

# SIMULATION OF RADIATION INDUCED MELTING AND SOLIDIFICATION IN THE BULK OF A TRANSLUCENT BUILDING FAÇADE

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## ABSTRACT

A translucent external wall system for solar space heating and daylighting is briefly presented. This system is composed of phase change material encapsulated in glass containers and a layer of transparent insulation material to reduce thermal losses to the environment. The melting process is induced by absorption of solar radiation in the bulk of the phase change material. In this article we focus on the one-dimensional mathematical-thermodynamic model of the store. The heat conduction and melting/solidification model with a term for the absorbed solar radiation employs continuous thermal properties of the phase change material. Based on this model a dynamic simulation program was developed, validated with measurements and successfully used for sensitivity analysis of system parameters. Results of these parameter studies are presented.

## 1. INTRODUCTION

In a national research project, a novel external wall system for solar space heating was investigated. This solar wall is composed of a translucent phase change material store covered by a transparent insulation which decreases the thermal losses to the environment. Since all the selected system components transmit visible light, this wall type can be used for daylighting purposes as well. The system employs an optical selective transmittance. Visible solar radiation is mainly transmitted, whereas invisible radiation is mainly absorbed and converted into heat, respectively phase change. Therefore, energy is stored and used for space heating purposes with a certain time delay. Figure 1 shows a vertical section through a prototype of this wall system with an overall thickness of about 280 mm. In this prototype wall, commercially available glass blocks were used as containers for the phase change material. A salt hydrate, calcium chloride hexahydrate with additions of other chlorides, was used as the storage medium. The melting enthalpy of this material is 192 kJ/kg and the mean melting temperature is 26.5 °C. For a more detailed description of the system we refer to [1] or [2]. For an overview about phase change materials we refer to Lane [3]. Recent results of research and application in

the domain of transparent insulation materials are available in [4].

This wall system was investigated experimentally and theoretically. The experimental investigations included spectral optical measurements on the storage material and long-term measurements on a prototype wall. The prototype system was built in a test facility and exposed to the natural climatic conditions for a five month period in the winter of 1993/94. About 60 physical parameters of the climate and the wall system were taken in time intervals of two minutes; mean values were stored in steps of one hour. These experiments are described in detail in reference [2]. The theoretical investigations performed until now include the development of thermodynamic and initial optical models of the system. A dynamical simulation program was developed which could be validated by long-term measurements on the prototype wall. Numerical simulations were carried out in order to study the dynamical behaviour of the system. In this article we will focus on the thermodynamic modelling of the phase change material store. Additionally we will present results of the system simulations.

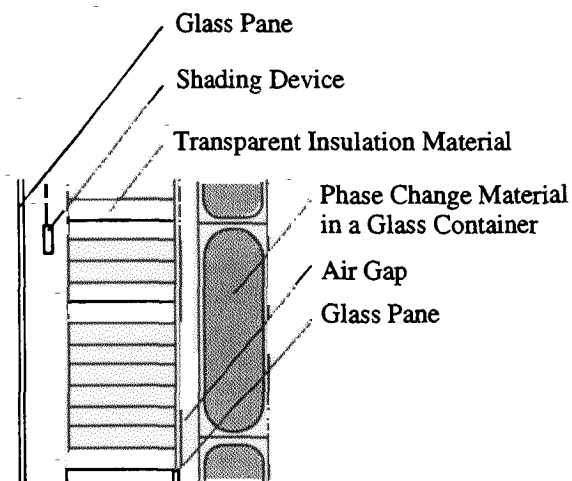


Fig. 1. External wall system for daylighting and solar space heating with translucent phase change material and transparent insulation.

## 2. MODELING OF THE THERMAL STORE

In many natural and technical processes melting and solidification occur. In the literature the mathematical formulation of this problem is named after Stefan [5], who studied the solidification of water in the polar sea at the end of the last century. Neumann [6] found an analytical solution to the problem for the case of a semi-infinite domain which is in an isothermal state at the initial time and is then exposed to a discontinuous temperature change at its boundary. In many practical applications, e.g. in solar energy engineering, the boundary conditions are stochastic and the problem has to be solved with the help of a computer. Several numerical methods are described in the literature. In general the thermal properties as functions of temperature used in these models are discontinuous at the melting temperature.

As already mentioned, in our experimental investigations we used a salt hydrate with additions of chlorides as phase change material for thermal storage purposes. Such mixtures do not show a sharply defined melting point but rather a melting region. In order to be able to describe the dynamic behaviour of such a material, a model was developed at our institute in which the thermal properties of the material are treated as continuous functions of temperature. This model was successfully tested in several applications. A detailed description of this continuous properties model is available in [7].

