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## SIMULTANEOUS CALCULATION OF HEAT, MOISTURE, AND AIR TRANSPORT IN A MODULAR SIMULATION ENVIRONMENT

#### Jarek KURNITSKI and Mika VUOLLE

HVAC Laboratory, Helsinki University of Technology, P.O. Box 4400, FIN-02015 HUT, Finland; jarek@cc.hut.fi; mika.vuolle@hut.fi

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**Abstract.** A new one-dimensional model for simultaneous heat, moisture, and air transport calculations in a modular simulation environment has been developed. The model supplements the indoor climate and energy model library that is used for building simulation. The model may be used as a single independent model or as a component of a large model system. The humidity by volume is used as a moisture transfer potential, enthalpy is calculated, condensation is taken into account and all equations are solved simultaneously. The models contain only equations and the general modelling language functions at the same time as a source code and a readable document. The model was validated against analytical solutions and an existing program.

Key words: simultaneous heat, moisture, and air transport, modular simulation environment, modelling language.

#### **1. INTRODUCTION**

Building simulation is widely used for energy and airflow calculations. In traditional programs the models are fixed and not editable. In modular simulation environments the models of basic components, such as walls, ducts, etc., are available and can be connected to create an arbitrary system, for example, the model of a building. The solver, model libraries, climatic data and end user's support with graphical user interface are essential parts of modular simulation environments. Commonly, one-dimensional models are used in building simulation. The 2D and 3D models may be also created, but the programs usually do not support effective and flexible grid generation used in computational fluid dynamics (CFD) programs. In the case of heat and moisture transport, 1D approach can be used successfully for real constructions if the air, heat, and

moisture flows can be described with sufficient accuracy by 1D flows. Simulation may be used as an alternative research method compared to laboratory experiments, field tests, and CFD, or may be combined with these. Modular simulation environment has certain advantages in comparison with traditional stand-alone heat and moisture (HAM) programs, made as a rule for research purposes. The stand-alone programs are effective in the cases they are created for. When even some minor changes are necessary, it may be impossible because the source code is usually not available. The changes are not easy to make either, due to complicated source code including numerical algorithms of the solver. That explains the large number of HAM programs with rather similar features - almost every research institute needs a program of its own. An important feature of modular simulation environment is a solver that is separated from the models. In a simulated system, the equations of whatever model can be replaced without making any change in the system description. Due to the modular structure, the changes can be easily made. Models contain only equations and links, variable and parameter definitions. General modelling language functions at the same time as a readable document and a source code. This makes it possible to collect completed models to model libraries that are understandable and can be applied by other users of the simulation environment. In this work a one-dimensional HAM model in a general modelling language is worked out and validated. It is competitive with traditional one-dimensional HAM programs, but gives advantages of a modular simulation environment. The model is compatible with other models of the indoor climate and energy (ICE) model library, which already includes moisture balance in air zone models.

## 2. MOISTURE TRANSFER IN A POROUS MATERIAL IN AIR CONTACT

## 2.1. Theoretical background

Building materials can be classified as hygroscopic and non-hygroscopic when they are in contact with moist air. All common building materials are porous. The pore volume (pore volume/bulk volume) occupies about 0.5% of the bulk volume in granite and up to 95% in mineral wool [<sup>1</sup>]. The pore system is as a rule complicated. For example, the pores may seem to be round at low magnification (×10), but the complicated microstructure actually appears at a higher magnification (×10 000) [<sup>1</sup>]. Complicated pore structure cannot be described by simple models like the capillary tube model, therefore it is reasonable to use in practice fully empirical approach.

The moisture is moving in vapour and liquid phase in the pores of the material. This is valid when the material is in air or water contact. Water vapour moves by vapour diffusion and with convective air flow if there is a gradient of the gas pressure  $P_{\rm g}$ . Liquid water and capillary condensed water can be

transported by the gradient of the pore water pressure  $P_1$  or by suction S. Absorbed water may migrate along surfaces in pores. At low relative humidity only diffusion occurs if air convection is not considered. At higher humidity the transport of moisture is a combination of diffusion, suction, and surface migration. When relative humidity is close to 100%, the suction dominates. In addition, these processes interact through evaporation/condensation and adsorption/desorption. Liquid water, flowing in a small pore, may evaporate in a large pore and flow as a vapour in it. In the next small pore the vapour may condense and continue movement in liquid phase again. Mathematically the moisture flow g'' (kg/m<sup>2</sup>/s) is described in all these cases by a Fick's type of relation where the flow is equal to the gradient of a state variable or flow potential multiplied by the moisture flow coefficient. In practice, there are two approaches to describe the moisture flow: moisture flow may be separated into vapour and liquid flows or it may be handled as a total flow. According to Claesson  $[^2]$ , the separation is often reasonable, but one must remember that there is no way to measure these two flows; only the total flow can be measured. In the well-known theory of Luikov  $[^3]$ , this separation is a cornerstone. A problem is to account for the heat of evaporation in the energy balance. In the theory of Luikov it is assumed that the fluxes are proportional with a constant coefficient of proportionality. Claesson states  $[^2]$  that there is no physical justification for this ad hoc assumption; in any real system, the ratio of these two flows will vary.

