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Hygrothermal simulation and risk evaluation - The impact of discretization on numerical results and performance

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Abstract. Regulations for modelling when deducting thermal simulations are represented in the standards [1]. However, the level of model detail regarding discretization in hygrothermal simulations and especially for evaluating the mould risk on surfaces of organic vapour barriers is almost never discussed. The presented approach shows that the chosen discretization of the simulation model is one of the most influencing factors for the risk analysis of surfaces of very fine layers, such as paper vapour barriers, in walls with interior insulation via hygrothermal simulations. To reduce the computational performance issues caused by very fine finite volume meshes [2], the hygrothermal properties of the connecting surfaces of the finite volumes can be calculated instead. For the risk analysis the VTT-Model was implemented in the hygrothermal simulation program HAM4D_VIE, followed by a comparison of the effect of discretization on the results of the surfaces of the vapour barrier. The results of the comparison are discussed with regard to numerical results and their qualitative impact on computational performance. The presented numerical model will be proposed as an alternative for risk analysis on surfaces of vapour barriers, where mould growth would either stay undetected or the necessary discretization with elements comes at the cost of computational performance.

1. Introduction
The VTT-Model is a well tested model for the risk evaluation of mould growth on surfaces. The results of the VTT-Model, called Mould Index, express the risk of visual findings and their visual representation on surfaces [3]. This is why it is necessary to choose a mesh fine enough so the results of the analysed cells can be representative of the real behaviour of the material surface. Especially when evaluating the risk of mould growth on the surface of vapour barriers with this model, the very fine elements needed in these locations come at cost of computational performance [2]. A possible solution for the numerical and performance issues caused in these places is to modify the connections between cells, where modifications such as vapour barriers are used in the building part. If the altered hygrothermal properties caused by the modifying factor in between the cell-surfaces are taken into account, comparable numerical results as in an only cell driven modelling approach can be achieved at a lower computational cost.
Only Cell Driven Approach

Cells And Modifications

Figure 1. Depiction of the hygrothermal model used in an only cell driven approach and in an approach where, e.g., vapour barriers are regarded as modifications with different water vapour permeances.

2. Expanding hygrothermal results to the surfaces of finite volume elements

The need for calculating the hygrothermal behaviour on surfaces of finite volume elements was experienced when implementing the VTT-Model as a tool for risk analysis in HAM4D_VIE in [4]. For the simulation model in HAM4D_VIE (validated in e.g. [5, 6]), vapour barriers are not modelled as separate cells, instead they are regarded as modifications between two cells, modifying the moisture and air transfer between those, Figure 1. This modelling approach is inspired by the thermal model used by Blomberg [7] in which Eftring’s work [8] is cited as a major influence.

Main focus was to expand the existing calculation model to provide the necessary input parameters for calculating the Mould Index on cell surfaces. This meant that the relative humidity in these locations needed to be evaluated. With the existing model in place, the most efficient approach was to use the results of the given cells, which already take modifications into account, and calculate them back to the surfaces of the cells in the sense of a straight line equation. This procedure is shown exemplarily in the x-direction for the cell surface AO (cf. Figure 1) for moisture transfer by diffusion.

If the vapour pressure on surfaces can be expressed as Equation (1),

\[ p_{v,O} = \frac{W_{p,vx,A} \cdot p_{v,A} + W_{p,vx,B} \cdot p_{v,B}}{W_{p,vx,A} + W_{p,vx,B}} \]

the water vapour permeance is given as

\[ W_{p,vx,A} = W_{p,x,A} \]
with $W_{p,x,A}$ defined as
\[ W_{p,x,A} = \frac{W_{p,x} \cdot 2}{dx}. \] (3)

If $W_{p,x,A} + W_{p,x,B} \neq 0$, the sum of the water vapour permeances has to be calculated as shown in Equation (4)
\[ W_{p,vx} = \frac{1}{1/W_{p,x,A} + 1/W_{p,x,B} + s d_{Barrier}}. \] (4)

At last we have to set $W_{p,x,A} = W_{p,vx}$.

Without leakages, the vapour pressure on surfaces in the direction of $x$ can be calculated through reshaping the Equation (5) for the moisture flow rate $G_{v,x}$
\[ G_{v,x} = W_{p,vx} \cdot (p_{v,A} - p_{v,B}) \cdot dy_A \cdot dz_A \] (5)
into
\[ p_{v,AO} = p_{v,A} - \frac{G_{v,x}}{W_{p,vx,A} \cdot dy_A \cdot dz_A} \] (6)
with $W_{p,vx,A}$ being the water vapour permeance of cells with vapour barriers in between them and $p_{v,AO}$ being the calculated vapour pressure on the surface of cell A with dimensions $dy_A$ and $dz_A$. The vapour pressure on the surface of the neighbouring cell B is derived in the same manner leading to Equation (7).
\[ p_{v,OB} = p_{v,B} + \frac{G_{v,x}}{W_{p,vx,B} \cdot dy_B \cdot dz_B} \] (7)

