A NON-DIMENSIONAL FE MODEL FOR THE SIMULATION OF HEAT CONDUCTION IN CONCRETE

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ABSTRACT. The simulation of heat conduction in concrete is fundamental to the assessment of the long-term performance of structural elements under the conditions of service. The phenomenon is conventionally described using a partial parabolic differential equation with thermal diffusivity as the transport parameter. Under ambient conditions, the thermal diffusivity value for concrete remains practically constant and hence the governing model is often taken to be linear. This study develops a non-dimensional form of the model to achieve computational efficiency and stability. The developed model subjected to constant temperature boundary conditions, has been subsequently analysed with a one-dimensional FE scheme based on a lumped mass matrix model developed through Galerkin's technique. The algorithm has been implemented through a C++ programme to simulate the evolution of temperature distribution in a dry concrete medium with siliceous aggregates. The effect of different thermal gradients (60-25, 40-25, 20-25, and 0-25°C) on the attainment of steady state over a medium length of 0.1 m has been evaluated. The comparison of the simulated steady state temperature profiles against standard analytical solution verifies the reliability of the developed scheme.

Keywords: Heat conduction, Concrete, FEA

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INTRODUCTION

The long-term performance of concrete structures is affected by the conditions of exposure to which they are subjected. The primary environmental factors that influence their performance are temperature, rainfall, relative humidity and wind speed. Quantification of the effects of these factors enables effective design of concrete structures for mechanical loading as well as endurance against environmental actions. The phenomena that degrades the durability of structural elements are often affected by the temperature outside as well as the temperature distribution within them [1,2,3], thus making the study of heat transfer an important facet in durability design of concrete. The study of heat transfer in structures and structural elements also serves many other purposes such as estimation of thermal stresses [4], determination of thermal comfort of buildings, design of HVAC system, and building energy consumption analysis [5]. Therefore, it is significant to study heat transfer in concrete structures and structural elements.

Heat transfer in a structural element can be defined as the flow of energy from high temperature region to low temperature region by one or more of the three modes: radiation, convection and conduction. Heat transfer at the surface takes place by convection and radiation after which heat flows within the element by conduction. Heat conduction in concrete depends upon its thermal conductivity and thermal capacity, both of which are strongly affected by the type of aggregates used [6]. Their dependence on aggregate type has been studied by many researchers and standard equations are available quantifying their dependence [7]. Apart from the type of aggregate used, the state of saturation of concrete and temperature are other factors that influences the rate of heat conduction in concrete [6,7,8]. Not only does moisture content influences the temperature distribution, but the presence of thermal gradient also affect the moisture distribution in concrete. Steeper temperature gradient stimulates greater effect on the moisture distribution [9]. Therefore, heat and moisture transfer in concrete can be regarded as a coupled phenomenon. The modelling of heat conduction in concrete to determine the temperature distribution will help in effective determination of moisture distribution, which will further aide towards efficient durability design of concrete structures. Over the relatively small range of temperature encountered in concrete structures during a year, it is usually adequate to assume that the thermal conductivity and thermal capacity are constant [10]. Thus, the governing equation for heat conduction in concrete is often taken as linear.

This study adopts a numerical approach towards the determination of temperature distribution in concrete. Numerical approach provides the flexibility of using different types of boundary conditions and different shape and size of the domain. The present study develops an FE model using Galerkin's weighted residual method for the solution of one-dimensional transient heat conduction in concrete adopting non-dimensional parameters and a lumped mass scheme. The use of non-dimensional parameters reduces the range of orders involved and hence minimizes the errors inherent in numerical computation. Since the errors in computation are also a result of the characteristics of the matrices involved, the implementation of a lumped mass scheme offers stable convergence and consistent result [11]. The FE scheme is implemented by developing a C++ programme for the simulation of temperature profiles within the considered domain. The developed numerical scheme is subjected to four different constant temperature boundary conditions. Further, the time required by each of the gradient to attain steady state is recorded and the temperature profile at that time is compared to the standard analytical solutions available for the problem. The

comparison of the simulated solution with the benchmark solution shows good convergence thus verifying the applicability of the developed FE scheme and C++ code for similar studies.

MODELLING OF HEAT TRANSFER IN CONCRETE

Governing Equation

The heat conduction equation is derived from Fourier's law and the law of conservation of energy. It can be stated as:

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(D_T \frac{\partial T}{\partial x} \right) \tag{1a}$$

The equation is a parabolic partial differential equation which is first order in time and second order in space. Thus, the solution of the governing equation requires an initial condition and two boundary conditions as input. Boundary conditions may either be specified as constant temperature value (Dirichlet/Essential boundary condition) or as heat flux (Neumann/Natural boundary condition).

