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The Application of Adjoint Sensitivity Theory to a Liquid Fuels Supply Model

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UCN-7969 (3 9-77)

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DEPARTMENT OF ENERGY

Printed in the United States of America. Available from
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road, Springfield, Virginia 22161
NTIS price codes—Printed Copy: A04; Microfiche A01

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ORNL/TM-8850

Contract No. W-7405-eng-26

Engineering Physics Division

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This Work Sponsored by
Office of Fossil Energy
U.S. Department of Energy

Date Published - September 1983

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ACKNOWLEDGMENTS

The authors are grateful to A. M. Perry and L. J. Hill of the Oab Ridge National Laboratory's Energy Division for their thorough review of the manuscript.

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Abstract—Adjoint sensitivity theory has been applied to a liquid fuels supply model to determine the sensitivity of calculated results to the parameters in the model. The power of the adjoint sensitivity methodology is that it provides, in principle, an efficient means of calculating the sensitivity, dR/dx, of any calculated result R to every parameter x in the model. The liquid fuel supply model considered is one of a class of models that may be constructed from the Generalized Equilibrium Modeling System (GEMS) developed by Decision Focus, Inc., Los Altos, California. It is shown that for this class of models the lengthy development effort that is usually associated with applying the adjoint sensitivity methodology can be avoided by using the GEMS program to evaluate the large number of partial derivatives that are needed to apply the methodology.

1. INTRODUCTION

In a previous paper,[1] subsequently referred to as 1, a model of liquid fuels supply (LFS) was presented and discussed. In another previous paper,[2] subsequently referred to as 2, adjoint sensitivity theory was shown to be applicable to large energy-economic models.

The advantage of adjoint sensitivity theory or methodology as described in 2 is that it provides, in principle, an efficient means of determining the sensitivity of a result of interest to all of the parameters that enter into the calculations. More precisely, if R is a result of interest obtained by solving a large set of nonlinear equations, the methodology provides, in principle, a means of calculating dR/dx, termed the sensitivity of R to x, for every parameter x that occurs in the equations that determine R. The qualifier "in principle" is introduced in the above two sentences because in applications such as those considered here, the very small sensitivities are difficult to calculate accurately and since they are of little interest no attempt is made to improve their accuracy. The complete list of sensitivities for a few results of interest provides a large amount of information about the model that could not be obtained without the adjoint methodology unless a prohibitively large amount of computing time were used.

The most elaborate use of the complete set of sensitivities is to combine them with error estimates for the model parameters to obtain uncertainty estimates for the calculated results.[3] This requires rather extensive information on parameter errors and in the case of energy-economic models has been carried out only approximately.[4]

Quite independent of uncertainties, however, the sensitivities are useful for purposes of data gathering and for determining whether a reformulation of the model is necessary or desirable. After all of the sensitivities have been calculated, it is a straightforward matter to determine the relatively small number of parameters that are contributing appreciably to a set of calculated results and then to examine the base case values for these parameters to determine if they can be improved. In a model such as the LFS model, which has approximately 1000 parameters, the task of determining accurate values for all of the parameters is formidable, and it is extremely helpful to have a measure of the importance of the parameters to aid one in considering the order in which parameter values in the model should be reconsidered for accuracy.

Another very significant point concerns the number of parameters in the model. The same parameter, e.g., return on equity, may occur at various places in the model, and it is a choice of the analyst as to whether this is one parameter or several parameters. The magnitude of the sensitivities of a result is, of course, dependent on this choice. By the method described here, it is possible to calculate a sensitivity for each individual parameter and then sum the sensitivities for any group of parameters that the analyst wishes to consider as a single parameter.

Finally, the information on which parameters have large sensitivities and which have small sensitivities is very useful in considering the manner in which the model is formulated. That is, if the parameter sensitivities are contrary to what is expected, then the model contains relations that were unperceived by the analyst and he must decide whether

these relations are valid or whether some reformulation of the model is desirable.

The disadvantage of the methodology as it was applied in 2 is that a large amount of analytic differentiation, and consequently a large development effort, is required before it can be applied. Furthermore, additional development work is required as often as the equations that specify the model change. In 2 it was pointed out that because of the modular structure of models constructed with the Generalized Equilibrium Modeling System (GEMS)[5] it was feasible to use numerical methods and the GEMS computer program to avoid much of the required development effort. These numerical methods have been implemented, and in this paper the results obtained using them to apply adjoint sensitivity theory to the LFS model described in 1 are presented and discussed.

In Section 2.A adjoint sensitivity theory as it is used in this paper is developed and discussed. In Section 2.B the liquid fuels supply model of 1 is briefly described. In Section 2.C the method is presented for evaluating, using the GEMS computer program, the partial derivatives required to apply the adjoint sensitivity methodology. In Section 2.D the results for which sensitivities have been calculated are defined. In Section 2.E the numerical details of obtaining the sensitivity results are given. Finally, in Section 3 the results are presented and discussed.

2. METHOD OF CALCULATION

2.A. Adjoint Sensitivity Theory

In this subsection the methodology of adjoint sensitivity theory as it is used in this paper is developed. A more complete development of the theory as it applies to energy-economic models will be found in 2,

and a more general development of the theory with references to its application in many fields will be found in the work of D. G. Cacuci.[6] In the application considered here, only algebraic equations occur so the discussion will be limited to this type of equation. The theory is, however, applicable to more general types of equations as indicated in Ref. 6.

Let the system under consideration be represented by N nonlinear equations in N unknowns, which may be written symbolically as

$$\overline{F}(\overline{P},\overline{x}) = 0 \tag{1}$$

where $\overline{F}$ is an N-vector function of the unknown dependent variable N-vector $\overline{P}$ and all of the parameters of the system are represented by $\overline{x}$. It is to be understood that the number of elements in $\overline{x}$ is not at all related to N and can be substantially larger, and all of the elements of $\overline{x}$ are, in principle, independent. In the following it will be assumed that for a specific choice of $\overline{x}$ a unique solution of Eq. (1) exists and is represented by $\overline{P}$. Thus, $\overline{P}$ is a function of $\overline{x}$.

Let R, called a response, represent any result of the calculations that is of interest. In particular, let

$$R = R(\overline{P},\overline{x}) \quad . \tag{2}$$

where $R(\overline{P},\overline{x})$ is any given nonlinear function of $\overline{P}$ and $\overline{x}$. The response R is a scalar that may be calculated from Eq. (2) when the solution $\overline{P}$ of Eq. (1) has been obtained for a given specification of $\overline{x}$.

