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Indoor Air Quality (IAQ) in the IBPSA Modelica Library (part II): Methodology of integration of new IAQ simulation models

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Abstract

The paper focuses on the simulation of indoor air quality (IAQ) for residential and tertiary buildings with the IBPSA modelica library. Developed methodologies for physical modeling of IAQ in the IBPSA library are first presented. Then, a case study of a room subject to external sources and internal production of pollutants, while interacting with several wall surfaces, has been assembled. Results were consistent compared to analytical and numerical solutions and simulations converged faster than a similar assembly built using the BuildSysPro-QAI modelica library. Finally, Effective Moisture Penetration Depth (EMPD) model has been integrated to evaluate the moisture interaction between walls and the air volume.

Key innovations

- Adding functions that transform data from concentrations to mass fractions using the density of the whole mixture (medium) and the inverse of this transformation.
- Introducing the notion of Particulate Matter Interval (PMI) to ensure a better representation of the inert particles’ diameter.
- Creating a new connector dedicated to the flow of air components to be used for IAQ related studies.
- Effective Moisture Penetration Depth (EMPD) model previously implemented in the BuildSysPro QAI modelica library (BSP-QAI) has been added to the IBPSA library.

Practical implications

- The open source IBPSA modelica library is required.
- A recent version of Dymola (2021 and later) is needed.

Introduction

The Modelica library developed by the International Building Performance Simulation Association (IBPSA) (https://build.openmodelica.org/Documentation/IBPSA.html) considers air components transported by an aeracual flow (gaseous pollutants and inert particles) as traces having no effect on the physical properties of the mixture with a negligible effect of the diffusive flows compared to the advective ones when air is in motion. A study done by Sayegh and al. (2023) confirmed the thermodynamical validity of these assumptions and thus showed that the modeling of IAQ in residential and tertiary buildings is possible with this modelica library. In this article, we skip to a more practical evaluation by presenting the methodology of integrating new models for IAQ studies in the IBPSA modelica library.

The library already contains several models for studies which consider aeraulic phenomena such as natural airflows and pressure profiles. Such models include air volumes, openings such as doors and orifices, air flow sources, etc. However, several other models dedicated for an IAQ study need to be added. These models include:

- Boundary conditions
- Scenarios of internal production of pollutants
- Pollutant/particle/humidity interaction between walls and the air volume

Method

The IBPSA library considers a trace \( i \) through its mass fractions \( C_i = \frac{m_i}{m_t} (kg_{trace}/kg_{air}) \) whereas the data given by commercial sensors are usually available in mass concentration \( \text{Rh}_{p_{i}} = \frac{m}{V} (kg_{trace}/m^3) \) in the case of gaseous pollutants, and in mass concentration \( \text{Rho}_{p_{i}} \) or particulate concentration \( N_{p_{i}} \) is available in mass fractions \( C_{i} \) and the inverse of this transformation when the concentration is needed while the mass fraction is available. These functions are listed in Figure 1.

![Figure 1: Functions added to transform concentrations to mass fractions and their inverses](image)

In each function, a relation is established between the mass fraction \( C_{i} \) and the available mass concentration of
a gaseous entity or inert particle \( (Rho_o \text{ or } Rho_{o2}) \) through the total density of the mixture (medium) \( Rho_i \) as shown in equation (1).

\[
C_i = \frac{m_i}{m_m} = \frac{m_i / V}{m_m / V} = \frac{Rho_i}{Rho_{o2}} \]

(1)

For example, if the medium is humid air, \( Rho_o = 1.2 \text{ kg/m}^3 \) is an approximate value of the total density of the mixture. Therefore, equation (1) is applied in function \( \text{Rho2C} \) where the pollutant’s mass concentration \( Rho_i \) is available and the mass fraction \( C_i \) of the gaseous pollutant is calculated.