At t = 0,

Initial condition:	$T(x=0) = T_{ini}(x)$	(1b)
Dirichlet boundary condition:	$T = T_1 \;\; at\; x = 0$ $T = T_2 \;\; at\; x = L$	(1c)
Neumann boundary condition:	$D_T \frac{\partial T}{\partial x} = q_1 \;\; at\; x = 0 \; and \; q_2 \;\; at\; x = L$	(1d)

Where, $T(°C)$ is temperature, $x(m)$ is the spatial distance*)*, $t(s)$ *is* time and D_T (m^2/s) is the heat transport parameter known as thermal diffusivity. T_1 *(°C)* and T_2 *(°C)* are the temperature at the two extreme boundaries, $T_{ini}(°C)$ is the initial temperature, $L(m)$ is the length of the domain and *q(W/m^2)* is the heat flux.

Thermal diffusivity is the transport parameter determining heat conduction in concrete. It is the ratio of thermal conductivity and thermal capacity. There are many studies oriented towards the determination of factors that influence the thermal conductivity and thermal capacity of concrete. Thermal conductivity is said to depend upon the mix proportioning, aggregate type, moisture status and unit weight of concrete in dry state [12,13]. Kim et al [14] experimentally studied the effect of various factors like age, volume of aggregate, water-cement ratio, temperature, moisture condition, admixtures, and fine aggregate fraction. They further developed a model including only those parameters which significantly affected the thermal conductivity of concrete. Also, there are models available in the literature to predict effective thermal conductivity of three phase mixtures like concrete such as the Krischer and Kroll model which is widely used for three phase system [15,16] and the Chaudhary and Bhandari model [17] which relates thermal conductivity to porosity and moisture content. The thermal conductivity *(K_T)* and thermal capacity *(C_T)* of concrete depends extensively on the type of coarse aggregate [7]. Table 1 and 2 summarizes the dependency of thermal conductivity and thermal capacity on types of aggregate and temperature for dry concrete [7].

Table 1 Dependence of thermal conductivity on aggregate type and temperature

AGGREGATE TYPE	TEMPERATURE RANGE $(°C)$	K_T $(Wm^{-1}\,°C^{-1})$
Siliceous aggregate	0 - 800	$(-0.00062T + 1.5)$
Carbonate aggregate	0 – 293	1.355
	Greater than 293	$(-0.00124T + 1.7162)$
Expanded shale aggregate	0-600	$(-0.0003958T + 0.0925$

Table 2 Dependence of thermal capacity on aggregate type and temperature

AGGREGATE TYPE	TEMPERATURE RANGE $(°C)$	C_T $(Jm^{-3}\,°C^{-1})$
Siliceous aggregate	0 – 200	$(0.005T + 1.7) \times 10^6$
Carbonate aggregate	0 – 400	2.566×10^6
	401 – 410	$(0.1765T - 68.034) \times 10^6$
Expanded Shale aggregate	0 – 400	(1.930×10^6)
	401 – 420	$(0.0772T - 28.95) \times 10^6$

The variation of thermal diffusivity in concrete within ambient temperature conditions is not very significant, therefore, thermal diffusivity is mostly taken as constant in the heat conduction analysis of concrete.

Non-Dimensional Representation

For implementation of the numerical scheme, the independent variables in equation (1a) are expressed in dimensionless terms in order to reduce the range of orders involved and minimize computational errors [18]. The following reduced variables are adopted for the formulation of the non-dimensional governing equation:

Reduced temperature: $$T_r = \frac{T - T_{\min}}{T_{\max} - T_{\min}} \quad (2a)$$

Reduced space variable: $$x_r = x/L \quad (2b)$$

Reduced time: $$t_r = \left(D_T * t/L^2\right) \quad (2c)$$

Restating equation (1a) in non-dimensional terms gives:

$$\frac{\partial T_r}{\partial t_r} = \frac{\partial^2 T_r}{\partial x_r^2} \quad (3)$$

Where, T_{min} $(°C)$ and T_{max} $(°C)$ are the minimum and maximum temperature respectively. The scrutiny of the final reduced governing equation shows that the thermal diffusivity term

which is of the order of 10^{-7} does not appear in the equation, thus reducing the range of order and minimizing the errors involved in numerical computation. This justifies the non-dimensionalization of the governing equation.