In the end the relative humidity can be calculated with the saturation pressure on the respective surfaces with Equations (8) and (9).
\[ \varphi_{AO} = \frac{p_{v,AO}}{p_{v,sat,O}} \] (8)
\[ \varphi_{OB} = \frac{p_{v,OB}}{p_{v,sat,O}} \] (9)

For proof of plausibility of the expanded model, the results of a simulation with stationary boundary conditions were compared to the results of a Glaser-calculation [9] with the same input parameters, which led to sufficient results. It has to be mentioned that this method doesn’t take possible moisture sorption isotherms of the vapour barrier into account, therefore, the response of the material is more dynamic and direct than compared to the only cell driven approach, where capacitive effects are not neglected, Figure 2. This could lead to possible over- or underestimation when evaluating the moisture behaviour of organic vapour barriers. Another simplification in this approach is the neglect of the influence of temperature conductivity caused by the barrier. For now saturation pressure on surfaces of cells is calculated using the temperature in place of the modification. Errors of these simplifications scale with the thickness of the vapour barrier. Therefore, to determine under which thresholds the simplified model can be used, a sensitivity analysis was carried out in which the thickness of the vapour barrier was varied in the simulation model, Figure 2 and Table 1. The analysis showed that the simplification especially impacts results regarding moisture transfer with a maximum error of approximately 10% for modifications with a thickness $\geq 10\, mm$. With regard to temperature results, the mean absolute percentage error stays under 1%, Table 1. To keep the deviation under 10%, it is recommended only to use the calculation model with modifications where the thickness is $\leq 5\, mm$ or materials with negligible capacitive properties. The influence of capacitive effects or the hygrothermal dependency of the vapour barrier properties and their computationally efficient implementation could be part of a future work.
Figure 2. Progress of the vapour pressure for an only cell driven approach compared to a model using cells and modifications. The results representative for one surface of the vapour barrier with different thicknesses are depicted.

Table 1. Mean absolute percentage error (MAPE) of the results using the model with cells and modifications compared to the results of an only cell driven approach. Different thicknesses of the vapour barrier are analysed with regard to hygrothermal results.

|                | MAPE$_{\text{Barrier}=1\text{mm}}$ | MAPE$_{\text{Barrier}=5\text{mm}}$ | MAPE$_{\text{Barrier}=10\text{mm}}$ |
|----------------|-----------------------------------|----------------------------------|----------------------------------|
| Vap. pressure  | 5.0%                              | 7.8%                             | 10.3%                            |
| Temperature    | 0.14%                             | 0.6%                             | 0.12%                            |
| Rel. Humidity  | 4.9%                              | 7.7%                             | 10.3%                            |

3. 1D models with varying levels of discretization
The model chosen for further discussion is derived from an in field measured building part in order to check the results of the simulation, especially after implementation of the VTT-Model, for plausibility. The discussed building part consists of a brick wall, where an interior insulation was installed for better thermal performance. Out of economical reasons mineral wool with building paper in front of the vapour barrier was chosen as the interior insulation solution, Figure 3. In combination with the indoor climate during the building process, the building part showed mould growth on the surface of the building paper next to the mineral wool, this is also indicated in Figure 3.

This leads to the question, how well can the behaviour of surfaces of vapour barriers be identified when modelling with an only cell driven approach, compared to a model with cells and modifications, and how well does the calculation perform in the sense of computational effort to achieve results necessary to detect malfunctions of a building part. For comprehensibility and the one dimensional nature of the problem, a 1D model was chosen for this comparison, shown in Figure 4, which only differs in the number of cells used for discretizing the layer of mineral wool and the chosen approach for modelling. Once the vapour barrier was modelled as a separate cell with a thickness of 1 mm and once it was modelled as a modification with the method discussed above.
Mould growth was found on the surface of the building paper facing the mineral wool.

Figure 3. 1D model of the brick wall with interior insulation. The layers are described from left to right, starting with the exterior plaster. The dashed line between mineral wool and plaster board indicates the location where mould growth was found on the surface of the vapour barrier (building paper).

Figure 4. 1D model of the brick wall with interior insulation in different forms of discretization (1 cell to 5 cells) of the layer of mineral wool.

4. Discussion of the results
In Figure 5, 6 and 7, the ordinate shows the scale of the Mould Index and the abscissa shows the x-coordinate to identify where the cells are situated in the model. The curves used stand for different levels of discretization of the mineral wool layer. Varying shading of the plot’s background indexes the different material layers. The results of the last time step of a one year simulation are depicted with markers showing the results of the cells. Because mould growth was only found on the outside surface (the surface of the vapour barrier next to the layer of mineral wool) of the building paper and for easier comparability between different levels of discretization, only the results of cells around the vapour barrier are plotted in the figures.

