FOURIER AND BIOT NUMBERS AND THE ACCURACY OF CONDUCTION MODELLING

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Abstract

Recent validation work has shown the importance of accurate modelling in order to bring together experimental results and predictions. A number of important areas were identified: heat transfer coefficient, edge effects, etc. This paper dwells on the latter.

After a short review of the associated theory the paper concentrates on the effects of Fourier and Biot numbers on the accuracy of the numerical approximation of the diffusion equation for heat flow through solid elements of buildings.

Since this is the most widely used method, the paper focusses on finite-difference modelling. However, the main conclusions are applicable to other numerical approaches as well.

By practical examples, representing typical building applications, it is demonstrated that it is easy to introduce - but also relatively easy to minimalize - errors due to space and time discretisation of building structures.

Symbols

B_i	Biot number ($h\,1/2d\,\lambda^{-1}$), -	α	thermal diffusivity($\lambda\rho^{-1}c^{-1}$), $m^2 s^{-1}$
c	specific heat, $J kg^{-1} K^{-1}$	ρ	density, $kg\,m^{-3}$
d	wall thickness, m	γ	implicit/ explicit weighting factor, -
d^*	effective thickness (($\alpha t_0 \pi^{-1})^{1/2}$, m	θ	temperature, $°C$
F_o	Fourier number ($\alpha \Delta t\, \Delta x^{-2}$), -	λ	thermal conductivity, $W\,m^{-1} K^{-1}$
h	convective heat transfer coefficient, $W\,m^{-2} K^{-2}$	Λ	growth factor, -
n	space step level		
s	time step level		
t	time, s		
t_0	cycle time, s		
x	space co-ordinate, m		

1. INTRODUCTION

Recent validation work (eg CEC 1989, Bloomfield 1992) has shown the importance of accurate modelling in order to bring together experimental results and predictions. A number of important areas were identified: heat transfer coefficient, edge effects, etc. This paper dwells on the latter.

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, this paper concentrates on the effects of various discretization schemes and nodal densities in terms of the effects on transient storage and surface temperature fluctuation. Since this is the most widely used method, here the focus is 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 this paper demonstrates the practical consequences by cases, representing typical building applications.
Many aspects of modelling are generic rather than application specific. This paper concentrates 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

There are many methods for the prediction of thermal conduction such as experimental, analytical, and numerical. Usually, the numerical method is prefered because of factors like versatility, simplicity, and costs. However, in numerical methods there is always a factor of uncertainty in the results. In order to minimize the uncertainty, it is important to understand how the error is created and propagates, ie the error sources and stability criteria of the adopted numerical scheme.

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

$$\frac{\partial \theta}{\partial t} = \alpha \, \frac{\partial^2 \theta}{\partial x^2} \tag{1}$$

where α 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 $B_i = h \, 0.5 \, d \, \lambda^{-1}$ (-)). If this number is much less than unity (say $B_i < 0.1$), then it is sufficient to use the so-called lumped capacitance method to obtain accurate results with minimal computational requirements. However, if B_i is not much less than unity, spatial effect must be considered, and some other method must be used; eg a numerical discretisation.

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:

$$\theta_n^{s+1} - \theta_n^s = F_o \gamma \, (\theta_{n+1}^{s+1} - 2\theta_n^{s+1} + \theta_{n-1}^{s+1}) + F_o(1-\gamma) \, (\theta_{n+1}^s - 2\theta_n^s + \theta_{n-1}^s) \tag{2a}$$

for internal nodes; while for boundary nodes:

$$\theta_n^{s+1} - \theta_n^s = 2 \, F_o \gamma \, (Bi \, \theta_{n-1}^{s+1} - (1 + Bi) \, \theta_n^s + \theta_{n+1}^{s+1}) + 2 \, F_o(1-\gamma) \, (Bi \, \theta_{n-1}^s - (1 + Bi)\theta_n^s + \theta_{n+1}^s) \tag{2b}$$

where F_o is the so-called Fourier number ($= \alpha \Delta t \, \Delta x^{-2}$ (-)), $\theta_n^s = \theta \, (\, n\Delta x \, , s\Delta t \,)$ and γ is a dimensionless parameter which must be chosen to be within the range $0 \le \gamma \le 1$. Setting $\gamma = 0, 1/2, 1$ results in respectively, the classic explicit, the Crank-Nicolson, or the fully implicit discretisation scheme.

