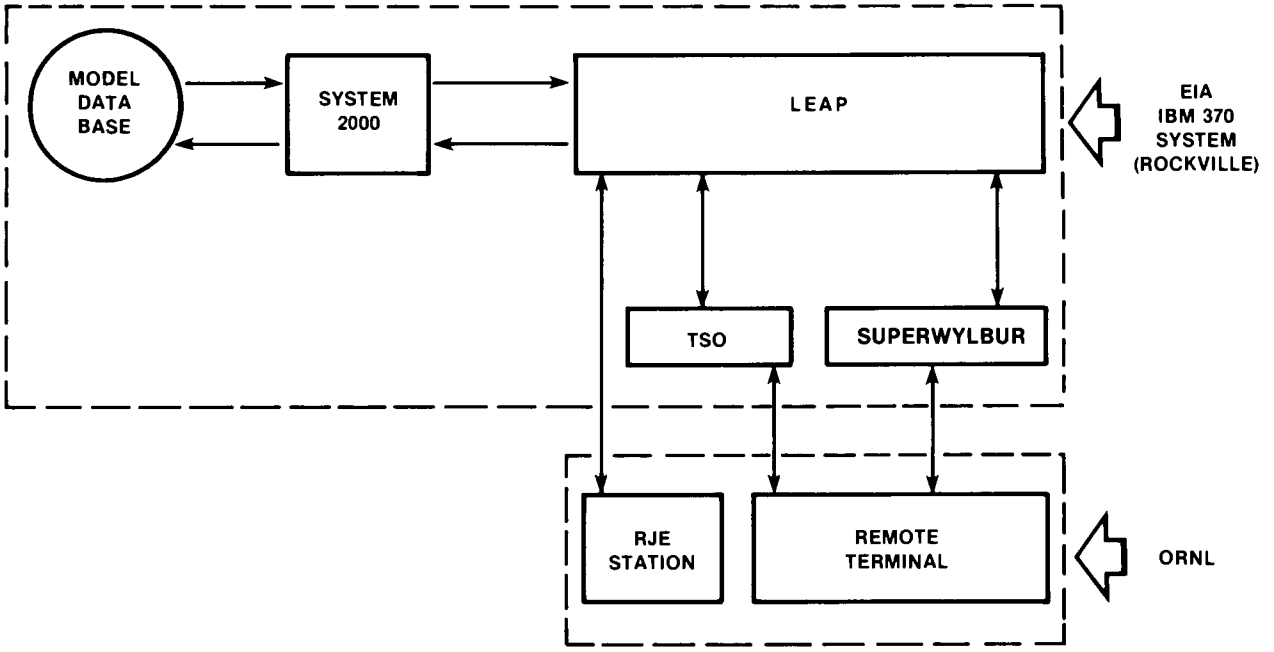


Figure A-1 ORNL/EIA communication link for model validation program

As with most major code systems the process of acquiring the necessary operational familiarity with the LEAP system represented a formidable challenge to project personnel In the early phases of the Model Validation Project the only LEAP "documentation" was the DFI reports describing the energy-economy modeling system and the computer modeling software (References 1 and 2, respectively) Although LEAP was developed within the context of the DFI system, the DFI documents did not describe the specific generic models that were linked together to form the hierarchical energy-economy networks for Models 22C and 88 nor did they describe how a user controls the LEAP simulation system during the solution and reporting processes Also the DFI documents did not identify where many of the equations inherent in the generic process models were programmed in the LEAP source subprogram Likewise, there was incomplete documentation of the FORTRAN names that represented the parameters in the equations or the labeled commons used to pass parameters between subprograms To add to the challenge, the LEAP code and the data bases for Models 22C and 88 were still being modified by EIA during the early phases of the ORNL project

Throughout the model validation project, the personnel of EIA's Long-Term Energy Analysis Division--J D Pearson, Director and his staff, S Cohen C Cornett M Hutzler and S Shaw--have provided invaluable assistance to ORNL personnel They have unselfishly shared their LEAP source decks, load modules, and data bases responded to innumerable questions, provided draft copies of evolving EIA LEAP documents, and provided "CLISTs"* for the LEAP system A draft copy of Cohen and Pearson's users manual,[4] which explains how to execute LEAP, if given a predefined energy-economy model generated by the S2K data basing system, has proved to be an invaluable guide to project operating personnel (As noted in the abstract of Reference 4, the report is intended for users who understand the LEAP methodology and the EIA computer facility, it is not intended as a LEAP primer)

2 LEAP--A Thumbnail Sketch from the Operator's Perspective

To describe the ORNL operating experience with LEAP and the auxiliary codes developed for the model validation project, we must define LEAP terminology by presenting a "thumbnail sketch" of the mechanics of executing LEAP Material for this section was taken from References 1, 2, and 4

LEAP comprises a set of generic models linked together in such a manner that an energy-economy network is formed The data transfer system acts as an interface between the code's logic and the data base storage system The storage system stores data in a hierarchical fashion in an attempt to provide flexibility with respect to model changes The data editing and display system (the EXECUTIVE) provides a

---

*A CLIST is a sequence of TSO commands in an executable format CLISTs are a convenient method for executing a series of frequently used TSO commands

link between the user and the LEAP system Complete editing of both input and output data files is possible through execution of the EXECUTIVE utility program Familiarity with the LEAP methodology and the data base management system (S2K) is necessary to effectively execute the LEAP load module

