ON THERMAL MODELLING OF WALLS AND SOLAR ENERGY APPLICATIONS

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ABSTRACT: after a short review of the theory associated with the numerical approximation of the diffusion equation for heat flow through solid elements of buildings, the paper concentrates on the effects of various discretisation schemes and nodal densities in terms of the effects on transient heat storage and surface temperature fluctuation. Since this is the most widely used method, the paper focuses on finite-difference modelling. However, the main conclusions are applicable to other numerical approaches as well. By practical applications, representing typical passive solar cases, it is demonstrated that it is easy to introduce - but also relatively easy to minimize - errors due to nodal discretisation of building structures.

Symbols

- $B_1$: Biot number ($h 1/2d \lambda^{-1}$)
- $d$: wall thickness, m
- $d'$: effective thickness ($2x_{th}^{-1}$)
- $m$: m
- $F_0$: Fourier number ($\tau h \Delta x^{-2}$)
- $h$: convective heat transfer coefficient, W m$^{-2}$K$^{-1}$
- $n$: space step level
- $s$: time step level
- $t$: cycle time, s
- $t_0$: cycle time, t
- $\alpha$: thermal diffusivity, $m^2$s$^{-1}$
- $\beta$: implicit/explicit weighing factor, -
- $\theta$: temperature, °C
- $\lambda$: thermal conductivity, W m$^{-1}$K$^{-1}$

1. INTRODUCTION

In (passive) solar applications in buildings, two effects are generally of major importance:
- the temporary - ie transient - storage of thermal energy in the building structure,
- the value and fluctuation of inside surface temperatures, since these greatly influence:
  1. thermal comfort of the occupants, and
  2. the re-distribution of solar energy (absorbed on internal surfaces) over the zone bounding surfaces.

A dynamic thermal (computer simulation) model of a building must incorporate a method for representing conduction heat flow in the solid elements of the building. This involves representing the continuous materials by a "network of nodes" and associated thermal capacities.

The number of nodes used must on the one hand be large enough to achieve a sufficient level of accuracy, but on the other hand be small enough to avoid excessive computational effort.

The accuracy not only depends on the number of nodes but also on the discretisation scheme. This problem is not new. The features of various numerical approximations to heat conduction can be found in textbooks and other literature. However the discussion is usually restricted to infinite or semi-infinite walls of a homogeneous material.

After a short review of the associated theory, we concentrate on the effects of various discretisation schemes and nodal densities in terms of the above two effects of transient storage and surface temperature fluctuation. Since this is the most widely used method, here we focus on finite-difference modelling.

In view of the scope of this conference, it does not seem appropriate to give a detailed theoretical treatment of the subject. Instead we want to demonstrate the practical consequences by cases, representing typical passive solar applications.

Many aspects of modelling are generic rather than application specific. This paper will concentrate on the generic as much as possible. Where specifics are required the point of reference will be the ESP-r building and plant energy simulation environment (Clarke 1985; Hensen 1991; Aasem et al. 1993).

2. BACKGROUND THEORY

The one-dimensional heat conduction equation may be written in the form

$$\frac{\partial \theta}{\partial t} = \alpha \frac{\partial^2 \theta}{\partial x^2}$$

where $\alpha$ is the thermal diffusivity. There are many different methods for dealing with it. As described in many textbooks (eg Incropera and DeWitt 1990), simplicity in approach is often a good starting point. Therefore the first thing to do is to calculate the Biot number (for a plane wall $B_1 = h0.5d \lambda^{-1}$). If this number is much less than unity (say $B_1 < 0.1$), then it is sufficient to use the so-called lumped capacitance method to obtain accurate results with minimal computational requirements. However, if $B_1$ is not much less than unity, spatial effect must be considered, and some other method must be used; eg a numerical approach.

As described by eg Waters and Wright (1985) there is, in principle, an infinite way of formulating a finite-difference (numerical) approximation to equation (1). No single or family of schemes is known to be superior. Many building thermal models use one of the comparatively simple difference schemes belonging to the family:

$$\theta^{n+1} - 2\theta^n + \theta^{n-1} = F_0 \theta^n (\Theta_{n+1} - 2\Theta_n + \Theta_{n-1}) + F_1 (1 - \gamma) (\Theta_{n+1} - 2\Theta_n + \Theta_{n-1})$$

where $F_0$ is the so-called Fourier number ($\tau h \Delta x^{-2}$), and $\gamma$ is a dimensionless parameter which must be chosen to be within the range $0 \leq \gamma \leq 1$. Setting $\gamma = 0$, 1/2, 1 gives respectively, the classic explicit, the Crank-Nicolson, and the fully implicit schemes.

