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Abstract:

This report presents the first of two deliverables related to WP 4 ‘Probabilistic assessment of interior insulation solutions’. The prime objective of WP4 is the development of an efficient strategy for the probabilistic hygrothermal assessment of interior insulation solutions. This deliverable reports on the outcomes from general developments within WP4 (Section 3), and from the specific activities within Task 4.1 (Section 2) and Task 4.3 (Section 4). Section 2 details the further developments of the deterministic hygrothermal assessment. Section 3 expands that towards probabilistic hygrothermal assessment. Section 4 finally focuses on efficient sequential Monte-Carlo sampling.

Keyword list: hygrothermal simulation, probabilistic assessment, sequential sampling
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Executive Summary

(Hans Janssen, KUL)

This report presents the first of two deliverables related to RIBuild’s WP 4 ‘Probabilistic assessment of interior insulation solutions’. The key objective of WP4 is the development of an efficient strategy for the probabilistic hygrothermal assessment of interior insulation solutions. That strategy involves Monte-Carlo-based repetitions of hygrothermal simulations, and hence requires an efficient deterministic hygrothermal simulator and an efficient probabilistic assessment approach. Prior to the initiation of the RIBuild project, both a deterministic simulator and a probabilistic methodology were already available. Their joint application to interior insulation solutions does however require further developments, primarily in relation to their numerical efficiency.

The various tasks in WP4 hence focus on efficiency improvements of both the deterministic simulator and the probabilistic methodology. Tasks 4.1 and 4.2 target the efficient one-, two- and three-dimensional simulation of heat, air and moisture transfer in building components, Tasks 4.3 and 4.4 aim for the efficient probabilistic assessment of hygrothermal performances based on these simulations. In the final Task 4.5, the developments of Tasks 4.1 to 4.4 are to be brought together in a final application example. This deliverable reports on the results from the general developments in WP4 (Section 3), and from the specific activities within Task 4.1 (Section 2) and Task 4.3 (Section 4). The future D4.2 is then to report on the outcomes of Task 4.2 and Task 4.4.

Section 2 details the further developments with respect to the deterministic hygrothermal assessment of interior insulation solutions, which was the prime target of Task 4.1. Within that Task, the Delphin hygrothermal simulation program has been significantly extended, concerning both effectiveness and efficiency. In relation to the former, the program has been extended to three-dimensional geometries, anisotropic material properties, and inclusion of air flow, each of which are important for the reliable hygrothermal assessment of internal insulation solutions. With respect to the latter, a modular solver framework, including iterative solver methods, has been implemented, greatly reducing the computational cost of the hygrothermal simulations.

Section 3 embeds that deterministic simulator into the probabilistic framework. To that end, a Matlab master code has been implemented, handling both preprocessing (assignment uncertain parameters, manipulation Delphin input files, execution hygrothermal simulations) and postprocessing (collection and quantification of output variables). Subsequently, the developed technique has been used in order to investigate a simplified balance model to integrate interior environment simulation in hygrothermal simulation models. Finally, the developed technique has been employed to study the performance of interior insulation solutions, both via one- and two-dimensional simulations. In relation to the latter, it was shown that both approaches yield different findings.

Section 4 finally focuses on the core of the probabilistic methodology, in particular efficient sequential Monte-Carlo sampling. In relation to this, the sampling efficiency of different low-discrepancy-based sampling schemes has been investigated, on the basis of simple mathematical functions as well as hygrothermal case studies. These revealed the Sobol series as the most dependable approach. In a subsequent study, approximate error quantification has been evaluated, based on randomized replications in combination with a standard-error-based estimator. It was shown that this estimator gives a reliable and conservative error quantification, which allows halting the simulations when a sufficient level of accuracy is reached.
1 Introduction

(Hans Janssen, KUL)

This report presents the first of two deliverables related to RIBuild’s WP 4 ‘Probabilistic assessment of interior insulation solutions’. The key objective of WP4 is the development of an efficient strategy for the probabilistic hygrothermal assessment of interior insulation solutions. The latter must proceed via numerical simulations, since a multitude of scenarios need to be judged quickly and cheaply. The overall strategy involves Monte-Carlo-based repetitions of hygrothermal simulations, and an efficient strategy hence requires an efficient deterministic hygrothermal simulator and an efficient probabilistic assessment methodology.

Prior to the initiation of the RIBuild project, both a deterministic simulator and a probabilistic methodology were already available, from previous research activities by respectively the Institute of Building Climatology of TU Dresden and the Building Physics Section of KU Leuven. Their joint application to interior insulation solutions did however require further developments, primarily in relation to their numerical efficiency. At that point in time indeed, the computational costs of such assessment of interior insulation solutions would highly exceed the time constraints of the RIBuild project.

The various tasks in WP4 hence focus on efficiency improvements of both the deterministic simulator and the probabilistic methodology. Tasks 4.1 and 4.2 target the efficient one-, two- and three-dimensional simulation of heat, air and moisture transfer in building components, Tasks 4.3 and 4.4 aim for the efficient probabilistic assessment of hygrothermal performances based on these simulations. In the final Task 4.5, the developments of Tasks 4.1 to 4.4 are to be brought together in a final application example.

The overall set-up of WP4 can be summarized as follows:

**Tasks**

- T4.1: an efficient 3D HAM simulation model
- T4.2: decomposition techniques in HAM simulation
- T4.3: sequential sampling for Monte Carlo analysis
- T4.4: surrogate models for HAM simulation
- T4.5: exemplary application illustration

**Deliverables**

- D4.1: basic probabilistic analysis (T4.1, T4.3)
- D4.2: metamodeling approaches (T4.2, T4.4)

The objectives and methodology for the different WP4 tasks can be formulated as follows:

- **Task 4.1: Numerical efficiency of hygrothermal simulation**
  Hygrothermal simulations with Delphin take on a double role in WP4: they may be applied directly in the probabilistic methodology for simple configurations, while they may be applied indirectly as a reference for the reduced-order and/or surrogate modelling for more complex configurations.
The currently available Delphin 5.8 allows one- and two-dimensional hygrothermal simulations making use of direct solvers for banded systems, with sufficient functionality and efficiency for simple configurations. The more complex configurations require three-dimensional functionalities and iterative solvers with preconditioning.

- **Task 4.2: Reduced-order models in hygrothermal simulation**
  Notwithstanding the potential efficiency gains targeted in Task 4.1, direct numerical simulation of heat, air and moisture transfer in building components will remain (relatively) computationally expensive, and alternatives need to be investigated. Task 4.2 aims for ‘model order reduction’ methods in that respect.

  The literature offers multiple references on the successful application of model order reduction methods for hygrothermal simulation, but most of these applications remain restricted to cases where linear heat and vapour transfer are the dominant mechanisms. Its applicability for the far more strongly non-linear liquid transfer – a dominant moisture transfer mechanism in most hygrothermal assessments of the internal insulation solutions – remains unknown, and that will form the prime research target of this task.

- **Task 4.3: Sequential sampling in probabilistic assessment**
  A sequential sampling strategy, merging replicated optimised Latin hypercubes and bootstrap-based error quantification, is presently the state-of-the-art concerning convergence efficiency and monitoring and forms the backbone of the probabilistic strategy. As currently independent optimal Latin hypercubes are combined, the rate of convergence is proportional to $n^{0.5}$, with $n$ the number of Monte Carlo samples. Theoretically though, quasi-Monte Carlo sampling schemes allow (far) higher convergence rates.

  To that aim, the replicated Latin hypercubes and bootstrap-based errors are to be abandoned in favour of low-discrepancy-based approaches combined with replication-based standard errors. In this task, different possible candidates for the actual low-discrepancy-based sampling schemes will be evaluated and compared, and their combinability with replication-based error quantification will equally be assessed.

- **Task 4.4: Surrogate modelling of hygrothermal performance**
  Static metamodels are at present a crucial element of the probabilistic methodology, in order to reduce the computational cost of the multi-level Monte Carlo sampling scheme. This surrogate modelling has however been restricted to static models: the models consider stationary outcomes only, and relate these directly to the variable input parameters. Their static character does however restrict their applicability.

  Dynamic surrogate models will greatly augment the potential of metamodels: explicit inclusion of the temporal variations of the hygrothermal conditions in the surrogate models makes them far more flexible. To this aim, recurrent neural networks are the first option to be examined. Alternatively approaches based on singular value decomposition or principal component analysis can be considered. Complementarily, the reduced-order models resulting from Task 4.2 may offer additional possibilities.

- **Task 4.5 Exemplary application on internal insulation case**
  WP6 targets a comprehensive comparative assessment of internal insulation solutions based on life cycle cost, combining the probabilistic assessment of hygrothermal performance
developed in WP4 with the quantification of life cycle costs of internal insulation’s benefits and damages formulated in WP5. To support the application of the WP4 techniques in such holistic evaluation, an illustrative application forms the concluding element of this work package.

In this illustration, a number of internal insulation solutions for external walls with embedded wooden beams, openings in the building envelope such as windows and doors etc., are evaluated via the developed probabilistic hygrothermal assessment strategy.

This deliverable reports on the outcomes from the general developments within WP4 (Section 3), and from the specific activities within Task 4.1 (Section 2) and Task 4.3 (Section 4). Section 2 reports on the further developments in relation to the deterministic hygrothermal assessment of interior insulation solutions. Section 3 expands that foundation toward the probabilistic hygrothermal assessment of interior insulation solution. And Section 4 then focuses on the core of the probabilistic assessment, specifically the efficient sequential Monte-Carlo sampling.
2 Deterministic hygrothermal modelling with Delphin

(Peggy Freudenberg, TUD)

2.1 General information

TU Dresden (IBK) was engaged with the further development of the modelling software DELPHIN, a sophisticated hygrothermal simulation tool, which is not only applied by researchers but also practitioners. DELPHIN is a hygrothermal simulation software resulting from long-time research and development activities at IBK (Institut für Bauklimatik), TU Dresden. The tool is able to simulate the transient heat- and moisture transport and storage of porous materials. Some advantages of DELPHIN are, in comparison to equivalent software tools, its sound physical basis and its high numerical efficiency for the evaluation of complex details, adverse boundary conditions etc. This potential raised the desire to extend the software to the third dimension and develop a completely new state-of-the-art in the field of hygrothermal modelling. However, this development requires fundamental improvements in different fields, e.g. the material model, geometry specification, performance (parallel computing) and results analysis (post-processing). The software capabilities and some aspects of the required extension are summed up in this paragraph.

2.2 Heat, air and moisture transfer modelling in DELPHIN

2.2.1 History and capabilities of Delphin

DELPHIN traces back to the theoretical work of professor J. Grunewald and the previous prototype software DIM from 1991. This early version was only able to simulate the one-dimensional transport and comprised the simulation core itself without graphical user interface. It was later on extended to the second dimension (DIM version 2) and completed with a graphical user interface for both, the model input (DELPHIN pre-processing: geometry, materials, boundary conditions etc.) and a results analysis (PostProc). A combination of all three software modules led to the research software tool DELPHIN (version 4, about 2001). The proceeding upgrading of new physical models, e.g. the modelling of salt transport within a research project in 2003, pushed the envelope of the software. A total restructuring of the source code became inevitable. A. Nicolai tackled this in 2003 within his doctoral research study about salt transport in porous media. The restructuring comprised a new development of the data model and the calculation engine as well as the reformation of the user interface (DELPHIN version 5). This was realized via C++ standard and Borland VCL library, at that time a fundamentally innovative standard. This sound framework enabled a number of further software extensions in the subsequent years. Currently, another improvement, a more powerful solver framework development, is in progress and partially incorporated in the software version DELPHIN 6. This modification has also become necessary concerning a specific tool extension, the three-dimensional modelling capability.

DELPHIN comprises an extensive physical model for the description of the coupled heat air and moisture transport in porous matters. It is based on dynamic equations for the modelling of energy and mass conservation. For these purposes, the microscopically inhomogeneous porous materials are regarded as homogeneous materials. This enables the balancing of spatially resolved energy and
mass densities depending on the associated transport and storage processes. Examples for the covered transport processes are heat transfer, vapour transfer and liquid water transfer.

### 2.2.2 Heat and Moisture Storage

Any material is able to store heat in its solid matrix. In addition, porous materials show the ability to store heat in the pore-encapsulated air, vapour or liquid water. This amount can be significant, due to the high heat storage capacity of water. Any rise in heat quantity causes either an increasing temperature level or a phase transition of the matter. The dependency of heat quantity increase and temperature increase is given with the specific heat capacity. Specific denotes the reference to a mass or volume unit. The same relationship is describable as a function if the change of water content and the according heat capacity increase, due to the replacement of less heat storing air with better storing water, is represented. Pore matrix, vapour and liquid water in the pores are in balance with each other. The surface properties of gaseous and liquid matter depend on each other. This appears in the shape of convex water surfaces in capillary pores where the curve shape results from the size of the pores and influences the vapour condensation and evaporation conditions. The higher the capillary forces are, the stronger is the curve shape and the lower is the vapour pressure above the tensioned surface (Kelvin equation). This decreases the relative humidity and thus the evaporation point of the tensioned liquid. A consequence of this dependency is the pore-diameter-depending and thus material specific ability of a material to store liquid water at a given relative humidity level of the environment. This ability is measured via exciccator experiments for particular relative humidity levels and results in the sorption isotherms for the entire hygroscopic range of approximately below 95%\(^1\). Above this level, liquid water (capillary condensate) is dominantly filling the pores and rising the water transport capabilities. A further filling process of the pore system in this over-hygroscopic range would require a disproportionately high capillary pressure, which is not producible with an increase in relative humidity. It requires another measurement technique, the pressure plate procedure. Different pressure steps are measured and yield specific balance water contents in the materials. All points are approximated with a so-called water retention curve, equivalent to the sorption isotherms in the hygroscopic range. Both approximated curves, water retention curve and sorption isotherm are convertible into each other and therefore united via the Kelvin equation. The resulting moisture storage function is applied for each moisture-storing material in the DELPHIN software and thus part of material database.

### 2.2.3 Heat Transport

Transfer of heat resp. energy is feasible via three different mechanisms, convection (fluids), radiation (any matter) and conduction (resting fluids, solid matters). The conductive heat transfer is seen as the leading transfer mechanism in (porous) building materials, although all three processes are participating. Consequently, Fourier’s law is applied to describe the transfer. It formulates the induced heat flux depending on the temperature gradient and a material property, the thermal conductivity. Thermal conductivity of a specific (porous) material is not a static value as it depends e.g. on the moisture content. A rising moisture content causes an increasing value of the thermal conductivity. This effect is primarily relevant for materials with a very low dry conductivity. It could therefore cause a remarkable performance loss in insulation materials. This dependency is covered in DELPHIN as the thermal conductivity function is also subject of the material library.

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\(^1\) Further details about the measurement procedure are subject of WP2 deliverables within this project.
Radiation and convection as remaining heat transfer mechanisms are considered for specific cases. An application case for both mechanisms, radiative and convective exchange, is a cavity. Radiative exchange between one cavity-directed material surface to the opposite side is calculated according to Stefan and Boltzmann’s law via temperature level, material emission coefficients and geometric composition. A further transport process via air movement within the cavity is given as convective mechanism, a process, which is always associated with the mass flow in a fluid.