If x is now defined to be a general element of $\overline{x}$, the sensitivity of R to x is defined to be dR/dx and the general problem of sensitivity

theory is to determine dR/dx for each and every element of $\overline{x}$. If Eq. (2) is differentiated with respect to x, then

$$dR/dx = \partial R/\partial x + \partial R/\partial \overline{P} \cdot \partial \overline{P}/\partial x \tag{3}$$

where $\partial R/\partial \overline{P}$ is a row vector having N elements and $\partial \overline{P}/\partial x$ is a column vector having N elements. It should be noted that dR/dx is the total drivative of R with respect to x in that all of the dependence of R on x is considered, but the derivative dR/dx is taken with all parameter values except x held fixed. Since R is by assumption a known function of $\overline{P}$ and $\overline{x}$, the quantity in Eq. (3) that must be determined to calculate dR/dx is the vector $\partial \overline{P}/\partial x$.

By differentiating Eq. (1)

$$\partial \overline{F}/\partial \overline{P} \cdot \partial \overline{P}/\partial x + \partial \overline{F}/\partial x = 0 \tag{4}$$

where $\partial \overline{F}/\partial \overline{P}$ is an N by N matrix. Since $\overline{F}$ is by assumption a known function of $\overline{P}$ and $\overline{x}$, Eq. (4) represents a large set of linear equations that may be solved to obtain $\partial \overline{P}/\partial x$. The difficulty in determining $\partial \overline{P}/\partial x$ from Eq. (4) and then dR/dx from Eq. (3) is that $\partial \overline{P}/\partial x$, as determined from Eq. (4), depends explicitly on x; therefore, the large set of equations in Eq. (4) must be resolved for each parameter x.

This difficulty can be circumvented by combining Eqs. (3) and (4) to yield

$$dR/dx = \partial R/\partial x - \overline{D} \cdot \partial \overline{F}/\partial x \tag{5}$$

where $\overline{D}$ is determined from the equation

$$\overline{D} \cdot \partial \overline{F}/\partial \overline{P} = \partial R/\partial \overline{P} \quad . \tag{6}$$

Equations (5) and (6) are the important results of adjoint sensitivity theory. Since both $\overline{F}$ and R are by assumption known functions of $\overline{P}$ and $\overline{x}$, Eq. (6) represents a large set of linear equations that may be solved to determine $\overline{D}$ and then dR/dx may be calculated from Eq. (5). However, $\overline{D}$ as determined by Eq. (6), does not depend explicitly on the particular element x that is used in Eq. (5); therefore, a single determination of $\overline{D}$ enables one to calculate dR/dx for every element x of $\overline{x}$. Equation (6) does depend on the response, R, and therefore a new determination of $\overline{D}$ is required for every R that is considered. Thus, by using Eqs. (5) and (6) rather than Eqs. (3) and (4) to determine dR/dx for every x in $\overline{x}$, the requirement that the large set of linear equations given by Eq. (4) be solved for each x has been replaced by the requirement that the large set of linear equations given by Eq. (6) be resolved for each response R to be considered. Therefore, the methodology is most useful when there are a large number of parameters and few results or responses of interest.

2.B. Liquid Fuels Supply (LFS) Model

The liquid fuels supply model considered here is the same as that described in detail in 1, so only a brief discussion of the model will be given. This model is a particular example of the models that may be constructed using the Generalized Equilibrium Modeling System.[5]

In Fig. 1 a schematic diagram of the LFS model is shown. Each type of geometric element in Fig. 1 represents a different type of activity, i.e., a different process submodel. Each geometric element contains a number that will be referred to as the activity or node number. Each

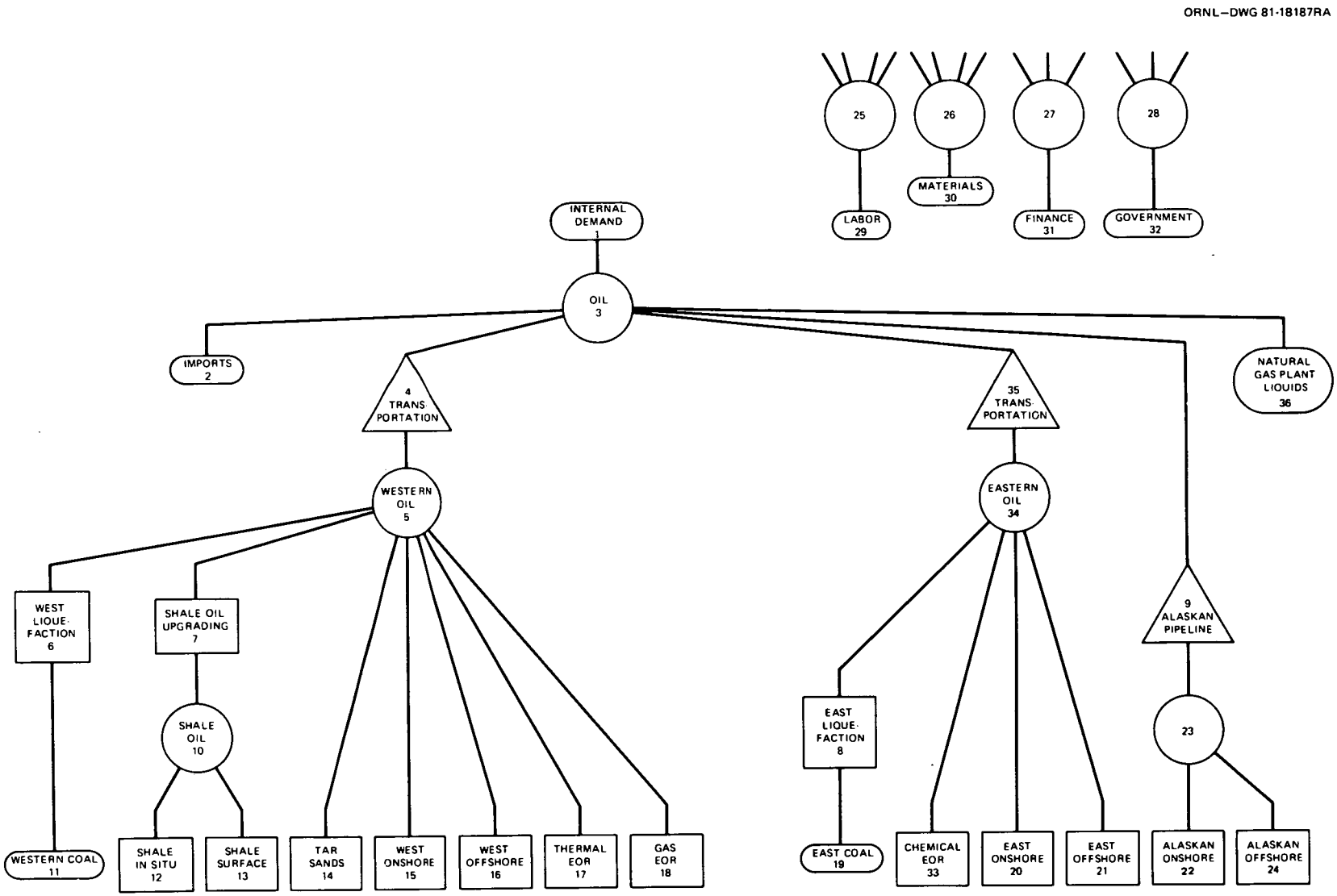

Fig. 1. Schematic diagram of LFS model.