In order to apply this model we have to make the following assumptions:

Thermal radiation in the bulk of the material and natural convection in the liquid phase are neglected.

The density is constant ( $\rho = \rho_{\text{liq}} = \rho_{\text{sol}}$ ).

The heat conductivity  $k$  and the specific heat  $c_p$  are continuous functions of temperature.

Effects of sub-cooling are neglected.

In the case of the mentioned external wall system (see fig. 1), we used a one-dimensional approach to describe the melting/solidification problem in the storage material. With Fourier's law of heat conduction and the energy conservation equation we obtain

$$\rho \cdot \frac{\partial h}{\partial t} + \frac{\partial}{\partial x} \left( -k \cdot \frac{\partial T}{\partial x} \right) + \frac{\partial G}{\partial x} = 0. \quad (1)$$

$x$  denotes the space co-ordinate,  $T$  the temperature,  $G$  the intensity of solar or short-wave radiation in the bulk of the material and  $h$  the specific enthalpy. The term for the volumetric heat source  $\partial G/\partial x$  has to be calculated with an optical model of the store, taking into consideration the spatial and spectral distribution

of the incident solar radiation and the spectral space-dependent optical properties of the storage medium [2]. The relation between specific enthalpy and specific heat is defined as

$$h(T) = \int_0^T c_p(T) dT \quad \text{and} \quad c_p(T) = \frac{dh}{dT} \quad (2)$$

Performing the inner derivative

$$\frac{\partial h}{\partial t} = \frac{dh}{dT} \cdot \frac{\partial T}{\partial t} \quad (3)$$

and using equation 2 and applying the product law of differential calculus one obtains

$$\rho \cdot c_p \cdot \frac{\partial T}{\partial t} - \frac{\partial k}{\partial x} \cdot \frac{\partial T}{\partial x} - k \cdot \frac{\partial^2 T}{\partial x^2} + \frac{\partial G}{\partial x} = 0. \quad (4)$$

The thermal diffusivity is

$$\alpha(T) = \frac{1}{\rho} \cdot \frac{k(T)}{c_p(T)} \quad (5)$$

The assumption of a constant density implies that no material transport has to be taken into account during the melting/solidification process. With equation 5 the following non-linear partial differential equation results:

$$\frac{\partial T}{\partial t} = \alpha(T) \cdot \left[ \frac{\partial^2 T}{\partial x^2} + \frac{1}{k(T)} \cdot \left( \frac{\partial k}{\partial x} \frac{\partial T}{\partial x} - \frac{\partial G}{\partial x} \right) \right], \quad (6)$$

$$q'_{\text{source}} = \frac{\partial G}{\partial x}$$

Figures 2 and 3 show four thermal properties of the phase change material which was used in our experimental investigations as functions of temperature. The empirical fit functions  $k(T)$  and  $c_p(T)$  were found by taking into consideration the known thermal properties in the pure solid and the pure liquid phase; additionally the melting enthalpy was known. These functions were used for system simulations.

Two boundary conditions belong to equation 6, given by the heat fluxes from the store to the transparent insulation respectively to the room

$$\left( -k(T) \cdot \frac{\partial T}{\partial x} \right) \Big|_{x=0} = q_{\text{TI}}$$

$$\left( -k(T) \cdot \frac{\partial T}{\partial x} \right) \Big|_{x=d} = q_{\text{room}} \quad (7)$$

and the initial condition

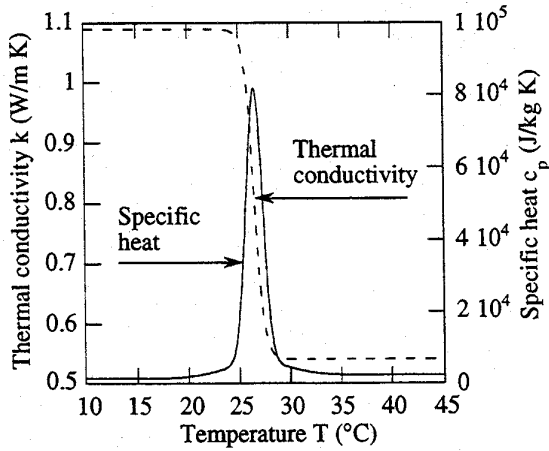


Fig. 2. Specific heat and thermal conductivity of a phase change material as a continuous function of temperature.