The accuracy of this family of schemes may be controlled by appropriate choice of $\gamma$ and $F_0$. The choice is restricted however by the need to ensure stability and the desirability of preventing oscillatory solutions. Figure 1, presented by Waters and Wright (1985) and due to Crandall (1955), illustrates the
regions of instability and oscillatory behaviour in the $\gamma - F_n$ plane, and shows the point were the spatial error is minimised (at $\gamma = 0.127$ and $F_n = 0.224$), which is in the region of stability and non-oscillation. Although in principle it is always possible to choose these values of $\gamma$ and $F_n$, this is often not very convenient when operating a general purpose building thermal model. Low accuracy calculations with minimal computational effort are often acceptable, but high accuracy should be possible when required. The most practical way of achieving this is to use long time steps (say 1 h) and large space increments for approximate calculations.

Many buildings contain thin layers of materials which are thermally important. Thus $F_n$ is often large. Typically for a 1-h time step $F_n$ may be in the range $1 < F_n < 100$, which is in turn suggests that it is preferable to choose $\gamma > 1/2$ to avoid stability problems.

Waters and Wright (1985) came to the conclusion that for these circumstances (where both $\gamma$ and $F_n$ are far from their optimum values) it is best to distribute the nodes in such a way that $F_n$ is everywhere the same. However, many thermal models do not offer such a facility. As will be demonstrated later it is not really necessary either.

With respect to distribution of nodes it is important to consider the heat wave penetration depth or effective thickness $d'$ which is that distance from the material surface where the amplitude of the cyclical temperature fluctuation at the surface is reduced to 1/e of its original value: $d' = \sqrt{\frac{\gamma}{\omega \rho c}}$, where $\gamma$ is the cycle time (at a depth of 3 $d'$ the amplitude will only be 5%). For instance a common material with $\alpha = 10^4 m^2 s^{-1}$ (eg insulation or concrete) and cycle times of 1 year, 1 day, 1 hour, and 1 minute respectively $d'$ will be 3.17 m, 0.17 m, 0.034 m, and 0.004 m. It will be obvious that in numerical simulation involving cyclical temperature fluctuations, there should be a node in the region of $d'$ otherwise any transient effects due to this fluctuation cannot be taken into account. In terms of the above example, suppose we have a concrete wall and study a 24 h fluctuation, then there should be a node representing the first 0.17 m of the wall. However if we study a 10 minute fluctuation (as is typical the case if a (solar) plant is involved), then there should even be a node representing the first 0.015 m.

Obviously there is a relation between $F_n$ and $d'$. If we would use a time step of $= t/10$ then $F_n = 1$ effectively means that $\Delta t = 0.56 d'$; for $F_n = 1/3$ we get $\Delta t = 0.97 d'$. If the time step would be $= t/24$ then $F_n = 1 = \Delta x = 0.36 d'$, and $F_n = 1/3 = \Delta x = 0.63 d'$.

For the boundary of a homogeneous layer (exposed surface layer) equation (2) is not applicable. Instead one employs discretisation of the incoming or outgoing heat flux which is then treated similar to (2). It is possible to devise various nodal schemes for an exposed boundary layer. Hoen (1987) tested various options and (from analytical validation of cases for which exact solutions exist) came to the conclusion that the results quite well represent the exact solution provided that the surface node does not have any heat capacity; ie the first node with heat capacity is "buried" in the material. As will be demonstrated later, this is however related to the Fourier number; ie when $F_n$ is chosen favourably a scheme employing a surface node with heat capacity does give accurate results.

3. APPLICATION

The above theory may best be illustrated by some practical demonstrations. For this we start from some typical homogeneous constructions which are quite common for buildings (including (passive) solar applications). The material properties and dimensions are collected in Table 1.

