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A STUDY OF THE OPTIMAL TRANSITION TEMPERATURE OF PCM WALLBOARD FOR SOLAR ENERGY STORAGE

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ABSTRACT

In this report, we consider the performance of wallboard impregnated with phase change material. An ideal setting is assumed and several measures of performance discussed. With a definition of optimal performance given, the performance with respect to variation of transition temperature is studied. Results are based on computer simulations of PCM wallboard with a standard stud wall construction.

We find the diurnal heat capacity to be overly sensitive to numerical errors for use in PCM applications. The other measures of performance, diurnal effectiveness, net collected to storage ratio, and absolute discharge flux, all indicate similar trends. It is shown that the optimal transition temperature of the PCM is strongly influenced by amount of solar flux absorbed by the PCM.

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1. INTRODUCTION

The energy storage system is an important component of any passive solar energy application to space heating. Passive solar buildings can take advantage of the thermal mass of walls ceiling and floors to store energy during the day for release at night when the maximum heating load occurs. Recent work with phase change materials (PCM's) embedded in wall board offers the possibility of easily installed thermal mass on many of the interior surfaces of a building [1,2].

The thermophysical properties of the PCM's under consideration are controllable in manufacture [6]. In particular, a phase change transition temperature can be obtained suitable for a particular solar application. McCabe [3,4] has studied this problem both numerically and analytically for storage cylinders. In this paper we study the optimal transition temperatures for two PCM's under a variety of circumstances. The two PCM's are the hydrated salt, calcium chloride hexahydrate ($CaCl_2 \cdot 6H_2O$) and the paraffin wax, n-Octadecane. The development of measures of performance is given in [3 and 4]. We adapt McCabe's measures to the wallboard case and present a numerical comparison of the measures.

The application is to the heating of a solar building. Neeper observes [2] that the area of walls and ceilings available for installation of PCM wallboard in a solar house may be up to three times the floor area. With reasonable load to collector ratios most of this area will not be directly illuminated and charging of the PCM will be by means of the convective coupling between the room air temperature and the wall surface temperature. Those surfaces that are directly illuminated or receive radiation from a directly illuminated surface must also be considered. Neeper estimates that with a $+/-5°F$ swing in room temperature the convectively coupled surfaces can store $40 Btu/ft^2$. The PCM wallboard receiving additional solar energy should be able to store and discharge all the energy it receives. Thus it may be desirable to have one kind of PCM wallboard in a solar greenhouse or sunspace and another kind in the interior rooms. Indeed, the optimal (in a sense we must discuss) thermophysical properties for the PCM wallboard will depend on all the conditions imposed on the wall. One might expect some difference between the behavior of an internal wall and an external wall. In the case of an internal wall there may be charging and discharging from both sides of the wall. For an external wall, the weather conditions and the amount of insulation may have an important effect.

In this paper these effects are discussed based on consideration of one square foot of a layered wall with PCM wallboard on one side. For exterior surfaces, a standard stud wall construction will be used. The response of the PCM wallboard to varying amounts of direct solar flux and typical external weather data will be shown. In the first section of the paper, we discuss measures of performance of the simple unit area of wall and define a sense in which the performance might be considered optimal. The numerical model used to evaluate performance is presented in the second section. The third section gives results computed from the numerical model.

2. PERFORMANCE MEASURES

For this discussion we restrict our attention to a unit area of PCM wallboard in a somewhat idealized solar structure. The wallboard covers a standard stud wall construction. For simplicity only the potential for heating will be considered. The important heat fluxes for charging are q_c, the convective flux from the room to the wall, and q_d, the directly absorbed flux from the direct solar or from the reradiation of hot objects in the room. The important flux for discharging will be only q_c. In addition, we take into account the heat flux due to convection, q_r, from the back side of the wall to the outside air or to the interior air. To further simplify the setting of our study we assume that the room air temperature and the incoming direct radiation follow an "ideal" pattern. We assume that the room air temperature is 65°F during the night and 75°F during the day. The period of day will be taken as 12 hours long and the direct flux input to the PCM wallboard will follow a sine curve with its maximum at noon. The amount of direct solar input to the wall over the diurnal cycle will be denoted by S_{amt}, with units of $\frac{Btu}{day-ft^2}$.