At each finite step in time there will be a difference between the exact solution of equation (1) and the numerical approximation according to equation (2). The total error is a combination of:

a) truncation errors, which result from replacing the derivatives in equation (1) by finite differences. This type of error can be minimized by using difference schemes of higher truncation error order, or by reducing the time or space increments.

b) rounding errors, which arise from performing the required computational operations with numerical values having limited number of significant digits. This type of error can be minimized by using

double precision arithmetic. In general, rounding errors are not significant as long as mathematical stability is satisfied.

c) "history" errors, which are due to errors introduced in preceding solution steps. This type of error is strongly dependent on the growth factor. For a more comprehensive description in the current context the reader is referred to (Nakhi 1993b), here only a brief description is given. The numerical behaviour of a set of equations can be classified according to the value of the growth factor (Λ) into four categories:

$$
\begin{array}{llll}
        & \Lambda & > 1   & \text{unbounded growth} \\
0 <   & \Lambda & < 1   & \text{steady decay} \\
-1 <   & \Lambda & < 0   & \text{stable oscillation} \\
        & \Lambda & < -1 & \text{unstable oscillation}
\end{array}
$$

So, for $|\Lambda| < 1$ the solution will be stable, and for $|\Lambda| < 0$ oscillation **may** occur.

In the neighbourhood of a discontinuity in the initial values, in the boundary values, and between initial values and boundary values the truncation error is usually severe. Therefore, if the growth factor at those discontinuities were negative, then an oscillation in the predicted temperature will occur with a rate of decay dependent on the magnitude of the growth factor. In general, the rate of decay or of growth of an error in the following steps is dependent on the growth factor to the power of the number of time steps after the error was introduced.

It can be proven easily, that for an implicitness of $0.5 \leq \gamma \leq 1.0$, the magnitude of the growth factor does not exceed 1 for all positive values of Fourier number F_o. However, as $F_o \rightarrow 0$ the growth factor goes to -1 for the Crank-Nicolson method[‡], and goes to 0 for the fully implicit method. When $F_o = 0.5$, the growth factor for the Crank-Nicolson method goes to 0. In general, the growth factor for any difference scheme according to equation (2) becomes zero when

$$
F_o = \frac{1}{4\,(1-\gamma)}
$$

and oscillation **may** occur for F_o values above that.

The accuracy of this family of schemes may be controlled by appropriate choice of γ and F_o. 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 γ-F_o plane, and shows the point were the spatial error is minimised (at $\gamma = 0.127$ and $F_o = 0.224$), which is in the region of stability and non-oscillation. Although in principle it is always possible to choose these values of γ and F_o, 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_o is often large. Typically for a 1-h time step F_o may be in the range $1 < F_o < 100$, which 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 γ and F_o are far from their optimum values) it is best to distribute the nodes in such a way that F_o is everywhere the same. However, this is very impractical.

[‡] on the other hand the truncation error order becomes $O(\Delta x^4)$
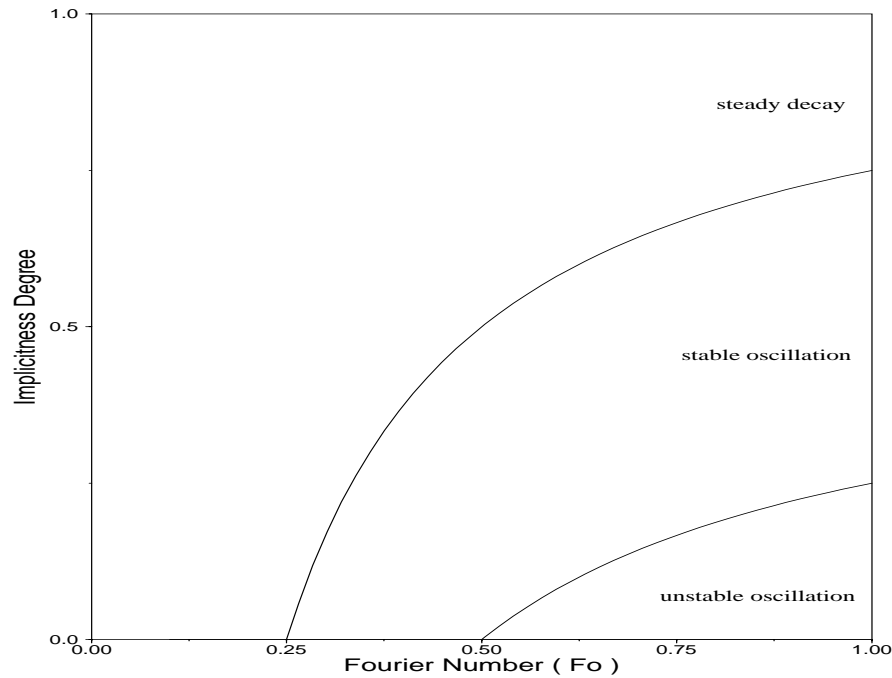
Figure 1 Weighting factor γ, vs F_o (from Waters and Wright 1985)