4.1. Results: Only Cell Driven Approach
Figure 5 shows marginal mould growth in the last mineral wool cell, maxing out in the highest discretization level, but still remaining smaller than 1, which is considered as the threshold before mould growth sets in [3]. The vapour barrier itself shows no risk of mould growth with a Mould Index equal to 0. With an only cell driven approach and when using the VTT-Model,
Figure 5. Results of the Mould Index for an only cell driven approach. The mineral wool layer (ranging from 27 to 39 cm), the vapour barrier (ranging from 39 to 39.1 cm) and the cell for the plasterboard on the inside (ranging from 39.1 to 40.35 cm) are shown.

no risk of mould growth can be detected in the building part.

To show the needed discretization to detect the mould growth on the surface of the vapour barrier, with an only cell driven approach, the models, whose results are discussed in Figure 6, where created. These models show an increasing discretization of the vapour barrier, ranging from 1 to 10 cells while the layer of mineral wool stays discretized with 5 cells. The results show that the detection of mould growth sets in when there are at least two cells used for modelling the vapour barrier, with the Mould Index being 1.5 in the first cell. In comparison, the model with cells and a modification, depicted in Figure 7, showed a Mould Index ranging from 5.1 to 5.6 in respect of the cells used for modelling the layer of mineral wool. The model with the only cell driven approach, even though it shows a rising tendency of the Mould Index for the first cell of the vapour barrier, converges to a Mould Index of 3.7 when 10 cells are used to discretize the layer of the vapour barrier. Although using two cells to model the vapour barrier shows a tendency alarming enough to question the building part as a whole in the sense of a risk analysis, the gravity of the malfunction, when classifying according to the scale of the Mould Index [3], is not depicted accurately and can lead to distorted conclusions when not enough cells are used to discretize the vapour barrier.

4.2. Results: Cells With Modification

Figure 7 shows almost the same mould growth in the last mineral wool cell, again, maxing out in the highest discretization level. In comparison to Figure 5, the Mould Index for the surface of the vapour barrier on the outside (Position of cell in x-direction depicted in Figure 7 = 39.0 cm), lies between 5.6, when discretizing with only one cell for the layer of mineral wool, and 5.1 for the highest level of discretization, in this model with 5 cells for the layer of mineral wool. On the other side of the vapour barrier (Position of cell in x-direction depicted in Figure 7 = 39.1 cm) the Mould Index degenerates to 0 again, which also could be seen at the building sight.

Because of the needed iterations to achieve convergence of the results in a finite volume element, the model, in which the vapour barrier was modelled as a cell, was already more
Figure 6. Results of the Mould Index for an only cell driven approach with the discretization of the vapour barrier ranging from 1 (CellDrivenApproach_MW_5C_VB_1C) to 10 cells (CellDrivenApproach_MW_5C_VB_10C).

Figure 7. Results of the Mould Index for the model with cells and modifications. The results of the mineral wool layer (ranging from 27 to 39 cm), the surface of the cell next to the vapour barrier (Position of cell in x-direction = 39.0 cm), the surface of the cell next to the plasterboard (Position of cell in x-direction = 39.1 cm) and the cell for the plasterboard on the inside (ranging from 39.1 to 40.35 cm) are shown.
laborious computationally than the model with cells and a modification. Even different levels of discretization of the mineral wool layer showed no effect on the result in the cell of the vapour barrier regarding the results of the Mould Index. This yields in the problem, that the only cell driven approach forces a discretization of the cell of the vapour barrier \( \text{thickness}_{\text{cell}} = 1 \text{mm} \), which slows down the calculation even more. The approach with cells and modifications is computationally more effortless, but seems to overestimate the risk of mould growth, when compared with the results of the highly discretized vapour barrier with an only cell driven approach.

5. Summary

With a simple one dimensional model it could be shown that the risk analysis of paper vapour barriers (done with the Mould Index from the VTT-Model) is only possible when acknowledging the different hygrothermal behaviour on opposed sides of the barrier. Especially for fast risk evaluations of these situations, the modelling with cells and modifications, representing vapour barriers as simplified hygrothermal behaviour altering connections between cells, seem like a numerically and computationally well-suited approach. It reduces the computational cost, which would otherwise come with discretizing the cells of a vapour barrier, to achieve results representative of the hygrothermal behaviour on their surfaces. For now, the presented method should only be used for qualitative risk estimations, as it seems to slightly over- or underestimate the mould growth on the surfaces because no moisture sorption isotherms of the vapour barrier are taken into account. The exploration of this simplification and its impact will be part of future work.

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