For each construction a number of simulations were performed. The case being studied concerned a sudden change in ambient temperature on either side of the construction. Initially there is a steady-state situation in which all temperatures (ambient and inside the construction) are equal to 0°C. At some point in time (say at $t = 0$), the ambient air temperature is suddenly raised to 20°C. There is no radiant heat exchange, and the convective heat transfer coefficients $h$ are assumed to be 3 W m$^{-2}$ K$^{-1}$.

All calculations were carried out with ESP-r, which is based on the control volume heat balance method. The current implementation assumes one-dimensional heat flow and uses a mixed implicit/explicit discretisation scheme with $\gamma = 0.5$, ie the Crank-Nicholson scheme. Each single layer of material (as introduced by the user) is represented by two surface nodes (each representing 1/4 of the layer's thermal capacitance) and one central node (representing 1/2 of the layer's thermal capacitance). The nodes are connected with two (equal) thermal resistances. Thus, in ESP-r, exposed surface layer nodes do represent a heat capacity. As will be demonstrated, this gives accurate results provided that the Fourier number is chosen favourably. The reason to use this type of nodal scheme in ESP-r is that it is "symmetrical" for each layer, which implies major numerical and implementation advantages. ESP-r has been subjected to a rigorous validation exercise (CEC 1989). From this the conclusions with respect to heat conduction, state that (after reviewing theory and solving techniques, and performing code checking, analytical tests and sensitivity studies) no major bugs were found with regard to ESP-r's conduction algorithm and overall solving strategy.

For the problem described above (ie plane wall with convection), Schneider (1955) provides an exact solution for the surface temperature $\theta_s$ in case of the lumped capacitance method:

$$\theta_s = \theta_{s0} + \Delta \theta (1 - e^{-2\omega t/\rho c})$$

(3)

where $\theta_{s0}$ denotes the initial temperature, $\Delta \theta$ the ambient temperature step change, and $d$ the wall thickness.

In case the lumped capacitance method is not applicable, Schneider (1955) provides as exact solution:

$$\theta_s = \theta_{s0} + \Delta \theta \left(1 - \sum_{m=1}^{\infty} \frac{\sin m\theta_s}{2m} + \sin 2m\theta_s e^{-\frac{2\omega t}{\rho c}} \cos m\theta_s \right)$$

(4)

where values for $m\theta_s$ can be found in Schneider (1955).
As indicated in the introduction there are two aspects which are of particular interest: the surface temperatures and the amount of stored heat.

3.1. Surface Temperatures

Let us first consider the surface temperatures. Figures 2, 3, and 4 show the surface temperature evolution for respectively the aluminium, insulation and concrete plane walls, after a 20 K step change in ambient temperature. In each case, the wall is modelled as a single layer, and different time steps were employed. For each case the Biot number and the Fourier numbers are indicated.

![Figure 2: Evolution of surface temperature for aluminium (B_t = 1.5 \times 10^{-5}) modelled as 1 layer, using different time steps](image)

The horizontal parts of the stair-case temperature lines, represent the average temperature during a time step as calculated. In case of the aluminium the Biot number is such that the lumped capacitance method would have been applicable. However since it is common to use the same method throughout in a general purpose building thermal model (as is the case in ESP-r) here the finite difference method was used. In the case of the aluminium we have very high Fourier numbers which probably cause the oscillatory behaviour (as predicted by Figure 1). Ideally, it should have been possible to refer to a fully implicit scheme in this case, as can be seen from Figure 1.

![Figure 3: Evolution of surface temperature for insulation (B_t = 3.3 -) modelled as 1 layer, using different time steps](image)

This oscillatory behaviour can also be seen in case of the insulation (Figure 3). However the oscillations disappear when the time step and hence $F_r$ decrease. In case of the concrete (Figure 4), there seems to be no distinction between the various time step lengths.

Simulations were performed for concrete using a time step of 3600 s, and modelled as 1, 2, or 3 layers. Although there was a range in $F_r$, the results were only slightly affected. The biggest differences occurring in the period immediately after the ambient temperature change.

Figure 5 shows the results for concrete using a time step of 60 s, and modelled as 1, 3, or 8 layers. From these results it is quite clear that if we are interested in small time steps, the number of layers is very important if we want to have accurate results for the surface temperature. As explained earlier there are two effects which play a role in this specific case: (1) the Fourier number, and (2) the fact that the surface node represents a heat capacity. Nevertheless, it may be clear from Figure 5, that if the Fourier number is chosen favourably, the results are quite accurate.