2.2.4 Vapour and Liquid Water Transport

Water vapour diffusion is driven by vapour pressure differences in adjacent air masses of any permeable construction. Vapour pressure raises with increasing vapour density (absolute water content) and temperature level. The relationship between vapour pressure gradient and resulting mass flux through a material is described via vapour conductivity. This property can also be expressed as vapour diffusion resistance factor, which sets the vapour conductivity of a particular material into relationship with the base vapour conductivity of air. Equivalent to thermal conductivity, vapour conductivity is not a constant and changes with liquid water content in a porous material. Starting at a relatively low level for low liquid water contents, the vapour conductivity increases until a maximum is reached. Vapour conductivity is derived from dry and wet cup measurements. If the water content of the porous material increases towards upper hygroscopic and overhygroscopic range, a decrease in vapour conductivity is recorded, which is caused by the reduction of vapour permeable pore space. A fully saturated material is finally not able to let the vapour pass and shows a vapour conductivity of Zero. The liquid water conductivity behaves inverted to vapour conductivity. It shows a very low value for low liquid water contents and increases continuously with increasing liquid water content. The functional description of this dependency is a complex procedure (see: Scheffler, 2008; Scheffler and Plagge, 2010), which also takes the moisture storage into account. A revision and a detailed description of this development are subject of WP2. The maximum of liquid water conductivity is many times higher than the maximum of vapour conductivity. Both functions are subject of the DELPHIN material specification.

2.2.5 Numerical Solution in DELPHIN 5

Several numerical solution methods have been applied for solving the coupled heat, air- and moisture transport in DELPHIN. The specific user-defined case (geometry, boundary conditions etc.) yields a HAMT-project-depending coupling or decoupling of the involved balance equations, more precisely the conservation equations for mass and energy. This coupling and the degree of freedom in the physical modelling determine the efficiency of a particular numerical solution method. The numerical solution method, which was applied in DELPHIN for the governing balance equation system is a control volume method (CVM). It indicates some advantages like the exact formulation of fluxes over the boundaries of the control volume and a more common numerical scheme. Some further simplifications like the restriction to orthogonal volume elements allow additional optimization of the numerical efficiency, pre- and post-processing.

The implementation of coupled heat- air and moisture transport in building constructions leads usually to a system of partial differential equations of parabolic type. These equations are transferred into a system of ordinary differential equations (ODE) via discretization of the spatial coordinates of the specific detail geometry. This enables the independent selection of primary state variables (unknowns) and driving potentials. The remaining time dependency of the state variables, which is included in the ordinary differential equations (ODE) is solved via time integration solver.
DELPHIN adopted the CVODE integrator, an open source code within the SUNDIALS package, written in C.

The solution approach via control volume method demands a balancing of involved state quantities in form of the energy- and mass flow densities for each volume element. These quantities are summarized in form of a vector for all volume elements. The computation of the time derivative equals the physical core element of DELPHIN. It requires four main work steps. The first step is the computation of all derived state variables, for example temperature or relative humidity or vapour partial pressure, and the computation of all required transport coefficients, for example thermal conductivity or liquid water conductivity, for each volume element separately. The second step is the computation of resulting heat and moisture fluxes between these volume elements and at the boundary of the geometry due to the defined boundary conditions. This has to be conducted for each element margin. A third step is needed for the computation of sources and sinks within the construction for each element. Finally, the state variable alteration rates (divergence) in each element are identified. They are computed as a balance of in and out-streaming fluxes as well as sinks and sources.

The computational implementation of this physical model is based on the DELPHIN data model. It includes a multitude of libraries for the material handling and characterization, the calculation of climate conditions for specific surface properties, the fundamental physical equations. The model is furthermore able to handle the interrelation of element patterns with connecting margins, the numeration of elements and the management of memory topologies, necessary for the data access. This part can be summarized as initialization process and equals up to 60% of the program code. Therefore, it is an essential component for the efficient data access during the simulation runtime.

### 2.3 Hygrothermal model extension towards three-dimensional geometries and anisotropic material properties

#### 2.3.1 Overview

The above explained numerical algorithms are deeply anchored in the DELPHIN 5 implementation. Time integrating method, matrix shape (bad matrix), solution approach for linear equation systems within the Newton-method (direct solution method, LU-factorization with backwards-decomposition) are fixed components of the program code. This proved to be a tight constraint concerning the 3D-extension of the software. It was handled with a newly developed IBK-solver platform. This platform shows a modular structure and embraces the multitude of program libraries, e.g. material model, post-processing, integrator (e.g. SUNDIALS), solver for the system of equations, supporting libraries (e.g. error handling) as well as the new components: integrator framework and functional mockup unit (FMU) support. These libraries can be accessed by several software products (DELPHIN, COND, THERAKLES, NANDRAD) likewise.

Based on this newly developed platform, DELPHIN 6 building simulation software was firstly implemented as DELPHIN 5 technology to allow a gradual composition of the modular source code. The new structure enabled an exchange of central numerical algorithms as for example the linear equation solver within the Newton algorithm. It allowed furthermore an extension of the former two-dimensional program version towards third dimension. This comprised the following tasks:

- Extension of the data model for the application of 3D-grids
• Extension of the output data format and post-processing adapter for 3D grids
• Restructuring of the initialization process (memory demand of the former implementation was too huge)
• Extension of the flux calculations between grid elements in three dimensions
• Memory access optimization during runtime
• Introduction of iterative solvers for linear equation systems (Krylow-subspace methods)
• Development and application of suitable matrix structures and pre-conditioners for 3D-heat air and moisture (HAM) simulations

### 2.3.2 Numerical methods

The data model extension focuses on the introduction of a third dimension (z-coordinates). In this context, the former ij-addressing (2D-grid) was widened out to ijk-addressing for the 3D-grid. The file format itself lists all assigned materials (material ID, material colour and material name), a grid table with the grid dimensions of all three spatial directions (x,y,z), the element geometry (grid index number, global grid coordinates of the centre of the grid cuboids) and index of the assigned material referring to the material list (material ID) and the boundary areas (middle points of the boundary areas). Further details about the modified geometry format and about the output file format are given in the technical report (Vogelsang and Nicolai, 2016).

![Figure 2-1: Spatial directions coordinate and index definition concerning the calculation grid in DELPHIN 6 (Vogelsang and Nicolai, 2016)](image)

An extension of the according initialization procedure for three-dimensional geometries yielded the problem of huge memory demand even for moderately complex geometries. It was impossible to keep the required geometry information and its corresponding reference structures simultaneously in the main memory. This required a splitting of the entire initialization process in order to handle it coordinate-separated. The new algorithm firstly initiates assignment matrices for x-coordinates and dissolves all associated references. After termination of the x-coordinates, the procedure continues with the assignment matrices for the y-dimension and so on.
During the calculation of heat and moisture fluxes between the grid elements also z-directed fluxes are calculated now. This required an extension about the third dimension in the computation of alteration rates for the heat- and moisture flux balance.

A vast challenge was the memory demand resulting from the conversion from 2D- to 3D-simulations with a subsequent conversion of data structures. One example is the modification of the previously summarized fluxes for construction-internal and exterior boundary conditions in one vector. This yielded the problem of an extended flux quantity number, due to the fact, that up to 20 flux quantities were required for each side (e.g. heat conduction, vapour diffusion, direct solar radiation, diffuse solar radiation, long-wave heat exchange, wind-driven rain). These quantities were fully deposited in the memory and recalled during runtime of the software. Two disadvantages resulted from this approach. Firstly, the memory demand increased enormously and secondly, the central processing unit (CPU) is slowed down due to the prolonged memory data transfer. The implemented restructuring of the data structure reduced the memory demand by approximately one third and speeded up the kernel loops remarkably.

Besides this optimization, the direct solution method for the linear equation systems turned out to be the most challenging obstacle for the realization of 3D-simulations. Memory demand and computing time, which are required for the LU-factorization of the band matrix, are increasing linearly with the band broadness and quadratically with the number of rows/columns of the matrix. Therefore a cubic complexity for 3D-cases exists which impedes the application of direct solution methods for non-trivial geometries. The chosen alternative is an iterative method for the solution of linear equation systems, which reduces the memory demand remarkably. State of the art in this field is Krylov- subspace iteration methods, specifically GMRES (generalized minimal residual) methods. These methods rely on the idea of a residual minimization, which remain in the equation system after insertion of an estimated solution. The method proceeds with a stepwise identification of vectors, which are orthogonal to each other. All vectors are consequently orthogonal to each other and the scalar resp. inner product of all vectors to all other vectors adds up to zero. It is possible to identify specific factors as multipliers for the vectors, which yield a nearly correct solution. This is realized via small equation systems and requires a sufficient quantity of vectors. The implementation of this method demands a detailed knowledge about the accurate settings and the corresponding performance impact and success. Challenge examples are the integration of this procedure into the Newton-system and the adaption of convergence tests. The finally implemented GMRES-method in DELPHIN 6 is generally applied for larger 2D problems and for all 3D problems.

Another approach for the optimization of iterative solution methods is the application of preconditioners. This can be explained for the example of a simple equation system \( Ax=b \) that should be solved. A left-side multiplication with the inverse of \( A \) yielded the solution \( A^{-1}Ax=x=A^{-1}b \). Indeed an exact calculation of the inverse is neither reasonable nor efficient. Instead, an approximation of the exact solution \( P \approx A^{-1} \) can be found and applied on the equation system. Hence, the iteration procedure includes a simpler problem. Such an approximation \( P \) is called preconditioner. DELPHIN uses the ILU preconditioner as standard for the Krylow- subspace methods (Vogelsang et al. 2014).

### 2.3.3 Specification of anisotropic material properties

DELPHIN was originally based on the macroscopic view on the properties of porous materials. Likewise all alternative HAMT models published in the past, the material properties were regarded
as homogeneous and thus independent on the direction of heat, air- and moisture transport. An involvement of directed material properties requires three main extensions of the software function volume:

- Computation algorithm: directional computation of transport coefficients along the three spatial directions x, y and z
- Data model: Extension about the ability to define material grain directions
- Material model and data base: extended file formats and extended computation functionality

Anisotropic properties of wood affect mainly its heat- and moisture transport characteristics. It is less relevant for the macroscopic quantification of moisture storage. Consequently, there is a necessity to account for this direction dependency of anisotropic material properties in the heat and moisture flux computation, which was previously explained.

For isotropic materials, the moisture flux between two adjacent volume elements is given as the product of the transport coefficient and the driving potential resp. gradient. For the example of liquid water flux $j^w$, the gradient could be the capillary pressure gradient $\nabla p_l$ and the transport coefficient could be the liquid water conductivity $K_l$.

$$j^w = K_l \cdot \nabla p_l$$  \hspace{1cm} (1)

Anisotropic materials show a direction-dependent transport coefficient, which differs between all three spatial directions: tangential, radial and longitudinal. To distinguish these dependencies, the material directions u, v and w are introduced. Depending on the location of the material within the coordinate system, a particular transport coefficient has to be considered. As explained in the previous text passages, DELPHIN applies rectangular grids and computes all fluxes solely along the main coordinate directions x, y and z. The transport coefficients have to be chosen in accordance to these directions. The following figure shows an example for this application where the transport coefficients differ depending on the material grain direction (u, v) and its orientation in the coordinate system (x, y) for the example of liquid water flux calculation.

![Figure 2-2: Application of directional transport coefficients for liquid water conductivity for differently oriented materials.](image_url)

A consideration of specific material grain directions within the modelled geometry is consequently essential for the exact application of directed material properties. This is realized via rotation matrix
in DELPHIN. This rotation matrix is applied on the tensor of the transport properties. Details about this approach are given in (Vogelsang and Nicolai, 2014).

The material model in DELPHIN equals the approach to derive coefficients and state-variable-depending functions for the constitutive equations of the transport theory from the lab-measured material parameters. This process requires a calibration routine to identify material functions for the moisture storage and transport. The resulting material functions are stored in a material file in form of a data table. During the data processing, the material file is scanned for defined key words that identify each parameter and function, values are memorized and required interim values are interpolated linearly. An extension of the material file requires therefore additional directional supplements for these key words and a corresponding material file structure that allows the definition of both, homogeneous and directional material properties. The latter spans bi- (u, v) or tri- (u, v, w) planar material orientations. The extended material file format for a three-dimensional material is given in the following example.

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**Figure 2-3: Extract from the material file for a three-dimensional anisotropic material (basic parameters)**
The previous example shows the definition of directional parameters. This is done by the help of direction suffixes for the second and third dimension (v, w). Consequently, the original file format for homogeneous materials was retained as it was abstained from suffix “u”. The same approach as for the base parameters given in the previous figure was chosen for the material functions. An extract of a three-dimensional parameterization of liquid water and vapour conductivity is shown in the following example. Details about the revised material file format are given in the technical report (Vogelsang and Nicolai, 2013).

![Figure 2-4: Extract from the material file for the example of an anisotropic material.](image)

As a second step for the definition of directed material properties, further information about the orientation of the material in the defined geometrical composition of the constructive detail is also required. This was originally done in a four-line assignment tag for each material block within the project file as the following example illustrates:

```xml
<Assignment type="Material" location="Element">
  <Reference>Spruce (Holzbalken, 192)</Reference>
  <Range>0 0 0 22</Range>
</Assignment>
```

![Figure 2-5: Assignment block for homogeneous materials in the DELPHIN project file.](image)

As previously explained, the assignment of directed material properties is based on the definition of rotation matrices. These matrices allow the link between the transport direction and the system coordinates of the project file. The assignment block in the project file is therefore extended about a mapping tag with a three-character value. This value lists the corresponding material direction u, v or w for each spatial direction (first value for x-dimension, second value for y and third value for z). The following file extract again shows the assignment tag of a material block. In this case, the material properties and functions are defined as u-values for the x-direction, v-values for the y-direction and again u-values for the z-direction.
Figure 2-6: Assignment block for anisotropic materials in the DELPHIN project file.

This spatial assignment is saved for each finite volume element and applied in each computation routine to derive the particular transport properties for each material according to the active transport directions. For the simple case of directly assigned orientations (as explained above), this is provided via selection of the valid plane. In the case of arbitrary rotated coordinates, this is realized via matrix multiplication with a resulting complex transformation matrix. To speed up the computation time, that is slowed due to the required trigonometrical functions, this part is shifted to the solver initialization process. This produces a pre-calculated 3x3 matrix which is applied to any transport direction with the following consequences for the computation algorithm with the following consequences for the computation algorithm:

- Heat- and moisture transport functions are calculated for all material orientations.
- The transformation matrix is applied and transformed functions are saved for each system coordinate.
- Any flux computation uses pre-calculated transport functions.

A meaningful pre-calculation and storage of manifold applied variables are essential implementation aspects for the provision of efficient simulation routines. The underlying definition and management of data structures should be suitable to allow a rapid access on pre-calculated parameters. Different implementation versions were tested and analysed. The selected version consists in the storage of all properties in each element for the system coordinate direction, already during the computation of the element-based state variables. These pre-calculated transport coefficients are applied as volume-weighted averages and multiplied with the gradient (driving potential).

2.3.4 Validation: academic joist end test

Although there is a multitude of thermal and hygrothermal validation cases (e.g. ISO 10211, ISO 15026, HAMSTAD) there is still a lack of proved reference data. Analytical solutions are only available for simple hygrothermal cases and only for one-dimensional transfer. There are no reference cases with analytical solutions covering anisotropic materials, two- or three-dimensional heat and moisture transfer. For this reason, an idealized experimental case was set up in order to produce measured reference data sets for the verification of the three-dimensional HAMT model in DELPHIN.