If the mass fraction is available and the mass concentration is required, function \( \text{C2Rho} \) is applied. It simply applies the inverse of equation (1) and multiplies the mass fraction by the density of the mixture. Equation (2) presents the applied equation

\[
Rho_i = C_i \times Rho_o \]

(2)

On the other hand, particles concentrations are sometimes expressed as a particulate concentration \( N_{p_i} \) rather than a mass concentration \( Rho_{p_i} \). This is because most particle sensors are based on the principle of light scattering which is used as a particles-counting unit. In these sensors, particles are transported in the air stream through a focused beam of visible or infrared light and the intensity of the scattered light in a selected direction is monitored by a photodetector to count the number of passing particles and their sizes. The readings are then converted to a particle mass concentration, assuming that the particles are spherical and have a constant bulk density and refractive index. This transformation is performed by proprietary algorithms and therefore no exact information on the methods is available (Feenstra et al., 2019).

In the methodology, functions \( N_{p2C} \) and \( C_{2Np} \) consider an additional step to transform the particle concentrations from particulate concentration \( N_{p_i} \) to mass concentration \( Rho_{p_i} \) before calculating the mass fraction \( C_i \) based on the previous equations. This step is shown in equation (3).

\[
Rho_{p_i} = N_{p_i} \times m_{p_i} = N_{p_i} \times Rho_{o} \times V_p \]

(3)

Following the approach commonly used in the literature and discussed by Feenstra (2019), the inert particles considered in this article are spherical with a fixed bulk density. A hypothesis is therefore taken where a theoretical density of \( Rho_p = 2000 \text{ kg/m}^3 \) is assigned to all particles and the volume of a particle is \( V_p = \frac{4}{3} \pi r^3 = \frac{\pi}{6} d_a^3 \) where \( d_a \) is the diameter of the particle. Thus, the relationship between the mass fraction of a particle and its particulate concentration is established by equation (4).

\[
C_i = \frac{Rho_{p_i}}{Rho_o} = \frac{Rho_{p_i} \times V_p}{Rho_o} \times N_{p_i} \]

(4)

Equation (4) is used in function \( N_{p2C} \) while its inverse is used in function \( C_{2Np} \) to calculate the particulate concentration \( N_{p_i} \) starting from the mass fraction of the trace \( C_i \).

However, inert particles are generally considered in categories, or classes of particles \( PM \), such as \( PM1, PM25 \) and \( PM10 \): in each category we consider all particles whose diameter \( d_a \) is smaller than the associated index (1 µm, 2.5 µm and 10 µm respectively). On the other hand, it is important to consider these particles with their different sizes because, in addition to calculating the volume \( V_p \), the diameter of the particle plays an important role in its deposition on a surface and its resuspension in air.

In order to take into consideration the different diameters \( d_a \) included in a PM category, the notion of Particulate Matter Interval (PMI) is introduced.

Each PMI contains the particles whose diameter is between two boundary values. As a consequence, the number of particles in the category \( PM#Y \) is the sum of the number of particles in intervals \( PMI#Y \) for \( Y \leq X \).

For example, five PMI intervals can be considered

- PMIF (very fine particles) which includes particles with diameter \( d_a \leq 0.1 \mu m \)
- PM1 which includes particles of diameter \( 0.1 \mu m \leq d_a < 1 \mu m \)
- PM25 which includes particles of diameter \( 1 \mu m \leq d_a < 2.5 \mu m \)
- PM10 which includes particles of diameter \( 2.5 \mu m \leq d_a < 10 \mu m \)
- PMIG which includes coarse particles of diameter greater than \( 10 \mu m \) \( d_a \geq 10 \mu m \)

Figure 2 shows the distribution of the PMI intervals (in blue) through the PM categories (in red).

\[ \text{Figure 2: The repartition of PMI intervals in the PM categories} \]

Finally, the particle volume \( V_p \) of a PMI interval (used in equations (3) and (4)) is calculated as the average particle volume of this interval. It is illustrated by equation (5).

\[
V_{p_{da2}} = \frac{1}{d_{a2} - d_{a1}} \int_{d_{a1}}^{d_{a2}} \frac{d}{6} d \pi d_a^4 \]

\[
= \frac{\pi}{24} (d_{a2}^4 - d_{a1}^4) \]

\[ \text{Integration of the IAQ models} \]

\[ \text{Integration of the boundary conditions model} \]

The functions presented in the previous section are included in a boundary condition model which describes
the levels of pollution around the studied system (input data is usually supplied by installed commercial sensors). Thus, directly transforming concentrations data into mass fractions $C_i$.