Formulation of Element-Level Governing Equation

The FE formulation of the reduced governing equation is carried out by applying Galerkin's weighted residual method on equation (3). The method involves multiplying the differential equation with weight function and then subsequently solving to obtain a weak form of the differential equation. The weighted residual statement for equation (3) is obtained as:

$$\int_0^l w_k \frac{\partial T_r}{\partial t_r} - \int_0^l w_k \frac{\partial^2 T_r}{\partial x_r^2} = 0 \tag{4a}$$

Where, w_k is the weight function, and l is the reduced element length in FE analysis.

Integrating equation (4a) by parts gives:

$$\int_0^l w_k \frac{\partial T_r}{\partial t_r} - \left[w_k \frac{\partial T_r}{\partial x_r} - \int_0^l \frac{\partial w_k}{\partial x_r} \frac{\partial T_r}{\partial x_r} \partial x_r \right] = 0 \tag{4b}$$

Considering linear elements with two nodes the interpolation function can be written as:

$$T_r = \left[\left(1 - \frac{x_r}{l}\right)\left(\frac{x_r}{l}\right) \right] \begin{Bmatrix} T_{r1} \\ T_{r2} \end{Bmatrix} = [H]\{d_e\} \tag{5a}$$

$$\frac{\partial T_r}{\partial x_r} = \begin{bmatrix} \frac{-1}{l} & \frac{1}{l} \end{bmatrix} \begin{Bmatrix} T_{r1} \\ T_{r2} \end{Bmatrix} = [B]\{d_e\} \tag{5b}$$

Where, $[H]$ is the interpolation matrix $\{d_e\}$ is the vector representing elemental degrees of freedom and $[B]$ is the gradient matrix. The weight functions in equation (4b) are now substituted as interpolation functions.

Therefore, substituting $\left(w_k = 1 - \frac{x_r}{l} \right)$ equation (4b) gives:

$$\begin{bmatrix} \frac{l}{3} & \frac{l}{6} \end{bmatrix} \{\dot{d}_e\} + \begin{bmatrix} \frac{1}{l} & \frac{-1}{l} \end{bmatrix} \{d_e\} = -\left. \frac{\partial T_r}{\partial x_r} \right|_{x_r = 0} \tag{6a}$$

Similarly, substituting $\left(w_k = \frac{x_r}{l} \right)$ in equation (4b) gives:

$$\begin{bmatrix} \frac{l}{6} & \frac{l}{3} \end{bmatrix} \{\dot{d}_e\} + \begin{bmatrix} -\frac{1}{l} & \frac{1}{l} \end{bmatrix} \{d_e\} = \left. \frac{\partial T_r}{\partial x_r} \right|_{x_r = l} \tag{6b}$$

The general element level governing equation is obtained by combining equation (6a) and (6b), and can be stated as:

$$\frac{l}{6}\begin{bmatrix}2 & 1\\ 1 & 2\end{bmatrix}\{\dot{d}_e\}+\frac{1}{l}\begin{bmatrix}1 & -1\\ -1 & 1\end{bmatrix}\{d_e\}=\begin{Bmatrix}-\left.\dfrac{\partial T_r}{\partial x_r}\right|_{x_r=0}\\ \left.\dfrac{\partial T_r}{\partial x_r}\right|_{x_r=l}\end{Bmatrix} \tag{7}$$

The element level semi-discrete governing equation can also be represented as:

$$[m]\{\dot{d}_e\}+[k]\{d_e\}=\{q\} \tag{8a}$$

Where, $[m]$ and $[k]$ are element level mass matrix and diffusivity matrix respectively. $\{d_e\}$ is the vector representing nodal temperature values and $\{q\}$ is the vector of nodal fluxes. Equation (8a) represents a semi-discrete form of the finite element formulation. In order to obtain a fully discretized scheme, equation (8a) needs to be solved further using finite difference method. In this study, Crank–Nicolson scheme has been used for complete discretization of the semi-discrete equation. Finally, the fully discretized scheme is states as:

$$\left([m]+0.5\Delta t_r[k]\right)\{d_e\}^{n+1}=\left([m]-0.5\Delta t_r[k]\right)\{d_e\}^{n}+0.5\Delta t_r\left(\{q\}^{n+1}+\{q\}^{n}\right) \tag{8b}$$

The element level fully discretized scheme can be assembled to form a global equation which can be represented in $[A]\{X\}=\{b\}$ form where:

$$[A]=[M]+0.5\Delta t_r[K] \tag{9a}$$

$$\{b\}=\left([M]-0.5\Delta t_r[K]\right)\{X\}^{n}+0.5\Delta t_r\left(\{Q\}^{n+1}+\{Q\}^{n}\right) \tag{9b}$$

Where, $[M]$ and $[K]$ are global mass and diffusivity matrix respectively, $\{X\}$ represents the global degree of freedom and $\{Q\}$ is the global vector for nodal fluxes.