activity number represents a distinct set of parameter values in the process submodels. The same parameter, e.g., return on equity, may occur at several different nodes. Unless otherwise indicated, it is assumed here that a parameter at a node is independent of all parameters at all other nodes. This will be discussed further in Section 3 where the results are given. The line joining two nodes is termed a link and the variables of the system (except for initial conditions)[1,2,5] are the quantities (in energy units) per year and the prices per unit energy on each link at ten representive time points (1980 to 2025 in five-year intervals). These quantities per year and prices per unit energy on the links are the elements of $\overline{P}$ that were used in Section 2.A.

The basic premise of models constructed with GEMS is that supply must equal demand at all times; i.e., all demand will be supplied at some price. The equations of the model may be solved by iteration to obtain the values of the system variables; then combinations of the system variables, i.e., responses of interest [see Eq. (2)], may easily be evaluated. In 1 several responses of interest were evaluated and compared with the National Energy Policy Plan.[7] Here, the interest will be not only in evaluating various responses but in determining the derivatives of these responses [see Eq. (5)] with respect to all of the parameters in the LFS model.

2.C. Evaluation of the Elements of $\partial\overline{F}/\partial\overline{P}$ and of $\partial\overline{F}/\partial x$

To apply adjoint sensitivity theory as formulated in Section 2.A, it is necessary to evaluate the elements of the matrix $\partial\overline{F}/\partial\overline{P}$ in Eq. (6) before $\overline{D}$ can be evaluated and to evaluate the elements of the vector $\partial\overline{F}/\partial x$ before dR/dx may be evaluated from Eq. (5). If the equations of

the model, Eq. (1), are known, it is a straightforward but time-consuming task to analytically differentiate the equations and numerically evaluate the results to obtain the required derivatives. In 2 (where there were over 4,000 equations) this procedure was followed, but it was pointed out that, in principle, the significant development time could be avoided by using the GEMS computer program[5] to directly estimate all of the needed partial derivatives. This numerical procedure, which has now been implemented and is used in obtaining the results presented later in this paper, is described below.

The numerical procedure will be illustrated by considering, for simplicity, a conversion process (rectangular box in Fig. 1) that has one input link and one output link. The procedure is applicable to all of the processes in the GEMS system,[2] for example, to allocation processes that have many input links, but the equations are somewhat more complicated than for the case considered here. If the activity number of this conversion process is designated by n, then the quantities and prices on the output link of this node may be designated as Q_{nJ}, P_{nJ} where J is an index that numbers the T time points considered in the model. Similarly, the quantities and prices on the input link of node n may be designated as Q_{InJ}, P_{InJ} where the subscript I is used to designate the input link to node n. The quantities Q_{nJ}, P_{nJ}, Q_{InJ}, and P_{InJ} for all J are all elements of the vector $\overline{P}$ that were introduced in Eq. (1).

In the GEMS system one may consider complicated network diagrams such as that shown in Fig. 1 or very simple network diagrams. In particular, a network diagram having only one node may be considered. Let us consider the situation when the conversion process at node n is the only

process in the network. For this very special case, the system variables will be P_{nJ}, Q_{InJ} for all J and the quantities Q_{nJ} (the demand), P_{InJ} (the feedstock price) for all J will be exogenous system parameters. That is, if Q_{nJ}, P_{InJ} for all J as well as all other parameters at node n are specified, then the GEMS computer program will determine P_{nJ}, Q_{InJ} for all J. The GEMS equations for the conversion process at node n are then of the form

$$P_{nJ}-G_{nJ}[Q_{n1},\ldots,Q_{nT},P_{In1},\ldots,P_{InT},x_{n1},\ldots,x_{np}] = 0 \qquad J = 1,T \qquad (7)$$

$$Q_{InJ}-H_{nJ}[Q_{n1},\ldots,Q_{nT},P_{In1},\ldots,P_{InT},x_{n1},\ldots x_{np}] = 0 \qquad J = 1,T \qquad (8)$$

where G_{nJ} and H_{nJ} are functions of Q_{nJ},P_{InJ} for all J and of all of the parameters (the total number of which is designated by p) that occur in the equations at node n. Each of the parameters, x_{nk}, is an element of $\overline{x}$ in Eq. (1).

The form of the equations at a node is not dependent on whether or not the node is included in a network, and thus Eqs. (7) and (8) are elements of the vector $\overline{F}$ introduced in Eq. (1). If Eqs. (7) and (8) are differentiated with respect to a particular parameter $x_{m\ell}$, where m is an activity number that may or may not be equal to n, one obtains

$$\frac{\partial P_{nJ}}{\partial x_{m\ell}} - \sum_{K=1}^{T} \frac{\partial G_{nJ}}{\partial Q_{nK}} \frac{\partial Q_{nK}}{\partial x_{m\ell}} - \sum_{K=1}^{T} \frac{\partial G_{nJ}}{\partial P_{InK}} \frac{\partial P_{InK}}{\partial x_{m\ell}} = \frac{\partial G_{nJ}}{\partial x_{m\ell}}, \qquad J = 1,T \qquad (9)$$

and

$$\frac{\partial Q_{InJ}}{\partial x_{m\ell}} - \sum_{K=1}^{T} \frac{\partial H_{nJ}}{\partial Q_{nK}} \frac{\partial Q_{nK}}{\partial x_{m\ell}} - \sum_{K=1}^{T} \frac{\partial H_{nJ}}{\partial P_{InK}} \frac{\partial P_{InK}}{\partial x_{m\ell}} = \frac{\partial H_{nJ}}{\partial x_{m\ell}} , \qquad J = 1,T . \quad (10)$$

Equations (9) and (10) are elements of the vector equations given as Eq. (4). Comparing Eqs. (9) and (10) with Eq. (4) shows that

$$\partial G_{nJ}/\partial Q_{nK},\ \partial G_{nJ}/\partial P_{InK},\ \partial H_{nJ}/\partial Q_{nK},\ \partial H_{nJ}/\partial P_{InK}$$

for all J and K are the elements of the matrix $\partial\overline{F}/\partial\overline{P}$ corresponding to node n. Note that P_{nJ}, Q_{nJ}, P_{InJ}, Q_{InJ} for all J are only a small fraction of the totality of all system variables, and since only derivatives of these variables with respect to $x_{m\ell}$ occur in Eqs. (9) and (10) for node n, many elements of the matrix $\partial\overline{F}/\partial\overline{P}$ for node n are zero. This is also true, as shown in 2, for nodes that represent something other than a conversion process, and one of the consequences of the modular structure of models constructed with the GEMS system is that the matrix $\partial\overline{F}/\partial\overline{P}$ is very sparse, that is, has many zero elements. This is important because the number of elements in $\partial\overline{F}/\partial\overline{P}$ that must be calculated is reduced and because the work of determining $\overline{D}$ from Eq. (6) is also reduced.