For gaseous pollutants, data are in the form of mass concentration $Rho_i$ therefore the Rho2C function is used. For particles, the mass fraction is calculated by the Rho2C function if the data are in the form of mass concentration $Rho_{pi}$, or the Np2C function if the particulate concentrations $N_{pi}$ are available.

**Integration of the internal production of pollutants/particles model**

A pollutant/particle production model is developed to consider its internal production due to different sources such as the physical activities of occupants either as an input profile from an external file or as a scenario of a fixed amplitude pulse. The available mass flow rate of gaseous pollutants is usually expressed in kg/s which is compatible with the IBPSA library models where the flow of traces is expressed in this unit. On the other hand, the data showing the production of particles are usually provided as particulate flow (particle/s). In this case, it will be transformed into mass flow rate by equation (6).

$$m_{pi} = N_{pi} \cdot \dot{m}_{pi} = N_{pi} \cdot Rho_{pi} \cdot V_p$$

(6)

**Integration of the Air/Wall interaction model**

Three air components are exchanged between an air volume and the adjacent wall surfaces: gaseous pollutants, inert particles and water vapor. The kinetics of the exchanges of gaseous pollutants between the air volume and the wall surface is represented by a couple of coefficients of adsorption $k_a$ and desorption $k_d$ (Tichenor, 1991) as shown in equation (7).

$$Q_{m_{ij}}(t) = \left(k_{a_{ij}} \cdot Rho_{o_{ij}}(t) - k_{d_{ij}} \cdot Rho_{s_{ij}}(t)\right) \cdot S_j$$

(7)

The adsorption coefficient $k_a$ and desorption coefficient $k_d$ are specific to each pollutant-material couple and can be determined experimentally in a chamber test (Tourreilles, 2015). The mass of pollutant per unit area $Rho_{o}$ is calculated from the mass flow rate of the pollutant $Q_m$ transferred from the air volume to the surface according to equation (8).

$$\frac{dRho_{o_{ij}}(t)}{dt} = \frac{Q_{m_{ij}}(t)}{S_j}$$

(8)

For inert particles, the Nazaroff model is used (Nazaroff, 2004). The balance of particles deposited and emitted on a surface is expressed in equation (9).

$$Q_{p_{ij}}(t) = \left(\nu_{d_{ij}} \cdot N_{p_{ij}}(t) - \nu_{r_{ij}} \cdot N_{p_{s_{ij}}}(t)\right) \cdot S_j$$

(9)

The number of particles deposited per unit area of the material $N_{p_{s_{ij}}}$ would be calculated from the particle flow rate deposited on the material surface $Q_p$ according to equation (10).

$$\frac{dN_{p_{s_{ij}}}(t)}{dt} = \frac{Q_{p_{ij}}(t)}{S_j}$$

(10)

The Nazaroff model states that the rates of deposition and resuspension $\nu_d$ and $\nu_r$ depend on a lot of factors. The deposition velocity $\nu_d$ is calculated from several coefficients, factors and constants that depend on the physical characteristics of air, the inclination of the wall, the friction velocity and the diameter and density of the particle. The friction velocity at the wall depends on the geometry of the room and the air velocity. For a mechanically ventilated room of classical size, the wall friction velocity is about 1 cm/s.

The resuspension velocity $\nu_r$ not only depends on the type of particle but on several other parameters such as the orientation of the wall, the nature of the surfaces involved and their reaction to the impact, the configuration of the room, the activity of the occupants and the history of particle deposition. Nevertheless, there is a lack of information concerning resuspension process. In this study, we have adopted a negligible empirical value of $\nu_r$ (10^{-10} s^{-1}). In practice, this low value assumes that the particles remain stuck to the wall surface.

Comparing the equations of Tichnor for gaseous pollutants (equation (7)) to that of Nazaroff for inert particles (equation (9)), it appears clearly that they are built in a similar way where the coefficient of adsorption $k_a$ (m/s) of gaseous pollutants is replaced by a velocity of deposition $\nu_d$ (m/s) while the coefficient of desorption $k_d$ (1/s) is replaced by the velocity of resuspension $\nu_r$ (1/s). Table 1 shows an analogy between the different terms of the two equations.