Formulation of Global Matrices

Consistent matrices

For the element level governing equation, the global matrices will be tridiagonal in nature and can be presented as:

$$M_{ij}=\begin{cases}2, \text{ for } i=j=1,m;\\ 4, \text{ for } i=j=2 \text{ to } (m-1);\\ 1, \text{ for } i=j=2 \text{ to } m,\ j=(i-1);\\ 1, \text{ for } i=1 \text{ to } (m-1),\ j=(i+1);\\ 0, \text{ for all other elements}\end{cases} \tag{10a}$$

$$K_{ij} = \begin{cases} 1, & for\ i = j = 1,m; \\ 2, & for\ i = j = 2\ to\ (m-1); \\ -1, & for\ i = j = 2\ to\ m,\ j = (i-1); \\ -1, & for\ i = 1\ to\ (m-1),\ j = (i+1); \\ 0, & for\ all\ other\ elements \end{cases} \quad (10b)$$

Where, m is the order of the matrices which is equal to the total number of unknowns. $M_{ij}\ and\ K_{ij}$ are global consistent mass matrix and diffusivity matrix respectively. i is the row index and j is the column index.

Lumped mass matrix

The convergence of the numerical solution of a partial differential equation and the accuracy of its results depends upon the characteristics of the matrices involved in computation along with the space and time discretization. The spatial oscillations in the results occur due to the characteristics of the $[A]$ matrix which comprises of the mass matrix and the diffusivity matrix. Neuman [19] used a central difference time stepping scheme on a parabolic partial differential equation and concluded that it is necessary to use a lumped mass matrix in order to achieve convergence and a stable solution especially in the case of unsaturated flow. Also, the adoption of lumped mass matrix occupies less storage space and therefore finer spatial discretization can be used. Ju et al [11] obtained FE solution for similar parabolic partial differential equation as the heat conduction equation with different types of elements for consistent and lumped mass matrix to draw a comparison. He found that while using a lumped mass scheme one can arbitrarily reduce the time step size at any time during the simulation to obtain a stable and convergent solution without changing the mesh structure. Also, he concluded that there is a significant difference in memory occupied and time required to simulate while using the consistent and lumped mass matrix with the latter ensuring faster computation and less storage occupancy. Sarkar et al [18] also concluded that the oscillations in the FE solution can be counteracted by forming diagonally dominant matrix. Additionally, the final $[A]$ matrix should not produce any negative element on the main diagonal. These constraints can be addressed by replacing the consistent mass matrix with lumped mass matrix. The constitution of the final lumped mass matrix is given in equation (11):

$$M_{ij} = \frac{l}{6}\begin{cases} 3, & for\ i = j = 1,m; \\ 6, & for\ i = j = 2\ to\ (m-1); \\ 0, & for\ all\ other\ elements \end{cases} \quad (11)$$

Here, M_{ij}^{L} represents the global lumped mass matrix.

SIMULATION OF HEAT CONDUCTION IN CONCRETE

Properties of the Physical Domain and Implementation of Numerical Scheme

For implementation of the numerical scheme, a case of dry concrete with siliceous coarse aggregate has been selected. The thermal diffusivity parameter for siliceous aggregate dry concrete can be computed as [7]:

$$D_T = \frac{-0.000625T + 1.5}{(0.005T + 1.7)\times 10^6} \tag{12}$$

The variation of the thermal diffusivity parameter for the temperature range adopted in this study $(0°\,C - 60°C)$ is not very significant. The coefficient of variation is 5.4%. Therefore, the thermal diffusivity is considered to have a constant value, which is the value of thermal diffusivity at $30°C$. A C++ programme was developed to facilitate the simulation of temperature distribution for four different temperature gradients $(60 - 25°C;\ 0 - 25°C;\ 40 - 25°C;\ 20 - 25°C)$ within the considered domain. In order to select a suitable mesh size, 1-hour simulation was carried out with increasing number of nodes. The reduced time step size adopted for this simulation is such that $\Delta t_r < (l^2/3)$ to ensure minimization of numerical oscillation [9]. Table 3 summarizes the parameters used for the simulation and Figure 1 shows
the variation of 1-hour temperature profile with number of nodes for two extreme gradients $(60 - 25^oC\ and\ 0 - 25^oC)$.