The first requirement of the storage system is that it be appropriately sized. That is, the latent heat storage capacity should be large enough to accommodate the amount of energy it will receive during the charging cycle. Based on simple considerations, and the assumption that the surface temperature of the wallboard does not differ from the transition temperature of the PCM by very much, the thickness, L, of the PCM wallboard should be at least

$$L = \frac{1}{\rho H} \left(S_{amt} - 12h(T_{cr} - 75) + 12U(\overline{T}_{day} - T_{cr}) \right). \tag{1}$$

In this equation, ρ, is the density of the material ($\frac{lbm}{ft^3}$), H is the latent heat of fusion ($\frac{Btu}{lbm}$), T_{cr} is the transition temperature (°F), and h is the heat transfer coefficient between the room air and the PCM wallboard. The last term represents the heat loss out the back of the one square foot of wall board to either to the outside air or to the room air. Here U is the overall coefficient of heat transfer for the wall construction and $\overline{T}_{day}$ is the average daytime temperature to which the back side of the wall couples. Similarly, we refer to the average night time temperature as $\overline{T}_{night}$

Having more storage capacity than required does not adversely affect the performance of the system. If there is not enough storage, the energy in effect spills over the storage and the temperature of the PCM will rise creating greater heat loss to the outside air. Thus for large amounts of direct flux the performance will degrade.

The second requirement of the storage system is that it be possible to get the stored energy out during the discharge cycle. By equating the amount of flux in during the day to the amount of flux out during the night one arrives at the following estimate for the phase transition temperature:

$$T_{cr} = \frac{h}{h+U}70 + \frac{U}{h+U}\left(\frac{\overline{T}_{day} + \overline{T}_{night}}{2}\right) + \frac{S_{amt}}{24(h+U)}. \tag{2}$$

In this expression h is again the heat transfer coefficient between the wall and the room air, U is the overall heat transfer coefficient of the wall. The expression makes clear the strong dependence of transition temperature on the amount of direct solar absorbed by the wallboard. Also the effect of insulation, small U values, is apparent. If the back of the wall couples to an interior air space with the same 75/65 temperature swing, the first two terms combine to give simply 70. The second term also shows some of the dependence on external weather conditions for the case of an exterior wall. The appropriate critical temperature for mild days is slightly higher than that for a cold day. The heat loss of the wall is less on mild days and the energy that should be discharged to the room is thus greater.

We hesitate to call the above two requirements measures of performance, but certainly any system that is sized inappropriately or fails to deliver its stored energy under design conditions would not perform well. Other measures have been introduced which characterize a storage system and correlate with its performance. Probably the simplest measure of performance is to rate the wallboard as a heater in terms of the number of Btu's one might expect a square foot of wallboard to give up during the night. We will refer to this measure as $q_{discharge}$. An optimized PCM would then be defined as one which gives up the maximum number of Btu's per night, with the maximum being taken over the range of transition temperatures.

McCabe [4] discusses three measures of performance, the Net-Collected-to-Storage ratio (NCSR), the diurnal heat capacity (dhc), and the diurnal effectiveness (ϵ_d). For the case of storage cylinders, he shows their dependence on dimensionless parameters such as the Stefan and Biot number. The Net-Collected-to-Storage Ratio is defined as the ratio of the total heat stored during charge to the amount of heat storage that is available from latent heat alone. For an ideally sized system this ratio should be one. If the system is undersized, there is energy tied up in sensible heat and the heat loss during the day will be high. A ratio larger than one is indicative of this situation. If the system is oversized, or if the solar input is less than expected, the ratio will be less than one. As noted before, the wallboard thickness being larger than required does not degrade performance. So the Net-Collected-to-Storage ratio is more a measure of sizing than system performance.