A model can be executed in either batch mode or interactive mode using TSO Data files required for batch or interactive execution of LEAP are the same The commands to specify the LEAP solution strategy the diagnostics to be generated during problem execution, and the required results--commands defined in Reference 4--can be used in both modes of executing LEAP

Input data for an energy-economy model is passed to the LEAP load module as a string file The network structure of the model input parameters and initial guesses of model results are contained in the string file A string file is created from the data base by "unloading" a model with the S2KUTIL CLIST (The CLIST was provided by S Cohen) The model can then be executed with the LEAP load module In general, one would READ the string file SETUP the problem SOLVE the problem and WRITE the resulting string file (Note that the solutions to a LEAP problem are placed in a string file) The resulting string file can then be "loaded" into the data base

Input parameters network structure, and model results can be displayed in tables by using the S2K EXECUTIVE The EXECUTIVE which is written in Programming Language Interface (PLI) produces two-dimensional "slices" of the data base in an easily interpretable format The EXECUTIVE can be executed interactively or in batch mode

Other methods used to obtain an edit of input parameters and model results are the REPORT and PERUSE functions and the data/report sub-commands of the SOLVE function The data/report subcommands of the SOLVE function and the REPORT function are used in batch mode The PERUSE function allows displaying of parameters in batch or interactive mode PERUSE can also be used to display model results at selected output links

Changes to parameters or network structure of a model can be made by using the EXECUTIVE Changes to parameters can also be made by using the PERUSE function If the EXECUTIVE is being used to invoke changes a new string file must subsequently be created and the problem must be set up and solved

PERUSE is most useful for temporary modifications to parameters The function is used during the execution phase of LEAP and does not require the a priori steps of interacting with the data base and creating a new string file However, some changes (i e network structure) cannot be made with PERUSE Not all changes can be made with either the EXECUTIVE or PERUSE If a change in the dimensional structure of the model is desired (e g changing a particular parameter from a specific to a generic process) then the LEAP source load modules and data base must all be modified

3 ORNL Operating Experience With Various Models

As described in Section IV Model 82 is simply Model 88 with more representative data from Model 22C used as input The actual process of changing the Model 88 parameters was performed by using the LEAP-EMS simulation system and the DFI Computer Modeling Software (CMS) system Use of different systems to prepare a model illustrates the versatility needed by LEAP operators The LEAP-EMS system edits string files with more ease and convenience than does the CMS system The cumbersome CMS system was used to change integer parameters in the data base because the LEAP-EMS system lacks such capability

After establishing a communication link for data transmission with the EIA facility--which sometimes must be done many times a day each time requiring from 1 to 45 min to establish the necessary phone line connections--Model 82 is executed in batch mode with the job input listed in Figure A-2 The example in the figure shows the execution of Model 82 on the EIA Rockville facility starting with an S2K string file on Logical Unit 2

Subsequent executions of Model 82 could begin from the saved file on Logical Unit 3 by using the command RESTORE, which restores the problem already set up from the point where it was saved For example if the solution was saved after the 25th iteration then RESTORE would restore the model in the condition it was in at the completion of Iteration 25 A subsequent SOLVE would be starting the 26th iteration

The execution time for the job shown in Figure A-2 was about 1 min 20 s (CPU) This time depends on the number of iterations and the computing system load at the time of execution

The JCL and input instructions shown in Figure A-2 could be used to execute Model 22C with a Model 22C string file on Logical Unit 2 and the appropriate data sets on Logical Units 3 and 4 Execution time for Model 22C depends largely on the number of iterations To simply restore a converged solution and perform one additional iteration to get a data/report requires about 1 min 30 s (CPU) However, if the solution is not converged, the CPU time required will depend on the number of iterations necessary to attain convergence (which could require multiple job submissions and user interaction) Model 22C runs through 10 iterations require about 10 min (CPU) A rough rule of thumb for estimating maximum CPU time for execution of Model 22C is 45 to 60 s per iteration and 2 min for a READ

To make changes to the data base and subsequently execute a model requires significantly more effort First one must interact with the EXECUTIVE system as described in Reference 2 Next an S2K string file is created by performing an S2K "unload " This is the string file that is subsequently "read" from Logical Unit 2 (Figure A-2)

As an example, the following steps would be required to change the initial resource cost for domestic oil in Model 82 and to execute the problem Initial resource cost for domestic oil appears in Model 82,

```
//QH5UMM82 JOB (6424 DO 1 50) 'LEAP-FROGS' TIME=(2 30)
/*ROUTE PRINT REMOTE30 <-----------------------------------------------a
//SOLVE EXEC PGM=EXEC REGION=2000K TIME=60 <----------------------------b
//STEPLIB DD DSN=CN6424 QH5 LEAP V2 LOAD DISP=SHR <---------------------c
//FT02F001 DD DSN=CN6424 QH5 LEAP MODEL82 STRING DATA DISP=SHR <---------d
//FT04F001 DD DSN=CN6424 QH5 LEAP MODELOT DATA DISP-( CATLG)
// SPACE=(TRK,(100,10)),UNIT=DASD,DCB=(RECPM=FB,LRECL=80,BLKSIZE=1600) <-e
//FT03F001 DD DSN=CN6424 QH5 LEAP SAVED MODEL82 DATA DISP=OLD
// SPACE=(TRK (420 70)) UNIT=DASK=(RECFM=VS BLKSIZE=3200) <--------------f
//FT06F001 DD SYSOUT=A
//FT05F001 DD *
READ                        */ READ SYSTEM 2K STRING FILE FROM FT02F001 --g
SETUP NETWORK ORDER         */ SETS THE PROBLEM UP FOR SOLUTION
SOLVE LOOP=25               */ EXECUTE 25 ITERATIONS OR UNTIL CONVERGENCE
SAVE                        */ SAVES A BINARY STRING FILE ON FT03F001
SOLVE LOOP=1 DATA REPORT    */ ONE MORE ITERATION TO PRINT FINAL RESULTS
END
/*
```