With respect to distribution of nodes a point of consideration is 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: $d^* = \sqrt{\alpha\, t_0/\pi}$, where t_0 is the cycle time (at a depth of 3 d^* the amplitude will only be 5%). For instance for a common material with $\alpha = 10^{-6}\, m^2 s^{-1}$ (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_o and d^*. If we would use a time step of $\approx t_0/10$ then $F_o = 1$ effectively means that $\Delta x \approx 0.56\, d^*$; for $F_o = 1/3$ we get $\Delta x \approx 0.97\, d^*$. If the time step would be $\approx t_0/24$ then $F_o = 1 \Rightarrow \Delta x \approx 0.36\, d^*$, and $F_o = 1/3 \Rightarrow \Delta x \approx 0.63\, d^*$.

3. IMPLEMENTATION

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 one central node (representing 1/2 of the layer's thermal capacitance), and two nodes at each boundary of the layer (representing 1/4 of the layer's thermal capacitance each). If such a node is on the interface with the next layer of material, then it also represents 1/4 of the next layer's thermal capacitance. Within a layer the nodes are connected with two (equal) thermal resistances. 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 bugs were found with regard to ESP-r's conduction algorithm and overall solving strategy.

Currently (and underlying this paper) work is under way (Nakhi 1993a) to develop a new grid generation technique to better represent inter-nodal conductivity and to enable a more explicit simulation of three dimensional phenomena such as thermal bridging and edge effects. Tasks of this work directly related to the current subject are:

1) Development of a one-dimensional dynamically adaptive grid generation technique which insures homogeneous internodal conductivity, and whose distribution of nodes is dependent on expected variable gradient.

2) Development of a three-dimensional grid generation technique to enable simulation of thermal bridging, and corner and edge effects within buildings.

3) A parallel effort will be to minimize some modelling error sources by enabling handling of variable thermal properties of building materials and by adapting direct-iterative and error equations techniques.

The current status of this work is that ESP-r now offers the following options with respect to discretisation and nodal placement:

- user selectable degree of implicitness $0.1 \leq \gamma \leq 1.0$;
- current default nodal placement where each user-defined layer is divided into 2 imaginary sub-layers, and one node is placed on each real or imaginary "interface" (see above);
- the user may assign any number of nodes for any individual layer in the problem;
- automatic node distribution according to the thickness and thermal diffusivity of each layer, and satisfying some user-specified reference Fourier number;
- dynamic updating of node distribution when the thermo-physical properties of any multi-layered construction are modified during the simulation (eg because of temperature or moisture dependence);
- replace a multi-layered construction with a lumped construction when the Biot number $B_i \leq 0.1$;
- distribute the nodes throughout the building according to the information given by a grid distribution file;

save the current grid distribution into a file;

4. 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 applications. The material properties and dimensions are collected in Table 1.

Table 1 Example construction materials

Property		Aluminium	Insulation	Concrete
thickness, d	m	0.002	0.10	0.20
conductivity, λ	$Wm^{-1}K^{-1}$	200	0.045	1.9
density, ρ	$kg\,m^{-3}$	2800	50	2300
specific heat, c	$J\,kg^{-1}K^{-1}$	880	840	840
thermal diffusivity, α	$10^{-6}m^2s^{-1}$	81.2	1.07	0.98

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 $3\,W\,m^{-2}K^{-2}$.

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

$$\theta_s = \theta_0 + \Delta\theta \ (1 - e^{-2\alpha t/\rho cd}) \tag{3}$$

where θ_0 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:

$$\theta_s = \theta_0 + \Delta\theta \ (1 - 4 \sum_{n=1}^{\infty} \frac{\sin m_n}{2m_n + \sin 2m_n} \ e^{-m_n^2 \alpha \frac{t}{(d/2)^2}} \cos m_n \tag{4}$$

where values for m_n 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.