The diurnal heat capacity, originally introduced by Balcomb [5], takes account of both the energy stored and the variation in surface temperature of the storage unit. Balcomb introduced the measure for sensible heat storage applications. McCabe [3] modified the definition so that it might also apply to latent heat storage. With this modification the diurnal heat capacity of the wall is the ratio of the amount of heat stored during the charge cycle to the difference in surface temperatures of the wallboard multiplied by the surface heat transfer coefficient. Since it has a singularity when the surface temperature remains constant, there are serious problems with the use of this measure of performance. Of course, with PCM wallboard, a constant surface temperature equal to the phase transition temperature is what we would like to achieve. As we will see, the diurnal heat capacity is overly sensitive to problem parameters and thus is not recommended as a numerical indicator of optimality.

Probably to overcome the problems with the diurnal heat capacity, McCabe also introduced a measure he calls the diurnal effectiveness, ϵ_d. This is the ratio of the convective discharge of the actual system to the convective discharge of an ideal system in which the energy is transferred at a constant rate. The ideal PCM wallboard system would discharge through the night maintaining a surface temperature of T_{cr}. The diurnal effectiveness is thus a measure of how far from ideal the actual discharge flux is. One would like to attain effectivenesses close to one. A number less than one indicates that the surface temperature has dropped below the critical temperature and that probably the PCM has totally discharged. Numbers greater than one might also be seen but they are anomalous.

Using the definition of optimal in terms of the discharge flux at night, we would like to compute the value of T_{cr} for a range of solar inputs. Then a computation of the above measures of performance for this "optimized" PCM wall, gives a comparison between the different measures.

3. A BRIEF DESCRIPTION OF THE NUMERICAL MODEL

The numerical model is based on the law of conservation of energy. As a pointwise statement, conservation of energy can be expressed as a partial differential equation involving the energy (or enthalpy) and the heat flux as

$$\rho \frac{\partial e}{\partial t} + \frac{\partial q}{\partial x} = 0. \qquad (3)$$

When discretized, or expressed in a control volume formulation, this takes the form

$$\frac{\partial e}{\partial t} = -\frac{q_r - q_l}{\Delta x}. \qquad (4)$$

The heat flux is expressed in terms of the temperature using the familiar Fourier's law, $q = -k \frac{\partial T}{\partial x}$. For the layered wall, the density of each layer is assumed to be constant though the conductivity, k, may change if the layer undergoes a change of phase. Each layer is divided into a number of control volumes with faces on the layer boundaries. Between layers we assume that temperature and flux are continuous. This gives rise to a resistive model for the conductivity at the interfaces. The time integration of Equation 4 is accomplished using an implicit Crank-Nicolson method. The non-linear equations resulting from the implicit time step are solved using Newton's method.

At each time step of the integration, information required to compute the measures of performance over a 24-hour period is gathered. The temperature/enthalpy profile of the wall may be output at fixed time intervals.

4. NUMERICAL RESULTS AND COMPARISON OF MEASURES OF PERFORMANCE

Using weather data for the first of the year from a Typical Meteorological Year weather tape and repeating the boundary conditions, the computer model was run until a periodic solution was reached. The starting point of the integration was at sunrise, 6 a.m., and the temperature profile through the wall at that time was computed from the steady state solution. Direct solar flux was a sine curve with the total number of Btu's absorbed during the day fixed by the parameter S_{amt}. On the last day of the simulation, day three, the data for the measures of performance were accumulated.

For each of the runs the wall construction was similar. A panel of PCM wallboard fronts a 3.5 inch insulating space (2×4 stud wall), followed by a half inch of asphalt sheathing board and a half inch of exterior wood siding. For interior walls, the construction had two panels of PCM wallboard separated by 3.5 inches of dead air. For interior walls the external temperature was assumed to be room temperature.