By comparing Eqs. (9) and (10) with Eq. (4) it can also be seen that $\partial G_{nJ}/\partial x_{n\ell}$ and $\partial H_{nJ}/\partial x_{n\ell}$ are the only nonzero elements of $\partial\overline{F}/\partial x$ when x is $x_{n\ell}$.

Using the GEMS computer program, the numerical estimation of the various partial derivatives discussed above is accomplished by considering Eqs. (7) and (8) in the very special situation when node n is the only node in a network diagram. By differentiating Eqs. (7) and (8) with respect to Q_{nK}, one obtains

$$\partial P_{nJ}/\partial Q_{nK} = \partial G_{nJ}/\partial Q_{nK} , \quad J = 1,T \tag{11}$$

and

$$\partial Q_{InJ}/\partial Q_{nK} = \partial H_{nJ}/\partial Q_{nK} . \quad J = 1,T . \tag{12}$$

Now, if a small change, ΔQ_{nK}, is made in Q_{nK} for a particular K, the GEMS program may be used to obtain the corresponding changes ΔP_{nJ} in P_{nJ} for all J and ΔQ_{InJ} in Q_{InJ} for all J. In like manner, if a small negative change $-\Delta Q_{nK}$ is made one may obtain from the program $\Delta P'_{nJ}$ and $\Delta Q'_{InJ}$. Then, $\partial G_{nJ}/\partial Q_{nK}$ and $\partial H_{nJ}/\partial Q_{nK}$ may from Eqs. (11) and (12) be approximated as

$$\partial G_{nJ}/\partial Q_{nK} = \Delta P_{nJ}-\Delta P'_{nJ}/2\Delta Q_{nK} , \quad J = 1,T \tag{13}$$

and

$$\partial H_{nJ}/\partial Q_{nK} = \Delta Q_{InJ}-\Delta Q'_{InJ}/2\Delta Q_{nK} , \quad J = 1,T . \tag{14}$$

The procedure may, of course, be repeated for all values of K.

Similarly, by making small perturbations in P_{InK} and x_{nk} and using the code to determine the corresponding changes in the system variables of node n when this node is considered to be the only node in the network, one may obtain estimates of the other partial derivatives for node n.

The above discussion is applicable in detail only to the case of a conversion node with one input and one output link, but it can be extended without difficulty (see 2) to all of the process submodels allowed in the GEMS system. Thus, by considering one node at a time, it is possible to determine from the GEMS program for any network diagram all of the nonzero partial derivatives that occur in the matrix $\partial\overline{F}/\partial\overline{P}$ and in

the vector $\partial\overline{F}/\partial x$. It must be emphasized that the considerations in this section serve only to determine the elements of $\partial\overline{F}/\partial\overline{P}$ and $\partial\overline{F}/\partial x$. It is still necessary to solve the set of equations given by Eq. (6) to determine $\overline{D}$ before Eq. (5) can be used to determine dR/dx for all x.

2.D. Responses of Interest

From Section 2.A it is clear that sensitivities, as considered here, are defined only with respect to a particular result or response of interest. As explained in Section 2.A, a response may be any function of the system variables and the system parameters. In this subsection the responses for which sensitivities will be presented and discussed in Section 3 are defined.

The first response considered is the ratio of the total quantity of oil imported in the 25-year period 1980 to 2005 to the total quantity of oil demanded in the same 25-year period. This response, R_{IQ}, may be written as

$$R_{IQ} = \frac{\sum_{J=1}^{5} Q_2(J)}{\sum_{J=1}^{5} Q_3(J)} \tag{15}$$

where

$Q_2(J)$ = the quantity of oil (energy) per year on the output link of activity 2 (see Fig. 1) at time J,

$Q_3(J)$ = the quantity of oil (energy) per year on the output link of activity 3, i.e., the link from activity 3 into internal demand (see Fig. 1), at time J,

J = 1 to 10 corresponding to the years 1980 to 2025 in 5-year intervals.

In the LFS model, quantities are measured in quadrillion Btu. Since supply is equal to demand in the LFS model, the quantity demanded per year may also be thought of as the quantity used per year.

The second response to be considered is the ratio of the total cost of imported oil in the period 1980 to 2005 to the total cost of oil demands in the same period. This response, R_{IP}, may be written

$$R_{IP} = \frac{\sum_{J=1}^{5} Q_2(J)P_2(J)}{\sum_{J=1}^{5} Q_3(J)P_3(J)} \tag{16}$$

where

$P_2(J)$ = the price per unit energy on the output link of activity 2 (see Fig. 1) at time J,

$P_3(J)$ = the price per unit energy on the output link of activity 3, i.e., the link from activity 3 into internal demand (see Fig. 1), at time J,

and the quantities $Q_2(J)$, $Q_3(J)$, and J are those defined in conjunction with Eq. (15). In the LFS model, prices per unit energy are measured in billions of 1980 dollars per quadrillion Btu. The responses R_{IQ} and R_{IP} are somewhat similar, but they differ in that R_{IP} depends explicitly on prices while R_{IQ} does not.

Next, six responses are defined that represent the fraction of the total demand in the year 2000 that is supplied by the various resource processes in Fig. 1. For onshore production, R_{ONS} is defined as

$$R_{ONS} = \frac{Q_{15}(5) + Q_{20}(5) + Q_{22}(5)}{Q_3(5)} \tag{17}$$

where 5 (=J) represents the year 2000. Similarly, for offshore, R_{OFS} is defined by

$$R_{OFS} = \frac{Q_{16}(5) + Q_{21}(5) + Q_{24}(5)}{Q_3(5)} ; \tag{18}$$

for enhanced oil recovery (EOR), R_{EOR} is defined by

$$R_{EOR} = \frac{Q_{17}(5) + Q_{18}(5) + Q_{33}(5)}{Q_3(5)} ; \tag{19}$$

for synthetic product, R_{SYN} is defined by

$$R_{SYN} = \frac{Q_6(5) + Q_8(5)}{Q_3(5)} ; \tag{20}$$

for production from shale and tar sands, R_{SHT} is defined by

$$R_{SHT} = \frac{Q_7(5) + Q_{14}(5)}{Q_3(5)} ; \tag{21}$$

and for imports, R_{IMP} is defined by

$$R_{IMP} = \frac{Q_2(5)}{Q_3(5)} . \tag{22}$$

2.E. Details of Numerical Calculations

The GEMS equations are very nonlinear and are solved by iteration so there is a limit to the accuracy of the calculated base case system variables. The base case solution used here was converged to .05% so this is approximately the accuracy to which the system variables are known and is at least very approximately the accuracy to which any response, R, is known.