4.1. Surface Temperatures

Concentrating on the surface temperatures first, 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.
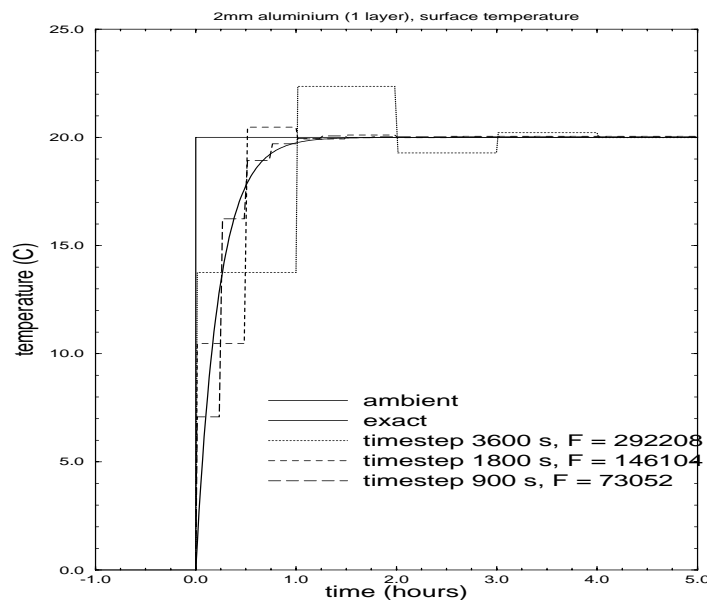

Figure 2 Evolution of surface temperature for a sheet of aluminium ($B_i = 1.5 \, 10^{-5}$ -) modelled as 1 layer, using different time steps

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
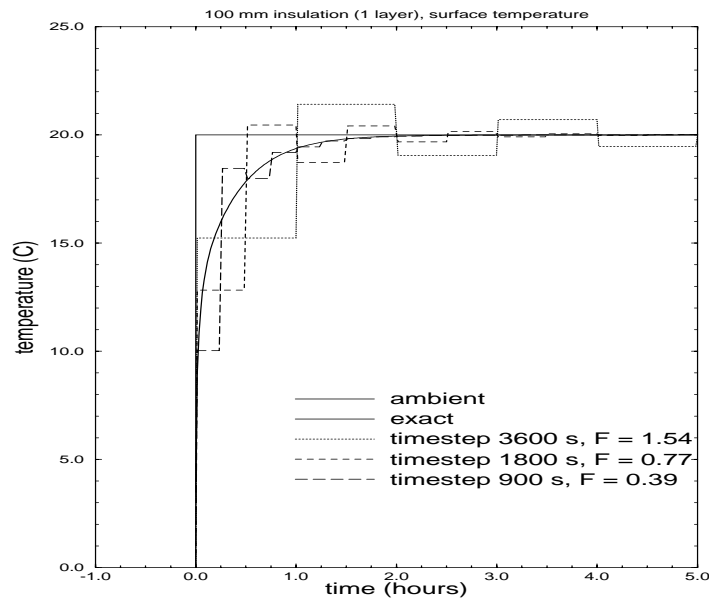
Figure 3 Evolution of surface temperature for a slab of insulation ($B_i = 3.3$ -) modelled as 1 layer, using different time steps
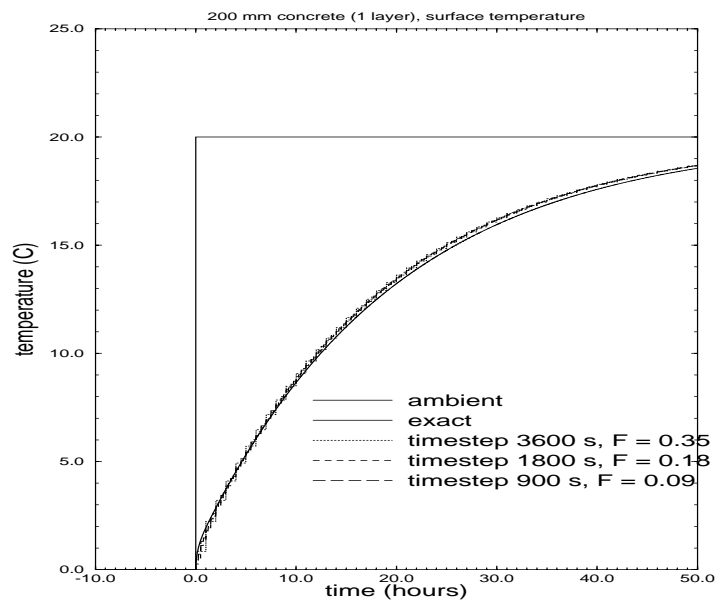

Figure 4 Evolution of surface temperature for a concrete slab ($B_i = 0.16$ -) modelled as 1 layer, using different time steps

scheme in this case, as can be seen from Figure 1.