Table 3 Data of parameters used in simulation

PARAMETER	VALUE
$D_T(m^2/s)$	8.0278×10^{-7}
$L\ (m)$	0.1
$T_{max}(°C)$	60
$T_{min}(°C)$	0

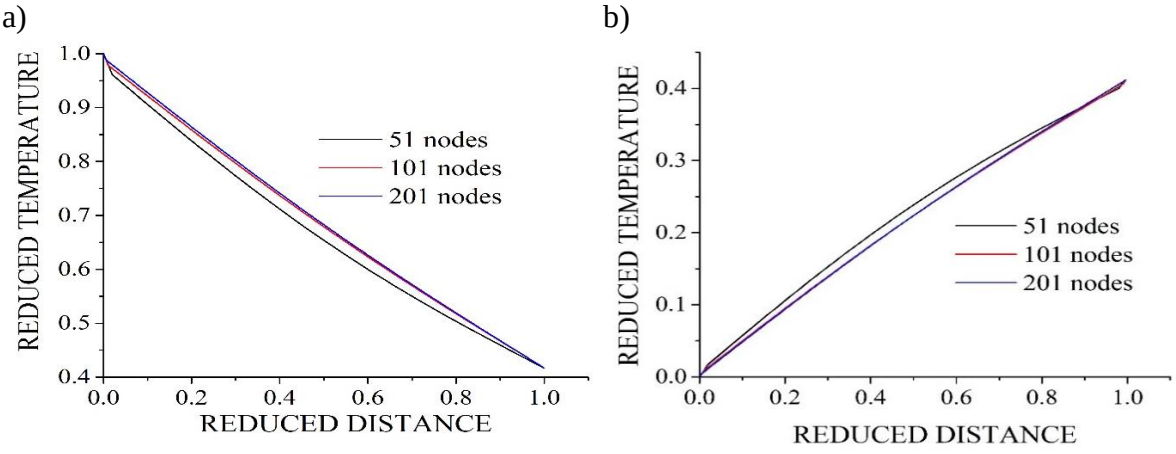

Figure 1 Variation of 1-hour temperature profile with number of nodes $(a)\ 60 - 25°C\ (b)\ 0 - 25°C$

Based on the mesh convergence study it can be concluded that normalized element length (l) equal to 0.005 (201 nodes) can be adopted for subsequent simulations as the temperature profile ceases to change with increase in number of elements beyond 200.

The reduced time step Δt_r is adopted such that $\Delta t_r = 0.99\, l^2$. This is done in order to achieve stable convergence and minimize numerical oscillations in the simulated profiles. Figure 2 shows the oscillations that are produced in the results when $\Delta t_r = 1.01\, l^2$ and the elimination of oscillation when $\Delta t_r = 0.99 l^2$ respectively.