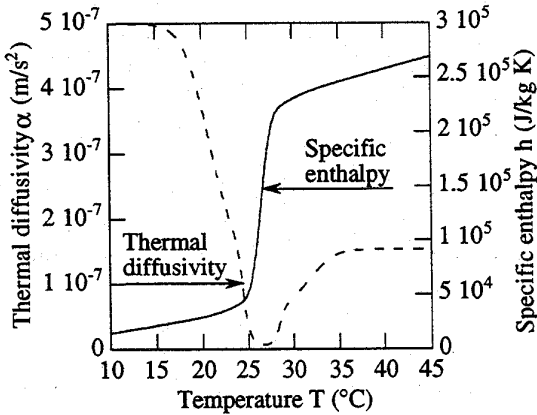


Fig. 3. Thermal diffusivity and specific enthalpy of a phase change material as a continuous function of temperature.

$$T(x)|_{t=0} = T_{\text{initial}}(x) \quad (8)$$

Equation 6 can be discretized in space and time

$$T_{m+1,n} = T_{m,n} + \alpha(T_{m,n}) \cdot \Delta t \cdot$$

$$\left\{ \frac{T_{m,n+1} - 2T_{m,n} + T_{m,n-1}}{(\Delta x)^2} + \frac{1}{k(T_{m,n})} \right. \\ \left. - \frac{[k(T_{m,n}) - k(T_{m,n-1})] \cdot [T_{m,n} - T_{m,n-1}]}{(\Delta x)^2} \right\} - \dot{q}'_{\text{source},m,n} \quad (9)$$

$m$  denotes the time step,  $n$  the space step and  $\dot{q}'_{\text{source},m,n}$  represents the discretized function of

the volumetric heat source due to the absorbed solar radiation in the storage medium.

Based upon this model a computer program was developed and tested by comparing the results of the simulations in a case in which an analytical solution was found by Neumann [6]. As already mentioned, Neumann developed a solution of the melting/solidification problem for the case of a semi-infinite domain which is initially at a constant temperature and then is exposed to a discontinuous temperature change at the boundary. We used values for the melting temperature, the melting enthalpy, the thermal conductivity and the density of calcium chloride hexahydrate with additives, which are available in reference [3]. In this test a fictitious enthalpy function was chosen, consisting of two exponential functions with the temperature difference  $\tau$  as a parameter for the width of the melting regime [7]. Within the temperature difference  $2\tau$  a share of  $1/e$  of the melting enthalpy is included. For  $\tau=0$  a discontinuous enthalpy function results which corresponds to the Neumann solution. We performed simulations with different widths of the melting regime  $\tau$ . For a decreasing  $\tau$ , the results converge as expected from the Neumann solution. Figure 4 illustrates the temperature as a function of the space co-ordinate. The discontinuity of the thermal properties in the case of the Neumann solution ( $\tau=0$ ) results in a kink in the temperature distribution.

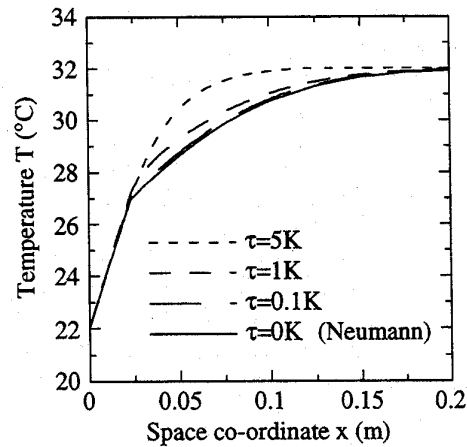


Fig. 4. Temperature distributions as a function of the space co-ordinate for different widths of the melting range. For very steep enthalpy functions, the Neumann solution can be obtained approximately. This temperature distribution shows a kink at the position of the melting front.

### 3. SIMULATION PROGRAM

In order to study the time-dependent behaviour of the system a simulation program was developed. The modular structure of the program, which is composed of four main procedures, is illustrated in figure 5. One of the main procedures has the task of solving the so-called Stefan problem. The programming language Pascal was used. Climatic data in time steps of one hour determine the boundary conditions of the system. To obtain numerical convergence in the Stefan problem procedure, this time step had to be divided further. With a time step of two seconds to solve the Stefan problem, the program ran successfully. Important output parameters are the intensity of the short-wave radiation transmitted into the backing room, the temperature distribution in the store and the energy fluxes from the store to the room, respectively to the environment.