NOTES

a REMOTE 30 is the ORNL RJE station

b EXEC is the member name for the LEAP load module in the partitioned data set (PDS) with the data set name CN6424 QH5 LEAP V2 LOAD

c Cataloged LEAP load module

d String file created by an S2K "UNLOAD" used to pass data from the data base to the LEAP code

e An S2K string file created by LEAP with the command WRITE this string file contains all model results as well as input data and can be "LOADED" into the data base

f A binary S2K string file created by LEAP this file is used for restarting if necessary

g The */ introduces a LEAP comment all information following the */ is ignored by the code

h Job input to execute on the EIA Rockville computing facility

Figure A-2 Input deck for batch mode execution of Model 82 [h]

table 5/3/, row 2 element 8 To change the value in the data base from the present 1 6 to 4 0, one would execute the EXECUTIVE This step could be done in batch mode or interactively with Cohen's EXECUTIVE CLIST the commands are the same, regardless of mode At ORNL, changes of this nature are generally made interactively The necessary commands are shown in Figure A-3 and table 5/3/ is shown in Figure A-4 The interaction time (wall clock) for making this change is about 20 to 30 min, however the RTAB command which returns the changed table to the data base, depends greatly on computing system load and has taken as long as 45 min

The next step is to create an S2K string file by using Cohen's S2KUTIL CLIST After the CLIST is executed, the command UNLOAD is given The user is then prompted for all other necessary information (e g , data set names) Time for UNLOADing a string file varies from about 15 min to 1 h, depending on computing system load and size of the model being unloaded

The model is then executed in batch mode by using JCL commands as shown in Figure A-2 Due to the computing region requirements for executing a LEAP model (approximately 2,000 000 bytes) and the computing time required to execute a typical case (generally greater than 2 min CPU), the EIA computing system places a LEAP job in a "job class," which usually results in the job being executed after normal working hours An average LEAP job turn-around of 20 to 24 h is the result of (1) the time required to access the EIA computing facility via FTS phone lines (2) the time required to prepare the data and submit a LEAP job (3) the "job class" limitation and (4) the limited project access to inhouse RJE equipment to retrieve the job printout

4 Code Development to Support Sensitivity Analysis by Screening Design

The LEAP source and load modules have been modified, and auxiliary codes have been developed to support sensitivity analysis The modifications to LEAP were in the PERUSE subroutine Programs CREST and FLOSS were developed for the statistical application of linear response surface methodology to determine sensitivities of LEAP input parameters to calculated prices and quantities

The PERUSE function allows the user to display and change model input parameters and to display model results without interacting with the data base management system An additional command was added to PERUSE which allows the user to write input parameters and model results to an external logical file in card images The addition of this command effectively allows access of model results by independent programs

As shown in Figures A-5 and A-6, the process for calculating sensitivities is a two-step procedure In the first step, CREST (Calculation of Random Numbers for Economic Sensitivities Testing Program) is executed N times, with each run varying selected model parameters randomly by ±X% (X is defined by the user) The "A" and "R" matrices for each run are written onto different logical files The "A"

```
EXEC EXEC CLIST
GMOD,82
GTAB,5/3/
C,E,2,8,4 00 <--------a
RTAB         <--------b
END
```

NOTES

a Change the element in row 2, column 8, to 4 0
b Return the table to the data base

Figure A-3 Sample LEAP commands to change a parameter in Model 82 table 5/3/

SPECIFIC PROCESS DATA

ATTRIBUTE

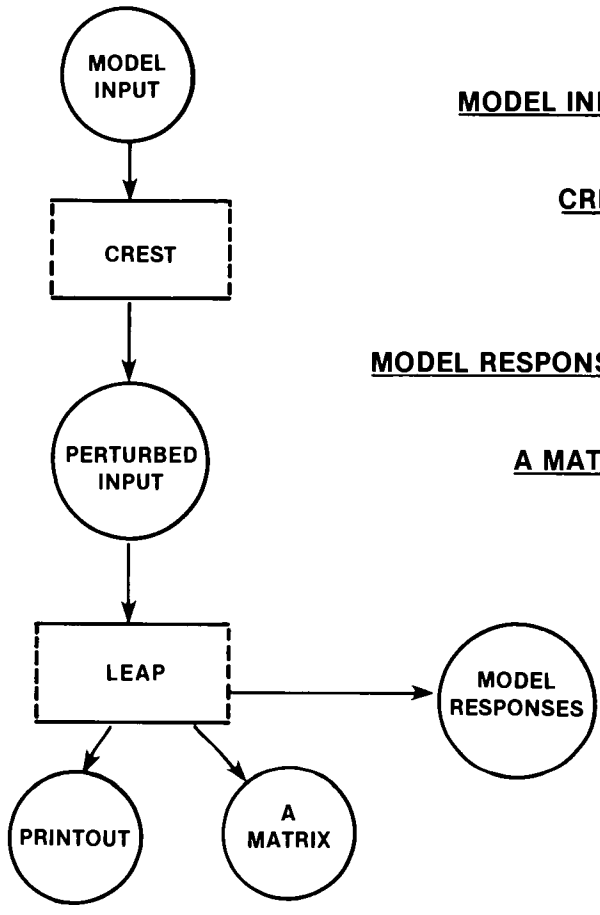
GP	Supply	PLANNING LEAD TIME	YEAR COMM AVAIL	CAPITAL TECH CH LIMIT	CHAR FACILITY LIFE	TAX LIFE	DEBT LIFE	EQUITY FINANCE FRACTION	INITIAL RESOURCE COST	BASE PRICE
Specific Process		1	2	3	4	5	6	7	8	9
Oil Supply 1	1	1	1975	1 0000	30	10	20	0 6500	1 2000	2 1699
Oil Supply 2	2	1	1930	1 0000	30	10	20	0 6500	1 6000	

