DOI:10.22337/2587-9618-2023-19-3-69-82

COUPLED HEAT AND MASS TRANSFER PROBLEM WITH DEPENDENT HEAT CONDUCTIVITY PROPERTIES AND ITS SEMI-ANALYTICAL SOLUTION

Vladimir N. Sidorov, Alim M. Primkulov

Moscow State University of Civil Engineering, Moscow, RUSSIA

Abstract: Present paper proposes a computation method for a coupled heat and mass transfer problem within the porous media where the heat conductivity properties of the media undergo changes caused by the mass transfer. Heat and mass transfer processes are coupled through the inclusion of evaporation and condensation phenomena which in turn require the solution to an another the vapour transfer problem. This complex coupled problem results in a system of both linear and non-linear second order partial differential equations that are spatially discretized by Finite Element Method. Temporal integration is carried out analytically. Thus, the proposed system of equations covering linear vapor transfer problem, linear filtration problem and non-linear heat transfer problem is transformed into a system of both linear and non-linear first order ordinary differential equations being solved by semi-analytical method. Picard approach of successive iterations is used for linearization of the equations. Convergent solution is achieved which is demonstrated on a sample problem herein below. Proposed method gives good insight on the processes taking place within the structures being subjected to temperature and vapor pressure gradients, including the residual effects of moisture accumulation, and assesses its impact on heat conductivity of materials that the structures consist of. Present study is a part of more extensive research on the application of semi-analytical methods in heat transfer problems, therefore it is not exhaustive and complete. Shortcomings of the method and its possible work-arounds as well as the topics for further studies are discussed in Conclusions and Further Studies section.

Keywords: Heat and mass transfer problem, coupled problem, non-linear, finite element method, semi-analytical method

СОВМЕСТНАЯ ЗАДАЧА ТЕПЛОМАССООБМЕНА С ЗАВИСИМЫМИ ТЕПЛОПРОВОДЯЩМИ СВОЙСТВАМИ И ЕЕ ПОЛУАНАЛИТИЧЕСКОЕ РЕШЕНИЕ

В.Н. Сидоров, А.М. Примкулов

Национальный исследовательский Московский государственный строительный университет, г. Москва, РОССИЯ

Аннотация: В настоящей работе предлагается метод расчета связанной задачи тепломассопереноса в пористых средах, когда свойства теплопроводности сред претерпевают изменения, вызванные массопереносом. Процессы тепло- и массопереноса связаны явлениями испарения и конденсации, что, в свою очередь, требует решения другой проблемы переноса пара. Эта сложная проблема приводит к системе как линейных, так и нелинейных дифференциальных уравнений в частных производных второго порядка, которые дискретизируются в соответствии с алгоритмом метода конечных элементов. Интегрирование по временной переменной выполняется аналитически. Таким образом, система дифференциальных уравнений, включающая линейное уравнение паропереноса, линейную задачу фильтрации и нелинейное уравнение теплопереноса, преобразуется в систему как линейных, так и нелинейных дифференциальных уравнений первого порядка, решаемых полуаналитическим путем. Для линеаризации уравнений используется подход Пикара последовательных итераций. Достигается сходящееся решение, что демонстрируется на примере задачи. Предложенный метод позволяет получить представление о теплофизических процессах, происходящих в конструкциях с учетом градиентов температуры и давления пара, в том числе об остаточных явлениях накопления влаги и оценить их влияние на теплопроводность материалов, из которых изготовлены конструкции. Настоящее исследование является частью более обширного исследования применения полуаналитических методов в задачах теплообмена, поэтому оно не является исчерпывающим и полным. Недостатки метода и его возможные обходные пути, а также темы для дальнейших исследований обсуждаются в разделе «Выводы и дальнейшие исследования».

Ключевые слова: задача тепломассопереноса, связанная задача, нелинейный метод, метод конечных элементов, полуаналитический метод.

1. INTRODUCTION

Multi layered exterior wall structures are widely used in modern buildings as they allow to achieve proper insulation properties as well as to have the desired interior and exterior appearance meanwhile be elegant, lightweight and be of sufficient strength and resilience. On the other hand, the study of physical processes taking place within such kind of walls are becoming, obviously, more complicated as the significantly varying material properties cause those physical processes to occur differently comparing to the homogenous single material wall structures. Multi-layered structures have extensively been studied both domestically and internationally with respect to their responses to varying indoor and outdoor conditions which have been reflected in building codes and manufacturer's design guidelines. Present study though, proposes a mathematical model that can quantitatively describe the processes in such structures with due account of their interactions and interdependence under the given boundary conditions.

In particular it reviews the heat transfer phenomenon within multi-layered wall structure in conjunction with the vapor transfer and the filtration occurring simultaneously and accounts their interactions.

Mathematical model that uses semi-analytical computation techniques is proposed to describe the process in such wall structures. Spatially, the model utilizes the Finite Element Method whereas the temporal variations are solved analytically.

Building Codes and Standards [1] contain various simplified computation methods for practical problems that, with due safety margin, account all negative factors that may develop within the structures thus allowing to design such structures in compliance with the serviceability requirements. The idea in those standard methods is to determine composition and geometric proportions of the structures that would withstand the extreme weather conditions of the region, assuming that at all other intermediate states of the weather the structure would perform adequately.

Main objective of present study is to couple the major physical processes happening in the wall within proposed mathematical model that will allow to calculate the immediate state of the structure under the given indoor and outdoor climate condition and including residual factors remained from the previous actions and solve such coupled problem. Hence the difference of the proposed heat and mass transfer model from standard computation methods is that the model describes accurately the immediate state of the wall.

2. RESEARCH METHODS

2.1. Wall Model

As a practical example let consider tri-layered wall structure consisting of inner and outer blockwork walls and heat insulation layer sandwiched in between. This structure is seemingly good case of the composite wall where the water condensation is very likely to occur. The insulation layer in the middle of the structure retains the majority of the heat thus causing the outer blockwork layer to be cooled down till almost the outdoor temperature. On the other hand, the same outer brickwall has a vapor transmissivity apparently lower than that of the middle insulation layer. These two factors jointly, under certain combination of boundary conditions, result in vapor condensation within the wall, that will consequentially adversely effect the heat transfer phenomena. Evaporation and condensation processes non-uniformly distribute the moist throughout the wall which creates a moisture gradient. Having the material filtration properties this gradient induces the filtration process within the wall. Condensation, evaporation and filtration processes combined form the ultimate moisture content distribution within the wall.