This simulation program was tested with long-term measurements on a prototype external wall. Over a long time period measurements and simulations were in agreement. These comparisons are documented in reference [2].

### 4. SIMULATION RESULTS

As an example demonstrating the system behaviour we took a time period of eight days in February from the semi-synthetic climatic data DRY (design reference year) for the location Zurich, Switzerland. Figure 6 illustrates the irradiance on a vertical south-oriented façade and the ambient temperature. The calculated response of the system is shown in the next two figures. In figure 7 one can see that the intensity of the transmitted short-wave radiation as a function of time has significant peaks corresponding to the irradiance in figure 6. Due to the phase change, the temperature in the store and the heat flux into the room is almost constant over a long period of time. The temperature in the room was assumed to be constant at 20 °C. In figure 8 the total energy flux into the room, composed of a flux of heat energy and a flux of short-wave radiation, is shown. After three sunny days, the fraction of melted material is higher than 0.8. As a result of this stored energy, the thermal losses through the south-oriented wall are very low during the following four days with low irradiance. In figure 8 the open state of the roller blind is marked by "1" and the closed state by "0". In order to minimize the thermal losses, the roller blind is closed during the night.

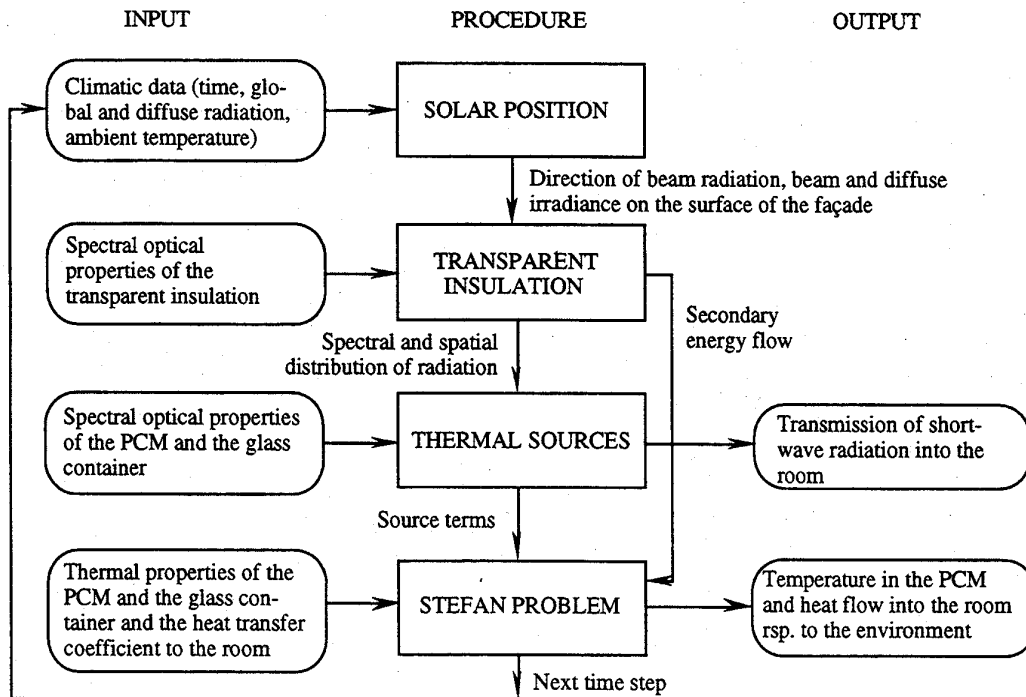


Fig. 5. Structure of the program which was used for simulation of the translucent wall. The program is divided into four main procedures. In the procedure "Stefan problem" the melting and solidification of the PCM is solved for stochastic boundary conditions.