The third day of simulation of a calcium chloride hexahydrate PCM wallboard is shown in Figure 1. Shown in the figure are the flux, q_r, from the back side of the wall to the outside air; q_l, the flux into the wall by direct illumination; q_{lc}, the convective flux from the all to the room air; and *epres*, the energy present in the wall. The PCM is responding to a direct flux of $300 \frac{Btu}{ft^2}$ per day and weather data is for the first of the year in Albuquerque, a cold day. The high temperature of the outside air is 45°F and the low is 18°F. Table 1 gives the maximum flux, temperature and energy values corresponding to unity in Figure 1. The energy present in the wall can be seen to rise from its starting value of zero to a peak at about 5 p.m. At that point charging from the direct flux is balanced by the losses from the back of the wall and the discharge convective flux to the room. The PCM gives heat to the room once the surface temperature of the PCM is higher than 75 degrees. The interior surface temperature is shown with the curve labeled t11. The exterior air temperature is shown with the curve labeled t_{nn}. When the surface temperature reaches the critical temperature of the PCM, 81°F, it stops until the PCM is fully charged. As can be seen, the PCM never fully charges.

Table 1 also gives values for the measures of performance associated with the PCM wallboard. Again, it is evident that the transition temperature of 81°F is not appropriate to the amount of solar flux received.

Table 1. Calcium Chloride Hexahydrate, 81°F

Maximum T_{11}	81.0	°F
Maximum q_c	-4.47	Btu
Maximum energy	103.3	
$q_{discharged}$	-119	Btu/night
q_{stored}	188	Btu/day
NCSR inverse	1.69	
dhc	4.24	
ϵ_d	0.24	

A similar case was run for *n*-Octadecane wax. Figure 2 shows the results of the simulation. Again due to the high critical temperature, 82.4°F, the discharge is rapid. Table 2 gives the maximum values of temperature, flux and energy appearing as unity in Figure 2, along with the computed measures of performance. The surface temperature during the charge cycle rises above the transition temperature of the material. This can be attributed to the low conductivity of the liquid paraffin wax. It also shows that care must be taken in numerical modeling of wax impregnated wallboard. In our calculations we have used five nodal points through the thickness of the wallboard.

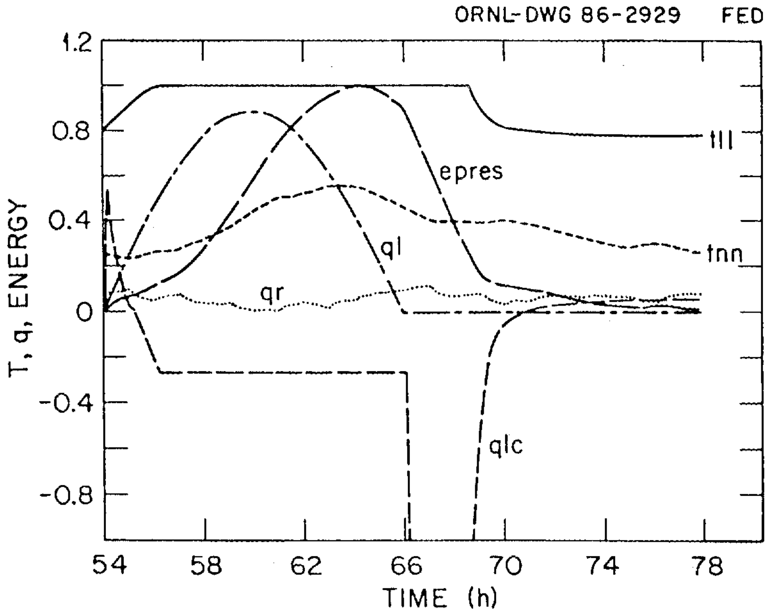

Figure 1. Diurnal cycle for calcium choloride hexahydrate with S_{amt} = 300 Btu/day, T_{cr} = 81°F. (Values normalized as per Table 1.)