ATTRIBUTE

GP	Supply	UNDISC RECOV AT BASE PRC	NEW RES AT TWICE BASE PRC	CAPITAL COST FRACTION	DEPOSIT DECLINE RATE	HALF DEP COST MULT	FULL DEP COST MULT	REGULA TORY POLICY	FINAL/ INITIAL COST
Specific Process		10	11	12	13	14	15	16	17
Oil Supply	1	121 0000	186 2000	0 8000	0 0998	1 0000	1 0000	0	2 1600
Oil Supply	2	308 0000	473 0000	0 8000	0 1338	1 0000	1 0000	0	1 8793

Table 5/3/ (Specific Process Data)
Model 82 <1401 10/22/79> Prod to Access 2 0 1 3 0 0 0 0 0 0 0

Figure A-4 Model 82 table 5/3/



MODEL INPUT — MODEL IS SET UP WITH PARAMETERS TO BE VARIED

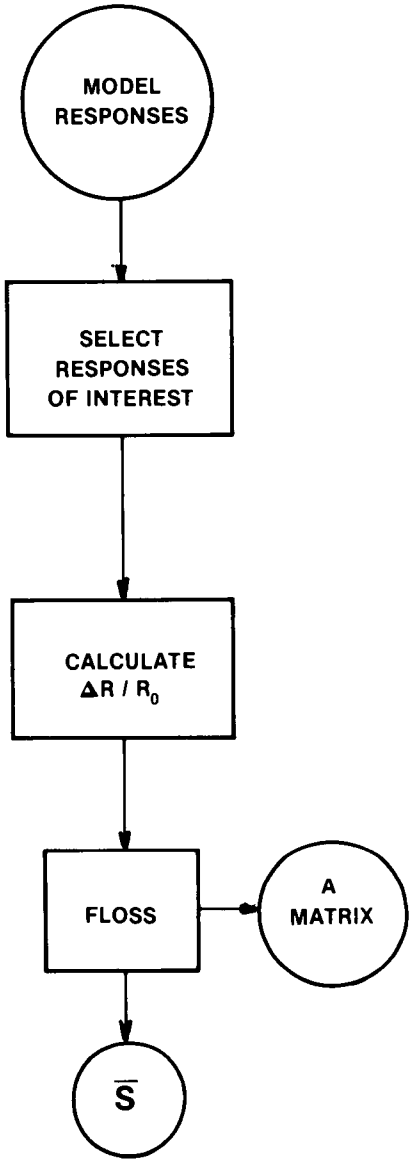
CREST — READS THE INPUT FILE AND PERTURBS THE CHOSEN PARAMETER BY ±X% (X IS DEFINED BY THE USER)

MODEL RESPONSES — PRICES AND QUANTITIES AT EACH NODE

A MATRIX — EACH ELEMENT IS ±1 INDICATING WHETHER THE CORRESPONDING PARAMETER WAS PERTURBED UP OR DOWN

CREST CALCULATION OF RANDOM NUMBERS FOR ECONOMIC SENSITIVITIES TESTING PROGRAM

Figure A-5 CREST--a code to perturb input parameters to LEAP



MODEL RESPONSES FROM N RUNS OF CREST LEAP

FLOSS SOLVES THE EQUATION

$$\bar{S} \cong A^T (AA^T)^{-1} R$$

Figure A-6 FLOSS--a code to calculate relative sensitivities

matrix consists of M ±1's, where M is the number of parameters being perturbed The random sequence of ±1's specifies the pattern used to perturb the parameters for each run The "R" vector is prices and quantities calculated by LEAP

In the second step, FLOSS (Fluctuated Leap Output Sensitivity Matrix Solver) sifts through the "R" vector to find the responses of interest selected by the user The fractional change in response ($\Delta R/R_0$) is calculated by the code FLOSS then calculates the sensitivities S for the N runs, M parameters, and the selected responses by means of the equation

$$S \cong A^T(AA^T)^{-1}R \qquad \text{(A 1)}$$

FLOSS then ranks the sensitivities by absolute value and lists the ranked sensitivities and standard deviations in an easily interpretable format

5 Getting Started - Again

Project operating personnel are frequently asked the following questions

1 How long would it take an individual to learn how to modify a LEAP data base and execute a model at ORNL?

If the individual is guided through the learning process by trained personnel, a conservative estimate of the time required to learn the LEAP system and to execute a model "independently" is 2 months This estimate assumes initial familiarity with IBM operating systems and time-sharing terminals but no familiarity with LEAP methodology