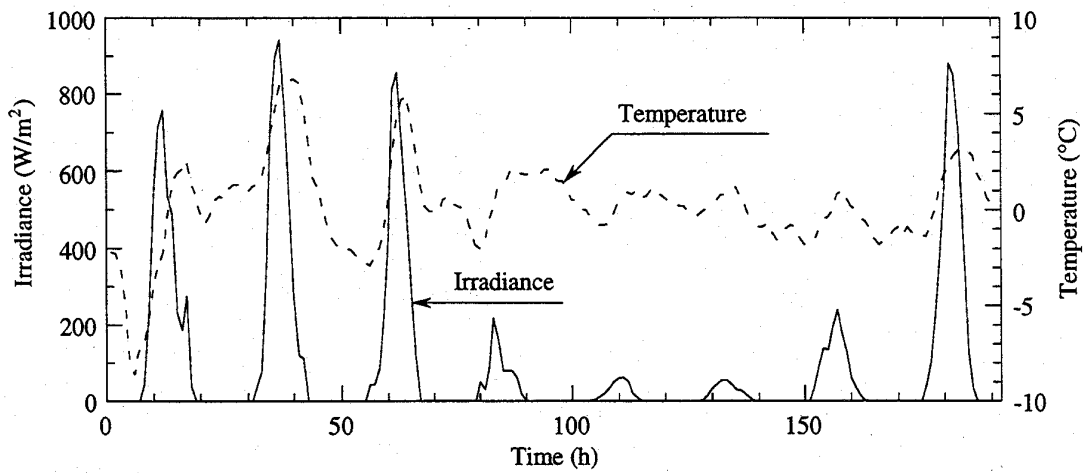


Fig. 6. Irradiance on vertical south-oriented surface and ambient temperature during eight days in February for the location Zurich, Switzerland (design reference year).

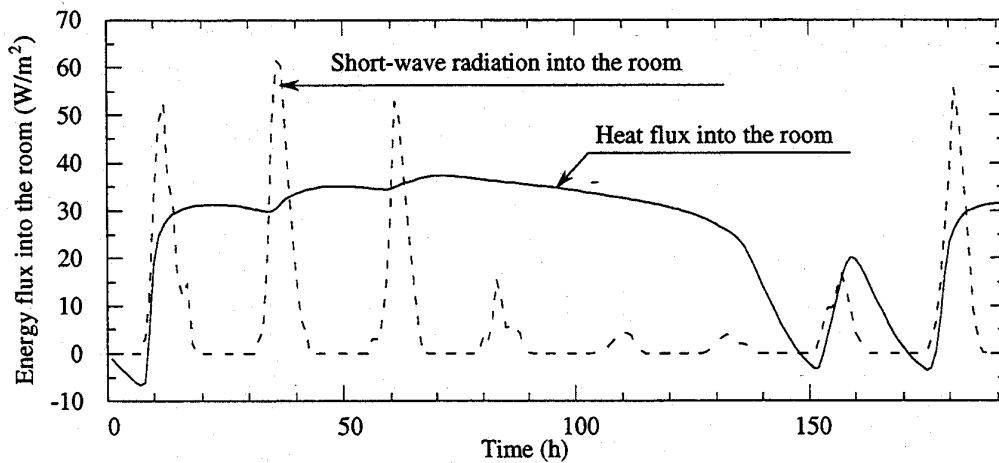


Fig. 7. Calculated "heat flux into the room" and "short-wave radiation into the room" as a function of time. The climate from fig. 6 was used as input for the simulation.

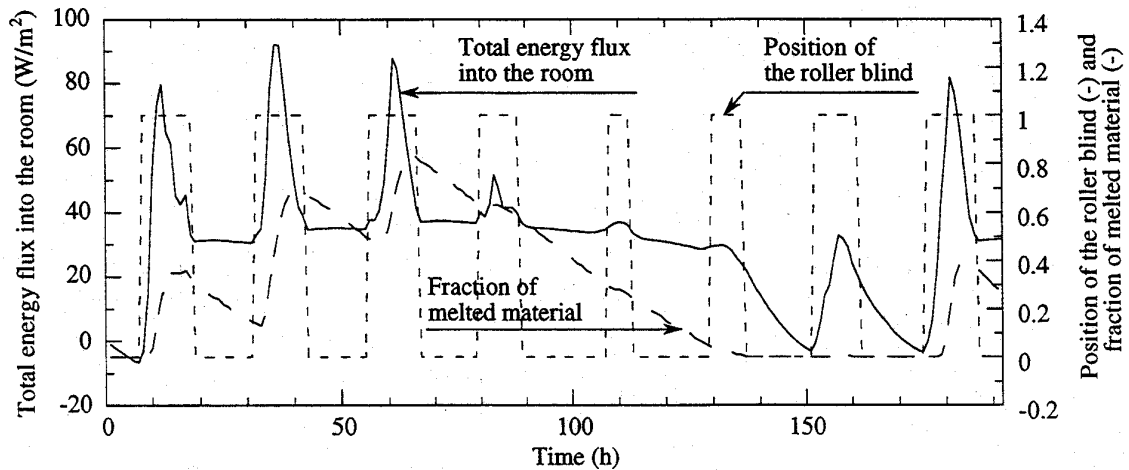


Fig. 8. Calculated "total energy flux into the room", "fraction of melted material" and "position of the roller blind" as a function of time. The climate from fig. 6 was used as input for the simulation.