**Table 1: Analogy between the Tichnor and Nazaroff equation terms**

<table>
<thead>
<tr>
<th>Tichnor (equation 7)</th>
<th>Nazaroff (equation 13)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flow of pollutants $Q_m$ (kg/s)</td>
<td>Flow of particles $Q_p$ (particle/s)</td>
</tr>
<tr>
<td>Coefficient of adsorption $k_a$ (m/s)</td>
<td>Velocity of deposit $\nu_d$ (m/s)</td>
</tr>
<tr>
<td>Coefficient of desorption $k_d$ (1/s)</td>
<td>Velocity of resuspension $\nu_r$ (1/s)</td>
</tr>
<tr>
<td>Mass concentration of pollutant in air $Rho$ (kg/m³)</td>
<td>Particulate concentration of particle in air $N_p$ (particle/m³)</td>
</tr>
<tr>
<td>Mass concentration of pollutant on wall surface $Rho_o$ (kg/m²)</td>
<td>Particulate concentration of particle on wall surface $N_{p_s}$ (particle/m²)</td>
</tr>
</tbody>
</table>

Hence, a study applied on the gaseous pollutants can be assumed to be applicable on the particles with different values of fixed coefficients especially considering the fact that the IBPSA library considers both air components (gaseous pollutants and inert particles) as traces that perform similarly with no impact on the physical state of the mixture. Therefore, for simplicity, a single gaseous pollutant is considered in the case study presented in this paper, however the study can be generalized to include a vector of pollutants and particles.

An air/wall interaction model is therefore developed. This model contains the Tichenor and Nazaroff equations and all the required constants and coefficients. The model is placed between the wall and the air volume. On one side, this model is connected to the thermal port of the wall to
transfer the information related to its thermal state and on the other side, to the air volume to transfer the information related to the aeraulic state of the medium. This interaction model is therefore a kind of bridge between a thermal state and an aeraulic state. However, due to the limitations related to the nature of the aeraulic connector in the IBPSA modelica library which is based on the Stream principle while the thermal port is based on the Flow principle, it is not possible to directly make this bridge between the aeraulic and the thermal port. This is due to the fact that Stream connectors give singularities if all flows in the connector are equal to zero (see https://specification.modelica.org/streams/stream-connectors.html for more information on Stream connectors).

Therefore, a modification has been applied on the air volume model present in the IBPSA library. A new IAQ connector of type Flow dedicated to the transport of air components is created and added to the volume model. Thanks to this new connector, the wall and volume models can be connected and thus exchange information related to the state of the medium and the surface without causing singularities due to zero mass flows when connecting a thermal connector to an aeraulic connector. Figure 3 shows the IAQ section added to the IBPSA volume model and the new IAQ connector related to transport of air components (appearing in green).

![Figure 3: Modified IBPSA air volume model](image)

**Case study**

The three developed IAQ models in addition to other aeraulic models already existing in the IBPSA modelica library are assembled to form a case study that represents a theoretical room confined within three walls and subject to a scenario of pollution. For simplicity a single vertically oriented wall model will represent all vertical walls, and two horizontally oriented walls representing the ceiling and the floor of the room. Figure 4 shows the graphical interface of the assembly. At the center, the modified volume model is given a volume \( V = 62.5 \text{ m}^3 \) and is connected through a trace input connector to a model of a scenario of an internal production of pollutants. On the other hand, the aeraulic connector of the volume is connected to an inlet orifice subject to a scenario of a forced flow of polluted air by an IBPSA air flow source model, and an outlet orifice which is in turn connected to an IBPSA model of fixed boundary conditions. Finally, the IAQ connector of the volume model is connected to the three walls of surfaces \( S = 15 \text{ m}^2 \) through the models of interaction between the walls and the volume (the equations of Tichnor and Nazaroff and given coefficients and constants are included in this model).