2 How much time would be required to develop and implement an energy-economy model?

There are several levels of model building Modifying the network structure or adding processes or sectors in an existing model is a much simpler task than creating a model initially Starting with a LEAP model a modeler familiar with LEAP methodology and DFI documentation could create and implement a changed model in 2 to 4 man-months, however, time greatly depends on the changes required and the complexity of the model

An energy-economy model has never been initially created at ORNL, and all aspects of creating such a model are not fully understood Therefore, we are not able to estimate the time for initially developing and implementing an energy-economy model

3 Can the LEAP system be installed on the ORNL computing system?

There are several factors which inhibit code transportability The data base management system used by LEAP (S2K) is proprietary and not available at ORNL Two IBM 3033 computers, each with 8 megabytes of memory, are included in the ORNL computing system However, jobs requiring 2,000 000 bytes of memory would normally be executed after normal working hours The present ORNL system restricts TSO users to regions of 270 000 bytes of memory Since both LEAP and S2K require 270 000 bytes it would not be possible to execute LEAP interactively at ORNL

REFERENCES FOR APPENDIX A

1 R J Adler et al , The DFI Energy-Economy Modeling System, Decision Focus, Inc Palo Alto, California (1978)

2 E G Cazalet et al , The DFI Computer Modeling Software (CMS) Decision Focus, Inc Palo Alto, California (1978)

3 Optimum Systems, Inc , User's Guide to the EIA Service Facility prepared for U S Department of Energy, Energy Information Administration Rockville, Maryland (1979)

4 S Cohen and J D Pearson The LEAP-EMS Users Manual, U S Department of Energy Energy Information Administration, Office of Long-Term Energy Analysis Division (in preparation)

APPENDIX B
ADDITIONAL EQUATIONS OF BASIC CONVERSION PROCESS

The equations of the basic conversion process were presented and discussed in Section V Expressions for three quantities that were not given in Section V--present value of capital cost $N_C(j)$ the discount factor $D(j\ k)$ and the prices beyond the last global time point considered $P(j)$ for $j > N_p + N$--are given here

1 Present Value of Capital Cost

As in Section V, the equations for determining the present value of capital cost $N_C(j)$ are given without explanation as to the derivation Such an explanation can be found in Reference 1 of Section V Because the equations are so lengthy they are written for simplicity for the case when the time-varying discount factors are not treated in complete generality (i e in the terminology of Reference 1 Section V NSHORT = 1) The equations given here are those used in Models 22C and 82

The present value of capital cost may be written as

$$N_C(j) = \frac{1}{1-f_T}[V_p(E_q\ j) + V_p(P_{rn}\ j)] + V_p(I_{nt},j) + V_p(P_t\ j) - \frac{f_T}{1-f_T}[V_p(D_t\ j)] - \frac{1}{1-f_T}[V_p(I_{tc}\ j)] \tag{B 1}$$

where

V_p = an operator that gives the present value at time j of the first argument in the bracket,

E_q = equity,

P_{rn} = principal

I_{nt} = interest

P_t = property tax,

D_t = depreciation for income tax purposes,

I_{tc} = investment tax credit

f_T = income tax rate

The present value of equity may be written as

$$V_p(E_q\ J) = \left[\sum_{\ell=1}^{2} E_{q\ell}(J_1)\right] \prod_{k=J_1}^{J-1} [1 + r_e(k)]^{\Delta} \tag{B 2}$$

$$+ \left[\sum_{\ell=1}^{2} E_{q\ell}(J_2)\right] \prod_{k=J_2}^{J-1} [1 + r_e(k)]^{\Delta} \qquad J - \frac{L}{\Delta} \geq N_p + 1_{\Delta}$$

where

$$J_1 = \text{Int}\ [J - \frac{L}{\Delta}] \tag{B 3}$$

$$J_2 = J_1 + 1 \tag{B 4}$$

$$E_{q\ell}(J_1) = f_E p_\ell(J_1) b_\ell(J) e_{\ell 1}(J_1, J_2) \qquad J_1 \geq N_p + 1$$

$$E_{q\ell}(J_2) = f_E p_\ell(J_2) b_\ell(J) e_{\ell 2}(J_1\ J_2) \qquad J_2 \geq N_p + 2\ , \tag{B 5}$$

where

$$\begin{aligned}
b_\ell(J) &= b_\ell[h_\infty + (1 - h_\infty)(1 - \beta_c)]^{t_I + (J-1)\Delta - t_A} && t_I + (J-1)\Delta > t_A \geqq t_I + (N_p)\Delta \\
&= b_\ell[h_\infty + (1 - h_\infty)(1 - \beta_c)]^{(J-1)\Delta - N_p\Delta} && t_I + (J-1)\Delta > t_A \\
& && t_I + (N_p)\Delta \geqq t_A \\
&= b_\ell\{1 + [t_A - t_I - (J-1)\Delta]\rho\} && t_A \geqq t_I + N_p\Delta \qquad \text{(B 6)} \\
& && \quad \geqq t_I + J\Delta \\
&= b_\ell\{h_\infty + (1 - h_\infty)(1 - \beta_c)^{t_A - t_I - N_p\Delta} && t_A \leqq t_I\ N_p\Delta \\
& && \quad > t_I + (J-1)\Delta \\
&\quad + [t_A - t_I - (N_p)\Delta]\rho\}
\end{aligned}$$