To carry out the evaluation of the elements of the matrix $\partial\overline{F}/\partial\overline{P}$ and of the vector $\partial\overline{F}/\partial x$ for the LFS as described in Section 2.C, it is necessary to specify small perturbations in the system parameters at each node. If the size of the perturbation is too small, then spurious results will be obtained because the change in the system variables induced by the perturbation may be too small to be meaningful because of the accuracy to which the system variables were determined. If, on the other hand, the perturbation is too large, one may be out of the linear range and the approximation of derivatives by finite differences may not be accurate. In obtaining the results presented here, a perturbation of 1% was used for noninteger parameters and a perturbation of unity was used for integer parameters. In the case of integer data elements, the perturbation used is the smallest perturbation allowed without modification of the GEMS system. It should be noted that there is no necessity for choosing the perturbation to be the same fraction (.01) for all parameters at all nodes, but this was done here.

To obtain sensitivities, it is necessary to solve, for each response considered, the large set of linear equations represented by Eq. (6). In the LFS model there are 461 variables and slightly over 1000 parameters.

Because of the modular structure of models constructed with GEMS (see Section 2.C), the matrix $\partial\overline{F}/\partial\overline{P}$ has, in principle, only 11,874 nonzero elements. Very efficient FORTRAN programs are available for the numerical solution of large sets of linear equations involving a sparse matrix. In the work reported here, the program written by J. S. Duff was used.[8] Once $\overline{D}$ has been obtained for a given response it is straightforward to calculate the derivatives of the response, dR/dx, for all parameters, x, in the model. The small sensitivities are not at all accurate because of the convergence criteria used in the base case and because of the size of the perturbation used. It is, in principle, possible to improve the accuracy of the small sensitivities, but since the magnitude of these sensitivities are of little interest this has not been done.

An estimate of the validity of the calculated sensitivity for any specific parameter can also be obtained without recourse to adjoint theory by changing the parameter x by an amount Δx and calculating $\Delta R/\Delta x$ by completely repeating the model calculations. This procedure is too costly to be carried out for very many parameters, but it does provide a means of verifying some of the sensitivities obtained by adjoint theory. Such comparisons will be presented in the next section of this paper. The sensitivities obtained by direct calculations were carried out using a 10% perturbation in the base case parameter values except when a 10% increase would give a parameter value that was out of its allowed range and then a -10% perturbation was used.

In comparing the sensitivities of different parameters it is usually more meaningful to consider relative sensitivities defined by (x/R)(dR/dx) where x and R are the base case values. The relative sensitivity may be

interpreted as the percent increase in the response due to a one percent increase in the parameter value. In the next section the results are presented and discussed in terms of relative sensitivities.

3. RESULTS AND DISCUSSION

Calculations have been carried out to determine the relative sensitivities of the responses defined in Section 2.D. In this section, only the largest relative sensitivities are presented and discussed. It is to be understood, however, that for each response the relative sensitivities have been calculated for every parameter in the system equations; thus, those parameters that are considered in this section are known to be the parameters with the largest absolute relative sensitivities for each response. It is to be noted, however, that the relative sensitivities presented here are obtained assuming that all of the parameter in the model are independent. If a parameter that occurs at several nodes, such as return on equity, is assumed to be the same parameter, then the sensitivity of a response for this parameter must be obtained by summing the sensitivities of the response for this parameter at each node over all of the nodes in which the parameter occurs. This procedure will, in general, change the ordering of the sensitivities on the basis of absolute magnitude. Since all of the individual sensitivities have been calculated, it is straightforward to carry out any desired summations, but this has not been done in obtaining the results presented here. Such summations are often very instructive, but because of partial cancellation by positive and negative sensitivities they are often difficult to interpret if the individual sensitivities that enter into summation are not also presented.

The calculated results (10 largest sensitivities) for responses R_{IQ} and R_{IP} defined in Section 2.D are given in Table 1. The first column describes the parameter, x, being considered. Information on the meaning of the parameters considered in Table 1 is given in the discussion below. A more lengthy discussion of the meaning of the parameter will be found in 1 and in Ref. 5. The second and fourth columns give the relative sensitivities, obtained by adjoint calculations, of the responses R_{IQ} and R_{IP}, respectively, to the parameter x. The third and fifth columns give the relative sensitivities, obtained by direct calculations, of the responses R_{IQ} and R_{IP}, respectively, to the parameter x. When no entry occurs in columns 3 and 5, it means that no direct calculations were performed. In column 2 the relative sensitivities are shown in the order of decreasing absolute value, and this determines the order in which the sensitivities are given in column 4.

The responses R_{IQ} and R_{IP} are similar and so are considered together, but they are also somewhat different in that R_{IP} depends explicitly on prices and R_{IQ} does not. By comparing the values in columns 2 and 4 of Table 1, it can be seen that the relative sensitivities of the two responses are very similar for all of the parameter values considered in the table. In considering the values of the relative sensitivities, it should be remembered that the relative sensitivity is the percent change in the response for a 1% increase in the parameter value in the base case. The magnitudes of the absolute relative sensitivities in Table 1 vary from approximately 0.20 to approximately 2.5. Whether or not these are large sensitivities depends to a considerable extent on the magnitude

Table 1. Relative sensitivities of the responses R_{IQ} and R_{IP}.†

Data element x	Relative sensitivity $\frac{x}{R_{IQ}} \frac{dR_{IQ}}{dx}$ Adjoint	Direct	$\frac{x}{R_{IP}} \frac{dR_{IP}}{dx}$ Adjoint	Direct
Efficiency of western oil transportation (4)‡	-2.52	-2.58	-2.37	-2.42
Price of imported oil in 1985 (2)	-1.16		-1.08	
Efficiency of Alaskan oil transportation (9)	-0.68	-0.69	-0.66	-0.66
Price of imported oil in 1990 (2)	-0.66		-0.72	
Efficiency of eastern oil transportation (35)	-0.63	-0.64	-0.60	-0.60
Base price of west onshore oil (15)	0.43	0.44	0.41	0.41
New resources at twice base price for west onshore oil (15)	-0.34	-0.35	-0.33	-0.32
Price of imported oil in 1995 (2)	-0.30		-0.33	
Total quantity of oil demanded in 1990 (3)	0.24		0.25	
Specific capital cost of west liquefaction (6)	0.22	0.22	0.20	0.20

†R_{IQ} is the ratio of the quantity of oil imported in the years 1980 to to 2005 to the total quantity of oil demanded in these years, and R_{IP} is the ratio of the total cost of imported oil in the years 1980 to 2005 to the total cost of the oil demanded in these years. Equations defining R_{IQ} and R_{IP} are given in Section 2.D. (In the base case, R_{IQ} = 0.28 and R_{IP} = 0.28.)