![Figure 4: Modelica assembly of the case study: a room subject to polluted air renewal and a scenario of internal production of pollutants.](image)

A model of an air renewal rate scenario \( Q_{v_{in}} \) in addition to a model of an external concentration scenario \( \text{Rho}_{e} \) is connected to the Forced_air source model. The function Rho2C is present in the external concentration scenario model \( \text{Rho}_{e} \) to transform this value from mass concentration to mass fraction before being transferred to the source model.

In this example, eight days profiles of the three scenarios models (air renewal rate \( Q_{v_{in}} \), internal production of pollutants \( \text{Source} \) and external concentration of pollutants \( \text{Rho}_{e} \)) are considered and shown in Figure 5 in blue, orange and green respectively. They represent all the possible combinations and are either zero or as follows \( Q_{v_{in}} = 8.68056 \times 10^{-3} \text{ m}^3/\text{s} \); \( \text{Source} = 3.6 \times 10^{-7} \text{ kg/s} \); \( \text{Rho}_{e} = 1.35 \times 10^{-6} \text{ kg/m}^3 \)

The results obtained by the IBPSA model are compared to analytical and numerical solutions coded in Python.

**Numerical solution**

The numerical solution is found by numerically integrating the following system of differential equations, given two initial values \( \text{Rho}(t = 0) = \text{Rho}_{0} \) and \( \text{Rho}_{0j}(t = 0) = \text{Rho}_{0j0} \) for all \( j \leq n \). In this case study, three walls are considered so \( n = 3 \).

\[
V \frac{d\text{Rho}}{dt} = Q_{v_{in}} (\text{Rho}_{e} - \text{Rho}) + \text{Source} - \sum_{j=1}^{3} \left( k_{aj} \text{Rho} - k_{dj} \text{Rho}_{s_{j}} \right) S_{j} \tag{11}
\]

\[
S_{j} \frac{d\text{Rho}_{s_{j}}}{dt} = \left( k_{aj} \text{Rho} - k_{dj} \text{Rho}_{s_{j}} \right) S_{j} \text{ for all } j \tag{12}
\]

**Analytical solution**

The system of equations (11) and (12) can be translated to a matrix as shown in equation (13).

\[
\dot{\text{C}} = A \cdot \text{C} + \text{K}
\]
Figure 5: Scenarios of air renewal rate, internal production of pollutants and external concentration of pollutants

Figure 6: Comparison between analytical, numerical and IAQ IBPSA assembly solutions. Top left: Volume concentration. Top right: Surface concentration of wall 1. Bottom left: Surface concentration of wall 2. Bottom right: Surface concentration of wall 3.

With

\[
A = \begin{bmatrix}
\frac{Q v_{in} + k a \cdot \sum_{j=1}^{n} S_j}{V} & \frac{k d_1 \cdot S_1}{V} & \ldots & \frac{k d_n \cdot S_n}{V} \\
k a & -k d_1 & \ldots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
k a & 0 & \ldots & -k d_n
\end{bmatrix};
\]

\[
C = \begin{bmatrix}
Rho \\
Rho_1 \\
\vdots \\
Rho_{2n}
\end{bmatrix}
\]

And

\[
K = \begin{bmatrix}
V \\
0 \\
\vdots \\
0
\end{bmatrix}
\]

Assuming that all coefficients \(k_{d_j}\) as well as \(Q v_{in}\) are constant and nonzero over the time interval \([0; T]\), therefore \(\det(A) \neq 0\) and hence \(A\) is invertible. Thus, we obtain the following analytical solution on this interval

\[
\hat{C} = \exp(At) \cdot \left( C_{t=0} + A^{-1} \cdot \hat{K} \right) - A^{-1} \cdot \hat{K}
\]

(14)

In the case where \(Q v_{in} = 0\), we can consider that \(Q v_{in} = \varepsilon \cdot k a \cdot \sum_{j=1}^{n} S_j\) in a way to keep the invertibility of the matrix \(A\) with \(\varepsilon = 10^{-6}\) for example.