One dimensional mathematical model, where the spatial argument varies along the thickness of the wall might be used to build the relationships between the processes. Physical model of above-mentioned tri-layered wall structure is depicted in Fig.1. The total wall thickness is L whereas the width of each individual layer is $\frac{L}{3}$.

Left hand side of the composite wall faces with the indoor environment varying within the range of positive temperatures while the right-hand side contacts the outdoor environment with the range of temperatures that may have also the negative values.

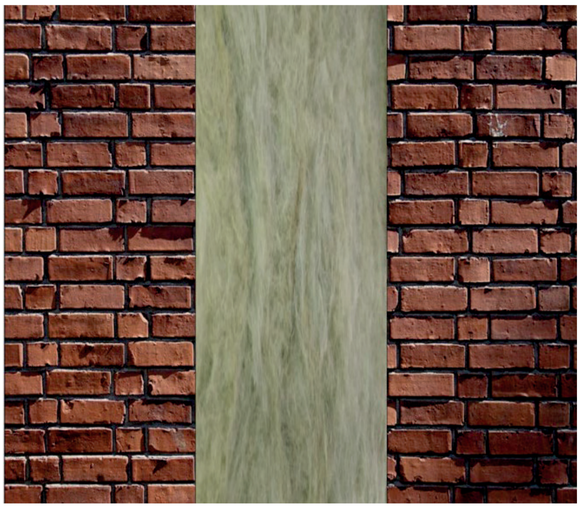


Figure 1. Multi layered wall structure

Indoor and outdoor temperatures are not constant with time as was noted earlier. Let assume that they are given as functions of time:

$$\phi_{in} = \Phi_{in}(t) \qquad (1)$$
$$\phi_{out} = \Phi_{out}(t) \qquad (2)$$

where, ϕ_{in}, ϕ_{out} - indoor and outdoor temperatures; Φ_{in}, Φ_{out} - some functions of t; t - time. Similarly, the indoor and outdoor partial vapor pressures are varying with time and can be described as:

$$p_{v,in} = P_{v,in}(t) \qquad (3)$$
$$p_{v,out} = P_{v,out}(t) \qquad (4)$$

where $p_{v,in}, p_{v,out}$ - indoor and outdoor vapor pressures; $P_{v,in}, P_{v,out}$ - some functions of t; t - time.

All major material properties such as heat conductivities, vapor transmission resistivities, liquid moist filtration properties that appear as parameters in mathematical model are also known and given.

2.2. Physical Processes

The physical model as it is shown on Fig.1 can be described as a finite domain consisting of:

- porous media composed of inner blockwork wall, heat insulation and outer blockwork wall all with its own individual properties - the skeleton;
- moist in its liquid phase (water) which defines the moisture content of the skeleton;
- humid air (binary gas) consisting of air and water vapor mixture.

Having the boundary conditions as specified in section 2.1 above, the processes taking place within the wall can be described as follows:

Mass transfer

This process includes the transfer of the binary gas and liquid water through the skeleton as well as the moist phase changes such as condensation as transformation of vapor into liquid water and the evaporation as transformation of liquid water into vapor. This mass transfer may happen due to the following causes:

a) At microscopic level (so called molecular transfer):

– Diffusion due to temperature gradient (as per Fick's law);

– Diffusion due to vapor concentration gradient;

– Diffusion due to chemical potential gradient;

– Osmosis caused transfers.
b) At macroscopic level (so called convection transfer):
– Capillarity adsorption transfer;
– Pressure gradient transfer (including hydraulic gradient);
– Gravity induced transfer.

Heat transfer

Heat transfer within the same domain occurs due to the following factors:
a) At microscopic level (so called molecular transfer):
– Heat diffusion induced by the difference of temperatures between the skeleton, the air/vapor and/or the liquid water;
– Heat transfer due to change in Enthalpy of the skeleton in the result of moisture content change;
b) At macroscopic level (so called convection transfer):
– Heat transfer induced by temperature gradient and the conductive properties of the media;
– Heat transfer due to moisture phase change (evaporation/condensation);
– Heat transfer due to radiation;
– Heat sink/sources at the boundaries of the domain (derivative boundary conditions).

Detailed discussion of each of above listed processes can be found in [2].

2.3. Heat and Mass Transfer Equations

Physical processes described in 2.1 - 2.2 may occur simultaneously or in various combinations thereof. Also, each of them may have impact in different magnitude on the temperature distribution in the wall. General approach in heat and mass transfer practical problems is to select the relevant processes individually, considering the particularities of that specific problem and evaluating the effect that the process may have on the result. Nonetheless the common property of all those processes is that they can be easily incorporated into the governing equation as a separate term. Hence, in most general form the equations describing heat and mass transfer can be written as:

$$\lambda_{m1,m2,m3}\frac{\partial u_{(1,2,3)}}{\partial t} = -\frac{\partial}{\partial x}\left(\sum_{i=1}^{N_m} D_{(m1,m2,m3)_i}\frac{\partial u}{\partial x}\right) - \sum_{i=1}^{M_m} V_{(m1,m2,m3)_i}\frac{\partial u}{\partial x} + \sum_{i=1}^{K_m} Q_{(m1,m2,m3)_i} \qquad (5)$$

$$\lambda_h\frac{\partial \phi}{\partial t} = \frac{\partial}{\partial x}\left(\sum_{i=1}^{N_h} D_{(h)_i}\frac{\partial \phi}{\partial x}\right) - \sum_{i=1}^{M_h} V_{(h)_i}\frac{\partial \phi}{\partial x} + Q_h \qquad (6)$$

where, m1, m2, m3 indices denote the mass transfer of vapor, liquid and solid masses respectively; u - mass being transferred; N_m, M_m, K_m - number of physical processes included into mass transfer problem, viz. N_m – number of processes occurring due to diffusion, M_m – number of processes occurring due to convection, K_m– number of processes occurring due to mass source or sinks (see mass transfer in 2.2); $\lambda_{m1,m2,m3}, D_{(m1,m2,m3)}, V_{(m1,m2,m3)}$ - material properties of relevant physical process of the mass transfer (e.g. $\lambda_{m1,m2,m3}$ – retarding coefficients of mass transfer, $D_{(m1,m2,m3)}$ – mass transfer permeability coefficients, $V_{(m1,m2,m3)}$ – mass transfer velocity); $Q_{(m1,m2,m3)}$ - mass source/sink (e.g. evaporation, condensation rates etc.) along the model and at the boundaries; h index denotes the heat transfer problem; ϕ - temperature; N_h, M_h - number of physical processes included into heat transfer problem (see heat transfer in 2.2); λ_h, D_h, V_h - material properties of relevant physical process of the heat transfer; Q_h - heat source/sink rate; t - temporal variable; x - spatial variable.