In the following, the moisture flow equations are written for total flow. This is justifiable since moisture permeability measured with typical methods like cup or gamma ray test characterizes the total moisture flow. A piece of the porous material in humid air is characterized in general case by three independent state variables:

 $P_{g}$ , gas pressure [Pa]

T, temperature [K]

moisture state variable

According to Claesson [<sup>2</sup>], the moisture state variable can be one of the following variables:

 $\nu$ , humidity by volume of the air [kg/m<sup>3</sup><sub>air</sub>]

*p*, water vapour pressure [Pa]

 $\varphi$ , relative humidity

 $P_1$ , pore water pressure [Pa]

 $S = P_g - P_1$ , suction [Pa]

*u*, moisture content by mass [kg<sub>w</sub>/kg<sub>dry</sub>]

 $w = \rho_{drv} u$ , moisture content by volume [kg<sub>w</sub>/m<sup>3</sup>]

 $\mu_{\rm w}$ , chemical potential of the water [J/kg]

This is justified due to relations between these variables. The relation between p and v is according to the universal gas law

$$p = v \frac{RT}{M_{\rm w}},\tag{1}$$

where R is the universal gas constant (R = 8.314 J/mol/K) and  $M_w$  is molecular weight of water ( $M_w = 0.018$  kg/mol).

Kelvin's law relates the pore water pressure  $P_1$  to the relative humidity:

$$P_1 = p_s(T) + \frac{RT\rho_w}{M_w} \ln(\varphi), \tag{2}$$

where  $p_s$  is saturated water vapour pressure and  $\rho_w$  is density of water  $(\rho_w \cong 1000 \text{ kg/m}^3)$ . The chemical potential of the water has following form:

$$\mu_{w}(p,T) = \mu_{w0}(T) + \frac{RT}{M_{w}} \ln(\varphi).$$
(3)

When the temperature T and the gas pressure  $P_g$  are constant, there is one independent variable that determines the moisture state. It may be any of the variables v, p,  $\varphi$ , w, u, and  $P_1$ , or any function of these variables. Fick's law for 1D steady-state flow with the humidity by volume as potential is:

$$g = -\delta_{\nu}(\varphi)\frac{\mathrm{d}\nu}{\mathrm{d}x}.$$
(4)

Here, flow coefficient  $\delta_{\nu}(\varphi)$  is moisture permeability with regard to humidity by volume [m<sup>2</sup>/s]. If temperature is not constant, we have two independent state variables (when gas pressure  $P_g$  is constant). Common choice of variables is either  $\varphi$  and T or w and T, as they can be directly measured. Another choice is p and  $P_1$ , since these variables are primary physical causes of diffusion and liquid flow. In principle, whatever combination of the two moisture state variables may be used due to relations (1), (2), and (3) between moisture state variables and temperature. When we add temperature state variable to Eq. (4), we get

$$g = -\delta_{\nu}^{T} \frac{\mathrm{d}\nu}{\mathrm{d}x} - \delta_{T}^{\nu} \frac{\mathrm{d}T}{\mathrm{d}x},\tag{5}$$

where the subscript of the flow coefficient denotes the corresponding potential and the superscript the second potential used in the equation. Here the flow coefficients are functions of two variables. In general, Eq. (5) means that in non-isothermal cases two potentials are needed to describe moisture transfer. In practice, Eq. (5) cannot be used since only isothermal material data are available. To use available material data  $[^{4,5}]$  in calculations, temperature dependence has to be neglected, i.e., we have to use Eq. (4). This simplification is justified in the

case of lightweight constructions, but in certain cases, such as massive stone constructions, it may not give satisfactory results (commonly two potentials are used in such cases).

## 2.2. Equations and simplifications used in existing programs

There is a number of existing codes, mainly research tools, some of these with quite similar features. In [<sup>6</sup>], the overview of models and codes is given and 37 computer codes are listed. This number includes also very simple codes. Only 8 of the 37 codes are generally available, i.e., are sold or given to interested users. Here we shall focus on the moisture balance equations of three programs: 1D-HAM, MATCH, and WUFIZ.

1. The model 1D-HAM (Lund University, Department of Building Physics) [<sup>7,8</sup>] is a basic model that includes heat, air and moisture transfer in one dimension. For describing the moisture transfer as potentials, humidity by volume  $\nu$  and corresponding flow coefficient  $\delta_{\nu}$  are selectively used. Heat flux and moisture flow equations are in the following form

$$q = -\lambda \frac{\partial T}{\partial x} + q_{\rm a} C_{\rm a} T, \tag{6}$$

$$g = -\delta_{\nu} \frac{\partial \nu}{\partial x} + q_{\rm a} \nu, \tag{7}$$

where q is heat flux [W/m<sup>2</sup>],  $\lambda$  – thermal conductivity [W/m/K],  $q_a$  – airflow rate [m<sup>3</sup>/m<sup>2</sup>/s], and  $C_a$  – volumetric heat capacity of air [J/m<sup>3</sup>/K]. Since airflow rate is constant during each time step, only energy and moisture balance equations are needed. The balance equations are:

$$C\frac{\partial T}{\partial t} = -\frac{\partial q}{\partial x},$$

$$\frac{\partial w}{\partial t} = -\frac{\partial g}{\partial x},$$
(8)

where *C* is the volumetric heat capacity of the material.