Results

Figure 6 shows a comparison between the three solutions (analytical in blue, numerical in orange and IAQ IBPSA assembly in green). The figure shows the profiles of the volume concentration of the pollutant and its surface concentration on each of the three walls (all concentrations are initialized at zero \(Rho_0 = 0\ kg/m^3\); \(Rho_{o_j} = 0\ kg/m^2\)). The curves superpose and therefore confirming the accuracy of the IBPSA assembly solution, assuming that the numerical solution in Python remains indisputable.

Comparison with a modelica BSP-QAI assembly

The same case study of an air volume under forced ventilation and interactions with three walls is done using BSP-QAI models, a BuildSysPro modelica library (https://build.openmodelica.org/Documentation/BuildSysPro.html) that has been developed during two PhD theses in a collaboration between the University of La Rochelle France and the R&D Lab of Electricity of France EDF (Toureilles, 2015, Picard, 2019). The results were exact with a significant difference in the
computational time. It took 0.015 secs for the IBPSA model to converge while it took 152 secs for the BSP-QAI assembly using a Cvode solver with a tolerance of $10^{-8}$ as shown in Table 2. The simulation time using the IBPSA assembly was up to 10000 times faster than the BuildSysPro QAI one.

Table 2: Computational time between the IBPSA and BSP QAI assembly simulation

<table>
<thead>
<tr>
<th></th>
<th>Integration CPU-time</th>
<th>Initialization CPU-time</th>
</tr>
</thead>
<tbody>
<tr>
<td>BSP QAI</td>
<td>152 s</td>
<td>0.043 s</td>
</tr>
<tr>
<td>IBPSA</td>
<td>0.015 s</td>
<td>0 s</td>
</tr>
<tr>
<td>Ratio</td>
<td>10133 times</td>
<td>-</td>
</tr>
</tbody>
</table>

The time saved is achieved thanks to a simplification used in the IBPSA models (unlike the BSP-QAI models) which neglects directly very small pressure differences and thus the mass flow rate is zero in those cases. Figure 7 shows a comparison between the mass flow rates recorded during the eight days simulation with the IBPSA assembly (in blue) and the BSP-QAI assembly (BSP in red). A zoom on day 1 is also shown in the figure where the comparison between the pressure differences $dP$ obtained with the two assemblies shows that the IBPSA assembly neglects directly minor differences while in the case of BSP-QAI they are still considered, causing therefore a higher computational time in those intervals.

The model (shown in Figure 8) assumes that two layers of material (of thickness $d_{\text{EMPD}_1}$ & $d_{\text{EMPD}_2}$ ) interact dynamically with periodic variations of the interior humidity. These thicknesses are proportional to the square root of the stress period $\tau$. Two zones are considered depending on this period, for the short-term period, zone $\text{zone}_{\text{surf}}$ of thickness $d_{\text{EMPD}_1}$ and for the long-term period, zone $\text{zone}_{\text{deep}}$ of thickness $d_{\text{EMPD}_2}$. The calculation of each $d_{\text{EMPD}}$ is performed according to equation (15).

$$d_{\text{EMPD}} = \sqrt{\frac{\text{diameter mat} \cdot \tau \cdot \text{surf paral}}{\pi \cdot \text{rhov mat} \cdot \text{sorpsd paral} \cdot \text{rhop mat} \cdot \text{surf}}}$$ (15)

The equations used by the EMPD model have been added to the modelica Air/wall interaction model alongside with the Tichnor and Nazaroff equations. A detailed explanation of the EMPD model is presented by Picard (2015) who integrated it in the BSP-QAI library. Figures 9 and 10 show a comparison between the results obtained with the BSP-QAI assembly (different shades of purple) and the developed IBPSA-IAQ assembly (different shades of green) using a single wall instead of three (for simplicity). Figure 9 shows the water vapor densities in the different zones (air volume $\text{Rhov}_{\text{zone}}$, short-term zone $\text{Rhov}_{\text{surf}}$ and long-term zone $\text{Rhov}_{\text{deep}}$). Figure 10 shows the mass flow rates of the vapor from the air volume to the short-term zone $\phi_{\text{surf}}$ and from the short-term zone to the long-term zone $\phi_{\text{deep}}$. All curves in both figures pairwise superpose, indicating therefore that the two modelica libraries give the same results.