For the sake of simplicity, the present paper focuses on macroscopic level processes only as they have more significant effect on temperature distribution within the topic problem, namely: convection due to temperature gradient; mass transfer due to vapor pressure and hydraulic gradients. However, it is straightforward to incorporate all the others processes as well with its associated physical parameters. Having this simplification made, the governing equations shall take the following form:

Liquid phase moisture transfer - filtration.

$$\frac{\partial h}{\partial t} = k_f\frac{\partial^2 h}{\partial x^2} + Q_f \overset{FEM}{\Longrightarrow} \{\dot{h}\} = [C_h]\{h\} + \{F\} \qquad (7)$$

where, h - mass content of liquid water, in kg per unit volume in m^3 of the skeleton; k_f - permeability coefficient, constant value for each material and does not change in time, in $\frac{m}{sec}$; Q_f - liquid water source/sink – a function accounting the incoming or outgoing moist, in m^3/sec; $\overset{FEM}{\Longrightarrow}$ - Finite element (matrix) transformation of the governing differential equation; $\{h\},\{\dot{h}\}$ - vectors of mass contents and its time derivatives values at the finite element nodes; $[C_h],\{F\}$ - Finite Element transformed matrix and vector that discretely models $k_f\frac{\partial^2}{\partial x^2}$ operator and water source/sink function Q_f in filtration equation.

Partial vapor pressure distribution

$$\frac{\partial p}{\partial t}=k_v\frac{\partial^2 p}{\partial x^2}+Q_p\overset{FEM}{\Longrightarrow}\{\dot{p}\}=[C_p]\{p\}+\{P\} \qquad (8)$$

where, p - partial vapor pressure, in Pa; k_v - vapor conductivity coefficient, constant value for each material and does not change in time, in $\frac{kg}{m\ sec\ Pa}$; Q_p - boundary condition function that accounts the variation of partial vapor pressure at the boundaries, contact surfaces with indoor and outdoor environments, in $\frac{Pa}{sec}$; $\overset{FEM}{\Longrightarrow}$ - Finite element (matrix) transformation of governing differential equation; $\{p\},\{\dot{p}\}$ - vectors of vapor pressures and its time derivatives values at the finite element nodes; $[C_p],\{P\}$ - Finite Element transformed matrix and vector that discretely models $k_v\frac{\partial^2}{\partial x^2}$ operator and the boundary condition function Q_p in partial vapor pressure equation.

Heat transfer.

$$\frac{\partial \phi}{\partial t}=\frac{\partial}{\partial x}\left(D\big(f(\phi)\big)\frac{\partial \phi}{\partial x}\right)+Q_h\overset{FEM}{\Longrightarrow} \overset{FEM}{\Longrightarrow}\{\dot{\phi}\}=[C_t(t)]\{\phi\}+\{T\} \qquad (9)$$

where, ϕ – temperature, in ℃; $D\big(f(\phi)\big)$ - heat conductivity depending on some function of ϕ, individual for each material, in $\frac{W}{m\,℃}$; Q_h - heat source/sink that accounts the boundary conditions and heat transfer due to evaporation or condensation, in $\frac{kcal}{m^3\cdot hr}$; $\overset{FEM}{\Longrightarrow}$ - Finite element (matrix) transformation of governing heat transfer differential equation; $\{\phi\},\{\dot{\phi}\}$ - vectors of temperatures and its time derivatives values at the finite element nodes; $[C_\phi],\{T\}$ - Finite Element transformed matrix and vector that discretely model $\frac{\partial}{\partial x}\left(D\big(f(\phi)\big)\frac{\partial}{\partial x}\right)$ operator and Q_h function in heat transfer equation.

Heat transfer equation (9) shows the heat conductivity coefficient *D* being dependent on a function of temperature ϕ. Fig. 2 depicts the variation of heat conductivity property of a material with its moisture content as proposed by T.I. Rubashkina [6]. Similar relations are also given in other resources [2]. In order to establish the function *D,* it is necessary to build the relationship between the moisture content *W* and the temperature ϕ, as it will be shown later.

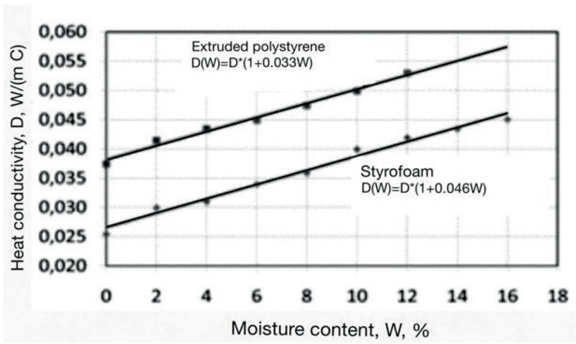


Figure 2. Heat conductivity D as a function of moisture content W

As it can be seen from Fig. 2 the moisture content of the wall material, which is, in our case, the solution to equation (7), changes the heat conductivity linearly. Then the solution to (9) explicitly depends on the solution of (7). Thus (7) and (9) should be solved jointly to obtain the temperature distribution within the media being adjusted to the moisture content. Linear relationship of material moisture content and its thermal conductivity can be defined as:

$$D\left(\frac{h(t)}{\rho_m}\right) = D_k \frac{h(t)}{\rho_m} + D_f \quad (10)$$

where, D_k, D_f - proportionality coefficients of linear relationship as in Fig.2 which are the constant values for each material; $h(t)$ - mass content of liquid water as a function of time t, to be determined by the solution of (7); ρ_m - dry density of the material.

Equation (7) includes the condensation/evaporation function Q_f which in turn depends on temperature. Hence the thermal conductivity D eventually non-linearly depends on temperature ϕ.