‡Numbers in parentheses are activity numbers as specified in Fig. 1.

of the uncertainties that are associated with the base case parameter values. However, even without considering uncertainties, it is very helpful to know which of the parameters have appreciable sensitivities With this information the analyst may direct his attention to obtaining reliable values for the rather small number of parameters having a significant influence on the results and for purposes of data gathering, at least, may ignore the very large number of parameters having no significant influence on the results. For the purpose of understanding the model, the parameters with very small sensitivities are of as much interest as those with large sensitivities.

The parameter with the largest sensitivity for both responses R_{IQ} and R_{IP} is the efficiency of western oil transportation. This parameter models the losses during transportation and the cost of transportation. An increase in this parameter would decrease the price of all western oil and would therefore make it more competitive with imported oil. Oil imports would then decrease and thus both responses being considered should decrease. This decrease is represented in Table 1 by the negative sign on the relative sensitivities in the first line of columns 2 and 4. Since western oil provides a substantial fraction of the oil demand in the period 1980 to 2005, it is not too surprising that the responses being considered should have a significant sensitivity to the efficiency of western oil transportation. However, the fact that for the responses considered, this efficiency of all of the parameters in the model has the largest relative sensitivity can be determined only by the methodology employed here. To a considerable extent, the importance of the efficiency of western oil transportation is a function of the model structure. That

is, it results from the fact that all western oil, which is a substantial fraction of the oil supply in the years 1980 to 2005, passes through the same transportation node. If more transportation nodes were used, i.e., if different transportation nodes were used for the various source of western oil, the significance of the efficiency of these individual transportation nodes would be reduced. One of the purposes of sensitivity theory is to indicate to the analyst that such structural importances are in the model so he may decide if they were intended or if some restructuring of the model is desirable.

The relative sensitivities obtained by direct calculations in the first line of Table 1 are in substantial agreement with the sensitivities obtained using adjoint methods. The small differences are due to errors introduced by approximating derivatives by finite differences in the calculations and by using a 10% perturbation in the direct calculations to preserve the numerical significance of calculated differences. The agreement between the adjoint and direct sensitivities throughout Table 1 is quite good and indicates that the numerical methods used to evaluate the partial derivatives in $\partial\overline{F}/\partial\overline{P}$ and $\partial\overline{F}/\partial x$ (see Section 2.C) are satisfactory.

The second, fourth, and eighth largest sensitivities in Table 1 are for the prices of imported oil in 1985, 1990, and 1995, respectively. In the LFS model the price of imported oil in all years is specified exogenously. The price of imported oil has a direct effect on the quantity of oil imported, so it is not surprising that the responses being considered have an appreciable sensitivity to these prices. The prices of

imported oil in the other model years are not shown in Table 1 because their relative sensitivities are less than the lowest relative sensitivities shown in the table. The prices of imported oil in the years 1985, 1990, and 1995 have larger sensitivities than the prices in later years because in the base case larger quantities of oil are imported in the early years. The price of imported oil in 1980 does not have an appreciable sensitivity because quantities in 1980 on the input links to all allocation processes are used as initial conditions in the model,[1,5] and this decreases the influence of this price. Finally, an increase in the price of imported oil in 1985, 1990, or 1995 should decrease the quantity of oil imported between 1980 and 2005, and this is indicated by the negative sensitivities for these parameters in Table 1.

The third and fifth largest sensitivities in Table 1 are for the efficiency of Alaskan and eastern oil transportation, respectively. This parameter was described above with regard to western oil transportation. An increase in the efficiency of either Alaskan oil transportation or eastern oil transportation decreases the price of oil from these sources and causes oil from these sources to be used in place of imported oil. Thus, for the responses R_{IQ} and R_{IP}, the relative sensitivities for these parameters would be expected to be negative and, in fact, are negative, as shown in Table 1.

The sixth and seventh largest relative sensitivities in Table 1 are parameters associated with the resource cost-supply curve that is input to the model for western onshore oil. To specify this curve, four parameters (initial resource cost, base resource price, undiscovered recoverable resources at base price, and new resources at twice base price)

must be specified.[1,5] Basically, the initial resource cost defines the overall normalization of the resource cost-supply curve and the other parameters are used to specify the shape of the curve. This shape is defined by

$$1 + A(\chi)^B$$

where χ is the cumulative resource commitment and A and B are constants that are determined from the last three parameters specified above.

As mentioned above, in the LFS model a substantial fraction of the total demand in the years 1980 to 2005 is supplied by western onshore oil, and therefore it is to be expected that the responses being considered would have appreciable sensitivities to the parameters that characterize the corresponding resource cost-supply curve. If the base price is increased, while the other parameters that define the resource cost-supply curve are held fixed, the resource curve is shifted upward. This increases the price of western onshore oil and makes it compete less favorably with imported oil. This causes imported oil to be used rather than western onshore oil, and thus the relative sensitivities for this parameter in Table 1 are positive. If, on the other hand, the parameter new resources at twice the base price is increased, the cost-supply curve is lowered and the sensitivities are negative as shown in Table 1.

The ninth sensitivity listed in Table 1 is the total quantity of oil demanded in 1990. In the LFS model the quantity of oil demanded is specified exogenously as a function of time.[1] The structure of the model is such that this demand must be satisfied at each and every model time-point, so it might be expected that the responses considered in Table 1

would have a significant sensitivity to these parameters. That is, if the demand for oil is increased in the years 1980 to 2005, when a significant fraction of the demand is satisfied by imported oil, it is to be expected that the amount of imported oil would increase. The quantities demanded in the years 1985, 1995, and 2000 are not included in Table 1 because only the 10 largest sensitivities are listed. The relative sensitivities of the responses R_{IQ} and R_{IP} to these additional parameters are just slightly less than the lowest value shown in Table 1.

The last sensitivity listed in Table 1 is the specific capital cost of a west liquefaction facility. This specific capital cost is a parameter in a conversion process, i.e., a process that converts one form of energy into another, such as coal to synthetic oil, that is used to model the capital cost of a facility of unit capacity.[1,5] If the specific capital cost of west liquefaction is increased, the price of oil from west liquefaction increases, and therefore this oil will compete less favorably with imported oil. Thus, more oil will be imported as indicated by the positive sensitivities of this parameter shown in Table 1.