The reference case is called “academic joist end test”. It includes different tests for an isolated block of wood in the proportions of a timber joist with dimensions of 0.1 m x 0.1 m in the cross section and about 0.5 m in the length. This joist end was placed in a climate chamber and exposed to a step-wise changing climate conditions. Resulting conditions within the timber sample were measured at different positions and depths. Initial conditions were set to an ambient temperature of 20°C and a relative humidity of 50% for a period of about one month. The change of boundary conditions equalled a rise to 90% relative humidity during ten minutes. This condition (20°C, 90%) was kept
over three days (72 hours) and then set back to the start level of 20°C and 50% where it remained for a several days. The duration of the whole experiment was finally about 50 days.

Conditions in the timber sample were measured at two different positions, one close to the side face (A) and one in the middle (M). Furthermore, four different depths were recorded, about 1 cm (1), 5 cm (2), 9 cm (3) and 17 cm (4) behind the front face of the beam end. In summary there were eight measurement positions, four in the middle axis in different depths (M1 to M4) and four at the margin in different depths (A1 to A4). The measurement points recorded temperature with a precision of ± 0.1 K via thermistor sensors (NTC) and relative humidity with a precision of ± 2 % via capacitive humidity sensors.

![Image](image_url)

**Figure 2-7:** Cross and longitudinal section through the „academic joist end“ with the keys and positions of the sensors.

![Image](image_url)

**Figure 2-8:** Photography of the „academic joist end“ with its sensors and sealed side surfaces (case 1) just before the placement in the climate chamber. The beam end sides were sealed with aluminium foil (vapour tightness) to control the transport directions.

A detailed analysis of the moisture transport direction was enabled with four different versions of this experiment. All of them were derived one after the other, each one lasting about 50 days. The first case was designed to analyse the moisture transfer in longitudinal direction. All side faces and the back face were sealed with a vapour-tight aluminium foil and only the front side remained uncoated. The second case included both, longitudinal and tangential transfer. In this case, one side face and the front face were kept open. This case was extended in the third experiment where two opposite sides and the front side were uncovered. Finally, in the last experiment, all side faces and
the front face were open. The resulting moisture transfer is consequently three-directional including longitudinal, tangential and radial fluxes.

Figure 2-9: Four validation test cases for the experimental evaluation of directed heat- and moisture transfer through the “academic joist end”. 1 (leftmost): front face uncovered, 2 (middle left): front face and one side face uncovered, 3 (middle right): front face and two opposite side faces uncovered, 4 (rightmost): all faces uncovered.

Figure 2-10 shows the accordance between simulated and measured relative humidity for the second test case, in which the front face and one side face are open. The agreement between measured and simulated curve is sufficient although there is a remarkable quality difference depending on the sensor depth. Sensor A1, which is located close to the front face at the margin of the side face, shows the best match. The domination of longitudinal moisture transfer over tangential transfer is therefore well followed by the simulation results. Sensors A2 and A3 show a retarded humidification course and thus lower moisture level at the peak point and furthermore a retarded drying behaviour. Sensor A4 was not displayed as the results were nearly congruent with A3.

Figure 2-10: Comparison between measured (thick lines) and simulated relative humidity for three different sensor positions at the margin of the timber sample for test case 2.

As sensors A2 and A3 are located at the same distance from the uncovered side face, the difference between the positions must be traced back to the influence of different transport properties for the different transport directions. Longitudinal moisture transport coefficients exceed the radial ones and are therefore causing a faster humidification close to the face front than at the deeper positions. This is well characterized by the simulation model, although the final level is overestimated by the simulation, especially for the deepest sensor (A3 resp. A4).
Different aspect might be the reason for this difference between measured and simulated curves. Material inhomogeneity can be excluded. First, the differences are systematic and not given for a single sensor. Secondly the timber piece was selected with high diligence concerning knotholes, cracks etc. and the same original sample piece was used for both, the climate chamber experiment and the material parameterization. Relevant reasons for the differences between simulation and measurement are therefore:

- Hysteresis of moisture storage. DELPHIN is based on desorption storage functions which are at a higher level than adsorption functions. For the example of the spruce, used in this experiment, there is a difference of 6 (desorption) to 4 (adsorption) vol.-% for an ambient relative humidity of 70%.
- Non-linearity of the timber. DELPHIN assumes idealized transport directions (x,y,z) which are not given in wood. Especially for tangentially there is an aversive transport process.
- Distribution processes between mobile and immobile phases within the material.
- Assumption of a permanent thermodynamic equilibrium in each volume element.

The analysis of the test cases was complemented with different strategies for the simulation settings as well as solver statistics that summarized convergence and failure details. A first modification of simulation settings was checked with a comparison between idealized and real boundary conditions. As in any other climate chamber experiment, the boundary conditions couldn’t be kept stable for the runtime of the experiments as fluctuations were given for both, temperature and relative humidity. The comparison of both scenarios yielded differences of below 2.4% relative humidity for the outermost sensor position. These short-time fluctuations are also influencing the simulation duration and cause a nearly tripled runtime compared to the idealized, stable conditions.

Another analysed simulation setting is the liquid water conductivity computation via Kirchhoff-potential or via liquid water conductivity. Both options were compared and yielded identical results but different durations of the simulation. Kirchhoff-potential was up to 10% faster than the liquid water conductivity approach.

Further settings were tested for case three of the joist end experiment. These tests included also the analysis of the inner sensors (M1 to M4) and covered variations of the thermal and hygric surface transfer coefficients as well as heat storage capacity and the vapour resistance factor of the timber. Thermal transfer coefficients were varied from about 4 to 11 W/m²K, vapour transfer coefficients from about 3·10⁻⁷ to 1·10⁻⁹ s/m. The impact of the thermal transfer coefficient on the resulting relative humidity level was about 1% and thus very low. A higher effect was obvious for the vapour transfer coefficient. The best accordance between measurements and simulation was given with a value of 3·10⁻⁸ s/m, while the thermal coefficient was fixed to 10 W/m²K. A modification of the storage capacity influenced the results only marginally. The adapted settings in test case 3 improved the accordance noticeable, although the quality difference over the depth of the material persisted. This raised the conclusion that the differences are a consequence of the moisture transport properties, which were laboriously measured and calibrated. Further experiments and simulations are needed to evaluate this.

The “academic joist end” test case produced valuable and meaningful results concerning the impact of different transport properties in different material grain orientations. Basically, the transport property impact is reproducible via DELPHIN 3D solver extension. The accordance level between
simulated and measured curves could be raised with further investigations of the 3D material model parameters and its impacts.

Figure 2-11: Comparison between measured and simulated relative humidity for four different sensor positions at the margin (A1: upper left figure, A3: upper right figure) and in the middle axis (M1: lower left figure, M3: lower right figure) of the timber sample for test case 3.

2.4 Hygrothermal model extension for the consideration of airflow

Air movements in the pore volume and within cavities are usually subject of a more dynamic process than the process of coupled heat and moisture transfer through the solid matter. A modification of the air pressure at the boundary of a construction causes typically a completely new (steady-state) air pressure field within a few seconds or minutes. Temperature and moisture fields take much longer to develop equilibrium states and require some hours, in the case of temperature modifications, up to some weeks or even months for changes in the relative humidity level. For the application field of building physics and the corresponding processes, it is not the focus to reproduce this dynamic nature of permanently changing pressure fields around the building. The main interest is the evaluation of the impact of airflow on the coupled heat- and moisture transfer in building details.

Starting with this focus, the dynamic heat and moisture transfer simulation requires an airflow field, which is only updated from time to time. The air mass balance, which is required for this approach, is consequently treated as quasi-steady-state differential equation (purely spatial derivation). In this manner, the simulation procedure computes the resulting airflow field for selected time points under consideration of the current boundary conditions. Buoyancy flow is equally computed with the current surface temperatures of the element faces. Computation of steady-state air flow fields is achieved via solution of linear equation systems. The model assumes basically laminar flow and neglects turbulences. An important aspect is a proper estimation of resulting flow velocities to get realistic convective surface transfer conditions for the coupled heat- and moisture transfer.
Several model extensions were necessary to include air flow computation in the DELPHIN solver. These are:

- Data model extension (e.g. definition of air pressure as boundary condition and field condition, reference pressure definition)
- Material model extension (e.g. air permeability properties)
- Computation algorithm in the DELPHIN solver

The definition of different air pressure levels at the boundary of a construction leads to a pressure decrease along the flow path that depends on the particular material air permeability, if a continuous air flow path through the construction is given.

In constructive details with unvented cavities air circulations arise due to the buoyancy forces. This might cause a substantial contribution for the heat and moisture transfer mechanisms. One example for such a construction is a tightened cavity at the joist end support within the masonry. The model should also cover these cases of cavities, which are surrounded by tight materials and own therefore no pressure difference at the boundary of the cavity itself. A consequence of this case would be a singular equation system due to a missing reference pressure. DELPHIN therefore features a possibility to define a reference pressure via sources and sinks model within a single element of the cavity. This enables the solution of the equation system and the resulting air velocities.

The extension of the material model was previously restricted to the introduction of a constant air permeability for a material. Unfortunately, the measurement of air permeability for the multitude of materials in the DELPHIN database was not realizable up to now. Thus, only a few measurement results are present which were adopted from literature sources. These measurements also do not cover the dependency of air permeability on the temperature and relative humidity level. This should be investigated in future research projects.

There are basically three different approaches for the implementation of air flow computation in the DELPHIN solver.

- Update of each single Newton-iteration step (hard coupling)
- Update in each new trial within the error control loop (for time point changes)
- Update after each successfully terminated simulation step (weak coupling)

These versions differ mainly in regard to the number of airflow fields to be calculated. The first approach causes a very frequent update of airflow field computation and results consequently in a remarkably increased simulation time. On the other hand, this approach provides a very exact mathematical solution within the allowed tolerances. The second approach causes an update of the airflow field for each time point change. This happened in each integration step and for each time step reduction action due to tolerance value exceedance or convergence failure. The computation of the airflow field uses the estimated solution (start solution) for the Newton procedure. For this approach, clearly less update steps are required. On the other hand the computed airflow field could differ stronger from the mathematically exact solution. This is expected for rapidly changing temperature and moisture distribution during the Newton-iteration. But this is seldom the case as a huge difference between the start estimate of the Newton procedure and the corrected convergence solution is always an indicator for a heavy integration error. The third approach in the list above causes an update of the flow field calculation after a terminated integration step. Consequently, the computed field is matching the temperature- and moisture distribution at the end of the integration step but it did not interact with it as it was not used for the actual calculation. This causes a flow...
field which drags one integration step behind the temperature and moisture field. For the example of strongly coupled temperature and airflow fields, this approach yields the same basic effect as an explicit integration procedure and leads to instable calculations. This could partly be compensated by the error test mechanism, which reduces the integration steps (increased number of time steps) and therefore the instabilities. Unfortunately, this leads similarly to the first approach to prolonged simulation periods although the number of airflow field calculations is much smaller than for the other two approaches.

All three approaches have been implemented into DELPHIN for test purposes. For the majority of test cases, the second approach (for each time point change) has proved to be a sufficient compromise between simulation runtime and precision of the simulation result (number of airflow field calculation steps). The first approach (hard coupling) can be recommended for extremely strong coupling of temperature and airflow fields. Application examples would be constructions with sheet metal, constructions with high temperature gradients or constructions with very high cavities resulting in very strong buoyancy airflows. The weak coupling approach shows its advantages for cases without buoyancy effects in form of a better performance and reduces simulation runtime.

For all three approaches, the impact of a modified Newton-procedure on the duration of the simulation has also been investigated. The linear equation system \( A\mathbf{p} = \mathbf{b} \) (\( \mathbf{p} \) equals the solution vector of the air pressures in all elements) was calculated via LU-factorization of the matrix \( A \) and successive backwards defragmentation. Even for complex geometries with a vast number of volume elements, the LU-factorization of the airflow equation system is very time consuming. An alternative is given with a root detection: \( F(\mathbf{p}) = A\mathbf{p} - \mathbf{b} = 0 \). This can be solved via Newton-procedure. The coefficient matrix of the Newton-procedure equals therein the matrix \( A \). If the matrix is updated, already the first step of the Newton-procedure is successful and yields the exact result. The effort is consequently equivalent to the direct solution of the equation system. It allows now to use the matrix \( A \) in factorized shape for several airflow calculations which avoids the elaborate LU-fragmentation step. On the other hand the matrix could be not perfectly updated and requires eventually several Newton steps. But finally this procedure is for common 2D-geometries much faster than an entire LU-fragmentation. It was therefore implemented in DELPHIN and led to a drastic increase of simulation runtime for the selected application cases (2D, moderately up to complex geometries, strong buoyancy flow). For 3D simulations the performance is not yet sufficient because the equation system for the computation of the airflow field is still done via direct solution algorithms (band matrix). A broad application in the field of engineering projects requires definitely further research activities.

\subsection{2.5 References}


3 Probabilistic hygrothermal modelling with Delphin

(Astrid Tijskens, KUL)

3.1 General information

The research on probabilistic modelling was conducted by Astrid Tijskens, who started in October 2015 as a PhD researcher at KU Leuven. This section gives a short overview of the progress of her work. To start, a general literature study (3 months) on hygrothermal damage patterns caused by interior insulation and on probabilistic modelling and metamodelling was performed, in order to get an overall understanding of the problem. Next, a probabilistic framework was developed, based on the methodology of Van Gelder (Van Gelder et al., 2014). In order to perform probabilistic studies with Delphin, a Matlab code was written which couples Delphin simulations in a Monte Carlo loop. Writing this code initially took about 6 months, though this is work in progress; often, new features are needed and implementing them can take a few hours to several days. Afterwards, literature on damage prediction models was reviewed (2 months), considering the probabilistic assessment of hygrothermal damage caused by interior insulation requires damage criteria. This resulted in the implementation of the updated VTT mould growth model and the VTT wood decay model in the probabilistic framework. Furthermore, a simplified dynamic zone model was developed (3 months), to enable taking into account more interior climate parameters the than the functionality of Delphin normally allows. Also, several probabilistic studies on interior insulation have been performed throughout the past year (5 months). In addition, two papers on the hygrothermal performance of interior insulation (Net Zero Energy Building symposium, October 20 2016; international WTA PhD symposium, September 14-16 2017) and a paper on the simplified hygrothermal dynamic zone model was written (11th Nordic Symposium on Building Physics, June 11-14 2017). To end, the first steps towards improving the calculation efficiency through metamodelling have been taken; a literature study on statistical learning has been started.

To start, an introduction to probabilistic modelling is given in section 3.2, explaining all principles applied in the probabilistic methodology. The application of this methodology on an interior insulation case study is described in section 3.3. Section 3.4 gives a detailed description and demonstration of the simplified hygrothermal dynamic zone model. To end, the findings from the current interior insulation studies are discussed in section 3.5.

3.2 Introduction to probabilistic modelling

Most studies on interior insulation make use of deterministic simulations, hence neglecting the inherent variability and uncertainty of geometries and configurations, of material and component properties, of internal loads and boundary conditions. A deterministic approach may hence lead to inconclusive analyses and non-optimal designs, and a probabilistic methodology is therefore to be preferred.