Moisture transfer problem (7) can be simplified by assuming that D_f is the heat conductivity property valued at the time $t = 0$, then the initial values for this problem will be a vector of zeros.

$$h(x, t = 0) = 0 \quad (11)$$

Accordingly, the solution of (7) will define the variation of moisture content throughout the wall at any given time $t = t_d$ in comparison to the initial values which are the moisture content at $t = 0$.

2.4. Evaporation and Condensation

In order to calculate the amount of moisture that condenses or evaporates within the wall a model proposed by Dalton [2] shall be utilized. Using the notation of the paper it can be expressed as:

$$\frac{dM}{dt} = \Theta A\left(x_p(t) - x_T(t)\right) \quad (12)$$

where, $\frac{dM}{dt}$ - rate of change of moisture in $\frac{kg}{hr}$; $\Theta = (25 + 19v)$ - evaporation/condensation coefficient in $\frac{kg}{m^2hr}$, where v - air flow velocity which is negligibly small for the topic problem and can be set to zero; A - contact area, assumed as unity, in m^2; $x_p(t)$ - air humidity as a ratio of vapor mass to dry air mass, in $\frac{kg}{kg}$; $x_T(t)$ - maximum air humidity as a ratio of saturated vapor mass at a given temperature to a dry air mass, in $\frac{kg}{kg}$.

Dalton model states that the condensation happens when $x_p(t) > x_T(t)$, or mass change rate $\frac{dM}{dt}$ is positive valued and the evaporation happens otherwise, when $\frac{dM}{dt}$ is negative valued.

It is a routine to show that $x_p(t)$ and $x_T(t)$ can be expressed by the following formulas, based on the ideal gas theory [5]:

$$x_p(t) = \frac{0.0022k_B}{p_{atm}m} p(t) \quad (13)$$

$$x_T(t) = \frac{0.0022k_B}{p_{atm}m} p_{vs}(t) \quad (14)$$

where, t – time, in hr; p_{atm} - absolute pressure (atmospheric pressure), assumed as 100 kPa; m - molecular mass of dry air, circa 4.81×10^{-26}kg; k_B - Bolzmann constant, 1.380649×10^{-23} $\frac{J}{°K}$; $p(t)$ – partial vapor pressure distribution within the wall, which is a solution to (8), in Pa; $p_{vs}(t)$ - saturated partial vapor pressure for a given temperature, in Pa, can be calculated by using the following formula in kPa (Magnus formula):

$$p_{vs}(t) = 610.94e^{\left(\frac{17.625\phi}{\phi+243.04}\right)} \quad (15)$$

where, ϕ - the temperature in °C; Equation (15) makes the saturated vapor pressure $p_{vs}(t)$ and consequently maximum air humidity $x_T(t)$ in (14) dependent on the temperature ϕ, hence the rate of change of moisture $\frac{dM}{dt}$ in (12) is also depends on temperature. Once equation (12) is established it can be incorporated into mass transfer problem (7) in form of mass sink or source function. Here the "sink" means the evaporation whereas "source" - the condensation. Namely:

$$Q_f = \frac{1}{\rho_w}\frac{dM}{dt} = \frac{1}{\rho_w}\Theta A\left(x_p(t) - x_T(t)\right) \quad (16)$$

where, ρ_w- density of water, in $\frac{kg}{m^3}$.
Function (16) accounts such phenomena as vapor transmission via its $x_p(t)$ term and heat transfer via its $x_T(t)$ term, while itself appears in mass transfer (filtration) problem (7). The filtration equation (7) in turn, redistributes the moisture within the wall due to hydraulic gradients and effects the heat conductivity value through (10).
The evaporation and the condensation phase change processes are also associated with the heat transfer as they are either endothermic as in case of evaporation consuming the heat from its surroundings, or exothermic as in condensation releasing the heat to its surroundings. Amount of heat consumed or released, is proportional to the amount of mass of water evaporated or condensed, i.e. it is proportional to (16). Then the heat sink/source function Q_h appearing in (5) can be written as:

$$Q_h = rQ_f \tag{17}$$

where, Q_f – moisture phase change (16); r - specific evaporation/condensation heat.
In [2] it is recommended the specific evaporation/condensation heat to be calculated as:

$$r = 595 - 0.55\phi \tag{18}$$

where, r - evaporation/condensation heat in kcal/kg; ϕ - temperature in °C.
Should r be assumed as a constant, say 595 kcal/kg, this simplification creates an error in the range of 2.0% - 2.5% in r value, which might be ignored. Alternatively (18) can be fully used in the calculations then an additional term occurs in (9) which needs to be handled as per finite element method procedure. Present study uses constant value for r.

2.5. Vapor Transfer
Vapor transfer problem, as it is defined in (8), with the boundary conditions (3), (4), after the finite element discretization, becomes a system of linear ordinary first order differential equations that have an analytical solution:

$$\{\dot{p}\} = [C_p]\{p\} + \{P\} \xrightarrow{solution}$$
$$\{p(t)\} = e^{[C_p]t}\{p_0\} + \int_0^t e^{[C_p](t-\xi)}\{P(\xi)\}\,d\xi \tag{19}$$

where, $\{p_0\}$ - is a vector of initial values (partial vapor pressure distribution within the wall at t = 0), which can be assumed as a linear interpolation between $p_{v,in}(0)$ and $p_{v,out}(0)$ as per given boundary conditions (3) and (4).
Vector notation $\{\cdot\}$ means that (19) results in a vector of nodal vapor pressure functions of time of the corresponding finite element model.
Boundary conditions (3) and (4) are assumed to be essential or Dirichlet boundary conditions.

2.6. Heat and Mass Transfer
Mass transfer or filtration problem (7) has the following finite element form:

$$\{\dot{h}\} = [C_p]\{h\} + \{F\} \tag{20}$$

Here the vector $\{F\}$ is a finite element transformed form of (16) thus it also depends on temperature through the link between (15) → (14) → (16). Therefore, in order to establish this function and solve (7) for a given time t_d, it is necessary to have the temperature distribution function $\phi(t)$. Should this function be guessed or somehow estimated then semi-analytical solution to (7) can be found as follows:

$$\{h^{\langle 0\rangle}(t)\} = e^{[C_h]t}\{h_0\} + \int_0^t e^{[C_h](t-\xi)}\{F^{\langle 0\rangle}(\xi)\}\,(\tag{21a}$$

$$\{h^{\langle 0\rangle}(t)\} = \int_0^t e^{[C_h](t-\xi)}\{F^{\langle 0\rangle}(\xi)\}\,d\xi \tag{21b}$$

as $\{h^{\langle 0\rangle}(t)\} = \{0\}$ according to (11), then (21b) can be used instead of more general (21a). As the function $h(t)$ depends on $\phi(t)$, which is the function we are looking for, then we have a non-linearity, as according to relationship (10), $h(t)$ values are needed to determine heat conductivity properties of the media. This non-linearity is resolved by using Picard iterative approach method. Angle brackets $\langle\cdot\rangle$ in $h^{\langle 0\rangle}(t)$ denote the iteration number.