The relative sensitivities of onshore oil production in the year 2000, R_{ONS}, offshore oil production in the year 2000, R_{OFS}, and oil production from enhanced oil recovery in the year 2000, R_{EOR}, are shown in Table 2. Similarly, the relative sensitivities of synthetic oil production in the year 2000, R_{SYN}, oil production from shale and tar sands in the year 2000, R_{SHT}, and imported oil in the year 2000, R_{IMP}, are shown in Table 3. Precise definitions of these responses are given in Section 2.D. For each response the data elements having the five largest absolute relative sensitivities are given in the order of decreasing absolute value.

Table 2. Relative sensitivities of onshore oil production in year 2000, R_{ONS}, offshore oil production in year 2000, R_{OFS}, and enhanced oil recovery production in year 2000, R_{EOR}.†

Data element x	$\frac{x}{R_{ONS}} \frac{dR_{ONS}}{dx}$	Data element x	$\frac{x}{R_{OFS}} \frac{dR_{OFS}}{dx}$	Data element x	$\frac{x}{R_{EOR}} \frac{dR_{EOR}}{dx}$
New resources at twice base price for west onshore oil (15)‡	0.68	Efficiency of Alaskan oil transportation (9)‡	2.52	Base price for thermal EOR (17)‡	-0.47
Initial resource cost for west onshore oil (15)	-0.54	Efficiency of western oil transportation (4)	-0.84	Return on equity for thermal EOR in year 2000 (17)	-0.47
Capital technological change limit for west onshore oil (15)	-0.43	Initial resource cost for Alaskan offshore oil (24)	-0.72	Efficiency of Alaskan oil transportation (9)	-0.45
Return on equity for west onshore oil in 2000 (15)	-0.43	Return on equity for Alaskan offshore oil in 1995 (24)	-0.45	Year of availability§ for thermal EOR (17)	0.44
Base price for west onshore oil (15)	-0.25	Return on equity for Alaskan offshore oil in 2005 (24)	0.34	Undiscovered recoverable resources at base price for thermal EOR (17)	0.40

†See section 2.D for a detailed definition of R_{ONS}, R_{OFS} and R_{EOR}. (In the base case, R_{ONS} = 0.33, R_{OFS} = 0.13, and R_{EOR} = 0.18.)

‡Numbers in parentheses are activity numbers as specified in Fig. 1.

§In this case, the relative sensitivity is defined by taking the parameter x to be the year of availability minus 1980.

Table 3. Relative sensitivities of synthetic oil production in year 2000, R_{SYN}, of oil production from shale and tar sands in year 2000, R_{SHT}, and of imported oil in year 2000, R_{IMP}.†

Data element x	$\frac{x}{R_{SYN}} \frac{dR_{SYN}}{dx}$	Data element x	$\frac{x}{R_{SHT}} \frac{dR_{SHT}}{dx}$	Data element x	$\frac{x}{R_{IMP}} \frac{dR_{IMP}}{dx}$
Efficiency of Alaskan oil transportation (9)‡	-2.21	Efficiency of shale oil upgrading (7)‡	2.87	Efficiency of western oil transportation (4)‡	-5.64
Specific capital cost of west liquefaction plant (6)	-2.05	Efficiency of western oil transportation (4)	1.66	Price of imported oil in 1995 (2)	-1.74
Availability of west liquefaction plant (6)	2.04	Efficiency of Alaskan oil transportation (9)	-1.27	Efficiency of Alaskan oil transportation (9)	-1.68
Variable operating cost of west liquefaction plant (6)	-1.98	Base price of surface shale oil (13)	-1.20	Price of imported oil in 2000	-1.54
Efficiency of shale oil upgrade (7)	-1.26	Capacity factor multiplier for shale oil upgrading (7)	-0.71	Efficiency of eastern oil transportation (27)	-1.43

†See section 2.C for a detailed definition of these responses. (In the base case, $R_{SYN} = 0.10$, $R_{SHT} = 0.10$, and $R_{IMP} = 0.12$.)

‡Numbers in parentheses are activity numbers as specified in Fig. 1.

It is to be noted that all of the sources of supply, except natural gas plant liquids, are included in one of the responses being considered. In general, it is to be expected that for a given response the parameters with the largest sensitivities are parameters characterizing activities that enter into the definition of the response. By considering the sensitivities given in Tables 2 and 3, it can be seen that this is often the case, but not always. Many of the resource process parameters that occur in Tables 2 and 3 have been described in conjunction with Table 1. In discussing Tables 2 and 3, the meaning of the parameters will be discussed only if they did not occur in Table 1.

In the case of the response R_{ONS}, all of the parameters shown are from west onshore oil production even though east onshore oil and Alaskan onshore oil are included in the definition of R_{ONS}. This is, to some extent, because in the year 2000 in the base case west onshore oil is producing a larger quantity than either east onshore or Alaskan onshore, but it may also be influenced by other factors such as transportation cost, etc.

In resource processes in GEMS, the change over time in the capital cost of a representative facility due to technological changes is modeled.[5] The parameter capital technological change limit is used in this modeling. If the capital technological change limit is increased, the capital cost and thus the price of west onshore oil increases. Therefore, less onshore oil is used and the relative sensitivity of R_{ONS} is negative as shown in Table 2.

The return on equity is, as the name implies, the required rate of returns on equity funds. In GEMS and in the LFS this rate is allowed to

change over time, i.e., must be specified at each of the model time points, therefore a separate relative sensitivity is calculated for the return on equity at each of the model time points.

In the case of the response R_{OFS}, three of the parameters with significant relative sensitivities in Table 2 are from Alaskan offshore production and the other two are from Alaskan and western oil transportation. West offshore and east offshore production are included in the response R_{OFS}, but parameters from these supply sources, i.e., parameters from activity numbers 16 and 21, do not appear in the list of the five largest relative sensitivities. Since Alaskan offshore oil production in the year 2000 provides a large part of the response R_{OFS} in the base case, it is understandable that an increase in the efficiency of Alaskan oil transportation should give a significant positive sensitivity. That is, an increase in the efficiency of Alaskan oil transportation decreases the price of the oil and causes more Alaskan offshore oil to be used. Note, however, that the sensitivity of R_{OFS} to the efficiency of western oil transportation is negative. An increase in this efficiency will increase the quantity of all western oil, including western offshore oil, used in 2000. This increase will decrease the amount of Alaskan oil used, and thus the amount of Alaskan offshore oil used in the year 2000. So the efficiency change will cause R_{OFS} to increase because of the increase in western offshore oil and to decrease because of the decrease in Alaskan offshore oil, and the negative sign on the sensitivity means that the decrease was larger than the increase. This is a case where it would have been difficult to predict even the sign of the sensitivity if only base case values were available.