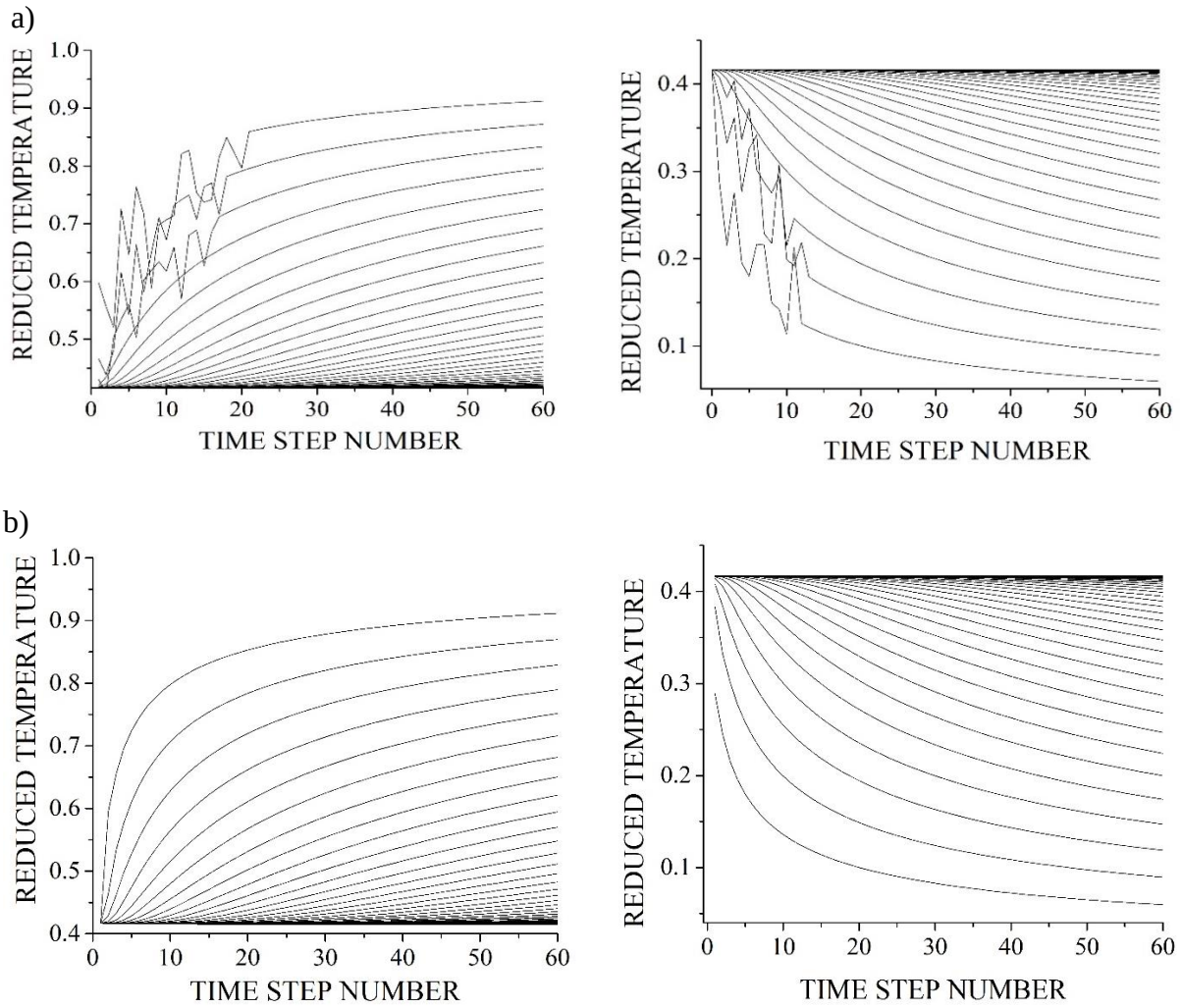

Figure 2 Effect of time step size on numerical stability for 200 elements for 60-25° and 0-25°C when a) $\Delta t_r = 1.01 l^2$ and b) $\Delta t_r = 0.99 l^2$

Thus, it is evident from Figure 2 that violation of the condition ($\Delta t_r < l^2$) leads to significant oscillation in the simulated results. For the purpose of this study, the reduced time step is such that $\Delta t_r = 0.99\, l^2$. Figure 3 represents the algorithm adopted for implementation of the FE scheme. Table 4 summarizes the results of the simulation and the time taken by each of the four gradients to attain steady state and Figure 4 shows the evolution of temperature profile for each gradient till steady state.