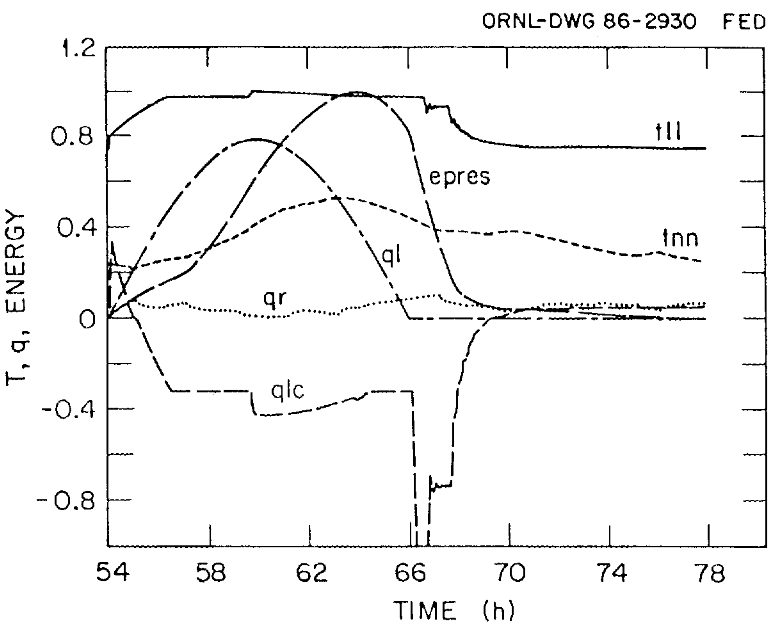

Figure 2. Diurnal Cycle for *n*-Octadecane. (Values normalized as per Table 2.)

Table 2. n-Octadecane, 82.4°F	
Maximum T_{11}	84.1 °F
Maximum q_c	-5.00 Btu
Maximum energy	281
$q_{discharged}$	-62.1 Btu/night
q_{stored}	129
NCSR inverse	1.71
dhc	2.43
ϵ_d	0.11

The primary numerical results of this study relate the transition temperature to the amount of absorbed direct flux. The following figures present this relation along with measures of performance of the system operating with the optimal transition temperature. The optimal transition temperature was obtained by maximizing the integral of the night-time discharge flux. Three day simulations were done to obtain each value of the objective function. The objective function, as dependent on the transition temperature, was minimized using a numerical minimization routine, FMIN. This routine uses a Golden section search method. The accuracy requested in this minimization was tol=1.e-2. The calculations were done on an IBM PC using FORTRAN double precision arithmetic.

Figures 3 and 4 show the normalized measures of performance and the optimal transition temperature associated with a given amount of directly absorbed flux on a one square foot panel of PCM wallboard. In these figures *de* is the diurnal effectivenss, *ncsri* is the inverse of the net collected to storage ratio, and *dhc* is the diurnal heat capacity. Both figures are based on runs using the January 1 weather data for Albuquerque. Figure 3 shows the calcium chloride hexahydrate system and Figure 4 shows the n-Octadecane system. The measures of performance show a degradation in performance when the amount of absorbed direct flux is above 360 Btu/day for the calcium chloride hexahydrate system and 200 Btu/day for the n-Octadecane system. This degradation represents sizing limitations of the half inch thick wallboard. A thicker wallboard would allow more latent heat storage. Though the diurnal heat capacity is overly sensitive to the surface temperature of the PCM, it does well in defining this sizing information. Tables 3 and 4 give the maximum values of the curves in Figures 3 and 4. This can be compared with the performance of the unoptimized systems given in Tables 1 and 2.