2. The program MATCH (TU Denmark, Thermal Insulation Laboratory) [<sup>9</sup>] introduces two potentials for the moisture flow: vapour pressure p and suction S (with corresponding flow coefficients  $\delta_p$  and  $D_s$ ); these variables are primary physical causes of diffusion and liquid flow. The moisture balance is without airflow term

$$\frac{\partial w}{\partial t} = \nabla \cdot \left( \delta_p \nabla p + D_S \nabla S \right). \tag{9}$$

The latest version of the program calculates airflow as well. Moisture balance (9) represents separation of the moisture flow into vapour and liquid flows. This separation may be taken as an approximation that is useful in non-isothermal cases and helps to use available material data [<sup>1</sup>]. Flow coefficients  $\delta_p$  and  $D_s$ 

are typically measured under isothermal conditions in air and water contact respectively. Vapour flow calculated with isothermal coefficient  $\delta_p$  is still temperature dependent due to temperature dependence of saturated vapour pressure.

3. The program WUFIZ (Fraunhofer Institute für Bauphysik) [<sup>10</sup>] uses also two potentials for moisture transfer, and airflow is not included in the moisture balance. The choice of potentials is interesting: for liquid flow the relative humidity  $\varphi$  and for vapour flow the vapour pressure p is used. The moisture balance is

$$\frac{\partial w}{\partial t} = \nabla \cdot \left( D_{\varphi} \nabla \varphi + \delta_{p} \nabla p \right). \tag{10}$$

This choice seems at first surprising, especially the use of relative humidity as the potential for liquid flow. Still, we have to remember that Kelvin's law [Eq. (2)] relates the pore water pressure  $P_1$  to the relative humidity. Thus, moisture balance equation (10) is similar to Eq. (9). This choice of potentials is based on numerous experiments. The flow coefficients are specified separately for water and air contact. WUFIZ has been carefully validated and it has given good results, for example, in the case of rain for external wall and massive stone structures.

In this chapter, three different selections of moisture flow potentials were considered. All of these are validated and used successfully. This demonstrates that moisture flow potential can be any of the state variables shown in Section 2.1. The selection of one or two potentials and the separation to liquid and vapour flows seems to be a question of available material data. While inside the material the moisture flow is mathematically described by Fick's type of relation, i.e., any of the moisture state variables can be used as potential and separation to liquid and vapour flows is therefore not justified, then on the boundary the water and air contact is different. Thereby flow coefficients are measured in air and water contact and it is logical to use separation, i.e., one potential for liquid flow and another potential for vapour flow. In addition, the only way to perform calculations is to neglect temperature dependence because non-isothermal material data is not available.

## 3. A NEW MODEL FOR HEAT AND MOISTURE TRANSFER

The purpose of the model of heat and moisture transfer (HAMWall) is to enable the calculation of moisture transfer in a general simulation environment and to offer an alternative to traditional stand-alone programs. HAMWall is made compatible with the ICE model library [<sup>11</sup>]. It can be used either as a single independent model or as a component of a bigger system. The common wall model RCWall may be simply replaced by HAMWall, and the room model which includes moisture balance and climate data, can be linked with it. It is considered that first of all there is a need for moisture calculations when building materials are in air contact. For this reason humidity by volume  $\nu$  is chosen to characterize the moisture transfer potential. This choice neglects temperature dependence but makes it possible to use most of the available material data – isothermal moisture permeability data measured in air contact.

## 3.1. Modular simulation environment

A modular simulation environment, IDA, has been developed by the Division of Building Services Engineering, KTH, and the Swedish Institute of Applied Mathematics, ITM [<sup>12</sup>]. The IDA environment has an interactive graphical modelling tool, IDA modeller. With the modeller, new systems can be created with a drag-and-drop feature. The models can be collected together to simulation systems in a hierarchical manner.

The core of the IDA is the IDA solver. It is a differential-algebraic solver which can handle algebraic loops. The integration method of the solver is the modified one-leg collocation method [<sup>13</sup>]. The solver has a variable timestep controlled by error estimation. The timestep during the integration can vary from several seconds up to several hours depending on the changes in the systems. With the variable timestep the calculation effort is put at the moments when it is needed. During nights, when there are no input signals, the solver may use a timestep of several hours without loosing the accuracy.

The solver can properly handle hysteresis and discontinuities. If the system changes its state between timesteps, the solver will decrease the timestep and localize the change. The solver is also input-output free, thus different versions of the same model are not needed. Further information on the solver can be found in  $[^{14}]$ .

The neutral model format (NMF) for the description of simulation models was first presented in 1989 [<sup>15</sup>]. NMF is a program independent language for modelling of dynamic systems using differential-algebraic equations.

The models are expressed in terms of equations and solving of them is left to the solver of the simulation environment. The variables and interconnections are introduced, too. When all variables are introduced with upper and lower limits, default values and units, the user of the models can adopt them more easily compared to traditional languages. A complete description of the NMF can be found in the NMF handbook [<sup>16</sup>].

Via translator, NMF modules can be used in several modular simulation environments. Translators are available from NMF to TRNSYS and HVACSIM+ [<sup>17</sup>]. Translators have also been developed for systems SPARK [<sup>18</sup>], IDA [<sup>19,20</sup>], ESACAP, and MS1.