![Figure 4: Evolution of surface temperature for concrete (B_t = 0.16 -) modelled as 1 layer, using different time steps](image)

3.2. Heat Storage

Apart from the surface temperatures, the transient storage of thermal energy in building constructions is of major importance. In our calculations we could calculate the heat flow to the wall from the temperature difference between ambient and surface, multiplied by the convective heat transfer coefficient $h$. Due to space constraint it is not possible to show the results here in graphical form, but only in tabular format.

Table 2 holds the total heat flow from ambient to the wall. It is the integral of the temporal heat flow over time. As such it also gives an indication of the accuracy of the integral of temperature evolution over time.

<table>
<thead>
<tr>
<th>Description</th>
<th>Aluminium</th>
<th>Insulation</th>
<th>Concrete</th>
</tr>
</thead>
<tbody>
<tr>
<td>exact</td>
<td>49.3</td>
<td>42.8</td>
<td>3984</td>
</tr>
<tr>
<td>$\Delta t = 3600$ s</td>
<td>39.8</td>
<td>44.1</td>
<td>3865</td>
</tr>
<tr>
<td>$\Delta t = 1800$ s</td>
<td>38.0</td>
<td>43.0</td>
<td>3864</td>
</tr>
<tr>
<td>$\Delta t = 900$ s</td>
<td>42.0</td>
<td>42.9</td>
<td>3864</td>
</tr>
</tbody>
</table>

From these results it is clear that in the case of aluminium, there is quite a large relative error (up to 25%). However the absolute
error is very small (for comparison: 10 kJ corresponds to the hourly heat output of a 3 W light bulb).

The accuracy (both relative and absolute) in case of the insulation is quite high. In case of the concrete we notice a heat deficiency of approximately 120 kJ m⁻². In this case the relative error is however quite small (about 3%). The heat deficiency results from the fact that the predictions of the surface temperatures are slightly too high as can be seen in Figure 4.

4. CONCLUSIONS

After a short review of the theory associated with numerical approximation of heat conduction through solid elements of buildings, practical effects of place and time discretisation parameters were demonstrated for materials common to (solar) applications in buildings.

The most important conclusions can be summarized in two groups. First the conclusions which are normally not under the control of a model’s user:

- It is preferable to choose a mixed implicit/explicit (γ > 1/2) discretisation scheme.
- In principle it is better if exposed boundary nodes do not represent thermal capacity.
- Implicit from the results follows that one has to be very careful when using simplified network models (were typically a number of walls will be represented by a single lumped capacitance node).
- The recommendations below should be automated as much as possible.

Conclusions and recommendations on aspects which may be under the control of the user:

- If it is a single wall you are interested in (or you have the ability to change a single wall’s approach in a whole building model), first determine the Biot number. Then if
  \[ B_t < 0.1 \] ( ), the lumped capacitance method will be most appropriate.
- Determine the “period time” associated with your problem, and make sure that the building model has a surface layer thickness, such that the first “buried” node at least represents the effective thickness \( d' \) of the wall.
- When simulating, set the time step such that you have enough detail within the period time; eg 1 h steps for daily fluctuations, 2 minute steps for 10 minute fluctuations, etc.

- Finally choose number of layers for the thermally important walls and time step, such that this leads to \( \gamma - F_x \) combinations, which are in the non-oscillatory region of Figure 1, preferably close to the line indicating a spatial truncation error of order \( \Delta x^2 \) (from Figure 1).

This implies that in case of the commonly used Crank-Nicolson scheme \( \gamma = 1/2 \), \( F_x = 1/2 \) would be a very appropriate choice. \( F_x = 1/2 \) also ensures that the above requirement with respect to \( d' \) is satisfied. When \( F_x < 1/2 \) (large capacitance layer and small time steps) the results will be non-oscillating but inaccurate, and it would be better to either sub-divide the associated layers or increase the time step. When \( F_x \gg 1/2 \) (usually in thin layers of material) the results will be oscillating and the temporal accuracy for the associated layers will drop. In that case it would be better to decrease the time step or to refer to a fully implicit scheme.

References