Table 3. Maximum Performance for $CaCl_2 \cdot 6H_2O$	
Maximum T_{cr}	77.87 °F
Maximum $q_{discharged}$	-298.4 Btu/night
Maximum q_{stored}	409.9 Btu/day
Maximum NCSR inverse	6.19
Maximum dhc	83.9
Maximum ϵ_d	0.98

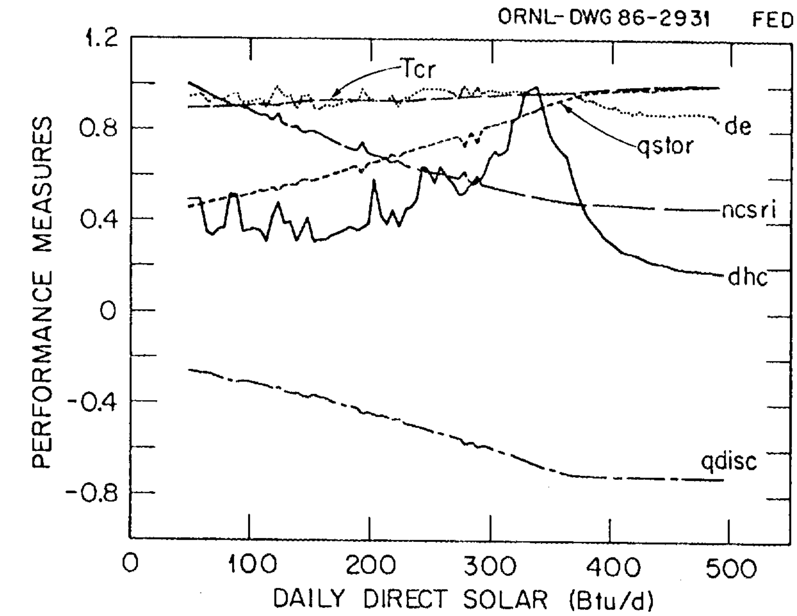

Figure 3. Measures of performance and optimal transition temperature for $CaCl_3 \cdot 6H_2O$.

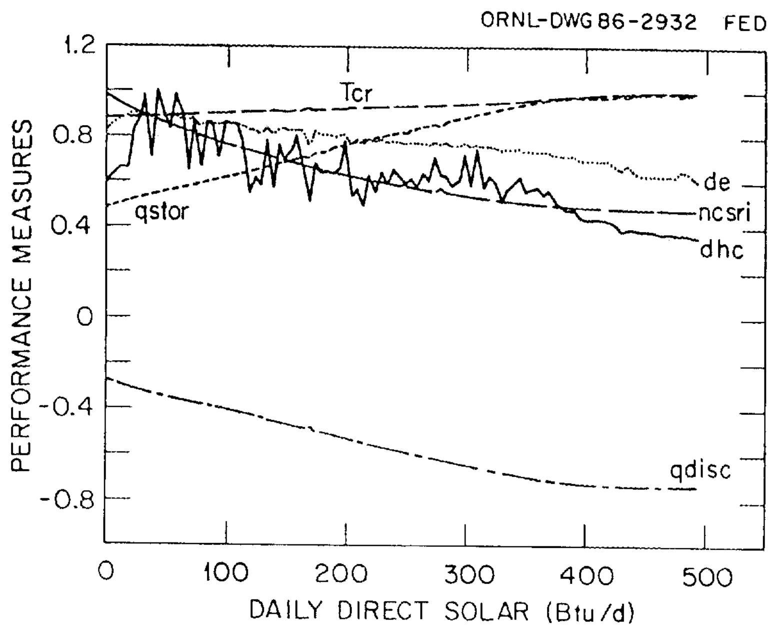

Figure 4. Measures of performance and optimal transition temperature for *n*-Octadecane.

Table 4. Maximum Performance for n -Octadecane	
Maximum T_{cr}	78.29 °F
Maximum $q_{discharged}$	-201.8 Btu/night
Maximum q_{stored}	273.6 Btu/day
Maximum NCSR inverse	1.69
Maximum dhc	12.3
Maximum ϵ_d	0.90

The optimal transition temperature is seen to increase linearly with the amount of absorbed direct flux received. Its value for no direct flux, the convectively charged case, is only slightly below the mean room air temperature. Its value for the absorbed solar flux of 350 Btu/day is 75.30°F in the calcium chloride hexahydrate system. In the n —Octadecane system, the value at 350 Btu/day is 75.06°F.