Finally, the exchange of water vapor between air volume and the room’s wall is introduced through the so-called EMPD (Effective Moisture Penetration Depth) model.
The article presented a developed methodology for integrating IAQ models within this modica library. A case study of a single room, in which the air volume interacts with several walls, and subject to different scenarios of external sources and internal production of pollutants has been assembled using the developed models. Results were consistent with analytical and numerical solutions calculated in Python in addition to a BSP-QAI modica assembly recording significantly lower computational time. The methodology of integration was based on three main approaches:

- The transformation of data from mass or particulate concentrations to mass fractions through functions that use the density of the whole mixture (medium) and their inverse.
- The application of the notion of PMI (particulate matter intervals) to ensure a better representation of the particle diameters when calculating the velocity of deposit of particles and their volumes.
- The creation of a new connector dedicated to the flow of air components and adding it to the air volume model already existing in the IBPSA modica library.

Finally, the humidity interaction between the walls and the air volume was modeled through the so-called EMPD (Effective Moisture Penetration Depth) model showing the same results as those calculated with the BSP-QAI modica library. Further developments will be done creating new models required for IAQ studies such as infiltrations and components of HVAC systems.

**Nomenclature**

- $C_i$ is the mass fraction of pollutant or particle $i$ in the air mixture [kg/trace/kg\text{air}]
- $m_i$ is the mass of pollutant or particle $i$ [kg]
- $m$ is the mass of the air mixture [kg]
- $m_{pi}$ is the mass of a particle $i$ [kg]
- $V$ is the volume of the air mixture [m$^3$]
- $Rho_{ci}$ is the mass concentration of pollutant or particle $i$ in the air mixture [kg/m$^3$]
- $Rho_{d}$ is the density of the air mixture [kg/m$^3$]
- $Rho_{p} = 2000$ is the theoretical density of the particles [kg/m$^3$]
- $Rho_{pi}$ is the mass concentration of particle $i$ in the air mixture [kg/m$^3$]
- $Rho_{sij}(t)$ is the mass of pollutant $i$ per unit area of material $j$ [kg/m$^2$]
- $N_{pi}$ is the particulate concentration of particle $i$ in air mixture [1/ m$^3$]
- $V_p$ is the volume of a particle $i$ [m$^3$]
- $V_{p_{abz}}$ is the average volume of a particle in the PMI interval indexed with the upper bound diameter $d_{a2}$ [m$^3$]
- $d_{a1}$ is the diameter of the lower bound of the PMI interval [m]
- $d_{a2}$ is the diameter of the upper bound of the PMI interval [m]
- $m_{pi}$ is the mass flow rate of particle $i$ in the air mixture [kg/s]
- $N_{pi}$ is the particle flow rate of particle $i$ in the air mixture [particle/s]
- $Q_{mi}(t)$ is the mass flow rate of pollutant $i$ exchanged between the air volume and the surface $j$ [kg/s]
- $K_{ai}$ is the adsorption coefficient associated with the pollutant $i$ / material $j$ pair [m/s]
- $k_{dij}$ is the desorption coefficient associated with the pollutant $i$ / material $j$ pair [1/s]
- $S_j$ is the surface of material $j$ considered [m$^2$]
- $Q_{pi}$ is the flow rate of particle $i$ deposited on the surface of material $j$ [1/s]
- $N_{p_{stij}}$ is the number of particle $i$ deposited per unit area of material $j$ [1/m$^2$]
- $v_{dij}$ is the deposition velocity of particle $i$ on the surface of material $j$ [m/s]
- $v_{r_{si}}$ is the resuspension velocity of particle $i$ from material $j$ [1/s]
- $d_{EMPD}$ is the thickness of the equivalent zone [m]
- $delta_{max}$ is the vapor permeability of the material [kg/m/s/Pa]
- $tau$ is the period of the considered harmonic water vapor stress [s]
- $P_{sat_{paroi}}$ is the saturation pressure of water vapor [Pa]
- $rho_{mat}$ is the density of the material [kg/m$^3$]
- $sorpslop = \frac{du}{dRH}$ is the slope of the sorption curve of the material where $u$ is the water content and $RH$ is the relative humidity [unitless]

**References**


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