In order to achieve the rapid convergence of the solution one may use the linear heat transfer equation to obtain the temperature distribution function as first iteration for Picard method. Namely, the equation can be assumed as:

$$\frac{\partial \phi}{\partial t} = D_f \frac{\partial^2 \phi}{dx^2} + Q_{hBC} \overset{FEM}{\Longrightarrow} \{\dot{\phi}\} = [C_\phi]\{\phi\} + \{T_{BC}\} \quad (22)$$

where, Q_{hBC} - are the function that includes only the boundary conditions (1) and (2); D_f - see (10); see (9) for others.

Unlike in (9) the matrix $[C_\phi]$ in (22) is not time dependent and just a matrix of constants

Semi-analytical solution to (22) has the following form:

$$\{\phi^{\langle 0 \rangle}(t)\} = e^{[C_\phi]t}\{\phi_0\} + \int_0^t e^{[C_\phi](t-\xi)}\{T_{BC}(\xi)\}\, d\xi \quad (23)$$

where, $\{\phi_0\}$ - is a vector of initial temperature distribution in the wall at time $t = 0$. Similarly to $\{p_0\}$, the initial values of $\{\phi_0\}$ in discrete nodes might be assumed as linear interpolation between $\left[\left(\phi_{in} = \Phi_{in}(0)\right) \cdots \left(\phi_{out} = \Phi_{out}(0)\right)\right]$ as per (1) and (2).

Having determined the temperature distribution function at first iteration by (23), one may define the mass transfer function by using (21b).

Each following iteration for heat transfer problem requires the solution of (9) which is linearized by the results of previous iteration and becomes the second order partial differential equation with variable coefficients. The solution to this equation has the form of:

$$\{\phi^{\langle i+1 \rangle}(t)\} = e^{\int_0^t [C^{\langle i \rangle}(\tau)]d\tau}\{\phi_0\} + e^{\int_0^t [C^{\langle i \rangle}(\tau)]d\tau} \int_0^t e^{-\int_0^\xi [C^{\langle i \rangle}(\tau)]d\tau} \{T^{\langle i \rangle}(\xi)\} d\xi \quad (24)$$

where, $[C^{\langle i \rangle}(\tau)]$ - the matrix which elements are the functions of time via (10); $\{T^{\langle i \rangle}(\xi)\}$ - a vector which elements are the functions of time that include the boundary conditions and heat source/sink as per (17); i - iteration number.

Both (22) and (9) have non-essential or Neumann boundary condition as given by (1) and (2).

2.7. Assumptions

All formulation described in sections above are based on the following assumptions:

a) At any given point within the domain and at any given moment of time, the porous media, the moisture in its vapor and liquid phases are all in local thermodynamic equilibrium, i.e. have the same temperatures along with other properties;

b) Porous media is none-deformable and homogeneous within each element of the material of the wall;

c) Gas phase (air and vapor) obeys the ideal gas law;

d) Heat transfer by radiation is negligible and ignored;

e) Moisture transfer due to gravity is ignored;

f) Condensation and evaporation phenomena do not change the initial moisture content of the skeleton significantly such that the degree of saturation of the porous media might be assumed as a constant within time $t \in [0 \cdots t_d]$, where t_d - is the design time.

2.8. Computation Workflow

Proposed formulation has been converted into a computation workflow that then is used for developing of the computer program. Conversion of governing partial differential equations into finite element equations is omitted here, as this can be found in many resources [3].

Computation steps:

Step 1

Form three finite element models with the identical spatial discretization, one for each of problems, i.e. vapor transmission, heat transfer and filtration problem;

Step 2

For a given initial vapor pressure distribution $\{p_0\}$ establish a function of $\{p\} = \{p(t)\}$ by using (19);

Step 3

For a given initial temperature values $\{\phi_0\}$ and by using (23) establish a function of $\{\phi\} = \{\phi^{\langle i \rangle}(t)\}$ where $i = 0$;

Step 4
Having the functions of $\{p\} = \{p(t)\}$ and $\{\phi\} = \{\phi^{\langle i \rangle}(t)\}$ determined on the current iteration, establish the functions $Q_f = Q_f(t)$ and $Q_h = Q_h(t)$ as per (16) and (17) accordingly;
Step 5
Solve filtration problem by using (21) to establish $\{h\} = \{h^{\langle i \rangle}(t)\}$;
Step 6
Establish the functions $D = D(\{h\})$ for the material conductivities by using (10);
Step 7
Solve the heat transfer problem with variable coefficients by using (24) incorporating the conductivity functions as per *Step 6* and the heat sink/source functions $Q_h = Q_h(t)$ as per *Step 4*;
Step 8
Compare the temperature distribution values for a given time $t = 0 + t_d$ using the results of *Step 7* with the values of temperature distribution function used at *Step 4*. Should the difference between the values are in excess of acceptable limit, return to *Step 4* at the following iteration $(i = i + 1)$ where use temperature distribution function $\{\phi\} = \{\phi^{\langle i+1 \rangle}(t)\}$ as it is obtained in *Step 7*. If the difference is less than the acceptable limit then the problem is solved.
Above workflow assumes the linearization of differential equation (9) by Picard method. This method has been preferred comparing to any others because it allows to monitor the iterative progress of every physical phenomenon happening within the model, be it filtration or heat transfer; and interpret them in the framework of boundary conditions and material properties.

3. PROBLEM DEFINITION, RESULTS AND DISCUSSIONS

3.1. Problem Definition

Wall model is assumed to be as in Fig.1. The goal is to calculate the distribution of temperatures within the wall at the given moment of time.