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_o 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 quite a range in F_o, the results were only slightly affected. The biggest differences occurring in the period immediately after the ambient temperature change.
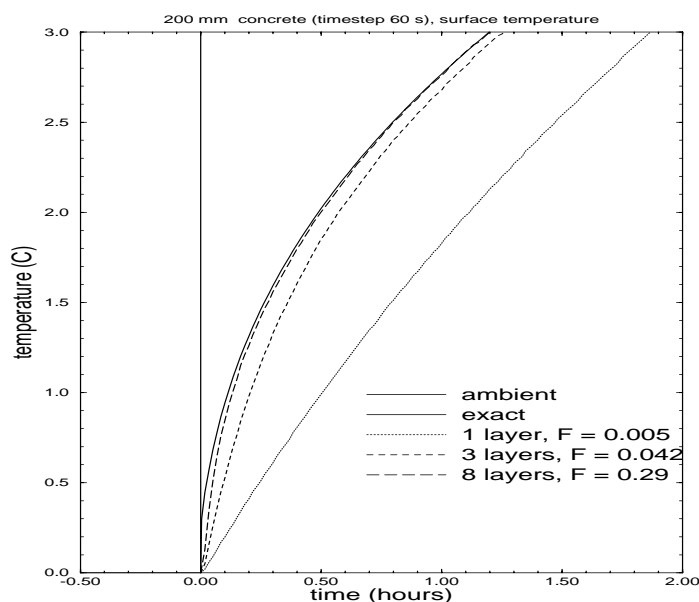

Figure 5 Evolution of surface temperature for concrete ($B_i = 0.16$ -) modelled with various numbers of layers, and using a time step of 60 *s*

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 growth factor (which, in case of the Crank-Nicolson method, goes to -1 when $F_0 \rightarrow 0$). From Figure 5 it may be clear that if the Fourier number is chosen favourably, the results are quit accurate.

4.2. Heat Storage

Apart from the surface temperatures, the transient storage of thermal energy in building constructions is of major importance. In the current work the heat flow to the wall is calculated 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 tabular.

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.

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

Table 2 Total heat ($kJ\ m^{-2}$) being stored in wall after 20 K step change of ambient temperature

Description	Aluminium	Insulation	Concrete
exact	49.3	42.8	3984
$\Delta t = 3600\ s$	39.8	44.1	3865
$\Delta t = 1800\ s$	38.0	43.0	3864
$\Delta t = 900\ s$	42.0	42.9	3864

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 the fact that the predictions of the surface temperatures are slightly too high as can be seen in Figure 4.

5. 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 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 (but are in the case of ESP-r):

•   It is preferable to choose a mixed implicit/ explicit ($\gamma > 1/2$) discretisation scheme.

•   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:

•   In case of a single wall (or when there is the option to change a single wall's approach in a whole building model), first determine the Biot number. Then if $B_i < 0.1$ (-), the lumped capacitance method will be most appropriate.

•   Decreasing the time step not always improves the accuracy. Sometimes it is preferable to decrease the space step. Apart from that it should be noted that the rate of change in required computation time relative to the number of time steps per hour is about unity; but the rate of change relative to the number of space steps is much less then unity.

•   However, decreasing the space step may result in loss of accuracy since the increase of the magnitude of the growth factor may offset the reduction in the truncation error.

A suggested approach might be:

•   Determine the "period time" associated with the 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 there is 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 γ - F_o combinations, which are in the non-oscillatory region of Figure 1, preferably close to the line indicating a spatial truncation error of order Δx^4 (h^4 in terms of Figure 1).
    This implies that in case of the commonly used Crank-Nicolson scheme ($\gamma = 1/2$), $F_o \approx 1/2$ would be a very appropriate choise. $F_o \approx 1/2$ also ensures that the above requirement with respect to d^* is satisfied. When $F_o \ll 1/2$ (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 $F_o \gg 1/2$ (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.

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