$$b_1 = S_C C_{LF} \tag{B 7}$$

$$b_2 = S_C(1 - C_{LF}) \tag{B 8}$$

$$e_{\ell 1}(J_1\ J_2) \quad \frac{p_\ell(J_2)\{[1\ r_e(J_1)]^\delta\ 1\}}{p_\ell(J_1)\{[1\ r_e(J_1)]^\Delta\ [1\ r_e(J_1)]^\delta\ \}+p_\ell(J_2)\{[1\ r_e(J_1)]^\delta\ 1\}} \tag{B 9}$$

$$e_{\ell 2}(J_1\ J_2) \quad \frac{p_\ell(J_1)\{[1\ r_e(J_1)]^\Delta\ [1\ r_e(J_1)]^\delta\ \}}{p_\ell(J_1)\{[1\ r_e(J_1)]^\Delta\ [1\ r_e(J_1)]^\delta\ \}+p_\ell(J_2)\{[1\ r_e(J_1)]^\delta\ 1\}} \tag{B 10}$$

where

f_E = fraction of the cost financed from equity

$h_\infty\ \beta_c\ \rho$ = input constants

$\delta = J_2\Delta - (J\Delta - L)$

$r_e(J)$ = return on equity at time J

L = time before the time of operation when capital is required

S_C = specific capital cost of a facility per unit capacity

C_{LF} = fraction of the specific capital cost that is due to the cost of labor

$p_\ell(J)$ = price as defined in conjunction with Eq (V 16)

If $J - L/\Delta < N_p + 1$ then Eq (B 2) becomes

$$V_p(E_q\ J) = \left[\sum_{\ell=1}^{2} E'_{q\ell}(N_p + 1)\right] \prod_{k=N_p+1}^{J-1} [1 - r_e(k)]^\Delta \tag{B 11}$$

where

$$E'_{q\ell}(N_p + 1) = f_E p_\ell(N_p + 1) b_\ell(J) \left[\frac{1+r_e(N_p+1)}{1+I'_f}\right]^{[N_p+1-(J-\frac{L}{\Delta})]\Delta} \tag{B 12}$$

where

I_f' = rate of inflation for times $j < N_p + 1$

To calculate the terms $V_p(P_{rn}\ j)$ and $V_p(I_{nt}\ j)$ in Eq (B 1), it is convenient to define them as

$$V_p(P_{rn}\ j) = V_p(P_{rno}\ j) + V_p(P_{rnc}\ j) \tag{B 13}$$

and

$$V_p(I_{nt},j) = V_p(I_{nto}\ j) + V_p(I_{ntc}\ j)\ , \tag{B 14}$$

where

$V_p(P_{rno}\ j)$ = present value at time j of the principal during operation

$V_p(P_{rnc}\ j)$ = present value at time j of the principal during construction

$V_p(I_{nto}\ j)$ = present value at time j of interest during operation

$V_p(I_{ntc}\ j)$ = present value at time j of interest during construction

Then

$$V_p(P_{rnc},j) = \left\{\sum_{\ell=1}^{2} B_{r\ell}(j_1)\right\} \frac{1}{D} \sum_{m=j_1}^{j-1} \alpha_1(m) \prod_{k=m}^{j-1} [1 + r_\ell(k)]^\Delta + \left\{\sum_{\ell=1}^{2} B_{r\ell}(j_2)\right\} \frac{1}{D} \sum_{m=j_2}^{j-1} \alpha_1(m) \prod_{k=m}^{j-1} [1 + r_\ell(k)]^\Delta \tag{B 15}$$

and

$$V_p(I_{ntc},j) = \left\{\sum_{\ell=1}^{2} B_{r\ell}(j_1)\right\} \sum_{m=j_1}^{j-1} \alpha_1(m) r_D(m) \left\{1 - \frac{(m-j_1)^\Delta}{D}\right\} \prod_{k=m}^{j-1} [1 + r_e(k)]^\Delta + \left\{\sum_{\ell=1}^{2} B_{r\ell}(j_2)\right\} \sum_{m=j_2}^{j-1} \alpha_1(m) r_D(m) \left\{1 - \frac{(m-j_2)^\Delta}{D}\right\} \prod_{k=m}^{j-1} [1 + r_e(k)]^\Delta \tag{B 16}$$

where

$$\alpha_1(J_1) = \frac{1 - \left[\frac{1}{1+r_e(J_1)}\right]^{\Delta}}{1 - \left[\frac{1}{1+r_e(J_1)}\right]} \tag{B 17}$$

$$B_{r\ell}(J_1) = (1 - f_E)p_\ell(J_1)b_\ell(J)b'_{\ell 1}(J_1\ J_2)\ ,$$
$$B_{r\ell}(J_2) = (1 - f_E)p_\ell(J_2)b_\ell(J)b'_{\ell 2}(J_1,J_2) \tag{B 18}$$

and where $b'_{\ell 1}(J_1\ J_2)$ and $b'_{\ell 2}(J_1,J_2)$ have the same form as $e_{\ell 1}(J_1\ J_2)$ and $e_{\ell 2}(J_1,J_2)$ given by Eqs (B 9) and (B 10) except that $r_e(J)$ is replaced by $r_D(J)$ (D = debt life and $r_D(J)$ = interest rate at time J)

Note that Eqs (B 15) and (B 16) do not have the same restrictions on J as does Eq (B 2), therefore Eqs (B 15) and (B 16) are to be used for $J < N_p + 1$ for which $p_\ell(J)$ must be defined The values are

$$p_\ell(J) = p_\ell(N_p + 1) \left(\frac{1}{1+1'_f}\right)^{(N_p+1-1)\Delta} \qquad J < N_p + 1 \tag{B 19}$$