#### **3.2.** Heat and moisture transfer equations

Since humidity by volume  $\nu$  was chosen for moisture transfer potential, the basic equations are similar to the model 1D-HAM (Section 2.2). For simplicity we shall not use in this section enthalpy, but it will be added in Section 3.3. If the flow directions shown in Fig. 1 are used, heat flux q'' and moisture flow g'' are as follows

$$q'' = -\lambda \frac{\partial T}{\partial x} + M''_{a}C_{a}(T - T_{\rm ref}), \qquad (11)$$

$$g'' = -\delta_{\nu} \frac{\partial \nu}{\partial x} + \frac{M_{a}''}{\rho_{a}} (\nu - \nu_{\rm ref}), \qquad (12)$$

where  $M''_{a}$  is air mass flow [kg/s/m<sup>2</sup>],  $T_{ref}$  is an arbitrary reference temperature,  $\rho_{a}$  is density of air [kg/m<sup>3</sup>], and  $\nu_{ref}$  is an arbitrary reference humidity by volume.

In the steady state, Eqs. (11) and (12) have analytical solutions which are used afterwards for validation of the model. For temperature the solution is well known

$$T(x) = T_1 + (T_2 - T_1) \frac{e^{x/L} - 1}{e^{l/L} - 1},$$
(13)

where the length L is given by

$$L = \frac{\lambda}{M_a'' C_a}.$$
 (14)

To obtain a solution for the moisture flow, we have to make the following replacement in Eqs. (13) and (14):

$$T \to \nu, \quad \lambda \to \delta_{\nu}, \quad C_{\rm a} \to \frac{1}{\rho_{\rm a}}.$$
 (15)





This follows from the similarity of Eqs. (11) and (12). For heat and moisture flow equations (11) and (12) we have energy and moisture balance in the form

$$\rho c_p \frac{\partial T}{\partial t} = -\frac{\partial q''}{\partial x} = -\frac{\partial}{\partial x} \left( -\lambda \frac{\partial T}{\partial x} + M_a'' C_a T \right) + h_{\text{vap}} \frac{\partial w}{\partial t}, \quad (16)$$

$$\frac{\partial w}{\partial t} = -\frac{\partial g''}{\partial x} = -\frac{\partial}{\partial x} \left( -\delta_v \frac{\partial v}{\partial x} + \frac{M_a''}{\rho_a} v \right), \tag{17}$$

where  $\rho$  is density of the material,  $c_p$  is the specific heat capacity of the material [J/kg/K], and  $h_{vap}$  is the latent heat of the vaporization [J/kg].

## 3.3. Model equations and parameters

Consider a numerical grid shown in Fig. 2 where each cell is described by two resistances R and one capacity C located in the middle of the cell; moisture content by volume w and diffusive moisture resistance Z characterize the moisture transfer. For each cell the material properties are defined. This means that each module can describe as many layers of the material as necessary.

Before we can write balance equations for cells, we have to write the entering and leaving heat and moisture flow equations for the cell *i*. For heat flux q, in Eq. (11) we add enthalpy of the moist air. We obtain

$$q_{i-1\to i} = \frac{A}{R_{i-1} + R_i} (T_{i-1} - T_i) + M_a H_{i-1} + g_{i-1\to i}^D h_{\text{vap}},$$

$$q_{i\to i+1} = \frac{A}{R_i + R_{i+1}} (T_i - T_{i+1}) + M_a H_i + g_{i\to i+1}^D h_{\text{vap}},$$
(18)

where A is area of the layer,  $R_i = l_i/2\lambda_i$  is the thermal resistance [m<sup>2</sup>K/W],  $l_i$  is thickness of the cell *i*, H is moist air enthalpy by mass [J/kg],  $g^D$  is diffusive moisture flow [kg/s], and  $h_{vap} = 2.5 \times 10^6$  J/kg. Use of the enthalpy means that



Fig. 2. Numerical grid and notations.

heat flow transported not only by dry air but also by vapour is taken into account. On the other hand, the use of enthalpy means more complex iteration.

The heat capacity for cell *i* is defined by  $C_i = A l_i \rho_i c_{pi}$  and the energy balance, based on Eq. (16), becomes

$$C_{i} \frac{\partial T_{i}}{\partial t} = \frac{A}{R_{i-1} + R_{i}} (T_{i-1} - T_{i}) - \frac{A}{R_{i} + R_{i+1}} (T_{i} - T_{i+1}) + M_{a} (H_{i-1} - H_{i}) + \Delta g_{i}^{D} h_{vap},$$
(19)

where  $\Delta g_i^D$  is the difference between entering and leaving diffusive moisture flows [includes two diffusive terms in Eq. (21)]. Moisture flow and balance equations are based on Eqs. (12) and (17). We have

$$g_{i \to i} = \frac{A}{Z_{i-1} + Z_i} (v_{i-1} - v_i) + \frac{M_a}{\rho_a} v_{i-1},$$

$$g_{i \to i+1} = \frac{A}{Z_i + Z_{i+1}} (v_i - v_{i+1}) + \frac{M_a}{\rho_a} v_i,$$
(20)

$$Al_{i}\frac{\partial w_{i}}{\partial t} = \frac{A}{Z_{i-1} + Z_{i}}(v_{i-1} - v_{i}) - \frac{A}{Z_{i} + Z_{i+1}}(v_{i} - v_{i+1}) + \frac{M_{a}}{\rho_{a}}(v_{i-1} - v_{i}), \quad (21)$$

where  $Z_i = l_i/2 \delta_{vi}$  is diffusive moisture resistance [s/m]. Normally, the density of the air  $\rho_a$  is calculated, which is a function of temperature and involves dry air and vapour. To simplify the calculations, constant air density 1.2 kg/m<sup>3</sup> may be used by parameter selection.