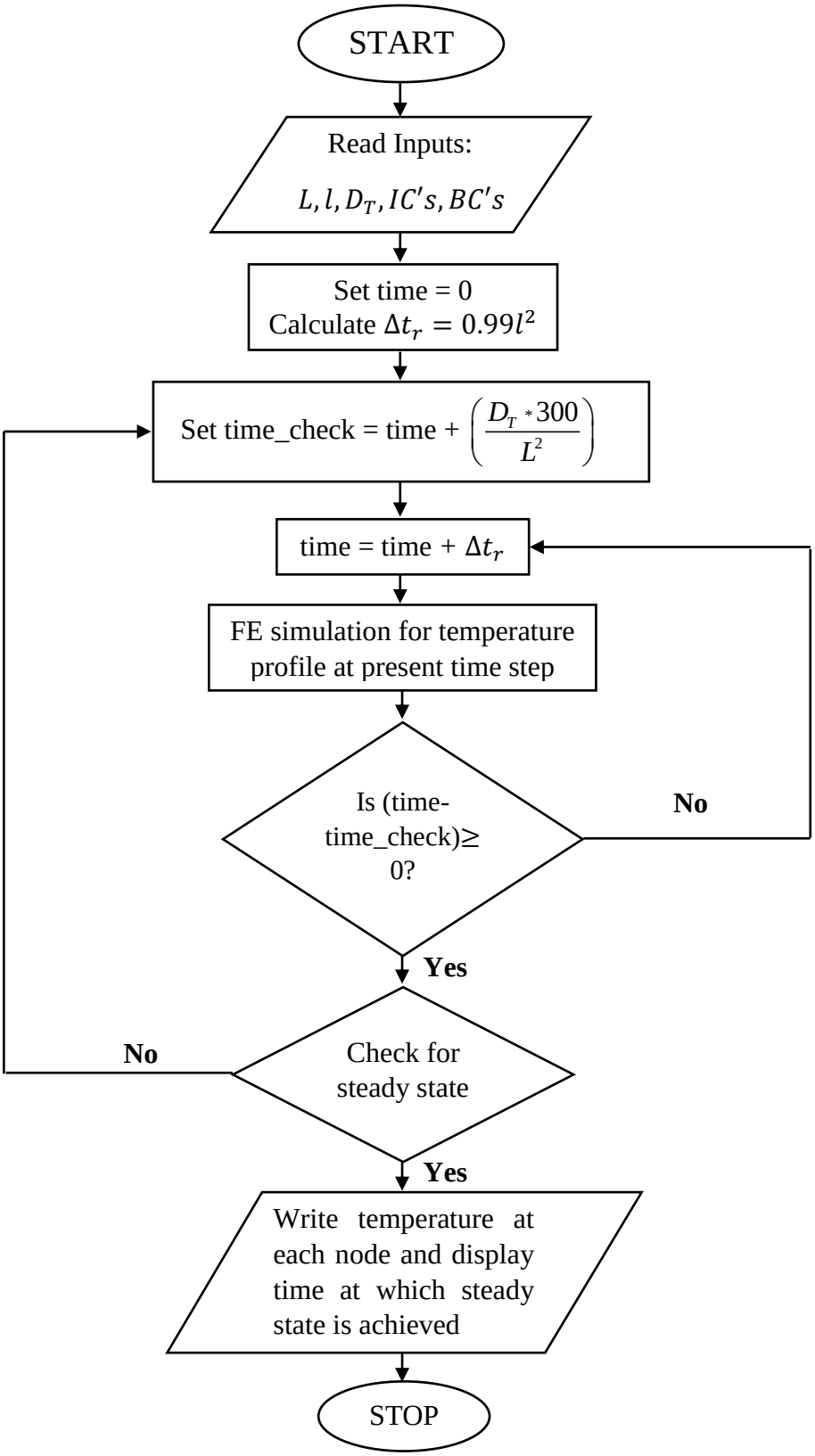

Figure 3 Algorithm for FE analysis of heat conduction in concrete

Table 4 Comparison of simulated parameters for different gradients

GRADIENT	NO. OF TIME-STEPS COMPUTED	TIME TAKEN FOR STEADY STATE (sec)
60 – 25 °C	30121	9271
0 – 25 °C	28110	8404
40 – 25 °C	26103	7804
20 – 25 °C	22089	6303