Two fundamental aspects of probabilistic modelling are uncertainty quantification and sensitivity analysis; to transform the variabilities of the input to the uncertainties of the output and to identify these input parameters that are most dominant in this transformation. Due to the complex, non-linear and transient character of most building performance problems, Monte Carlo-based techniques are often preferred for these goals. The Monte Carlo method refers to the repeated execution of a deterministic simulation model $f(x)$ for different values of the input parameters in
order to estimate the probability distribution of the output parameters. The Monte Carlo simulation can thus be presented by

\[ Y = f(X) \]

with \( X \in R^{n \times p} \) the input matrix and \( Y \in R^{n \times q} \) the output matrix, where \( n \) is the number of samples, \( p \) the number of input parameters and \( q \) the number of output parameters. Traditionally the \( n \) input parameter values are randomly selected according to their probability distributions, which can be discrete, uniform, normal, ... Therefore, a random value between 0 and 1 is selected and ascribed to the cumulative distribution function \( CDF(X_i) \) of the input parameter \( i \). The corresponding input parameter value can then be calculated using the inverse cumulative distribution function \( CDF^{-1}(X_i) \).

This way, also probabilities based on experimental data which can not be described by theoretical distributions are facilitated. Apart from random sampling, many other sampling strategies have been developed with the purpose of decreasing the number of samples needed to assure a reliable output distribution. Different sampling strategies and their efficiency will be discussed more in detail in section 4.

A probabilistic design methodology developed at the Building Physics section of KU Leuven (Van Gelder et al., 2014) is implemented and refined in RIBuild for the hygrothermal assessment of interior insulation measures. This probabilistic design methodology consists of four steps (see Figure 3-1): preprocessing, preliminary screening, updating and probabilistic design. These steps respectively select the input parameters and distributions (step 1), determine the most dominant input parameters and develop a metamodel to improve calculation efficiency (step 2), update the input distributions (step 3), and finally perform the actual probabilistic design (step 4). In the following paragraphs, these steps are discussed briefly; for a more detailed description, refer to (Van Gelder et al., 2014).

The actual probabilistic design (step 4) is performed through a Monte Carlo loop with a multi-layered sampling scheme (see Figure 3-1), which enables sorting parameters by their conceptual meaning. Contributing input parameters of the probabilistic design can be divided into three categories.

- **Design parameters**, such as the preferred insulation system or insulation thickness, are fully controllable. They are the unknown parameters in the design process, but once a design option is selected, the parameter values are known.
- **Inherently uncertain parameters**, such as the material properties and boundary conditions, are completely uncontrollable by the designer as their values are neither known in the design process nor after, but they can significantly influence the design performance. These parameters are ascribed to the uncertainty layer.
- **Scenario parameters** are inherently uncertain parameters dealing with potential scenarios for which an explicit evaluation is wanted, for example the user behaviour or the external climate load. These form the scenario layer.

By ascribing these parameter categories to a different layer in a multi-layered sampling scheme, all design options are subjected to the same uncertainties and a direct comparison for several scenarios is enabled. As a result, this probabilistic design can be used as an effective decision tool.

Prior to performing such a probabilistic design, the problem is first preprocessed (step 1) to select the output parameters needed for decision making. Contributing input parameters are
determined and fixed values or (provisional) input distributions are ascribed for respectively deterministic and probabilistic parameters.
Figure 3-1: Flowchart of the probabilistic design methodology (from Van Gelder et al., 2014)
Since the proposed multi-layered sampling scheme significantly increases the needed number of runs, time-consuming models are preferably replaced by a metamodel in the preliminary screening (step 2). Metamodels mimic the original, potentially time-intensive model with a simpler and faster surrogate model. To this purpose, training and validation sets are run in the original model to construct and validate the metamodel. Due to the extent of the multi-layered scheme, smaller sampling sets are used. These sets are also used to calculate sensitivity indices to rank the input parameters from most to least influencing the output distributions. Based on this sensitivity ranking, the provisional distributions of most influencing parameters are updated (step 3), while the less influencing parameters can be omitted. Limiting the number of parameters eases collecting the required input distributions as this can be time consuming. Moreover, this improves sampling efficiency and limits the number of considered design options in the multi-layered scheme. This stresses the importance of the preliminary screening in addition to the actual probabilistic design.

In the past work, the focus was mainly on the preprocessing (step 1) and the actual probabilistic design (step 4). The application of these two steps on interior insulation simulations with Delphin are discussed in the next section. The different elements of the preliminary screening (step 2) are part of future research.

### 3.3 Probabilistic modelling in Delphin

As Delphin is a deterministic simulation tool, it does not allow performing probabilistic analyses on its own; a global framework is needed to facilitate the probabilistic methodology described above. For this purpose, a Matlab code was developed which enables to define input parameter distributions, create a multi-layered sampling scheme, automatically change the sampled parameter values in Delphin, run the simulations and postprocess the output using damage prediction models. This section will cover the application of the previously described probabilistic methodology in the context of probabilistic assessment of the hygrothermal performance of a 1D wall with different interior insulation systems.

#### 3.3.1 Input parameters

As shown in Figure 3-1, the first step is to define the deterministic and probabilistic input parameters and their fixed values or (provisional) input distributions respectively. For a 1D wall with interior insulation, the characteristics and boundary conditions that are expected to influence the hygrothermal risks significantly are considered probabilistic and are shown in Table 3-1. Note that the chosen parameter distributions are provisional, as an example to explain the methodology, and should be updated based on the findings in WP2.

To deal with variability in climatic conditions, different exterior climates are included. Currently, only the Test Reference Years of three German climates are considered, since data of these climates was readily available. Of course, other climate locations can be included, as well as non-cyclic climate data (for example, a six-year data set). To incorporate variability in the wall conditions, uniform distributions of the wall orientation, the solar absorption and the exposure to wind-driven rain are considered. The wind-driven rain load can be calculated by the standard rain model of Delphin, or by using the catch ratio as described in (Blocken, 2002). The catch ratio relates the wind-driven rain (WDR) intensity on a building to the unobstructed horizontal rainfall intensity and is function of the reference wind speed and the horizontal rainfall intensity for a given position on the building façade and wind direction. In both models, variability in wall position and potential shelters, trees or surrounding buildings are reckoned with by the exposure factor. Additionally, a climate dependent normal distribution of the exterior convective heat transfer coefficient is
assumed, to take into account the variability in wind speed\(^2\). The exterior moisture transfer coefficient is related to the heat transfer coefficient through the Lewis relation. The properties of the brick wall itself are subjected to uncertainty as well. A large difference between the wall thickness of historical and traditional buildings exists. Therefore, a uniform distribution of the wall thickness is considered. Furthermore, as the brick material properties vary widely as well, different brick types are included. The characteristics of the currently used brick types can be found in Table 3-2 (Vereecken et al., 2015).

### Table 3-1: Probabilistic input parameters and distributions

<table>
<thead>
<tr>
<th>Input parameter</th>
<th>Input distribution</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Climatic conditions</strong></td>
<td></td>
</tr>
<tr>
<td>Meteorological climate data</td>
<td>D(Essen, Bremerhaven, Munich)</td>
</tr>
<tr>
<td>Convective heat transfer coefficient (h_{\text{conv}}) [W/m(^2)K]</td>
<td>Essen N(7.34, 2.11) Bremerhaven N(11.67, 3.17) Munich N(7.22, 1.77)</td>
</tr>
<tr>
<td>Moisture transfer coefficient (\beta ) [s/m]</td>
<td>7.7 (\cdot) 10(^{-9}) (h_{\text{conv}})</td>
</tr>
<tr>
<td><strong>Wall conditions</strong></td>
<td></td>
</tr>
<tr>
<td>Wall orientation [degree from north]</td>
<td>U(0, 360)</td>
</tr>
<tr>
<td>Solar absorption coefficient</td>
<td>U(0.4, 0.8)</td>
</tr>
<tr>
<td>Exposure factor WDR</td>
<td>U(0, 1.5)</td>
</tr>
<tr>
<td><strong>Brick layer</strong></td>
<td></td>
</tr>
<tr>
<td>Thickness [m]</td>
<td>U(0.15, 0.5)</td>
</tr>
<tr>
<td>Material</td>
<td>D(Brick 1, Brick 2, Brick 3)</td>
</tr>
</tbody>
</table>

Explanation of symbols used: U(a, b): uniform distribution between a and b; D(a, b): discrete uniform distribution with options a and b; N(\(\mu\), \(\sigma\)): normal distribution with mean value \(\mu\) and standard deviation \(\sigma\)

### Table 3-2: Brick type properties

<table>
<thead>
<tr>
<th>Material property</th>
<th>Brick 1</th>
<th>Brick 2</th>
<th>Brick 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Capillary absorption coeff. ([\text{kg}/\text{m}^2\text{s}^{0.5}])</td>
<td>0.125</td>
<td>0.46</td>
<td>0.04</td>
</tr>
<tr>
<td>Bulk density ([\text{kg}/\text{m}^3])</td>
<td>2087</td>
<td>1786</td>
<td>1080</td>
</tr>
<tr>
<td>Thermal capacity ([\text{J}/\text{kgK}])</td>
<td>870</td>
<td>1000</td>
<td>834</td>
</tr>
<tr>
<td>Dry thermal conductivity (\lambda_{\text{dry}}) [W/mK]*</td>
<td>0.9</td>
<td>1.08</td>
<td>0.996</td>
</tr>
<tr>
<td>Dry vapour resistance factor (\mu ) [-]</td>
<td>24.8</td>
<td>14.3</td>
<td>45.1</td>
</tr>
<tr>
<td>Capillary moisture content ([\text{kg}/\text{m}^3])</td>
<td>130</td>
<td>206.7</td>
<td>101</td>
</tr>
<tr>
<td>Saturation moisture content ([\text{kg}/\text{m}^3])</td>
<td>209</td>
<td>323</td>
<td>253</td>
</tr>
</tbody>
</table>

* Moisture dependent thermal conductivity: \(\lambda(w) = \lambda_{\text{dry}} + 0.56 \cdot w\) with \(w\) the moisture content in \(\text{m}^3/\text{m}^3\)

\(^2\) In future studies, this will be replaced by the Delphin boundary condition model ‘boundary layer with variable air velocity’, where the convective heat transfer coefficient is calculated according to \(h_{c} = h_{0} + k_{s} \cdot v_{\text{wind}}^{\text{ex}}\) (EN ISO 06946) and \(k_{s}\) is a sampled value between 1 and 8. This enables taking into account the transiency and variation of the wind speed directly, which is more accurate than the current approach.
In addition, variation in interior room conditions must be taken into account. Mainly two approaches are possible here. The first, and easiest, is the approach defined by the European Standards EN 15026 or EN 13788. In EN 15026, the interior temperature and relative humidity are dependent on the daily average exterior temperature. Two different humidity loads are defined to account for variability in building use. To avoid sudden ‘jumps’ between consecutive days, a running average could be used. In EN 13788, the interior humidity load is defined by an interior moisture excess in relation to the monthly average exterior temperature. Five different humidity classes are defined, for the interior temperature no values are given. The advantage of these European Standards is that they are fairly easy to use. However, the obtained interior climates have rather limited variability and thus do not consider all possible interior conditions. For a probabilistic study, this is rather undesirable. Therefore, a simplified dynamic zone model has been developed, which allows taking into account much more parameters, such as the ventilation rate, heat and moisture buffering capacity of the room, moisture production rate… With this zone model, a bigger variation on the interior climate can be obtained, thus ensuring the probabilistic analysis covers a broader variation in interior boundary conditions. The zone model is described in detail in section 3.4.

The remaining boundary conditions are all variables either with small variations or of less importance for the current study of a 1D wall. Therefore, these boundary conditions are treated deterministically. An overview of the deterministic boundary conditions is given in Table 3-3.

<table>
<thead>
<tr>
<th>Input parameter</th>
<th>Input value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Exterior surface</strong></td>
<td></td>
</tr>
<tr>
<td>Long wave emissivity</td>
<td>0.9</td>
</tr>
<tr>
<td><strong>Interior surface</strong></td>
<td></td>
</tr>
<tr>
<td>Total heat transfer coeff</td>
<td>8</td>
</tr>
<tr>
<td>Moisture transfer coeff</td>
<td>$3 \times 10^{-8}$</td>
</tr>
<tr>
<td><strong>Initial conditions</strong></td>
<td></td>
</tr>
<tr>
<td>Initial temperature [°C]</td>
<td>20</td>
</tr>
<tr>
<td>Initial relative humidity [%]</td>
<td>50</td>
</tr>
</tbody>
</table>

### 3.3.2 Output parameters and post-process

In order to assess whether damage will occur, damage criteria and prediction models are required. Typically, frost damage at the exterior surface, decay of embedded wooden beam ends, mould growth between masonry and insulation and mould growth on the interior surface are evaluated. The latter is especially important in case of thermal bridges (and thus of less importance in 1D simulations, as will be shown in the next section). Delphin, however, does not deliver outputs in the form of a damage prediction, but calculates the temperature, relative humidity, moisture content… and a post-processing of this output is thus required. In Delphin, only the specified outputs are saved during the simulation, and afterwards no additional data can be requested, so it is important to carefully define the required outputs beforehand. Moreover, requesting more output than needed is
detrimental, as more output significantly slows down the simulation time and complicates the post-processing. Therefore, after selecting the damage criteria, the corresponding prediction models determine the required Delphin outputs. Table 3-4 gives an overview of damage patterns, the currently used damage prediction models and the required Delphin outputs.

<table>
<thead>
<tr>
<th>Damage pattern</th>
<th>Prediction model</th>
<th>Required Delphin output</th>
</tr>
</thead>
<tbody>
<tr>
<td>Frost damage</td>
<td>Moist freeze-thaw cycles via Delphin Ice model</td>
<td>Freeze-thaw cycles, $MC_{sat}$</td>
</tr>
<tr>
<td></td>
<td>Moist freeze-thaw cycles via TU Dresden equation</td>
<td>$T$, $RH$, $MC_{sat}$</td>
</tr>
<tr>
<td>Decay of wooden beam ends</td>
<td>Number of hours that relative humidity exceeds critical limit</td>
<td>$RH$</td>
</tr>
<tr>
<td></td>
<td>VTT wood decay model</td>
<td>$T$, $RH$</td>
</tr>
<tr>
<td>Mould growth</td>
<td>Number of hours that relative humidity exceeds critical limit</td>
<td>$RH$</td>
</tr>
<tr>
<td></td>
<td>Updated VTT mould growth model</td>
<td>$T$, $RH$</td>
</tr>
</tbody>
</table>

The extra vapour diffusion resistance caused by the interior insulation system hinders an inward drying of the wall. Additionally, the lower temperature of the original wall structure results in a decreased drying potential towards the exterior. Hence, by applying interior insulation, the moisture content in the original wall structure will increase. This, in combination with the lower temperature results in an enlarged risk on frost damage (Maurenbrecher et al., 1998). Currently, the risk on frost damage is evaluated based on the number of moist freeze-thaw cycles per year at 0.5 cm from the exterior brick surface. The number of freeze-thaw cycles can be calculated either by the ice model of Delphin or by the TU Dresden equation criterion (Grunewald, 2016) during post-processing. The ice model calculates the number of freeze-thaw cycles internally, which has a negative impact on the calculation time. The TU Dresden equation criterion uses the temperature and relative humidity to calculate the number of freeze-thaw cycles during post-process, and is much faster. As the result of both models does not significantly differ, the TU Dresden equation criterion is used in general. A ‘moist’ freeze-thaw cycle is a freeze-thaw cycle that occurs in combination with a moisture content in the brick (in this case at 0.5 cm from the exterior surface) that is high enough to induce frost damage. In our studies, a moisture content higher than 25% of the saturated moisture content is assumed to be critical and thus to entail a risk on frost damage. Note that this is a rather arbitrary value, as currently no precise prediction criteria is at hand. Furthermore, the current frost damage prediction model does not take into account the duration below subfreezing temperatures while exceeding the critical moisture content.