The response R_{OFS} has significant sensitivities to the return on equity for Alaskan offshore oil in 1995 and 2005. It is interesting to note that these two sensitivities have opposite signs. The increase in return on equity in 1995 increases the price of Alaskan offshore oil in 2000 and causes less to be used. On the other hand, an increase in the return on equity in 2005 causes more Alaskan offshore oil to be used in 2000. The relative sensitivity for return on equity of Alaskan offshore oil in 2000 is not given in Table 2, but its value is -0.31, so it is only slightly smaller in magnitude than the last two sensitivities in column 4 of Table 2. In considering this relative sensitivity it is to be noted that the equations of the model are completely coupled in time so a change in a parameter value at a specific time can change the model solution at all previous and all future times.

For the response R_{EOR}, four of the high sensitivity parameters in Table 2 are from thermal EOR and the other is from Alaskan transportation. The significant sensitivity of R_{EOR} to the efficiency of Alaskan oil transportation is interesting because from the network diagram in Fig. 1 there is no obvious connection between thermal EOR and Alaskan oil transportation. However, there is a connection in that Alaskan oil competes with all other sources of oil at activity 3, but from this fact alone the importance of the efficiency of Alaskan oil transportation would not be apparent. It should be noted that five of the six responses in Tables 2 and 3 have a significant sensitivity to the efficiency of Alaskan oil transportation. This illustrates the power of adjoint sensitivity theory for pointing out specific parameters that are of unusual importance. In the year 2000 most of the EOR production is from thermal rather than gas

or chemical EOR; therefore, it is to be expected that the parameters from thermal EOR would show the highest sensitivities.

The parameter "year of availability" for a resource process is, as the name implies, the year when production is allowed to begin on a commercial scale. In the GEMS program this parameter is input as a specific year, e.g., 1985. To define the relative sensitivity, the parameter has been taken to be the year of availability minus 1980. In the model the year of availability for thermal EOR is 1985. If this year is increased, production is delayed for a few years, but in later years the price is lower because the resource has not been depleted as much and this causes an increase in the amount produced. The positive sensitivity of R_{EOR} in Table 2 to the year of availability for thermal EOR indicates that more is produced from thermal EOR in the year 2000 than would have been produced if the year of availability had not been changed.

The sensitivities for synthetic oil production, i.e., for the response R_{SYN}, are given in the second column of Table 3. Three of the five parameters given in column 1 of Table 3 are from west liquefaction, and the other two parameters are from Alaskan oil transportation and shale oil upgrading. The importance of the efficiency of Alaskan oil transportation has been indicated previously. West liquefaction is supplying somewhat more oil in 2000 than east liquefaction and this is primarily why the parameters from west liquefaction have the larger sensitivities. Parameters from east liquefaction have relative sensitivities that are not much smaller than those shown in the table. (For example, R_{SYN} has a relative sensitivity to the specific capital cost of east liquefaction of -0.70.)

The availability is a parameter in a conversion process that is used to model the fraction of the time that a facility is available for production. The variable operating cost is a parameter in a conversion process that is used to model the annual operating cost of a facility of unit capacity. An increase in the availability of a west liquefaction plant decreases the cost of the product, and thus the sensitivity of R_{SYN} to the availability of west liquefaction is positive as shown in Table 3. An increase in the variable operating cost of a liquefaction plant increases the cost of the product and therefore decreases the amount of the product used. Thus, the sensitivity of R_{SYN} to the variable operating cost is negative as shown in Table 3.

The efficiency is a parameter in a conversion process that models, as the name implies, the efficiency of converting one form of energy into another. From Fig. 1 it can be seen that oil from shale competes directly with oil from west liquefaction, and thus an increase in the efficiency of the production of oil from shale should decrease the response R_{SYN} as shown in Table 3.

The relative sensitivities for oil production from shale and tar sands, i.e., for the response R_{SHT}, are given in the fourth column of Table 3. Parameters from production from tar sands do not occur among the five largest sensitivities because tar sands production is small compared to production from shale in the base case. Similarly, production from shale in situ is small compared to production from surface shale. The efficiency of shale oil upgrading was discussed above in conjunction with the discussion of the response R_{SYN}. This efficiency has a very direct effect on all production from shale, and therefore the response

R_{SHT} also has appreciable sensitivities to the efficiency of western oil transportation and the efficiency of Alaskan oil transportation. The sensitivity to the efficiency of western oil transportation is positive since an increase in this parameter would cause more shale oil to be used. Conversely, the sensitivity of the efficiency of Alaskan oil transportation is negative because an increase in this parameter would cause less shale oil to be used.

The capacity factor of a facility in the GEMS conversion process is taken to be a function of the ratio of the operating cost at a given time to the price at the same time of the commodity being produced. The functional form is such that the capacity factor varies from its maximum to zero, depending on the ratio, and the capacity factor multiplier is a parameter that may be specified to determine the ratio at which the capacity factor is one-half of its maximum value. In the case of shale oil upgrading, an increase in the capacity factor multiplier decreases the capacity factor and thereby decreases the amount of oil produced from shale. Thus, the sensitivity of R_{SHT} to the capacity factor multiplier is negative as shown in Table 3.

The relative sensitivities of imported oil, i.e., of the response R_{IMP}, are shown in the sixth column of Table 3. The largest sensitivity is for the efficiency of western oil transportation. Note that this sensitivity of -5.64 is the largest sensitivity of any shown in Tables 1, 2, and 3. This means that the quantity of oil imported in the year 2000 would decrease by 5.64% if the efficiency of western oil transporation were increased by 1%. The importance of the efficiency of western oil transportation has been discussed previously. (See the discussion of the first entry in Table 1.)

The prices of imported oil at all time points considered in the LFS model are input parameters, and it is to be expected that the quantity of imported oil would be sensitive to these prices. Since the response R_{IMP} concerns the quantity of oil imported in the year 2000,one would expect this response to be sensitive to the price of oil in that year and this is the case.

The response is also sensitive to the price of imported oil in the year 1995. As stated previously, the equations of the model are completely coupled in time, so it is quite feasible for an increase in the price of imported oil in 1995 to decrease the quantity of imported oil in 2000.

SUMMARY

Adjoint sensitivity methodology has been applied to a specific liquid fuels supply model that contains 461 variables and slightly over 1000 parameters. The success of the application has been verified by comparing selected sensitivities obtained by adjoint calculations with sensitivities obtained by direct calculations. The power of the methodology lies in the fact that sensitivities for any result of interest can be obtained for all of the parameters of the model and thereby those parameters that give the largest and the smallest sensitivities can be determined. On the basis of the large sensitivity information, the analyst may direct his attention at obtaining more reliable values for the relatively small number of parameters that have a significant influence on the results. Both the large and the small sensitivities present information to the analyst on the manner in which the model is operating and may lead to new insight and to the desirability of reformulating various parts of the model.

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