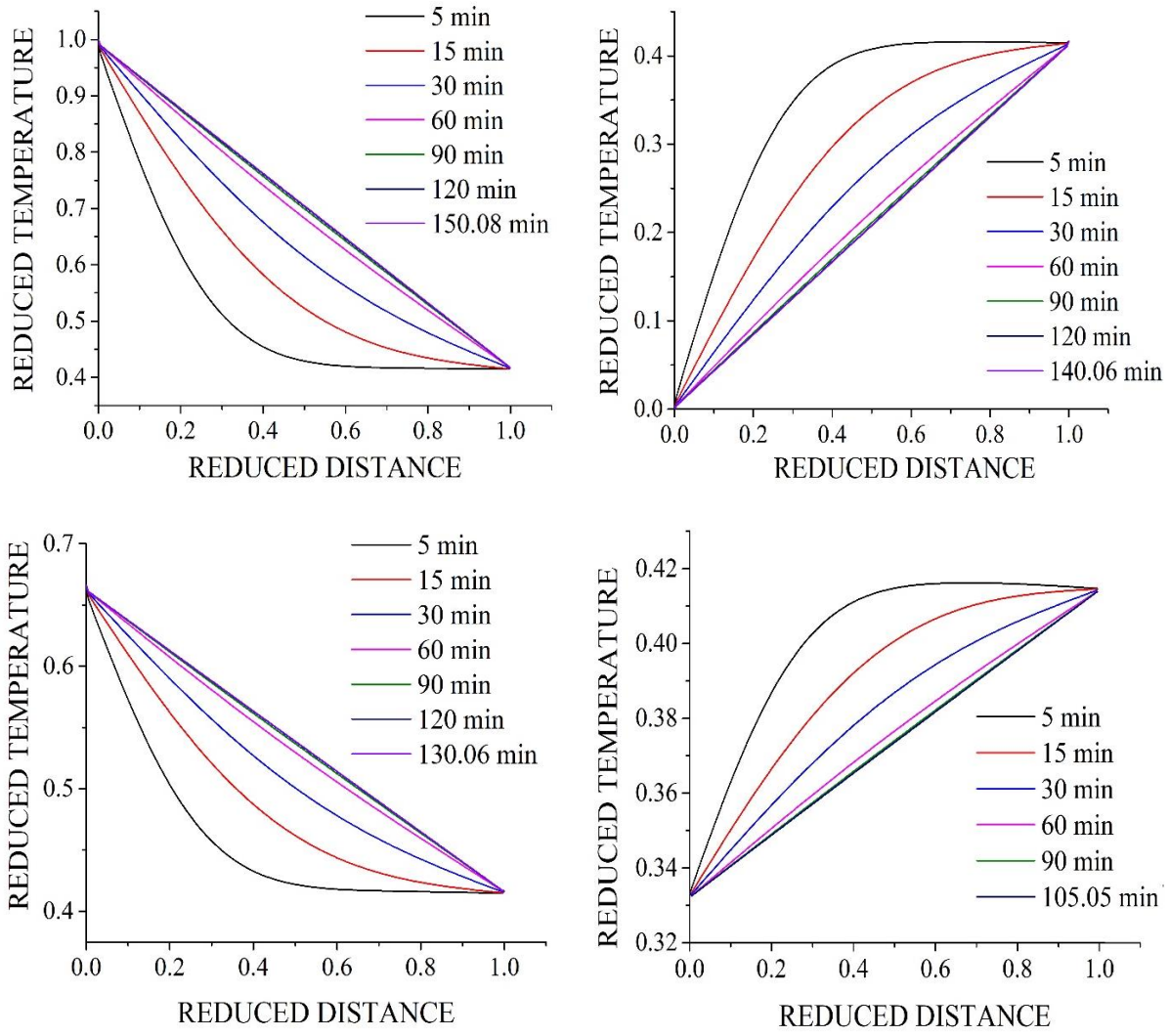

Figure 4 Temperature profile evolution till steady state for all gradients

Convergence and Verification of Numerical Scheme

The analytical solution for linear heat conduction problem for two different constant temperature boundary conditions is stated as [20]:

$$T = T_1 + (T_2 - T_1)\frac{x}{L} + \frac{2}{\pi}\sum_{n=1}^{\infty}\frac{T_2\cos n\pi - T_1}{n}\sin\frac{n\pi x}{L}\exp\left(\frac{-D_T n^2\pi^2 t}{L^2}\right) + \frac{4T_o}{\pi}\sum_{m=0}^{\infty}\frac{1}{2m+1}\sin\frac{(2m+1)\pi x}{L}\exp\left\{\frac{-D(2m+1)^2\pi^2 t}{L^2}\right\} \quad (13)$$

Where, $T_1(°C)$ and $T_2(°C)$ are temperature at the two extreme boundaries and $T_o(°C)$ is the initial condition.

The time taken by each of the simulated gradient to attain steady state is recorded, and the analytical solution to the governing equation is obtained by substituting the steady state time as input in equation (13). The difference between the simulated solution and benchmark solution is very less and the convergence achieved is good. Table 5 summarizes the error obtained in nodal values with respect to benchmark solution.

Table 5 Error in simulated nodal values with respect to benchmark solution at steady state

GRADIENT	AVERAGE ABSOLUTE PERCENTAGE DIFFERENCE (%)	ROOT MEAN SQUARE ERROR
60 – 25 °C	0.45	0.004107
0 – 25 °C	0.42	0.003937
40 – 25 °C	0.41	0.002762
20 – 25 °C	0.16	0.000718

CONCLUDING REMARKS

An assessment of the hygrothermal performance of structural concrete requires the modelling of heat and mass transfer processes. The modelling and simulation of these processes has remained an active area of research over the past several decades. The present study caters to the need of having insights into the algorithm of FE simulation of heat conduction in concrete by experimenting with a modified model stated using non-dimensional space, time and temperature variables and the associated time stepping scheme to ensure stable convergence. Robust application of FE simulation requires the implementation of various conditions as stated below:

1. The use of non-dimensional variables aides to reduce the range of orders involved thereby minimizing the computational errors and producing reliable results.

2. The occurrence of numerical instability is an inherent characteristic of the matrices involved in computation. Numerical oscillations can be minimized by adopting a lumped mass matrix and a suitable time stepping criteria. For the non- dimensional model formulated in this study, it is observed that adopting $\Delta t_r < l^2$ ensures smooth convergence.

3. The efficiency of the numerical scheme and the algorithm proposed in this study have been verified by comparing the simulated results with standard analytical solution. The comparison shows good match between the two results.

4. Although this work is limited to the simulation of heat conduction in concrete as a linear phenomenon, the identified concepts can be extended to the cases of non-linear transport processes, such as that of moisture movement in porous media.

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