The increased moisture content in the masonry wall might damage embedded wooden beam ends (Gnoth et al., 2005; Stopp and Strangfeld, 2006; Morelli and Svendsen, 2013). An indication of this risk can be made based on the number of hours that the relative humidity in the masonry at 5 cm from the insulation system exceeds the critical relative humidity for wood decay. For the critical

---

3 If several simulations run in parallel, the hard drive can be overloaded by writing all the output, resulting in a slower calculation of the simulations as they have to wait to write their output. This strongly depends on the specifications of the used computer; an SSD disk allows faster writing speed and thus is less prone to this problem.
relative humidity for wood decay, a relative humidity equal to 95% is assumed (Viitanen et al., 2011). Alternatively, the VTT wood decay model could be used, which calculates the percentage of mass loss of the wooden beam end based on the temperature and relative humidity (Viitanen et al., 2010). Note, however, that in a 1D wall study solely a rough indication of the wood decay risk is acquired, as two and three dimensional heat and moisture transport as well as potential air rotations around the wooden beam end are neglected.

At the interior surface and the interface between masonry and insulation, a too high relative humidity should be avoided, since this entails a risk on mould growth (Sedlbauer, 2002). The mould growth risk can be estimated by the number of hours that the surface relative humidity exceeds 80%, which is the lower limit of the critical relative humidity for mould growth according to (Viitanen et al., 2011). Alternatively, the VTT mould growth model can be used, which calculates the Mould Index based on the fluctuation of the temperature and relative humidity (Ojanen et al., 2010). The Mould Index is a value between 0 and 6, going from no growth to heavy and tight mould growth. In the updated VTT model, the expected material sensitivity to mould growth is implemented as well. In the current studies, the materials are always assumed to belong to the class ‘very sensitive’, hence the obtained results will be worst case.

Care should be taken with the currently used damage predictions, though, as they are not always reliable (Vereecken and Roels, 2012) and thus do not allow to define strict criteria of which level of damage is acceptable. This is especially the case for the wood decay model, as it is based on rather limited experimentations, and the rudimentary frost damage model. Therefore, in order to predict the hygrothermal performance of an interior insulation system accurately, further research on damage prediction models and their reliability is crucial, as part of WP 2. As soon as more accurate prediction models are investigated or developed, these can easily be implemented in the probabilistic framework.

3.3.3 Design options and multi-layered sampling scheme

The design options consist of the different insulation systems and thicknesses considered. In the current studies, only four insulation systems were included: (1) extruded polystyrene (XPS), (2) mineral wool with a vapour barrier, (3) calcium silicate, adhered to the brick wall with a 4 mm glue mortar, and (4) mineral wool with a smart vapour retarder. As an interior finishing layer, a 10 mm gypsum board is used, only the capillary active system (4) is rendered with a 10 mm plaster layer. For each insulation system, eight insulation thicknesses were considered: 1, 2, 4, 6, 10, 15, 20 and 30 cm. Hence, 33 options were analysed (4 interior insulation systems, with eight possible thicknesses + uninsulated reference wall). Of course, other insulation systems and thicknesses could be included as well. Though, keep in mind that an increase in design options implies a strong increase in simulation time, due to the multi-layered sampling scheme. Furthermore, until now only a 1D wall and a simple 2D wall with embedded wooden beam ends are considered. In the future, also thermal bridges in 2D and 3D could be included.

Once the design options are created, and the probabilistic input parameters and their probability distributions are defined, a multi-layered sampling scheme can be created. The number of samples should be chosen so that it is a multiple of all considered discrete input parameters, to ensure that all values have equal probability. Additionally, enough samples are needed in order to reach convergence of the output distributions, but as few samples as possible are wanted in order to reduce calculation time. This can be accomplished by sequentially adding small sample sets until
convergence is reached. In the current studies usually 108 samples were used, though convergence was not checked.

### 3.3.4 Evaluation of output

A deterministic simulation will generate one output for each examined damage pattern. A probabilistic analysis, however, results in as many outputs as samples used, for each design option. This large amount of data might complicate interpreting and comparing the results. Moreover, different representations of the same data might result in different conclusions. Therefore, a comprehensible and encompassing visual representation is necessary to allow drawing reliable conclusions.

A first option is using cumulative distribution functions. An empirical CDF plots each unique value of the considered parameter versus the percentage of values in the sample set that are less than or equal to it, and connects the points with a stepped line. Thus, the CDF of an output parameter P, or just distribution function of P, evaluated at x, is the probability that P will take a value less than or equal to x. CDF plots can be useful when comparing the distributions of a damage pattern across levels of the parameter P (e.g. different design options, wall thicknesses, exterior climates, …). However, this can easily become very complex when there are many different levels. Furthermore, CDF’s are hard to interpret intuitively, as they do not give an immediate overview of the performance.

Boxplots are a second option, and are frequently used. A boxplot (Figure 3-2) graphically depicts subsets of numerical data through their quartiles and usually have whiskers indicating variability outside the upper and lower quartiles. Outliers may be plotted as individual points. The spacing between the different parts of the box indicate the degree of dispersion (spread) and skewness (asymmetry) in the data. Boxplots are non-parametric: they display the variation of a statistical population without making any assumptions of the underlying statistical distribution. Hence, they are a simple way of summarizing the range of variation of a real-valued parameter across different subsets of data. However, their visual simplicity can hide a lot of important details about how the observations are distributed, such as in case of a multimodal distribution. A boxplot would not give any evidence of this multimodality, which might result in faulty conclusions. To overcome this multimodal distribution issue, variants on the boxplot have been developed which combine boxplots with nonparametric density estimates, such as the violin plot and the bean plot (Figure 3-2).

![Figure 3-2: Examples of a boxplot, a violin plot and a bean plot (from Pearson, 2011)](image)

A violin plot is similar to a boxplot with a rotated kernel density plot on each side. Typically violin plots will include markers for the median of the data and the interquartile range, as in standard box plots. Like box plots, violin plots are used to represent comparison of a parameter distribution
across different subsets of data. The latter is more informative than a plain box plot though, as the violin plot shows the full distribution of the data. A bean plot is an extension similar to violin plots but with some added features, such as the use of a variety of different kernel functions for density estimation, and the plotting of ‘bean lines’ corresponding to the observations of each individual value. Yet, these two box plot extensions have their disadvantages as well. Since they also plot the kernel density distribution, this distribution needs to be estimated and depending on the used parameter settings, this distribution might represent the true distribution accurately or not. Furthermore, these distribution estimates typically decay smoothly to zero and, as a result, extrapolate somewhat beyond the observed data range. This again might result in graphs that are difficult to interpret correctly.

A third option are dot plots, which are a form of one-dimensional scatterplots. It displays individual observations on a continuous scale using a dot (or other marker) and uses local displacements in a direction orthogonal to the scale in order to prevent dots from overlapping. Typical for dot plots, these displacements are increments of one dot width. Dot plots may be distinguished from histograms in that dots are not spaced uniformly along the horizontal axis. They are useful for highlighting clusters and gaps, as well as outliers. Hence, dot plots do not suffer from the multimodal distribution issue the way boxplots do. Their other advantage is the conservation of numerical information, as each observation is plotted as an individual dot. Hence, dot plots are a high variance, low bias data representation, and therefore are ideally suited for displaying moderate sized datasets when outliers and other irregularities are of interest. In case of larger data sets with discrete values, the frequency of an observation value can be visualised by proportionally scaling the dot size, instead of visualising each observation as a dot.

Apart from the visual interpretation of the simulation results, it is also important to define whether the insulation system performs within acceptable damage limits or not. Hence, strict criteria on how much damage is still acceptable are needed. However, given the accuracy of the current damage prediction models, this may prove to be rather difficult. Thus, the predicted damages should perhaps not be dealt with in an absolute way, but rather in a relative way, where the performance of the insulation system is compared to the performance of the uninsulated reference wall. This way, criteria are needed to define which changes in damage levels are still acceptable, rather than which damage level is acceptable. Currently, though, even defining the accepted increase in damage is rather challenging. Therefore, it is crucial this aspect is further investigated and discussed in WP 2.3 and WP 6.

### 3.4 Hygrothermal simplified dynamic zone model

This section was based on the recent paper by Tijskens et al. (2017).

#### 3.4.1 Introduction

When evaluating the hygrothermal performances of a building component, the question arises which interior boundary conditions to use in order to get reliable results. Building component simulation software, such as DELPHIN, can perform a powerful hygrothermal analysis but typically simplify the interior boundary conditions. Parameters such as the ventilation rate, vapour production, heat gains, and thermal and hygric inertia cannot be included. Building energy simulation (BES) software on the other hand, such as TRNSYS, is developed specifically to solve (multi) zonal energy balances. However, these software tools often have limited possibilities regarding building component analysis. Additionally, BES-models require more input parameters
and knowledge about the building, which is not always available. Furthermore, coupling building component analysis software to BES is often impractical. Consequently, most building component analysis are limited by defining an interior temperature and relative humidity only. Different approaches can be found in literature: indoor conditions are constant (dos Santos and Mendes, 2015; Sabera et al., 2012), or vary with the exterior temperature (Sabera et al., 2012; Künzel and Zirkelbach, 2013; Zhao et al., 2011, Pasztorya et al., 2012), as recommended by EN 15026 or ASHRAE 160, or an interior moisture excess is determined based on the exterior temperature (Changa and Kim, 2015), as specified in EN 13788. In reality, however, widely varying indoor conditions occur, depending on occupant behaviour and use. This might result in differing hygrothermal performance of the considered building component. Hence, improvement is possible by taking into account more realistic indoor climate parameters.

In the context of probabilistic modelling to investigate the hygrothermal risks of internally insulated walls, a simplified dynamic zone model has been developed to expand the functionality of DELPHIN 5.8. This zone model allows to incorporate more indoor climate parameters, in furtherance of a wider range of realistic indoor boundary conditions than proposed in EN 15026 or EN 13788.

**Nomenclature**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$</td>
<td>Surface</td>
<td>[m²]</td>
</tr>
<tr>
<td>$C_p$</td>
<td>Specific heat capacity</td>
<td>[J/kgK]</td>
</tr>
<tr>
<td>$d_p$</td>
<td>Penetration depth</td>
<td>[m]</td>
</tr>
<tr>
<td>$G$</td>
<td>Moisture flow</td>
<td>[kg/s]</td>
</tr>
<tr>
<td>$g_g$</td>
<td>Glass g-value [-]</td>
<td></td>
</tr>
<tr>
<td>$h$</td>
<td>Surface heat exchange coeff.</td>
<td>[W/m²K]</td>
</tr>
<tr>
<td>$H_{IR}$</td>
<td>Hygric capacity</td>
<td>[kg/m³%RH]</td>
</tr>
<tr>
<td>$H_s$</td>
<td>Solar radiation</td>
<td>[W/m²]</td>
</tr>
<tr>
<td>$n$</td>
<td>Ventilation rate</td>
<td>[h⁻¹]</td>
</tr>
<tr>
<td>$p_v$</td>
<td>Vapour pressure</td>
<td>[Pa]</td>
</tr>
<tr>
<td>$Q$</td>
<td>Heat flow</td>
<td>[W]</td>
</tr>
<tr>
<td>$q$</td>
<td>Heat flux</td>
<td>[W/m²]</td>
</tr>
<tr>
<td>$R_v$</td>
<td>Vapour gass constant</td>
<td>[J/kgK]</td>
</tr>
<tr>
<td>$T$</td>
<td>Temperature</td>
<td>[°C]</td>
</tr>
<tr>
<td>$U$</td>
<td>U-value</td>
<td>[W/m²K]</td>
</tr>
<tr>
<td>$V$</td>
<td>Volume</td>
<td>[m³]</td>
</tr>
<tr>
<td>$w$</td>
<td>Moisture content</td>
<td>[kg/m³]</td>
</tr>
<tr>
<td>$\beta$</td>
<td>Vapour diffusion exchange coeff.</td>
<td>[s/m]</td>
</tr>
<tr>
<td>$\delta$</td>
<td>Vapour permeability</td>
<td>[s]</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>Thermal conductivity</td>
<td>[W/mK]</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Volumetric mass density</td>
<td>[kg/m³]</td>
</tr>
</tbody>
</table>

### 3.4.2 Hygrothermal zone model

In the simplified zone model, the building component’s original interior boundary conditions (BC) are replaced by an air layer, as shown in Figure 3-3, which represents the interior zone and its hygrothermal properties. The air layer’s temperature and relative humidity are not defined, but will be controlled by its equivalent boundary conditions (BC*). In turn, the building component’s interior surface interacts with the air layer, in accordance with the latter’s properties. The air layer’s BC* will be defined by a heat- and moisture balance, as disclosed in the next two paragraphs.

![Figure 3-3](image)

**Figure 3-3:** (a) the original model geometry and (b) the zone model geometry, with an additional air layer and equivalent boundary conditions.
3.4.2.1 Heat transfer

The zonal heat balance is given by equation (1), with on the left hand side the solar heat gain and the interior heat gain; on the right hand side the ventilation heat loss, the transmission heat loss and the thermal buffering capacity, respectively. The buffering capacity includes the thermal capacity of both the air volume and interior surfaces.

\[ A \dot{g} g H_s + Q_{\text{int}} = 0.34 nV(T_i - T_e) + A_c U_c (T_i - T_{e,\text{eq}}) + (\rho_{\text{air}} C_{p,\text{air}} V + \rho_{\text{mat}} C_{p,\text{mat}} A_{\text{surf}} d_p) \frac{\partial T_i}{\partial t} \]  

(1)

\[ T_i \geq T_{\text{set}} \]  

(2)

This heat balance is solved numerically for the zone temperature \( T_i \) (dry bulb). The variable heating load is included by equation (2), which ensures \( T_i \) does not drop below the setpoint temperature \( T_{\text{set}} \). Because this unknown variable heat load cannot be assigned in DELPHIN, the heat balance cannot be solved automatically. Hence, the interior temperature is a precalculated hourly time series, in which the effects of the setpoint temperature, solar and interior heat gains, ventilation rate, transmission losses and thermal inertia are considered. This is the air layer’s BC* temperature \( T_{i}^* \). At the same time, a high heat exchange coefficient \( h_i \) (e.g. \( 10^5 \) W/m²K) is applied, in order to eliminate the resistance between air layer and BC*. Thus, the air layer temperature \( T_i \) equals the BC* temperature \( T_{i}^* \).