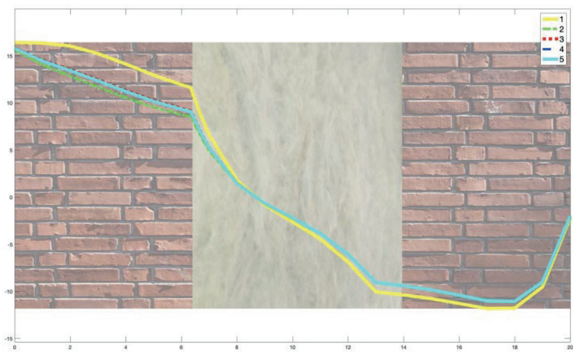
***Given*:**
Inner brickwall thickness $\frac{20}{3}$ m
Insulation thickness $\frac{20}{3}$ m
Outer brickwall thickness $\frac{20}{3}$ m
Structure thicknesses are deliberately selected as wide in order to demonstrate the non-linear behavior.
Brickwall properties:
Heat conductivity $D_f = 0.340 \frac{W}{m°C}$ and $D_m = 0.375 \frac{W}{m°C}$
Unit weight $\gamma_{wall} = 400 \frac{kg}{m^3}$
Vapor conductivity $k_{v_{wall}} = 0.17 \frac{mgr}{m\ hr\ Pa}$
Filtration permeability $k_{f_{wall}} = 0.17 \frac{m}{hr}$
Insulation layer properties:
Heat conductivity $D_f = 0.033 \frac{W}{m°C}$ and $D_m = 0.121 \frac{W}{m°C}$
Unit weight $\gamma_{wall} = 150 \frac{kg}{m^3}$
Vapor conductivity $k_{v_{wall}} = 0.5 \frac{mgr}{m\ hr\ Pa}$
Filtration permeability $k_{f_{wall}} = 1.5 \frac{m}{hr}$
Vapor pressure boundary conditions:

$$p_{v,in} = 873 + 50 \sin\left(\frac{\pi t}{12}\right), \text{ in } Pa$$
$$p_{v,out} = 378 + 314 \sin\left(\frac{\pi t}{50}\right), \text{ in } Pa$$

Temperature boundary conditions:

$$\phi_{in} = 20 + 4 \sin\left(\frac{\pi t}{12}\right), \text{ in } °C$$
$$\phi_{out} = -5 + 15 \sin\left(\frac{\pi t}{12}\right), \text{ in } °C$$

Design time period $t_d = 20hr$.
Below are the figures showing the temperatures, vapor pressure and moisture change variations throughout the wall in their successive iterations.



<u>Figure 3.</u> Temperature distribution within the wall at time $t = 20hr$. 1,2,3,4,5 – distribution curves for respective iteration.

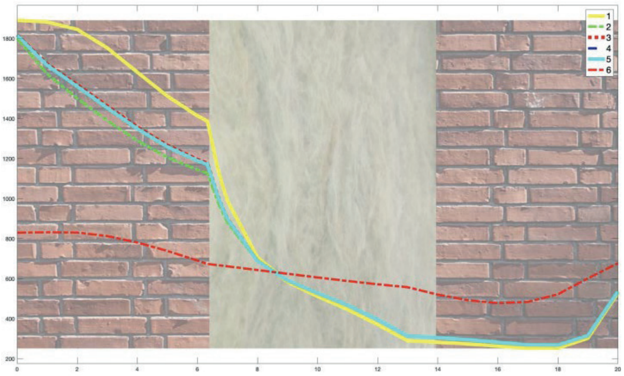


Figure 4. Saturated vapor pressure distribution within the wall at time $t = 20hr$. 1,2,3,4,5 – distribution curves for respective iteration. 6 - vapor pressure distribution as per vapour transit problem.

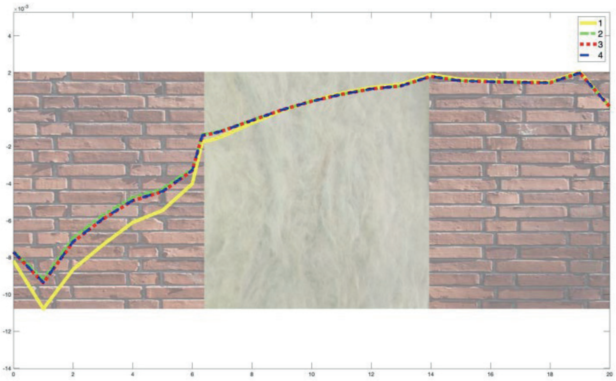


Figure 5. Moisture content variation curves at $t = 20hr$. 1,2,3,4,5 – distribution curves for respective iteration.

Calculation is considered as converged and completed when the following criterion is satisfied:

$$\frac{\left\|\phi^{\langle i\rangle}(t_d) - \phi^{\langle i-1\rangle}(t_d)\right\|_2}{\left\|\phi^{\langle i\rangle}(t_d)\right\|_2 + 1} \leq \epsilon_r$$

where, $\phi^{\langle i\rangle}(t_d), \phi^{\langle i-1\rangle}(t_d)$ – are i^{th} and $(i-1)^{th}$ iterations for temperature distribution functions evaluated at $t = t_d$; ϵ_r – allowable error (assumed to be 0.001); $\|\cdot\|_2$ - second norm of respective vector.

3.2. Discussions

The problem solved in Section 3.1 above has demonstrated how the solution iteratively has been found as per proposed workflow. Red dashed line 6 in Fig.4 represents the vapor pressure distribution at time $t_d = 20hr$ obtained by solving vapour transit problem (19). Yellow solid line 1 (Fig.4) is the saturated vapor pressure values being calculated based on linear heat transfer problem (see yellow line 1 in Fig. 3). The difference between red line 6 and yellow line 1 constitutes the evaporation if it is negative valued and condensation if it is positive valued. Point of intersection corresponds to the Dew Point temperature. The filtration problem (7) solved by accounting this difference results in moisture variation distribution as shown by yellow line 1 in Fig.5.

As the linear relationship is proposed in (Fig.2), the moisture content defines the heat conductivity property of respective material in tri-layered wall structure.