So far, the flow directions of q, g, and  $M_a$  shown in Fig. 2 are used. It can be seen from the balance equations (19) and (21) that diffusive terms are symmetrical, i.e., they will be the same also for the opposite flow direction. The convective terms (with  $M_a$ ) are not symmetrical and will be different if flow direction of  $M_a$  is opposite. It means that the direction of  $M_a$  should be checked and correct convective terms used. This is easily done in the NMF code and the complete balance equations of the inner cells are shown in the Appendix. It can be seen as well that the NMF code is compact and the equations are transparent. The balance equations of the first and the last cell are similar to the equations of inner cells, only the surface values (introduced in Section 3.6) are used.

## 3.4. Sorption isotherm and moisture permeability

For many materials moisture permeability depends on the relative humidity. This dependence may be given by using an equation recommended in [<sup>21</sup>]:

$$\delta_{\nu} = \delta^0 + B \left(\frac{\varphi}{100}\right)^C,\tag{22}$$

where  $\delta^0$ , *B* and *C* are constants. To use constant value for the permeability, it has to be written in place of  $\delta^0$  and the constant *B* should be equal to zero.

To solve the moisture balance equation (21), it is necessary to define the sorption isotherm, i.e., the relation between water content of the material and relative humidity of air  $w = w(\varphi)$ . The sorption isotherm may be defined in the hygroscopic range by two lines as shown in Fig. 3 or, alternatively, by the logarithmic equation

$$w = \frac{W_1 - \ln(W_2 - \ln\varphi)}{W_3},$$
(23)

where  $\varphi$  is relative humidity, and  $W_i$  are constants. This equation is recommended in [<sup>22</sup>] for wood and it is valid in the range about 5–100%. When Eq. (23) is used, it is assumed that relative humidity always exceeds the lower limit value. If not, one can easily add an additional constant term to (23) that will compensate negative values when relative humidity is below the lower limit. Other equations can also be used; for example, the equation used in MATCH [<sup>9</sup>] is as follows

$$w = w_{\max} \left( 1 - \ln \varphi / W_4 \right)^{-1/W_5}, \tag{24}$$

where  $w_{\text{max}}$  is upper hygroscopic limit value of the moisture content (at 100% relative humidity, Fig. 3), and  $W_4$  and  $W_5$  are constants.

If the linear model is used, we have the following equations  $[^7]$ 

$$w = \frac{\varphi}{\varphi_{*}} w_{*}, \qquad 0 < \varphi \le \varphi_{*},$$

$$w = w_{*} + \frac{\varphi - \varphi_{*}}{100 - \varphi_{*}} (w_{\max} - w_{*}), \qquad \varphi_{*} < \varphi \le 100\%.$$
(25)



Fig. 3. Linear approximation of the sorption isotherm.

Definition of the sorption isotherm at 100% of relative humidity during condensation (the vertical line in Fig. 3) is discussed in the next section.

## 3.5. Condensation

Consider a situation where calculated humidity by volume will exceed saturated humidity by volume in cell *i*. In the previous cell i-1 condensation did not occur, diffusive moisture flow and mass flow direction is from i-1 to i $(v_{i-1} > v_i)$  and in cell i+1 condensation may occur or not. This situation is shown in Fig. 4. It means that relative humidity in cell *i* will exceed 100%. This will occur during condensation if it is not taken into account in the equations. To calculate condensation, the amount of condensed water should be added to moisture content of the cell *i*. Entering and leaving moisture flows in Fig. 4 are the same as in Eq. (20) since the condensation algorithm should ensure that the value of  $v_i$  will not exceed the saturated value. For condensed flow we can write, using flow directions shown in Fig. 4,

$$g_{i}^{\text{cond}} = \frac{A}{Z_{i} + Z_{i+1}} \left( v_{i} - v_{i}^{s} \right) + \frac{M_{a}}{\rho_{ai}} \left( v_{i} - v_{i}^{s} \right), \tag{26}$$

where moisture flow corresponding to the difference  $(v_i - v_i^s)$  will condense. The condensation will increase moisture content of the material and a condensation term  $g_i^{\text{cond}} \frac{\Delta t}{Al_i}$  [kg/m<sup>3</sup>] should be added to the equation of the sorption isotherm [Eq. (23) or (25)]. If this is done, the humidity by volume in cell *i*, in case of condensation, will be equal to saturated humidity by volume,  $v_i = v_i^s$ . This means that moisture balance equation (21) is valid without any change.