It is also assumed that

$$r_D(J) = r_D(N_p + 1) \qquad J < N_p + 1 \tag{B 20}$$

and

$$r_e(J) = r_e(N_p + 1) \qquad J < N_p + 1 \tag{B 21}$$

Furthermore,

$$V_p(P_{rno}\ J) = B'_o\overline{r}_D \sum_{m=J}^{Int[D_N]} \alpha_1(m) \prod_{k=J}^{m-1} \left(\frac{1}{1+r_e(k)}\right)^{\Delta}\ , \tag{B 22}$$

and

$$V_p(I_{nto},J) = B_o'\bar{r}_D \sum_{m=J}^{Int[D_N]} \alpha_1(m) \left(1 - \frac{(m-J)\Delta}{D_N}\right) \prod_{k=J}^{m-1} \left[\frac{1}{1+r_e(k)}\right]^{\Delta} \tag{B 23}$$

where

$$\prod_{J}^{J-1} = 1 \tag{B 24}$$

$$B_o'(J) = \left\{ \left[\sum_{\ell=1}^{2} B_{r\ell}(J_1)\right] \left[1 - \frac{(J-J_1)\Delta}{D}\right] + \left[\sum_{\ell=1}^{2} B_{r\ell}(J_2)\right] \left[1 - \frac{(J-J_2)\Delta}{D}\right] \right\} \tag{B 25}$$

$$\bar{r}_D = \frac{r_D(J_1)\left[\sum_{\ell=1}^{2} B_{r\ell}(J_1)\right] + r_D(J_2)\left[\sum_{\ell=1}^{2} B_{r\ell}(J_2)\right]}{\left[\sum_{\ell=1}^{2} B_{r\ell}(J_1) + \sum_{\ell=1}^{2} B_{r\ell}(J_2)\right]}, \tag{B 26}$$

$$D_N = \frac{B_o'(J)}{\left[\sum_{\ell=1}^{2} B_{r\ell}(J_1) + \sum_{\ell=1}^{2} B_{r\ell}(J_2)\right]} \tag{B 27}$$

The present value of property taxes may be written as

$$V_p(P_t\ J) = B(J\ J)(p_{rt}) \sum_{m=J}^{1+\mathrm{Int}\left[\frac{L_c}{\Delta}\right]} \alpha_1(m)\ \frac{I(m)}{I(J)} \prod_{k=J}^{m-1} \left[\frac{1}{1+r_e(k)}\right]^{\Delta}, \quad \text{(B 28)}$$

where

$$B(J,J) = \sum_{\ell=1}^{2} [E_{q\ell}(J_1) + E_{q\ell}(J_2) + B_{r\ell}(J_1) + B_{r\ell}(J_2)] \quad \text{(B 29)}$$

P_{rt} = property tax rate

$I(J)$ = assessed value inflator that is input to the code as a function of time J

The present value of depreciation for income tax purposes may be written

$$V_p(D_t\ J) = B(J\ J) \sum_{m=J}^{1+\mathrm{Int}\left[\frac{T_L}{\Delta}\right]} \alpha_1(m) R(J + 1 - m) \prod_{k=J}^{m-1} \left[\frac{1}{1+r_e(k)}\right]^{\Delta}, \quad \text{(B 30)}$$

$$U(k\Delta) = \left(1 - \frac{2}{T_L}\right)^{k\Delta} \quad \text{(B 31)}$$

$$R(m) = \frac{U(m\Delta) - U[(m-1)\Delta]}{\Delta}, \quad \text{(B 32)}$$

where T_L = tax life of the facility and $B(J\ J)$ is given by Eq (B 29)

Finally the present value of the investment tax credit is given by

$$V_p(I_{tc}\ J) = I_{tcr}\left\{\left[\sum_{\ell=1}^{2} E_{q\ell}(J_1) + B_{r\ell}(J_1)\right]\prod_{k=J_1}^{J-1}[1 + r_e(k)]^{\Delta} + \left[\sum_{\ell=1}^{2} E_{q\ell}(J_2) + B_{r\ell}(J_2)\right]\prod_{k=J_2}^{J-1}[1 + r_e(k)]^{\Delta}\right\} \qquad J - \frac{L}{\Delta} \geq N_p + 1\ , \tag{B 33}$$

$$V_p(I_{tc}\ J) = I_{tcr}\left\{\left[\sum_{\ell=1}^{2} E'_{q\ell}(N_p + 1)\right]\prod_{k=N_p+1}^{J-1}[1 + r_e(k)]^{\Delta} + \left[\sum_{\ell=1}^{2} B_{r\ell}(J_1)\right]\prod_{k=J_1}^{J-1}[1 + r_e(k)]^{\Delta} + \left[\sum_{\ell=1}^{2} B_{r\ell}(J_2)\right]\prod_{k=J_2}^{J-1}[1 + r_e(k)]^{\Delta}\right\} \qquad J - \frac{L}{\Delta} < N_p + 1 \tag{B 34}$$

where I_{tcr} = investment tax credit rate

2 Discount Factor D(j k)

The discount factor D(j,k) that occurs in Eq (V 6) has the form

$$D(j,k) = \alpha_1(k) \prod_{m=j}^{k-1} \left[\frac{1}{1+r_e(m)} \right]^{\Delta} \tag{B 35}$$

The simplification concerning time-varying discount factors that was introduced in Section B 1 has been used to obtain Eq (B 35)