	Oct	Nov	Dec	Jan	Feb	Mar	Apr
$\bar{\vartheta} (^{\circ}\text{C})$	10.0	3.9	1.7	-0.4	0.3	5.6	8.3
$\overline{G}_{\text{tot}} (\text{W} / \text{m}^2)$	98.6	64.1	48.4	66.8	100.3	123.3	126.1
$\bar{q} (\text{W} / \text{m}^2)$	37	23	13	24	34	42	40
$\bar{\eta} (-)$	0.38	0.36	0.27	0.36	0.34	0.34	0.32

Tab. 1. This table shows the monthly mean values of the ambient temperature  $\bar{\vartheta}$  and the irradiance on a vertical surface  $\overline{G}_{\text{tot}}$  for the location Zurich, Switzerland. The climatic data stem from the design reference year DRY. The variable  $\bar{q}$  stands for the monthly mean energy flux into the building and  $\bar{\eta}(-)$  for the monthly system efficiency.

Keeping the other parameters of the prototype fixed, we varied only the mean melting temperature. As a result we plotted the "fraction of time with an energy gain" and the "total energy flowing through the wall" normalized with the absolute values of our prototype wall as a function of the mean melting temperature. The climatic data stem from the design reference year DRY from November 1th to January 31th for the location Zurich, Switzerland. Figure 9 shows the results of these simulations.

In comparison with the mean melting temperature of the phase change material in the prototype wall, which is about 26.5 °C, a lower mean melting temperature would lead to a higher fraction of time with an energy gain for the building. However in this case, a decrease of the total energy flowing into the building would occur. An optimization of the mean melting temperature has to take into account the thermodynamic behaviour of the building. Table 1 shows monthly mean values of ambient temperature and irradiance for the mentioned set of climatic data. Monthly mean values of the total energy flux into the room and mean values of the system efficiency are also tabulated. Due to optical and thermal losses, only about one third of the energy of the incident solar radiation can be used.

## 5. CONCLUSIONS AND OUTLOOK

In order to study the dynamic behaviour of a novel external wall system for daylighting and solar space heating, the continuous properties model was successfully applied to describe the melting/solidification problem in the phase change material store. The investigations showed that this wall system is more than just a day/night storage device. For example, with the system parameters of the prototype it is

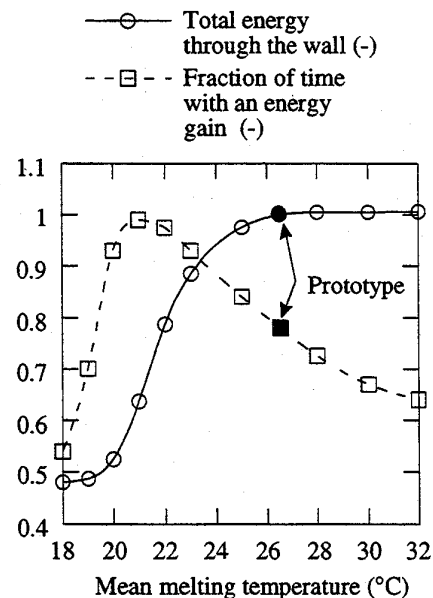


Fig. 9. Results of simulation runs from November 1th to January 31th. The climatic data stem from the design reference year DRY. The vertical axis shows the "relative total energy flowing through the wall" and the "fraction of time with an energy gain" normalized with the absolute values of our prototype wall as a function of the mean melting temperature.

possible to eliminate almost all heat losses through the wall to the environment, during a four day period with very low irradiance in winter time, assuming a high fraction of melted material at the beginning. Thanks to the promising results, we will continue our investigations on the system. At present, we are attempting to improve our knowledge concerning the optical processes in the phase change material store

by further experimental and theoretical investigations. In the new models, we take into account multiple scattering at low temperatures in the bulk of the crystalline storage material. A Monte Carlo method was chosen to study the propagation of light in the storage medium. These more detailed models are necessary in order to provide better fundamentals for further sensitivity analysis of optical system parameters.

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## NOMENCLATURE

$\alpha$	thermal diffusivity
$\rho$	density
$\tau$	width of the melting regime (temperature difference)
$c_p$	specific heat
G	irradiance
h	specific enthalpy
k	thermal conductivity
t	time
T	temperature
$\dot{q}_{\text{source}}$	volumetric heat source
x	space co-ordinate
<i>Indices:</i>	
n	space step
m	time step