Next, the heat exchange between the air layer and the building component’s interior surface needs to be specified. Since the interior surface is no longer subjected to BC, the surface resistance is not taken into account. This can be corrected by altering the thermal properties of the air layer material. In the original model, the heat flux between the interior surface and BC is calculated by equation (3). Note that the building component’s geometry is discretised, as DELPHIN employs the finite element method, and that DELPHIN does not take into account the surface element’s resistance. In the zone model, the heat flux between the interior surface and air layer is calculated by equation (4). The subscripts \( al \) and \( se \) refer to the air layer and surface element respectively.

\[ q_{\text{conv}} = h_i (T_{si} - T_i) \]  

(3)

\[ q_{\text{cond}} = \frac{1}{\lambda_{al}} \frac{d_{al}^2}{d_{se}} (T_{si} - T_i) \]  

(4)

Combining equation (3) and (4) results in the following formula for the thermal conductivity \( \lambda \) of the air layer. Note that the surface element’s resistance is neglected, due to its small thickness (0.1 mm).

\[ \lambda_{al} = h_i \frac{d_{al}}{2} \]  

(5)

3.4.2.2 Moisture transfer

The zonal moisture balance can be described by equation (6), where the right hand side describes the vapour flux through ventilation, the interior vapour production and the vapour flux through the building component, respectively. The left hand side represents the hygric buffering capacity of the zone. This buffering capacity includes both the capacity of the air volume and the hygric capacity \( HIR \) of the interior surfaces and objects (Janssen and Roels, 2009; Vereecken et al., 2011).
\[ \frac{V}{R_v T_i} \frac{\partial p_{vi}}{\partial t} = \frac{nV}{3600 R_v T_i} (p_{ve} - p_{vi}) + G_{vp} + G_{\text{trans}} \]  

(6)

The approach here is different compared to the heat balance; the moisture balance will be solved numerically by DELPHIN, rather than precalculated. The hygric buffering will be taken into account by altering the moisture sorption curve of the air layer (see next paragraph). The vapour transport through the wall will be calculated by DELPHIN, and thus can be omitted from the moisture balance hereafter. Consequently, only the vapour flux through ventilation and the vapour production must be implemented through the air layer’s BC*. In the original model, the moisture flux \( g_v \) between interior surface and BC is calculated by equation (7). This must equal the vapour flux through ventilation and vapour production in the air layer, given by equation (8).

\[ g_v = \beta_i (p_{vi} - p_{vesi}) \]  

(7)

\[ g_v = \frac{1}{A_{\text{wall}}} \frac{nV}{3600 R_v T_i} \left( (p_{ve} + G_{vp} \cdot \frac{3600 R_v T_i}{nV}) - p_{vi} \right) \]  

(8)

Combining equation (7) and (8) results in the formulas for the equivalent vapour diffusion exchange coefficient \( \beta_i^* \) (equation (9)) and the equivalent vapour pressure \( p_{vi}^* \) (equation (10)), which define the air layer’s BC*.

\[ \beta_i^* = \frac{1}{A_{\text{wall}}} \frac{nV}{3600 R_v T_i} \]  

(9)

\[ p_{vi}^* = p_{ve} + G_{vp} \cdot \frac{3600 R_v T_i}{nV} \]  

(10)

Next, the air layer’s moisture properties still need to be adjusted. The buffering capacity of the fictitious air layer needs to equal the buffering capacity of the whole zone. To do so, the moisture sorption curve of the air layer is adjusted by adding the moisture buffering capacity \( HIR \) of the zone to the sorption curve of air and subsequently multiplying by the scale factor \( V_{\text{zone}}/V_{\text{al}} \). The resulting formula is given by equation (11). It is important the air layer has a sufficient volume (thickness), so no moisture content \( w_{al} \) larger than 1 m³/m³ is obtained.

\[ w_{al} = \left( RH \cdot p_{vi, sat} \frac{V_{\text{zone}}}{V_{\text{al}}} + RH \cdot 100 \cdot HIR \right) \]  

(11)

Finally, the vapour exchange between the air layer and the building component’s interior surface needs to be specified. Analogous to the heat exchange, the vapour flux between interior surface and BC must be equal to the vapour flux between interior surface and air layer, as stated by equation (12). This leads to equation (13) for the vapour permeability of the air layer \( \delta_{al} \). Again, the surface element’s resistance is neglected, due to its small thickness.

\[ g_v = \beta_i (p_{vesi} - p_{vi}) \equiv \frac{1}{\delta_{al}^2} \left( p_{vesi} - p_{vi} \right) \]  

(12)

\[ \delta_{al} = \beta_i \frac{d_{al}}{2} \]  

(13)

### 3.4.3 Comparison with EN 15028 and EN 13788

To compare the zone model indoor climate with EN 15026 and EN 13788 interior boundary conditions, a south oriented massive masonry wall with interior insulation is taken as example. The
meteorological data of Bremerhaven is used and inside, a kitchen with open floor plan is considered. Table 3-5 shows the zone model input parameter values. By way of comparison, two different ventilation rates are applied. In both cases, the ventilation rate is halved when the exterior temperature drops below 12°C and doubled when the interior temperature exceeds 23°C. The thermal and hygric inertia correspond to brick walls with plaster, a concrete floor slab with tiles and a wooden beam ceiling with plasterboard finishing (Vereecken et al., 2011). The hourly vapour production and interior heat gains are given in Figure 3-4.

### Table 3-5: Input parameters for the zone model and used values

<table>
<thead>
<tr>
<th>Input parameter</th>
<th>Input value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Room dimensions W x D x H [m]</td>
<td>6 x 10 x 2.5</td>
</tr>
<tr>
<td>Setpoint temperature 6-22h/22-6h [°C]</td>
<td>20/18</td>
</tr>
<tr>
<td>Window surface fraction [-]</td>
<td>0.3</td>
</tr>
<tr>
<td>g-value glass [-]</td>
<td>0.6</td>
</tr>
<tr>
<td>Ventilation rate [1/h]</td>
<td>0.5; 1</td>
</tr>
<tr>
<td>Number of persons [-]</td>
<td>2</td>
</tr>
<tr>
<td>Thermal inertia $M$ [J/m³K]</td>
<td>$187 \times 10^3$</td>
</tr>
<tr>
<td>Hygric inertia $HIR$ [kg/m³%RH]</td>
<td>0.737</td>
</tr>
</tbody>
</table>

**Figure 3-4:** (a) hourly vapour production; (b) hourly interior heat gains.
Figure 3-5: (a) daily mean interior temperature; (b) daily mean interior relative humidity.

Figure 3-6: (a) variation of the vapour excess with the monthly mean exterior temperature; (b) variation of the interior relative humidity with the daily mean exterior temperature.

Figure 3-5 shows the daily mean interior climate. As can be seen, the zone model temperature and relative humidity are subjected to more fluctuations. This can be attributed to the hourly calculation, in contrast to EN 15026, where daily averages are used. In Figure 3-6, the zone model climate is compared to the climate classes of EN 13788 and EN 15026; the agreement is quite well. Nevertheless, the same room with different parameter values (in this case, the ventilation rate) does not belong to the same climate class. The same building use can thus result in different humidity loads, depending on the used parameter values. This, in combination with more fluctuations, could lead to different hygrothermal risk predictions, compared to the EN 15026 or EN 13788 indoor climates; especially in case of thermal bridges and mould growth on the interior surface. However, this has not been investigated in the current study.

3.4.4 Discussion and conclusion

The current hygrothermal zone model has some limitations. Firstly, the heat balance is pre-calculated due to the variable heating load. As a consequence, the heat transmission through the
building component is estimated using its U-value, which ignores reduced thermal insulation due to an increased moisture content and all transient effects of the massive structure. Secondly, not all air layer and surface element thicknesses give accurate results. When the air layer is too small, the moisture retention curve might show moisture contents above 1 m³/m³; if the air layer is too large though, this can result in inaccurate fluxes as the air layer is not discretized. At the same time, if the surface element is too large, its resistance is no longer negligible and the calculated fluxes will again be less accurate. An air layer thickness of 100 mm and surface element thickness of 0.1 mm suffice in most cases. Thirdly, the zone model requires more input parameters in comparison with the European standards. When performing deterministic case-unspecific simulations, this might prove a difficulty. In such cases, it might be better to reach for the European standards. However, in case of a probabilistic assessment, a broader variety of interior climates can be obtained, which can lead to more reliable performance predictions. To conclude, when higher accuracy for the interior climate is required, this simplified zone model can be an adequate alternative to complex building energy simulation software.

3.5 Performance of interior insulation

3.5.1 1D wall

A probabilistic assessment is performed for a massive brick wall renovated with different interior insulation systems. The probabilistic methodology described in section 3.3 is applied; the same input and output parameters are used. Different wall thicknesses are considered, as well as different interior and exterior conditions. Four insulation systems are studied: (1) extruded polystyrene (XPS), (2) mineral wool with a vapour barrier, (3) calcium silicate, adhered to the brick wall with a 4 mm glue mortar, and (4) mineral wool with a smart vapour retarder. As an interior finishing layer, a 10 mm gypsum board is used, only the capillary active system (3) is rendered with a 10 mm plaster layer. For each insulation system, eight insulation thicknesses are considered: 1, 2, 4, 6, 10, 15, 20 and 30 cm. Hence, 33 options are analysed (4 interior insulation systems, with 8 possible thicknesses + uninsulated reference wall). This study limits to a 1D cross section of the wall, so no construction details such as corners or embedded wooden beam ends are modelled. Furthermore, the masonry wall is simplified to a single isotropic brick layer; no mortar joints are modelled. To exclude potential influence of starting conditions, the simulations are started on September 1st; data from these first four months is not used. After this initialization period, the simulations run for another three years. During these three years the temperature and relative humidity on the specified positions (see Figure 3-7 and section 3.3.2) are monitored. Additionally, the heat flux through the wall is monitored during the third year.

Figure 3-7: Vertical section of the 1D wall composition with positions of damage monitoring indicated
3.5.1.1 Heat loss

Figure 3-8 shows the total heat loss during the heating season in the third year, from October 1st to April 30th, as a function of the dry thermal resistance of the insulation systems. Due to its higher thermal conductivity, the capillary active system yields a lower dry thermal resistance than the other insulation systems of identical thicknesses. Moreover, the spread in total heat loss found for the walls with the capillary active system is much larger than found for the vapour tight insulation systems and outliers are much more probable for the former system. This large spread and presence of outliers for the capillary active system is due to the potential moisture accumulation in the insulation material. Hence, it can be concluded that the vapour tight systems perform most robust with respect to the thermal performance of the wall. Additionally, the spread in total heat loss decreases for all insulation systems as the insulation thickness increases. Note also that a thermal resistance above approximately 4 m²K/W does not further reduce the heat losses significantly, and thus is often not worth it – especially because it involves a reduction in floor area.

![Graph showing heat loss](image)

**Figure 3-8: Boxplot of the total heat loss during the heating season (Oct 1 – Apr 30), as a function of the dry thermal resistance of the insulation systems and the reference wall (in grey). The 75th percentile for XPS is plotted in black and, for comparison, repeated in the other panels in grey.**
The influence of the input parameters on the output distributions was determined based on an additional sensitivity analysis with scatter plots and Spearman’s rank correlation coefficients. To get a complete view on the influence of all input parameters, some of them were investigated in a combined form. The wind-driven rain load, for example, is a combination of the exterior climate, the orientation and the catch ratio factor. The influence of the masonry characteristics is analysed based on a combined parameter \( A_{\text{cap}}/(w_{\text{cap}} \cdot d_{\text{brick}}) \) as well, indicated as the moisture penetration factor (Vereecken et al., 2015). A larger capillary absorption coefficient \( A_{\text{cap}} \) (kg/m²s) facilitates the moisture uptake in the brick layer and the larger the capillary moisture content \( w_{\text{cap}} \) (kg/m²), the more moisture can be stored in the brick. Hence, the ratio of both characteristics \( A_{\text{cap}}/w_{\text{cap}} \) influences the inward movement of the moisture front. In addition, the time needed for the moisture to reach the warm side of the masonry wall depends on the masonry thickness \( d_{\text{brick}} \) (m). A high moisture penetration factor means a larger risk for the moisture to reach the warm side of the masonry. The masonry vapour diffusion thickness \( s_d \) (m) is a combination of the vapour permeability \( \mu \) and the masonry thickness \( d_{\text{brick}} \) (m). Other input parameters were investigated as well, but were less dominant and thus will not be discussed.
Figure 3-9: Scatter plot of the total heat loss as a function of the yearly rain load. For each insulation system (columns) and thickness (rows), the Spearman’s rank correlation coefficients $r_s$ are given.
Figure 3-10: Scatter plot of the total heat loss as a function of the moisture penetration factor. For each insulation system (columns) and thickness (rows), the Spearman’s rank correlation coefficients $r_s$ are given.
The sensitivity analysis showed the wind-driven rain load to have a significant influence on the heat loss in case of a capillary active insulation system, as shown in Figure 3-9. For the reference wall (in grey), a positive regression is found between the rain load and the total heat loss, though the correlation is rather small. For the capillary active system, a better correlation can be observed, while for the XPS and MW insulation systems the influence of the rain load is negligible. Indeed, the CaSi insulation system has the capacity to accumulate moisture, which is not the case for the vapour tight systems. Furthermore, the ease with which moisture is transported towards the warm side of the masonry is expected to influence the heat loss as well. The influence of the moisture penetration factor on the heat loss is shown in Figure 3-10. As expected, a positive regression is found, though less pronounced for the insulated walls. The larger correlation between the moisture penetration factor and the total heat loss for the reference wall is obvious since the thermal resistance of this wall assembly is solely obtained by the masonry. Similar, in case of smaller insulation thicknesses, the thermal resistance of the masonry wall (which is proportional to \(d_{brick}\)) will have a larger share in the total thermal resistance of the wall assembly.

Based these findings, it can be concluded that – regarding the heat loss – a capillary active insulation is more sensitive to wind-driven rain. This phenomenon is furthermore independent of the brick characteristics; even in case of a low moisture penetration factor (i.e. no fast moistening of the outer wall leaf), a high rain load could result in an extra heat loss. Thus, the thermal resistance of a capillary active insulation system can only be fully exploited on walls with a low wind-driven rain load.

### 3.5.1.2 Frost damage

As described in section 3.3.2, the frost damage is evaluated based on the amount of moist freeze-thaw cycles, shown in Figure 3-11. In case of a vapour tight insulation system, a larger number of moist freeze-thaw cycles than found for the reference wall might be induced. This is already the case when applying only 1 cm of insulation, but is especially notable with increasing insulation thickness. For the capillary active insulation system, this increase is much less pronounced. Note, however, that for all insulation systems and thicknesses, the median is still zero moist freeze-thaw cycles.

The influence of the rain load and the moisture penetration factor on the number of moist freeze-thaw cycles is visualised in Figure 3-12 and Figure 3-13. Whereas the graphs for the capillary active system shows a similar behaviour as observed for the reference wall, this is not the case for the walls with a vapour tight system. For the latter insulation systems, a high rain load clearly results in a larger number of moist freeze-thaw cycles. In addition, a negative correlation between the number of moist freeze-thaw cycles and the moisture penetration factor is found. The lower the value for \(A_{cap}/w_{cap}\), the less easily moisture is transported inward. Hence, more moisture is stored near the outer surface, which could induce more moist cycles. The Spearman’s rank correlation coefficients are however too small to draw definite conclusions.
Figure 3-11: Boxplot of the number of moist freeze-thaw cycles (\(w > 0.25w_{sat}\)) in the third year, as a function of the dry thermal resistance of the insulation systems and the reference wall (in grey).
Figure 3-12: Scatter plot of the number of moist freeze-thaw cycles as a function of the yearly rain load. For each insulation system (columns) and thickness (rows), the Spearman’s rank correlation coefficients \( r_s \) are given.
Figure 3-13: Scatter plot of the number of moist freeze-thaw cycles as a function of the moisture penetration factor. For each insulation system (columns) and thickness (rows), the Spearman’s rank correlation coefficients $r_s$ are given.
3.5.1.3 Mould growth on the interior surface

To estimate the mould growth risk on the interior surface, two performance indicators are evaluated in the third simulation year: the number of hours that the relative humidity on the interior surface exceeds 80% and the maximal Mould Index on the interior surface. In the VTT mould model, the interior surface was assumed to be ‘very sensitive’ to mould growth. Both performance indicators are shown in Figure 3-14 and Figure 3-15, as a function of the dry thermal resistance of the different insulation systems. For the walls with a vapour tight interior insulation system, the indoor surface relative humidity does not reach 80%, nor is the Mould Index of level 0 exceeded. Due to the high vapour resistance and the low liquid permeability of the vapour tight insulation system, the moisture stored in the masonry wall cannot be transported towards the indoor surface. In case of CaSi insulation, however, moisture in the masonry wall can be transported inwards. In some of the studied boundary conditions and for thinner insulation thicknesses, this result in an exceedance of the lower limit of relative humidity for mould growth. Though, note that for all insulation thicknesses, a lower mould growth risk is observed than for the reference wall.