3 Prices $P_T(j)$ for $j \geqq N_p + N$

The prices $P_T(j)$ for $j \geqq N_p + N$ that occur in Eq (V 6) and equations to determine the prices must be specified The equations used are

$$P_T(j) = \left[V(j) - \left(\frac{1}{1+r_c} \right)^{\Delta} V(j+1) \right] \frac{1 - \left(\frac{1}{1+r_c} \right)}{1 - \left(\frac{1}{1+r_c} \right)^{\Delta}} \tag{B 36}$$

$$N_p + N \leq j \leq 2N_p + N - 1 ,$$

where

$$r_c = \frac{r_e(N_p+N) - I_f}{1+I_f} , \tag{B 37}$$

$$V(j) = V_C(j) + V_0'(j) \tag{B 38}$$

The term $V_0'(J)$ is expressed as

$$V_0'(J) = \frac{1 - \left(\frac{1}{1+r_c}\right)^{\Delta}}{1 - \left(\frac{1}{1+r_c}\right)} \sum_{\ell=1}^{2} \{[1-\delta_\ell{}^3]V_0 f_\ell p_\ell (N_p + N)(1 + I_f)^{[J-(N_p+N)]\Delta}$$

$$+ \delta_\ell^3 \; T_{EF}{}^{-1} P_I (N_p + N)\,(1 + I_f)^{[J-(N_p + N)]\Delta}$$

$$\{g_{\infty\ell} B_1 \chi_\infty(Z_1) + g_{\infty\ell} B_2 \chi_\infty(Z_2) \qquad \text{(B 39)}$$

$$+ [1 - g_{\infty\ell}][1 + \alpha_\ell]^{[t_I+(J-1)\Delta-t_A]} B_1 \chi_\infty(Z_3)$$

$$+ [1 - g_{\infty\ell}][1 + \alpha_\ell]^{[t_I+(J-1)\Delta-t_A]} B_2 \chi_\infty(Z_4)\} \quad ,$$

where

$$B_1 = f_{\infty\ell}\{\psi_C(y_1\, n_L - 1) + a_{o\ell}\, \Delta\psi_L(y_1\, n_L - 1)\} \qquad \text{(B 40)}$$

$$B_2 = [1 - f_{\infty\ell}][1 - \alpha_\ell]^{[t_I + (J-1)\Delta-t_A]}$$

$$\{\chi_C[y_{2\ell}\, n_L - 1)] + a_o \Delta\psi_L[y_{2\ell}\, n_L - 1]\}$$

where

$$n_L = 1 + \text{Int}\left[\frac{L_c}{\Delta}\right] \qquad \text{(B 41)}$$

$$y_1 = \left[\frac{1}{1+r_c}\right]^{\Delta} \quad , \qquad \text{(B 42)}$$

$$y_2 = (1 - \alpha_\ell)^{\Delta}\, y_1 \qquad \text{(B 43)}$$

$$\psi_\infty(y) = \frac{1}{1-y} \qquad \text{(B 44)}$$

$$\psi_C(x\, n_L - 1) = \frac{1-X^{n_L-1}}{1-X} \qquad \text{(B 45)}$$

$$\psi_L(x\ n_L - 1) = \frac{1+(n_L-1)X^{n_L} - n_L X^{n_L-1}}{(1-X)^2} \tag{B 46}$$

$$Z_1 = \left[\frac{1}{1+r_c}\right]^{n_L\Delta} \tag{B 47}$$

$$Z_2(\ell) = (1 - \alpha_\ell)^{n_L\Delta} \left[\frac{1}{1+r_c}\right]^{n_L\Delta} \tag{B 48}$$

$$Z_3(\ell) = Z_2(\ell) \tag{B 49}$$

$$Z_4(\ell) = (1 - \alpha_\ell)^{n_L\Delta} \quad (1 - \alpha_\ell)^{n_L\Delta} \left(\frac{1}{1+r_c}\right)^{n_L\Delta} \tag{B 50}$$

The term $a_{o\ell}$ in Eqs (B 40) and (B 41) for $\ell = 1$ and 2 is a constant to be obtained by approximating the function $f_A(J)$ given by Eq (V 17) to be of the form

$$f_A(J) = 1 + a_{o\ell} J\Delta \tag{B 51}$$

In the present LEAP code $a_{01} = a_{22} = 0$ For $\ell = 3$ the function $f_A(J)$ is not used [see Eq (V 20)] and thus $a_{03} = 0$ always Furthermore

$$V_C(J) = \frac{N_C'(J)}{\beta} \left\{ 1 + \frac{1}{h_\infty + (1-h_\infty)(1-\beta_c)^{t_I+(J-1)\Delta-t_A}} \right\}$$

$$\left\{ h_\infty[\psi_\infty(W_1) - 1] + (1 - h_\infty)(1 - \beta_c)^{t_I+(J-1)\Delta-t_A} [\psi_\infty(W_w)-1] \right\} \tag{B 52}$$

where

$$W_1 = \left[\frac{1}{1+r_c}\right]^{n_L \Delta} \tag{B 53}$$

$$W_2 = (1 - \beta_c)^{n_L \Delta} \left(\frac{1}{1+r_c}\right)^{n_L \Delta} \tag{B 54}$$

$$N_C'(J) = N_C(N_p + N)(1 + I_f)^{[J-(N_p+N)]\Delta} \tag{B 55}$$

and thus $P_T(J)$ in Eq (B 36) can be determined

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