However, compared to Eq. (26), it is numerically much more stable to take condensation into account by defining water uptake with the sorption isotherm. Relative humidity will never exceed 100% if sorption isotherm is defined to be vertical at 100% relative humidity. This was tested by comparing the results with the results calculated using Eq. (26). The output was identical with both methods. In calculations, first we have to know when condensation starts. For that purpose, in IDA the event-function may be used. If condensation has started, the solver will go backwards in time to find out the exact moment when condensation started. The formulation of the event-function is shown in the Appendix. When condensation starts, the sorption isotherm is almost vertical

$$w_i = w_{\max,i} + (\varphi_i - 100)1000w_{\max,i}.$$
 (27)

Equation (27) means that, for example, relative humidity 100.1% (i.e. 0.1% error) will correspond to moisture content a hundred times the hygroscopic limit value. If the logarithmic equation (23) is used instead of Eq. (25), the value at 100% should be given as  $w_{\max,i}$ . This is used in the last part of the sorption isotherm [Eq. (27)]. Sorption isotherm written in NMF is shown in the Appendix. In the tested cases it was possible to calculate condensation both with linear [Eq. (25)] and logarithmic [Eq. (23)] sorption curves without any numerical difficulties.

### 3.6. Input and output flows on the boundary surfaces and links

Equations of the boundary cells determine how the module can be linked with other modules, in particular with those of the room model. It should be noted that a HAMWall module starts and ends with a surface and contains equations only for the solid material between these surfaces. Thus, heat transfer coefficients belong to the room model. Consider a situation on the left boundary of the model, shown in Fig. 5. Here, positive flow directions are shown,  $T_r$ ,  $H_r$ ,  $F_r$ , and  $P_r$  are air temperature, enthalpy, absolute humidity and total pressure in the room;  $T_a$ ,  $H_a$ , and  $v_a$  are surface temperature, air enthalpy and humidity by





volume on the surface. In Fig. 5,  $g_r$  is moisture flow from room model to HAMWall and it equals to moisture flow g in HAMWall that involves both diffusion and convection. There is no moisture resistance on the surface. Neither is surface moisture resistance included in HAMWall to make it possible to link two HAMWall models. Heat flow from the room model to HAMWall is divided into two parts:  $Q_a$  represents convective and radiation heat transfer, and  $Q_{\rm hf} = M_a H_r$  heat flow carried by airflow.

According to Fig. 5, boundary equations are

$$Q_{a} + Q_{hf} = \frac{A}{R_{l}} (T_{a} - T_{l}) + M_{a} H_{a} + g_{d} h_{vap},$$

$$g_{r} = \frac{A}{Z_{l}} (v_{a} - v_{l}) + M_{a} F_{r},$$
(28)

where  $g_d = A(v_a - v_1)/Z_1$  is diffusive moisture flow. As  $Q_{hf}$  is not defined in the room model, it should be included in the HAMWall. From Eq. (28) follows

$$Q_{\rm a} = \frac{A}{R_{\rm l}} (T_{\rm a} - T_{\rm l}) + M_{\rm a} (H_{\rm a} - H_{\rm r}) + g_{\rm d} h_{\rm vap}.$$
(29)

The convective term in Eq. (29),  $M_a(H_a - H_r)$ , depends on the direction of airflow. If the direction of  $M_a$  is opposite, this term obtains negative sign.

The situation on the right boundary of the model is similar to the left one shown in Fig. 5. Only positive directions of  $Q_a$ ,  $Q_{hf}$ , and  $g_r$  are opposite.

#### 4. VALIDATION OF THE MODEL AND EXAMPLES

### 4.1. Analytical solutions

In steady state, the temperature distribution of a material layer is given by Eq. (13). Insertion of (15) into (13) gives the distribution of humidity by volume. Consider a material layer (20 cm of mineral wool) with the following properties and boundary conditions:

$$L = 0.2 \text{ m}$$

$$\lambda = 0.05 \text{ W/m/K}, \delta_v = 1.5 \times 10^{-5} \text{ m}^2/\text{s}$$

$$T_{\rm o} = 15^{\circ}{\rm C}, T_{\rm b} = 5^{\circ}{\rm C}$$

$$v_{a} = 0.01 \text{ kg/m}^{3}, v_{b} = 0.001 \text{ kg/m}^{3}$$

Analytical solution is compared with the model calculations in Figs. 6 and 7.



Fig. 6. Temperature distribution at airflow  $M''_{a} = 5 \times 10^{-4} \text{ kg/m}^{2}/\text{s}$  by different number of cells in the model.



Fig. 7. Distribution of humidity by volume at  $M''_{a} = 5 \times 10^{-4}$  kg/m<sup>2</sup>/s by different number of cells in the model.

Maximum error in temperature is 2.1% with 8 cells, 1.2% with 16 cells, and 0.6% with 32 cells. In the humidity by volume, maximum error is 11% with 8 cells, 7.1% with 16 cells, and 4.2% with 32 cells. The error depends on the airflow rate and at smaller airflow it is smaller. In Table 1 the maximum error is shown at three airflow rates for the case with 16 cells.