![Figure 3-14: Dotplot with frequencies of the number of hours that the relative humidity on the interior surface exceeds 80% during the third simulation year, as a function of the dry thermal resistance of the different insulation systems. The grey lines connect the samples with identical boundary conditions. The black line indicates the 75th percentile of the distribution for each insulation system.](image)
Figure 3-15: Dotplot with frequencies of the maximal Mould Index on the interior surface during the third simulation year, as a function of the dry thermal resistance of the different insulation systems. The grey lines connect the samples with identical boundary conditions. The black line indicates the 75th percentile of the distribution for each insulation system.

Figure 3-16 and Figure 3-17 show the influence of the rain load and the moisture penetration factor on the maximal Mould Index. While the rain load seems to have a large impact for the reference wall and the capillary active insulation system, this is not the case for the vapour tight systems. Though, also for larger CaSi thicknesses this effect is less notable. The same tendency can be observed for the correlation with the moisture penetration factor. A high rain load, especially in combination with a high moisture penetration factor, might result in a high indoor surface relative humidity. Note, however, that the Mould Index for both the reference wall and the capillary active insulation system does not exceed level 2, which corresponds to mould growth still invisible to the naked eye (Viitanen et al. 2015). Furthermore, after applying a capillary active insulation system, mould growth was only found for boundary conditions that also caused mould growth on the reference wall; though, a higher indoor surface relative humidity or a longer period exposed to a high indoor surface relative humidity after applying the interior insulation is not impossible.
Figure 3-16: Scatter plot of the maximal Mould Index on the interior surface during the third year, as a function of the yearly rain load. For each insulation system (columns) and thickness (rows), the Spearman’s rank correlation coefficients $r_s$ are given.
Figure 3-17: Scatter plot of the maximal Mould Index on the interior surface during the third year, as a function of the moisture penetration factor. For each insulation system (columns) and thickness (rows), the Spearman’s rank correlation coefficients $r_s$ are given.
3.5.1.4  Mould growth between masonry and interior insulation

The number of hours that the relative humidity on the interface between the masonry wall and insulation system exceeds 80% and the maximal Mould Index on the interface during the third simulation year are shown in Figure 3-18 and Figure 3-19 respectively, as a function of the dry thermal resistance of the different insulation systems. When applying a vapour tight insulation system, it is clear that the moisture content at the interface increases strongly; due to the high vapour resistance and the low liquid permeability of the vapour tight insulation system, the moisture in the masonry wall can only dry out outwards. Note that the number of hours exceeding the critical relative humidity and the Mould Index increase most for the first centimetres of insulation, and stay almost constant above an R-value of approximately 2 m²K/W. A capillary active insulation system, on the other hand, is more vapour permeable and thus allows the moisture to dry out inwards. However, as the CaSi insulation thickness increases, the vapour permeability of the insulation decreases, and a higher moisture content at the interface is observed. Thus, the increased vapour resistance due to the larger insulation thickness becomes more notable. This effect is also shown in the moisture profiles described in section 3.5.1.6. For the reference wall, a relatively high number of hours are found for a number of cases, due to a high wind-driven rain load (see further), though the Mould Index remains below level 2 in all cases but one. Keep in mind that to calculate the Mould Index the sensitivity class ‘very sensitive’ was used (see section 3.3.2), which might overestimate the mould growth risk.

The influence of the rain load and the moisture penetration factor on the maximal Mould Index is shown in Figure 3-20 and Figure 3-21 respectively. The rain load is found to have an important effect on all wall assemblies, as indicated by the high Spearman’s rank correlation coefficients. For the moisture penetration factor a positive correlation is found as well, though the impact seems less distinct. For all insulation systems, a high Mould Index is possible even for a low moisture penetration factor.
Figure 3-18: Dotplot with frequencies of the number of hours that the relative humidity on the interface between masonry and interior insulation system exceeds 80% during the third simulation year, as a function of the dry thermal resistance. The grey lines connect the samples with identical boundary conditions. The black line indicates the 75th percentile of the distribution for each insulation system.
Figure 3-19: Dotplot with frequencies of the maximal Mould Index on the interface between masonry and interior insulation system during the third simulation year, as a function of the dry thermal resistance. The grey lines connect the samples with identical boundary conditions. The black line indicates the 75th percentile of the distribution for each insulation system.
Figure 3-20: Scatter plot of the maximal Mould Index on the interface between masonry and insulation during the third year, as a function of the yearly rain load. For each insulation system (columns) and thickness (rows), the Spearman’s rank correlation coefficients $r_s$ are given.
Figure 3-21: Scatter plot of the maximal Mould Index on the interface between masonry and insulation during the third year, as a function of the moisture penetration factor. For each insulation system (columns) and thickness (rows), the Spearman’s rank correlation coefficients $r_s$ are given.
3.5.1.5 Decay of wooden beam ends

The number of hours that the relative humidity in the brick at 5 cm from the interior brick surface exceeds 95% is shown in Figure 3-22. Additionally, the VTT wood decay model was used to calculate the wood mass loss of the wooden beam ends after the third simulation year, shown in Figure 3-23. For all wall assemblies, including the reference wall, a relative humidity higher than 95% during the whole year (8760 h) is possible, as is a 100% wood mass loss. This is important to keep in mind when interpreting the results for the insulated walls, as this indicates that the wood decay model is not very accurate. After applying an interior insulation system, the wood decay risk is found to increase, especially for the vapour tight systems. In addition, similar to the mould growth risk on the interface between masonry and insulation, the first centimetres of insulation induce the largest increase in wood decay risk; above an R-value of approximately 2 m²K/W, the risk does not increase much further. The capillary active insulation system, on the other hand, seems to perform more in line with the reference wall. A slight increase of the risk is noted for the first centimetres of insulation; only the larger insulation thicknesses result in a significantly higher risk, although still much lower than for the vapour tight insulation systems. Hence, this indicates that a vapour tight system is the most risky technique when wooden beam ends are present.

![Figure 3-22: Dotplot with frequencies of the number of hours that the relative humidity at the wooden beam ends exceeds 95% during the third simulation year, as a function of the dry thermal resistance. The grey lines connect the samples with identical boundary conditions. The black line indicates the 75th percentile of the distribution for each insulation system.](image-url)
Figure 3-23: Dotplot with frequencies of the wood mass loss of the wooden beam ends after the third simulation year, as a function of the dry thermal resistance. The grey lines connect the samples with identical boundary conditions. The black line indicates the 75th percentile of the distribution for each insulation system.

The rain load is found to have an important influence on the wood decay risk, as shown in Figure 3-24. A clear positive regression can be observed and high Spearman’s rank correlation coefficients are noted. Note however that a high wood mass loss might occur for a rather limited rain load as well, especially in case of a thicker vapour tight insulation. Though, similar to the mould growth risk at the interface between masonry wall and insulation the correlation with the moisture penetration factor is less clear (Figure 3-25). Although a positive regression is found, it is too small to draw definite conclusions.
Figure 3-24: Scatter plot of the wood mass loss at the wooden beam end after the third year, as a function of the yearly rain load. For each insulation system (columns) and thickness (rows), the Spearman’s rank correlation coefficients $r_s$ are given.
Figure 3-25: Scatter plot of the wood mass loss at the wooden beam end after the third year, as a function of the moisture penetration factor. For each insulation system (columns) and thickness (rows), the Spearman’s rank correlation coefficients $r_s$ are given.
3.5.1.6 Temperature, relative humidity and moisture content profiles

The temperature (T), relative humidity (RH) and moisture content (MC) profiles during the third simulation year of one sample are shown in Figure 3-26 and Figure 3-27, for the capillary active and XPS insulation respectively. It is apparent that the RH and MC profiles at the inner part of the brick wall are higher in case of a vapour tight insulation system. For the capillary active insulation system, the RH and MC are more in line with the findings for the reference wall. This can be accredited to the high vapour permeability of CaSi, which allows the wall to dry out inwards. Consequently, as shown in section 3.5.1.5, embedded wooden ends show less decay risk when a capillary active insulation system is applied. Nevertheless, a considerable rise in RH and MC is seen for larger CaSi insulation thicknesses. This suggests that the decreasing vapour permeability due to an increasing insulation thickness has a significant impact on the drying potential of the wall, resulting in a higher wood decay risk and mould growth risk on the interface between masonry and insulation. Figure 3-27 shows a similar tendency for the vapour tight insulation system, although less pronounced; since the high vapour resistance of 1 cm XPS already reduces the drying potential substantially, a further decrease in vapour permeability has a smaller relative impact. Furthermore, the RH and MC are found to decrease if the vapour resistance of the masonry wall is lowered to a value more in line with a brick-mortar composition ($\mu = 5$) (Hens, 2015), while keeping the other input parameters fixed. This is shown in Figure 3-28 and Figure 3-29. This results in a lower wood decay and mould growth risk for both insulation systems as well as for the uninsulated reference wall. Additionally, in case of the capillary active insulation, the influence of the insulation thickness is less apparent for higher masonry vapour permeability. This correlation of the masonry vapour permeability and damage risk was not clearly distinguishable in the sensitivity analysis. However, it is possible that other probabilistic characteristics and boundary conditions, such as the wind-driven rain load and the masonry liquid permeability, overshadowed the influence of the masonry vapour permeability. Regarding the moist-freeze thaw cycles, Figure 3-26 clearly shows that, in case of a capillary active insulation, the MC at the outer part of the wall only differs much from the reference wall for larger insulation thickness. This effect, in combination with a lower exterior surface temperature for larger insulation thickness, results in an increased number of moist freeze-thaw cycles for larger insulation thicknesses. In case of a vapour tight insulation system, a significant increase in MC is seen as soon as 1 cm of insulation is applied, due to the decreased drying potential. Hence, the critical saturated moisture content for frost damage will be exceeded more often. As a consequence, a vapour tight insulation results in a higher number of moist freeze-thaw cycles.
Figure 3-26: The average temperature, relative humidity and moisture profiles during January, April, July and October for one sample of calcium silicate insulation. The profiles of the reference wall are indicated in grey.
Figure 3-27: The average temperature, relative humidity and moisture profiles during January, April, July and October for one sample of XPS insulation. The profiles of the reference wall are indicated in grey.
Figure 3-28: The average temperature, relative humidity and moisture profiles during January, April, July and October for one sample of calcium silicate insulation with reduced masonry vapour resistance ($\mu = 5$). The profiles of the reference wall are indicated in grey.
Figure 3-29: The average temperature, relative humidity and moisture profiles during January, April, July and October for one sample of XPS insulation with reduced masonry vapour resistance ($\mu = 5$). The profiles of the reference wall are indicated in grey.
3.5.1.7 Discussion and conclusion

From the findings above, it is clear that applying any type of interior insulation might result in damage, even for a small insulation thickness. Vapour tight insulation systems were found to have a higher masonry moisture content and relative humidity, which lead to an increased number of moist freeze-thaw cycles, a higher risk for mould growth between the masonry and insulation system and a higher decay risk for wooden beam ends. In case of a capillary active insulation system, the results regarding frost damage, mould growth and wood decay were more in line with the uninsulated reference wall. Nevertheless, larger CaSi thicknesses resulted in an increased damage risk, due to an increasing vapour resistance. Some remarks need to be considered, though. First of all, a realistic input is of vital importance, as the output is determined by the input. Hence, caution is required when applying the current observations while dealing with other boundary conditions. The current results showed the significant impact of wind-driven rain on the performance of the interior insulation systems; hence, other conclusions might be possible for more dry climates. Furthermore, the current study contains some simplifications and assumptions. To start, no wooden beam ends were modelled, thus excluding potential air rotations around the beam ends which might result in a different moisture distribution. Secondly, the masonry was assumed a single isotropic brick layer, and the brick properties were considered representative for the masonry. However, results showed that a higher vapour permeability resulted in a significantly lower RH and MC, and consequently a lower wood decay risk. This stresses the importance of a correct characterisation of masonry walls. In order to obtain reliable results regarding the applicability of interior insulation, the influence of the masonry vapour permeability requires further investigation. To end, it should be noted that the used performance indicators do not give a quantitative analysis of the risk; this would require more accurate damage prediction models, which are currently not available.

To conclude, the current results show increasing hygrothermal damages for increasing thicknesses of insulation, already from the first centimetre onward. This implies that strict criteria are needed on how much mould growth, wood rot and frost damage is acceptable. However, given the (in)accuracy of the current damage prediction models, this may be a difficult definition. As already mentioned in section 3.3.2, the current results indicate that the predicted damages should perhaps not be dealt with in an absolute way, but rather in a relative way, compared to the uninsulated reference wall.
3.5.2 2D wall with embedded wooden beam ends

A first rudimentary 2D study has been performed, where the embedded wooden beam ends are modelled. Due to simulation time restrictions (one 2D simulation can take 1 to 48 hours to run), only the reference wall and XPS and CaSi insulation with 15 cm thickness were simulated. Note that full contact between the masonry and wooden beam end is assumed, thus imposing perfect capillary contact and excluding air rotations around the beam ends. Furthermore, only one type of wood (spruce) and one dimension (width of 6.5 cm, depth of 5 cm) were considered. Hence, these results can only give a rough indication of the differences between 1D and 2D conditions and should not be seen as true hygrothermal performance, nor can they serve as a guide to decision-making.