To illustrate the dependence of the optimal transition temperature on weather data, Figure 5 shows a mild winter day with high temperatures in the 60's and lows in the high 30's. The transition temperatures are slightly higher than the severe day case. The difference is not dramatic because of the good insulating value of the wall. For S_{amt} = 350 Btu/day, the optimal transition temperature for calcium chloride hexahydrate is 75.70°F. Maximum values are given in Table 5.

Table 5. Maximum Performance for $CaCl_2 \cdot 6H_2O$ Mild Day	
Maximum T_{cr}	78.15 °F
Maximum $q_{discharged}$	-310.7 Btu/night
Maximum q_{stored}	394.1 Btu/day
Maximum NCSR inverse	2.20
Maximum dhc	65.9
Maximum ϵ_d	0.98

The diurnal effectiveness remains high for any of the optimized systems. It begins to degrade only when the sizing problem manifests itself. As a measure of performance, it is equivalent to the optimality measure introduced with the discharge flux. The net collected to storage ratio is displayed using the inverse of its value. This again gives sizing information but does not offer much help in determining optimal performance for a given size.

5. CONCLUSIONS

We conclude that the diurnal effectiveness and the diurnal heat capacities are qualitatively different measures of the performance of a latent heat solar energy storage system. For the PCM wallboard it is possible to get very high diurnal efficiencies by

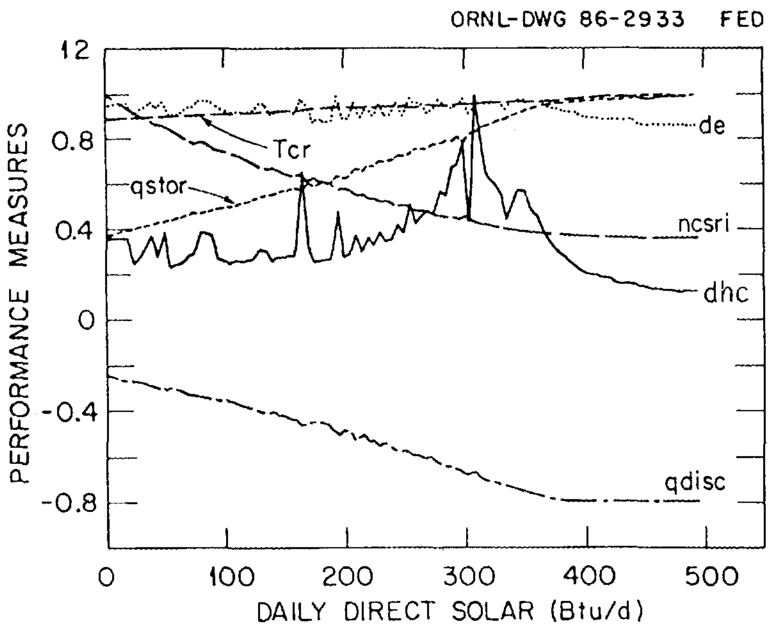

Figure 5. Measures of performance and optimal transition temperature for $CaCl_2 \cdot 6H_20$ on a mild day.

choosing the transition temperature to match the amount of direct flux received. The optimal transition temperature of a PCM wallboard can be seen to depend on the amount of solar flux the wallboard absorbs and the losses due to poor insulation or severe weather conditions. The optimal curve as computed by numerical simulation is linear for appropriately sized systems. Since this is the functional form predicted by the simple analysis of the first section, it would be reasonable to calibrate the simple expression with experimental results and use it instead of a numerical simulation for the design of solar structures using PCM wallboard. It would also appear that the effect of external weather conditions on the optimal transition temperature is not drastic. This will be particularly true for a well insulated wall. As a consequence, it should be possible for manufacturers of PCM wallboard to design wallboard taking into account only the amount of direct flux that a panel will receive.

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