Table 1. The effect of airflow rate on the maximum error in the case of 16 cells

$M''_{a}$ , kg/m <sup>2</sup> /s	10 <sup>-4</sup>	$5 \times 10^{-4}$	10 <sup>-3</sup>
Error in temperature, %	0.08	1.2	3.1
Error in humidity, %	0.77	7.1	11.2

# 4.2. Comparison with 1D-HAM

In the following, a simple problem of exfiltration and infiltration is solved both with IDA and 1D-HAM (see Section 2.2). Exactly the same material properties for moisture permeability  $\delta_{\nu}$ , sorption isotherm model [Eq. (24)], and air density 1.2 kg/m<sup>3</sup> are used. Consider a wall structure with 13 mm plasterboard on the warm side, 150 mm mineral wool, and 10 mm plasterboard on the cold side. Inner plasterboard is considered to be rather vapour tight (painted or vapour barrier used), but at the same time the wall is not airtight. The leakage airflow is proportional to pressure difference and equals 1 l/s/m<sup>2</sup> at 20 Pa. For plasterboard  $\delta_{\nu} = 3 \times 10^{-6} \text{ m}^2/\text{s}$ ,  $\lambda = 0.23 \text{ W/m/K}$  and sorption isotherm with  $\varphi_* = 94\%$ ,  $w_* = 9.5 \text{ kg/m}^3$ , and  $w_{\text{max}} = 30 \text{ kg/m}^3$  is used. The data for the mineral wool is:  $\delta_{\nu} = 18 \times 10^{-6} \text{ m}^2/\text{s}$ ,  $\lambda = 0.045 \text{ W/m/K}$ ,  $\varphi_* = 25\%$ ,  $w_* = 0.2 \text{ kg/m}^3$ , and  $w_{\text{max}} = 0.25 \text{ kg/m}^3$ . For inner plasterboard, which was considered to be more vapour-tight,  $\delta_{\nu} = 10^{-7} \text{ m}^2/\text{s}$  is used. The model involves 10 cells: 1st cell for inner plasterboard (l = 13 mm), 5 cells for mineral wool (cells 2–6, l = 30 mm) and 4 cells for external plasterboard (cells 7 and 8, l = 1 mm, and cells 9 and 10, l = 4 mm).

At t = 0, all materials are dry and the moisture content corresponds to about 20% relative humidity. After a day on the warm surface  $\varphi = 30.8\%$ ,  $F_r = 0.0045$  kg/kg for IDA and  $v_r = 0.0054$  kg/m<sup>3</sup> for 1D-HAM, and the temperature is 20°C; on the cold surface  $\varphi = 90.2\%$ ,  $F_r = 0.0034$  kg/kg,  $v_1 = 0.00413$  kg/m<sup>3</sup> and temperature is 0°C. This period lasts 4 days and there is no pressure difference across the wall. During the next 2 day period (t = 121-168 h) humidity and temperature on boundaries remain the same, but the pressure difference 20 Pa will cause an exfiltration 1 l/s/m<sup>2</sup>. During the last 5 day period (t = 169-288 h) the opposite pressure difference 20 Pa will cause infiltration 1 l/s/m<sup>2</sup>. In Fig. 8, dynamics of the relative humidity on the condensation surface in the first cell of the external plasterboard (cell 7) is shown. Figure 9 shows the corresponding moisture content of cells 7 and 8.

It can be seen that the level of relative humidity calculated with 1D-HAM is lower. Due to that reason, the drying of the external plasterboard is more rapid as compared to IDA. This is due to different equations used for saturated vapour pressure calculations in IDA and 1D-HAM (IDA uses ASHRAE's equations



Fig. 8. Relative humidity in the first cell (cell 7) of the external plasterboard.



Fig. 9. Moisture content of the first two cells (cells 7 and 8) of the external plasterboard.

 $[^{23}]$ ). When boundary conditions of 1D-HAM were slightly changed, i.e., in 1D-HAM humidity by volume on both surfaces was increased by 0.22 g/m<sup>3</sup>, the results agree better (Figs. 8 and 9, 1D-HAM<sup>\*</sup> denotes the case with changed boundary conditions).

#### 4.3. Dynamic simulation of a large system

In Sections 4.1 and 4.2 the HAMWall model was used as a separate model. Here the model is used as a part of a larger system – a model of ICE application which represents an office or residential building with all necessary models and data. This is done by replacing the external wall model RCWall with HAMWall. The wall structure described in Section 4.2 is used. We consider a 20 m<sup>2</sup> office room with 2 persons and corresponding moisture, heat, and CO<sub>2</sub> sources and the climate data of Helsinki. The ventilation runs at every workday from 6 am to 5 pm with an air change rate of 10 l/s/pers which causes 1 l/s/m<sup>2</sup> exfiltration airflow through the external wall. Rest of the time the air change rates 2 l/s/pers and 0.2 l/s/m<sup>2</sup> infiltration are caused by an exhaust fan. It is presumed that wind does not affect pressure conditions and air change inside the room. The results of the all the year round simulation are shown in Fig. 10.

The calculations were made also for 4 and 6 persons. It can be seen that the moisture load of 2 persons did not cause condensation. Relative humidity is most of the time below 80%. Condensation was achieved with the moisture load of 5 persons. In cases of 4 and 6 persons, the turning point in sorption isotherm at relative humidity 94% can be found from the relative humidity curves. In Fig. 11 relative humidity and moisture content on condensation surface (inner surface of the external plasterboard) are shown during one week in December for 2 and 6 persons. There is the condensation on the 14th, 15th, and 16th. Moisture content and relative humidity follow the presence of people in both cases – a sharp rise takes place during office hours.



**Fig. 10.** Duration curves of relative humidity in the first cell of the external plasterboard (cell 7, in contact with insulation) when moisture load corresponds to 2, 4, and 6 persons, and corresponding outdoor temperature variation for 6 persons duration curve.