When all corrected values of heat conductivities D and heat sink/source functions Q_h are entered into heat transfer problem (9) and solved by (24) the temperature distribution curve in second iteration is obtained, which is represented by green dashed curve 2 in Fig.3 and as the saturated vapor pressure distribution curve 2 in Fig.4. As it can be seen, the temperatures within the wall from inner face till Dew Point location (a point of intersection of 1,2,3,4,5 curves with curve 6 in Fig.4) have decreased, comparing to the previous iteration, thereafter the temperatures are increased. This can be explained as follows:

- The wall, up until the Dew Point location experiences the evaporation which results in drying out of the wall material thus decreasing its conductivities as per (10). The lower the heat conductivity the higher the resistance to heat transfer, and the better its insulation properties. Also, the heat is partially consumed to compensate the evaporation heat. Therefore, the combined effect of reduced moisture content and the evaporation heat consumption explains why the temperature drops within this zone of the wall.
- Once the Dew Point location is crossed, evaporation changes into the condensation which increases the moisture content which in

turn increases the conductivity. The higher the conductivity the more the heat is transferred. Additionally, there is a heat expel due to the condensation process. Yet again, the combined effect of these two processes results in increase of the wall temperature comparing to its previous iteration.

Having calculated the temperature distribution functions by solving the non-linear problem in $t \in [0, t_d]$, these functions are used for the next iteration. The iterations fine-tune the evaporation and condensation amounts until the stabilized temperature distribution is achieved. These iterations are shown in different colors on the respective figures.

4. CONCLUSIONS

Proposed semi-analytical formulation and computation workflow give a powerful tool to calculate practical the mass and heat transfer problems in multi-layered structures taking into account the interaction in between the key physical processes. Finite element conversion of differential equations allows to define and incorporate many other phenomena mentioned in section 2.1 above thus making the formulation a universal tool.

However, the formulation has also some shortcomings that should be kept in mind while using it. They are briefly discussed below:

a) Unrestricted Moisture Content Change

Linear relationship as defined in (10) is continuous with practically no upper and lower bounds. Computationally the argument of (10) may take such a value that would make the heat conductivity value or the total moisture content less than minimum allowable values. Similarly, the moisture content may rise largely such that the material would not be able to hold that amount of liquid water.

The problem of excessive and negative valued moisture content in the model can be overcame by introducing the limiting values for moisture content for each material comprising the wall structure. In such case the equation (10) shall take the following form:

$$D\left(\frac{h(t)}{\rho_m}\right) = \begin{cases} D_{min};\ \forall W = \dfrac{h(t)}{\rho_m} < W_{min} \\ D_k \dfrac{h(t)}{\rho_m} + D_f;\ \forall W = \dfrac{h(t)}{\rho_m} \in [W_{min}, W_{max}] \\ D_{max};\ \forall W = \dfrac{h(t)}{\rho_m} > W_{min} \end{cases} \quad (25)$$

where, W_{min}, W_{max} - are respectively minimum and maximum moisture content that respective material may have; D_{min}, D_{max} - are respectively minimum and maximum heat conductivity coefficients of respective material.

b) Limitation of Saturation Degree during the Evaporation and the Condensation

Among the other assumptions made in formulation, one regarding the constant degree of saturation is arguable. Excessive condensation and evaporation will inevitably either fill in the voids of the material fully (till maximum degree) or dry it out till minimum possible moisture content. Dalton's model, as described in section 2.4, defines the amount of condensation or evaporation based on the contact area A as noted in (12) which is an area of interface surface between the liquid water and the air. Having assumed the saturation degree as constant, the contact area A becomes constant throughout the material as well. However, the saturation degree and thus the contact area at evaporation zone of the model may decrease, whereas it may increase at the condensation zone. Accordingly, the total amount of moist being evaporated should decrease as the material becomes drier and is actually less than that obtained by proposed calculation, whereas the total amount of condensation should increase and be more that it is calculated. This has an effect on temperature distribution as well. By intuition one may assume that the temperatures all throughout the wall would be slightly higher comparing to those obtained by proposed calculation.

The way to overcome this shortcoming is to introduce a function that would calculate the saturation degree in space and time and incorporate that function into the computation workflow.

Apparently, the saturation degree should be a function of moisture content $h(t)$ or $Sr = Sr(h)$, where Sr is a saturation degree having its value within a range of $[0 \cdots 1]$. Assuming at time $t = 0$ the saturation degree of the material to be $Sr = Sr_0$ then (16) can be rewritten as:

$$Q_f = \frac{1}{\rho_w}\frac{dM}{dt} = \underbrace{\frac{1}{\rho_w}\Theta A Sr_0\big(x_p(t) - x_T(t)\big)}_{1^{st}\ term-sink/soource\ function} + \underbrace{\frac{1}{\rho_w}\Theta \mathrm{A}\left(x_p(t) - x_T(t)\right)Sr(h)}_{2^{nd}\ term\ -to\ be\ included\ into\ FEM} \quad (26)$$

Here, 1^{st} term in (26) is similar to (16) and is included into filtration calculations in accordance with proposed workflow. 2^{nd} term can be further developed by assumption:

$$Sr(h) = \alpha h \quad (27)$$

where, α - is some proportionality coefficient. Then second term will change the filtration governing equation (7) to the following form:

$$\frac{\partial h}{\partial t} = k_f\frac{\partial^2 h}{\partial x^2} + G(t)h + Q_{f1} \quad (28)$$

where,

$$G(t) = \frac{1}{\rho_w}\Theta \mathrm{A}\alpha\left(x_p(t) - x_T(t)\right)$$

Q_{f1}- is first term of right-hand side of (26).

This modification to filtration equation makes it a differential equation with variable coefficients. Accordingly, it will require the relevant solution method.

c) Filtration Formulation in Unsaturated Media

Filtration equation (16), even with the modifications as proposed in (b) above, does not accurately describe the flow happening within the wall. In [2] it is proposed to use the specific moisture content which is equal to

$$u = \frac{h(t)}{\rho_m}$$

and use relevant mass transfer coefficient of the media that includes the pore saturation degree as well. This is a kind of generalization of filtration phenomenon. However, should the filtration within the unsaturated media (the skeleton) be described in form of the equation similar to (7) that equation would become more complicated and non-linear. By intuition one may say that the proposed computation method gives conservative results as it assumes that flow occurs in a constant saturation degree, thus this non-linearity is ignored and the computation is simplified. The evaporation/condensation rate may account the saturation degree effect, if the modification as proposed in (b) is used, whereas for filtration problem the saturation degree effect is ignored posing inconsistency. The numerous computations being run for various initial conditions and using the materials properties that are common in construction industry, showed that mass transfer due to filtration is relatively small comparing to the condensation and evaporation, therefore one may assume that the saturation degree effect, if ignored in filtration problem only, may constitute an error within the permissible limits. Nonetheless this topic has to be investigated further.

d) Ice formation

Another phenomenon that has not been included into calculations is the ice formation within the part of the wall which has negative Celsius temperatures as well the liquid water properties within porous media which may vary at low temperature. In [1] it is proposed to introduce a coefficient ϵ_{ice} that reduces the function (16) at low temperatures such that it is correcting both filtration and heat transfer problems. Further investigations on the way how to include these factors into the calculations need to be done.

REFERENCES

1. SP 50.13330.2012 Thermal protection of buildings.
2. **A.B. Lykov**, Teoriya teploprovodnosti. [Heat transfer theory] // High Education, Moscow 1967. (In Russian).

3. **L.J. Segerlind.** Applied Finite Element Analysis. New York: John Wiley & Sons., 1984.
4. **C.H. Forsberg.** Heat Transfer Principles and Applications. London: Academic Press, Elsevier Inc., 2021.
5. ***Van P. Carey***. Liquid-Vapor Phase-Change Phenomena. An Introduction to the Thermophysics of Vaporization and Condensation Processes in Heat Transfer Equipment. 3rd edition. CRC Press, 2020.
6. **V.N. Kupriyanov, A.M. Yuzmukhametov, I.Sh. Safin**. Vliyaniye vlagi na teploprovodnost' steno-vykh materialov. Sostoyaniye voprosa. [Influence of moisture on the thermal conductivity of wall materials. Question status.] // Proceedings of KSUAU No. 1(39). Building structures of buildings and structures. 2017.
7. **H.P. Langtangen, K.A. Mardal.** Introduction to Numerical Methods for Variational Problems. Cham: Springer Nature Switzerland, 2019.
8. **P.V. O'Neil.** Advanced Engineering Mathematics. Boston: PWS Publishing Company, 1995.
9. **J.N. Reddy.** An Introduction to Nonlinear Finite Element Analysis with applications to heat transfer, fluid mechanics, and solid mechanics. 2nd edition. Oxford University Press, Oxford, 2015.
10. **K.P. Zubarev.** Using Discrete-Continuous Approach for the Solution of Unsteady-State Moisture Transfer Equation for Multilayer Building Walls. International Journal for Computational Civil and Structural Engineering. v.17, i.2, 2021, pp. 50 -57.
11. ***V.N. Sidorov*, *S.M. Mackewicz*.** Solving Unsteady Boundary Value Problems Using Discrete-Analytic Method for Non-Iterative Simulation of Temperature Processes in Time. Key Engineering Materials, Vol. 685, pp. 211-216, Trans Tech Publications Ltd., 2016 ISSN: 1013-9826 DOI: 10.4028/www.scientific.net/KEM.685.211

СПИСОК ЛИТЕРАТУРЫ

1. СП 50.13330.2012 Тепловая защита зданий.
2. **А.В Лыков**. Теория теплопроводности. Высшая школа, М., 1967.
3. ***L.J. Segerlind***. Applied Finite Element Analysis. New York: John Wiley & Sons., 1984.
4. **C.H. Forsberg**. Heat Transfer Principles and Applications. London: Academic Press, Elsevier Inc., 2021.
5. **Van P.Carey**. Liquid-Vapor Phase-Change Phenomena. An Introduction to the Thermophysics of Vaporization and Condensation Processes in Heat Transfer Equipment. 3rd edition. CRC Press, 2020.
6. **В.Н. Куприянов, А.М. Юзмухаметов, И.Ш. Сафин**. Влияние влаги на теплопроводность стеновых материалов. Состояние вопроса. // Известия КГАСУ №1(39). Строительные конструкции здания и сооружения. 2017.
7. **H.P. Langtangen, K.A. Mardal**. Introduction to Numerical Methods for Variational Problems. Cham: Springer Nature Switzerland, 2019.
8. **P.V. O'Neil.** Advanced Engineering Mathematics. Boston: PWS Publishing Company, 1995.
9. **J.N. Reddy.** An Introduction to Nonlinear Finite Element Analysis with applications to heat transfer, fluid mechanics, and solid mechanics. 2nd edition. Oxford University Press, Oxford, 2015.
10. **К.П. Зубарев.** Использование дискретно-континуального подхода к решению уравнения нестационарного влагопереноса в многослойных стенах зданий.
11. **V.N. Sidorov, S.M. Mackewicz.** Solving Unsteady Boundary Value Problems Using Discrete-Analytic Method for Non-Iterative Simulation of Temperature Processes in Time. Key Engineering Materials, Vol. 685, pp. 211-216, Trans Tech Publications Ltd., 2016 ISSN: 1013-9826. DOI: 10.4028/www.scientific.net/KEM.685.211

Vladimir N. Sidorov, Doctor of Engineering Science, member of Russian Academy of Architecture and Construction Sciences, head of a department, Department of Computer Science and Applied Mathematics, Moscow State University of Civil Engineering (MGSU), 26, Yaroslavl highway, Moscow, 129337, SidorovVN@mgsu.ru, 8-495-183-59-94;

Alim M. Primkulov, Master of Science, postgraduate student, Department of Computer Science and Applied Mathematics, Institute of Digital Technologies and Modeling in Construction, Moscow State University of Civil Engineering (MGSU), 26, Yaroslavl highway, Moscow, 129337, a.primkulov@prodim.ru, +7(926)907-75-94.

Владимир Николаевич Сидоров, доктор технических наук, член-корреспондент РААСН, заведующий кафедрой, кафедра информатики и прикладной математики, Федеральное государственное бюджетное образовательное учреждение высшего образования "Национальный исследовательский Московский государственный строительный университет" (НИУ МГСУ), 129337, г. Москва, Ярославское шоссе, д. 26, SidorovVN@mgsu.ru, 8-495-183-59-94;

Алим Махмудович Примкулов, аспирант, кафедра информатики и прикладной математики, Институт цифровых технологий и моделирования в строительстве, Федеральное государственное бюджетное образовательное учреждение высшего образования "Национальный исследовательский Московский государственный строительный университет" (НИУ МГСУ), 129337, г. Москва, Ярославское шоссе, д. 26, a.primkulov@prodim.ru, +7(926)907-75-94.