## 5. DISCUSSION

There are two intricate questions related to moisture transfer calculation methods: the choice of the moisture transfer potential and the separation of moisture flow into vapour and liquid flows. Claesson [<sup>2</sup>] has shown that two potentials are needed in non-isothermal cases to describe moisture transfer. It is also known that in practice only total moisture flow can be measured and, thus, separation into vapour and liquid flows is not justified. Nevertheless, available material data will dictate the answers to these questions. Since there is no non-isothermal material data available, the only way to perform calculations is to neglect temperature dependence. Separation into two flows seems to be also reasonable because material data are typically measured in air or water contact. In this work, the humidity by volume was chosen for moisture transfer potential, as this choice allows to use most of the available material data.

The developed model should be taken as a first step for simultaneous heat, moisture, and air transport calculations in a modular simulation environment. It was developed to offer a flexible and effective alternative for traditional standalone programs. As in ICE zone-models the moisture balance equations were already used for air, it was a logical step to develop the model for porous media. The model uses effectively the features of the simulation environment; despite of calculating air density, enthalpy, and condensation, the source code is very transparent. The length of the source code of HAMWall is less than five pages and without routine variable and parameter definitions less than three pages. This means that any changes can easily be done – the code is readable and short. For example, it would be easy for IDA users to change the equation of the sorption isotherm or moisture permeability, to add a second potential or even the hysteresis of sorption.

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#### APPENDIX

## EXAMPLES OF THE NMF CODE USED IN THE HAMWall MODEL

```
/* Balance equations of the inner cells
   FOR i=2, (n-1)
     QC[i] := IF MaPos > 0.5 THEN
               Ma*(H[i-1]-H[i])
             ELSE
               Ma*(H[i]-H[i+1])
             END_IF;
     gC[i] := IF MaPos > 0.5 THEN
               Ma*(v[i-1]/rhoa[i-1]-v[i]/rhoa[i])
             ELSE
               Ma*(v[i]/rhoa[i]-v[i+1]/rhoa[i+1])
             END IF;
     QD[i] := A/(R[i] + R[i-1])*(T[i-1] - T[i]) + A/(R[i])
+ R[i+1])*(T[i+1]-T[i]);
    gD[i] := A/(Z[i] + Z[i-1])*(v[i-1] - v[i]) + A/(Z[i])
               + Z[i+1])*(v[i+1]-v[i]);
    C[i] * T'[i] = QD[i] + QC[i] + gD[i] * HF_VAP;
     l[i] *A*w'[i] = gD[i] + gC[i];
END FOR;
```

Here *MaPos* equal to 1 indicates positive, and equal to 0 negative  $M_a$ . Local variables are used for convective and diffusive terms, QC[i] and gC[i] for convective heat and moisture flow terms, QD[i] and gD[i] for diffusive heat and moisture flow terms. T' and w' are time derivatives of temperature and moisture content.

Here the value of *CondOn* is changed from 0 to 1 when the moisture content exceeds the hygroscopic limit value *w*2.

```
END_FOR;
```

Here parameter *linSor* determines which equation for the sorption isotherm is used [*linSor* = 0 - Eq.(23), and *linSor* = 1 - Eq.(25)].

/\*Input and output flows on the boundary surfaces\*/

```
gaD := A/Z[1] * (va - v[1]);
gbD := A/Z[n] * (vb - v[n]);
       QLeak1 = IF MaPos > 0.5 THEN
                                        Ma * H1
                                  ELSE
Ma * Ha
                                  END_IF + gaD * HF_VAP;
      QLeak2 = IF MaPos > 0.5 THEN
                                      - Ma * Hb
                                   ELSE
                                     - Ma * H2
                                   END IF + gbD*HF VAP;
HumF1 = IF MaPos > 0.5 THEN
                                         Ma * Hum1
                                   ELSE
                                         Ma * v[1]/rhoa[1]
                                   END IF + gaD;
      HumF2 = IF MaPos > 0.5 THEN
                                      - Ma * v[n]/Rhoa[n]
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                                     - Ma *Hum2
          END_IF + gbD;
       Qa = A/R[1] * (Ta - T[1]) + IF MaPos > 0.5 THEN Ma*(Ha-H1) ELSE Ma
                        * (H[1]-Ha) END_IF + gaD * HF_VAP;
       Qb = A/R[n] * (Tb - T[n]) - IF MaPos > 0.5 THEN Ma*(H[n]-Hb) ELSE Ma
         * (Hb-H2) END_IF + gbD * HF_VAP;
```

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## SOOJUS-, NIISKUS- JA ÕHUÜLEKANDE SAMAAEGNE ARVUTAMINE MODULAARSES SIMULATSIOONIKESKKONNAS

## Jarek KURNITSKI ja Mika VUOLLE

On välja töötatud uus ühedimensiooniline mudel poorse materjali soojus-, niiskus- ja õhuülekande samaaegseks arvutamiseks modulaarses simulatsioonikeskkonnas. Niiskuse liikumise potentsiaaliks on võetud absoluutne niiskus mahu järgi, samuti on arvestatud entalpiat ja kondenseerumist. Mudelit on kontrollitud analüütiliste lahendite ja ühe tuntud programmi abil. Mudel täiendab sisekliima ja energia mudelikogumikku, mida kasutatakse hoonete arvutisimulatsiooniks. Seda võib rakendada kas iseseisvana või suure mudelisüsteemi ühe komponendina, mis lubab realiseerida kõiki modulaarse simulatsioonikeskkonna võimalusi.

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