3.5.2.1 Heat loss

Figure 3-31 shows the heat loss through 1m² wall during the heating season (October 1st to April 30th) for the reference wall and the XPS and CaSi insulation systems. For comparison, the 1D results are included as well. For the reference wall and the capillary active insulation system, the impact of the wooden beam ends seems rather limited, while in case of the XPS system, the heat loss does increase. Indeed, as XPS has a lower thermal conductivity than CaSi, the relative increase in heat loss is bigger for the XPS insulation system. Though, the absolute difference between the 1D and 2D XPS situation is similar in magnitude as for the CaSi insulation system. Furthermore, a larger spread is observed for the 2D XPS situation, which might be caused the thermal bridge due to the wooden beam end and the moisture content in the wall: a higher moisture content will result in a higher heat loss via the wooden beam end.
3.5.2.2 Frost damage

The number of moist freeze-thaw cycles is shown in Figure 3-32. In case of the vapour tight insulation, slightly fewer moist freeze-thaw cycles are observed due to the somewhat higher heat loss. The impact is limited however, for the reference wall and the capillary active insulation system as well.
3.5.2.3 Mould growth on the interior surface

Figure 3-33 (left) shows the number of hours that the relative humidity on the interior surface exceeds 80%, Figure 3-33 (right) shows the maximal Mould Index on the interior surface during the third simulation year. These graphs indicate that around the wooden beam, a higher mould growth risk is observed than in the 1D situation, especially for the XPS insulation system. Due to a lower vapour resistance where the wooden beam pierces the vapour tight insulation, moisture stored in the wall can now more easily dry out inwards. This drying effect is magnified by the assumption of perfect capillary contact between the masonry and wooden beam end, as this allows liquid moisture transport via the wooden beam end; in absence of this capillary contact, moisture transport is only possible through diffusion. Due to the increased liquid moisture transport, a higher surface relative humidity around the wooden beam end is observed; in combination with a lower surface temperature due to the thermal bridge, this might result in mould growth for some of the boundary conditions.
3.5.2.4 Mould growth between masonry and interior insulation

The risk for mould growth on the interface between masonry and insulation in shown in Figure 3-34. In case of the reference wall and the capillary active insulation system, a small increase in risk is found. For the XPS insulation system, however, a decrease is found, although the risk is still higher compared to the reference wall and CaSi insulation system. The wooden beam piercing the vapour tight insulation results locally in a higher vapour permeability, as well as a higher liquid moisture transport due to the assumed capillary contact. Hence, the masonry wall can dry out inwards, more that in the 1D situation, resulting in a lower Mould Index. Though, note that for some boundary conditions a strong increase in mould growth risk is found, even if no or little mould growth was observed in the 1D situation. Possibly the increased interface temperature and relative humidity, allowing more mould activity, might be the cause of this, though this has not been investigated enough to draw definite conclusions.
Figure 3-34: Dotplot with frequencies of (left) the number of hours that the relative humidity on the interface between masonry and insulation exceeds 80% and (right) the maximal Mould Index on the interface between masonry and insulation, during the third simulation year, in the 1D and 2D situation. The grey lines connect the samples with identical boundary conditions. The black asterisk indicates the 75th percentile of the distribution.

3.5.2.5 Decay of wooden beam ends

Figure 3-35 (left) shows the number of hours that the relative humidity at the wooden beam ends exceeds 95%. Figure 3-35 (right) shows the wood mass loss after the third simulation year. Here, a lower wood decay risk is found for all wall assemblies. Although, in some cases a higher decay risk is found than in the 1D situation. Again, a lower vapour resistance at the wooden beam allows the masonry wall to dry out more inwards, thus a lower wood decay risk is observed. Keep in mind, however, that a perfect contact between masonry and wooden beam end was assumed, thus excluding air rotations around the beam ends, which might result in a different moisture distribution. Furthermore, the assumed capillary contact allows a significantly higher moisture transport from the masonry into the wooden beam end, evidently resulting in a higher relative humidity and thus wood mass loss.
Figure 3.5: Dotplot with frequencies of (left) the number of hours that the relative humidity at the wooden beam ends exceeds 95% and (right) the wood mass loss, during the third simulation year, in the 1D and 2D situation. The grey lines connect the samples with identical boundary conditions. The black asterisk indicates the 75th percentile of the distribution.

### 3.5.2.6 Conclusion

This rudimentary 2D study showed that the 2D damage predictions can differ significantly from the 1D simulations. Though, due to the number of assumptions and simplifications in this preliminary analysis, a further in-depth study is required, in order to draw definite conclusions on whether an interior insulation system performs within acceptable damage limits or not when wooden beam ends are present.

### 3.6 Conclusion

In this section, the description and the application of the probabilistic assessment of the hygrothermal performances of interior insulation solutions is presented. Initially, the overall probabilistic approach has been explained, with focus on the multi-level sampling scheme that is applied. The coupling with the Delphin simulation environment has been established via a Matlab...
code, automating the sampling of the input parameters, the simulation of the different cases, and the post-processing of the outputs. As the variability of the indoor climate is a critical aspect, a Delphin-integrated interior-environment model has been developed as well. To end, the outcomes from exemplary interior insulation studies have been discussed.

These outcomes should be interpreted with care, as they are not representative for the whole spectrum of internal insulation applications. First and foremost, the basic configuration is an unrendered brick masonry wall, which hence easily absorbs all incoming wind-driven rain. Configurations with paint or render may react strongly differently to the application of internal insulation. Moreover, the taken distributions for the different probabilistic parameters are restricted, given that only 3 brick types and 3 climate sets have been used, as well as approximations for many other parameters.

However, some important lessons can be taken away from these exemplary interior insulation studies: it was shown there that the rain load has a strong impact on the result of the performance assessment, that multi-dimensional simulations lead to other outcomes than one-dimensional simulations, and that the damage criteria also result in significant potential damage for the reference construction (without internal insulation). These observations are to be taken into account in the overall interior insulation performance assessment in RIBuild’s WP6.
3.7 References


4 Sequential sampling for probabilistic analysis

(Tianfeng Hou, KUL)

4.1 General Information

The research on sequential sampling was carried out by Tianfeng Hou, who started in October 2015 as a Ph.D student at KU Leuven. In this section, a brief overview of the progress of his work will be provided. First, a literature review about the sequential sampling based on quasi-Monte Carlo methods and the framework of probabilistic analysis of building performance was conducted, which took about 4 months. Next, in order to obtain a deeper understanding of the fundamental properties and practical applications of different quasi-Monte Carlo methods, a case study based on simple numerical functions was performed, on which roughly 4 months were spent, including implementing different quasi-Monte Carlo sequences and their related randomization strategies. In this part of the research, different quasi-Monte Carlo sequences were compared, with respect to their sampling efficiency and the accuracy of their error estimation strategies. At the end of this interval, an internal report has been compiled. In addition, in order to investigate the performance of quasi-Monte Carlo methods with respect to the applications in building physics, a case study of the heat loss through a masonry wall was performed, which required some 5 months. In this case study, the distribution of heat loss was quantified by estimating its mean and standard deviation. The sampling efficiency and the accuracy of related error estimation techniques of different sampling strategies were compared. A paper about using quasi-Monte Carlo based probabilistic assessment of wall heat loss was accepted by the 11th Nordic Symposium on Building Physics. Consequently, complementary to the thermal analysis, a hygrothermal analysis with four outputs and seven input parameters was performed, and for which roughly 3 months were invested. Furthermore, in order to illustrate the potential factors which may degrade the performance of quasi-Monte Carlo methods, a Gaussian kernel smoother analysis for our hygrothermal case study was proposed, in which some 2 months were invested. At last, besides of the sequential sampling, some activities related to improving calculation efficiency through model order reduction have been performed, including a literature study on proper orthogonal decomposition and proper generalized decomposition, and a case study of using proper orthogonal decomposition for solving the heat transport equation. These activities took approximately 4 months, however, since this is not part of the current deliverable, it will not be discussed here.

In this report, first a general introduction of sequential sampling for probabilistic analysis is put forward, followed by the sampling strategies with focus on potential problems that they may bring in (Section 4.2). Subsequently, to firstly discuss which factors may influence the sampling efficiency of quasi-Monte Carlo methods, two simple numerical test functions with different number of dimensions and different order of smoothness are put forward as mathematical case study (Section 4.3). Next, the hygrothermal calculation object and the use of quasi-Monte Carlo for uncertainty analysis based on two building physical case studies will be proposed (Section 4.4). In the first part of this section, the sampling efficiency of these sequential sampling methods is investigated (Section 4.4.2), and a conclusion of which sampling scheme has the highest efficiency is provided. Subsequently, to study the potential factors which may degrade the performance of quasi-Monte Carlo methods, a Gaussian Kernel smoother analysis is proposed (Section 4.4.3). Finally, the accuracy of the error estimation method is investigated (Section 4.4.4), culminating in conclusions on the optimal sequential sampling scheme (Section 4.5).
4.2 Introduction

The use of numerical simulations for hygrothermal performance assessment is becoming progressively more common. However, since significant uncertainties exist for most input variables, a stochastic approach providing a probability distribution of the outputs is of crucial importance. In building physics, a variety of probabilistic modelling approaches for uncertainty propagation hence have been developed over the last decades (Hokoi and Matsumoto, 1988). Among them, sampling-based uncertainty propagation through Monte-Carlo approaches is the most versatile and widely used, because of its general applicability and typical robustness (Janssen, 2013). The essential idea of this method is to repeat execution of a deterministic core simulation with randomly selected values of the input parameters, in order to obtain the probability distribution of the targeted outputs. However, in cases where that deterministic core simulation is (relatively) time consuming, the number of needed repetitions should be minimized. In that respect, three criteria are crucial. Firstly the sampling scheme should be as efficient as possible, which can be described as using a minimal number of runs to obtain a desired accuracy level. Based on the work of (Niederreiter, 1978), a sampling scheme with a greater uniformity of its sampling points will have a faster rate of convergence and is hence considered to be more efficient. Secondly, monitoring sampling convergence should be possible, in other words, estimation of the accuracy of the result should be feasible. Such error estimation allows terminating the Monte Carlo analysis when a desired accuracy has been reached. And thirdly, sequential additions of single samples should be possible, because it guarantees a maximal reduction of the computational expense of the Monte Carlo analysis. By doing so, a desired accuracy of the outcomes can be reached with a truly minimal number of repetitions.

The current state of the art in building physics in that respect is replicated optimized Latin hypercube sampling (Janssen, 2013), wherein smaller sub-designs are sequentially added to reach the desired number of runs n, instead of using a single n-run optimized Latin hypercube design. In addition, each of these sub-designs is an optimized Latin hypercube design, which takes a Latin hypercube sampling as the initial design, and then iteratively optimizes the location of sample points by using the enhanced stochastic evolutionary algorithm (Husslage, et al). Due to the superiority of optimized Latin hypercube sampling over standard Monte Carlo and Latin hypercube sampling (Janssen, 2013), the sampling efficiency of the replicated optimized Latin hypercube sampling is thus guaranteed. Moreover, the replicated designs allow estimating the error of Monte Carlo analysis, since the standard error of these sub-designs can be obtained by applying the ‘sample splitting’ bootstrap method (Janssen, 2013).

This approach satisfies the first two criteria, but is not wholly in line with the third demand, as blocks of samples, instead of single samples, are sequentially added. And more critically, the main drawback of this method is that correlations may exist between the smaller sub-designs, given that each small sub-design is optimized via the same algorithm. These correlations may in turn lead to a bias for the error estimation as well as to a decline of the sampling convergence rate.

Instead of the replicated optimized Latin hypercube sampling, quasi-Monte Carlo methods (or QMC methods in short), which are typically constructed based on low-discrepancy sequences, can also be used for efficient uncertainty propagation. There are two main families of QMC methods: lattice rules and digital nets, which represent different approaches to achieve uniformity of the points. We will use both lattice rules and digital nets to construct quasi-Monte Carlo sampling schemes for uncertainty propagation, exemplified through mathematical and building physical case studies.
4.2.1 Sampling strategies and randomization

In this report, a Monte-Carlo-based uncertainty analysis is applied for propagating the variations of the input to the variations of the output. Standard Monte Carlo methods use pseudo-random sequences of size \( n \) to quantify the probability distribution of the target outcomes, which typically provide a convergence rate of \( O(n^{-1/2}) \) (Glasserman, 2013). In contrast, quasi-random sequences are constructed with quasi-Monte Carlo methods, which can offer a better uniformity than the random sequence, resultant uniformly covering the domain of interest more quickly, and thus yielding a convergence rate of \( O((\log n)^d/n) \) for functions with sufficient smoothness (Glasserman, 2013). As mentioned before, there are two main families of quasi-Monte Carlo methods: lattice rules and digital nets, which are constructed by different approaches to achieve the desired uniformity of the points. More details on lattice rules and digital nets can be found in (Dick and Pillichshammer, 2010). Before we move to using quasi-Monte Carlo methods for building physical applications, it is important to mention three crucial challenges of quasi-Monte Carlo as well as to explain how these difficulties can be overcome.

First, contrary to standard Monte Carlo, which uses independent random samples to estimate the probability distribution of the target outcomes, quasi-Monte Carlo methods apply deterministic quasi-random sequences. Thus, the conventional error estimation method based on the central limit theory is not valid for quasi-Monte Carlo methods (Snyder, 2000). Secondly, in order to have quasi-Monte Carlo outperform standard Monte Carlo with respect to sampling efficiency, \( O((\log n)^d/n) \) needs to be smaller than \( O(n^{-1/2}) \). Hence, \( d \) should be relatively small and \( n \) should be relatively large (Caflisch, 1998). Thirdly, quasi-Monte Carlo methods are found to lose efficiency when the deterministic core simulation does not behave smoothly (Moskowitz and Caflisch, 1996).

To overcome the first challenge, randomization techniques can be applied to get multiple independent quasi-random sequences, and in this way confidence intervals for the results can be constructed based on the standard error. An overview of different randomization techniques for quasi-Monte Carlo integration can be found in (L’Ecuyer and Lemieux, 2005). With respect to the second challenge, (Van Gelder, 2014) shows that in many building physical engineering problems, even though the number of the total input parameters may be large, the number of effective parameters is usually fairly small. And based on (Wang and Fang, 2003), for low-effective-dimension problems, the randomized quasi-Monte Carlo sequences can still perform much better than standard Monte Carlo, even for large \( d \). For the third challenge, a limited smoothness commonly occurs in building physical simulation, as discrete parameters (such as different materials and climates) are often involved, which may introduce discontinuity in the behavior of the
core simulation. However, in this analysis, we actually found that the even though discrete parameters are included in the analysis, quasi-Monte Carlo methods can still outperform the standard Monte Carlo method, as long as these discrete parameters do not dominantly impact the uncertainty analysis.

Apart from optimized Latin hypercube designs, three other quasi-random sequences – Sobol (Sobol’, 1967), Niederreiter-Xing (Xing and Niederreiter, 1995) and Good Lattice (Sloan and Joe, 1994) – are applied and compared. Here, the Sobol and Niederreiter-Xing sequences are examples of digital nets, while the Good Lattice sequence is constructed by lattice rules. For randomization, the Sobol sequence applies a random linear scramble combined with a random digital shift (Matoušek, 1998). On the other hand, the Good Lattice and Niederreiter-Xing sequences are randomized through Cranley-Patterson shifting (Cranley and Patterson, 1976) and digital shifting (L’Ecuyer and Lemieux, 2005), respectively. Moreover, all three low-discrepancy sequences are in base 2, and the Good Lattice sequence applied here has been optimized for an unanchored Sobolev space for up to \(2^{13}\) points.

### 4.2.1.1 Sampling strategies

**Lattice points**

The construction of Lattice rules has been introduced by (Korobov, 1959, 1960) and (Hlawka, 1962), and the core idea is to use a generating vector to obtain a set of points that are uniformly distributed over the \(d\)-dimensional domain. A rank-1 lattice rule with \(n\) sampling points takes the form:

\[
Q_n(f) = \frac{1}{n} \sum_{k=0}^{n-1} f\left(\frac{k\mathbf{z}}{n}\right) = \frac{1}{n} \sum_{k=0}^{n-1} f\left(\frac{kn \mod n}{n}\right)
\]  

(1)

The integer vector \(\mathbf{z} = (z_1, ..., z_s)\) is the generating vector and the braces around the vector indicate that we take the fractional parts of each component in the vector. For theoretical analysis we often assume that \(n\) is prime to simplify some number theory arguments. For practical application we often take \(n\) to be a power of 2. The total number of possible choices for the generating vector is then \((n-1)^s\) and \((n/2)^s\), respectively (Kuo and Nuyens, 2016). The quality of the lattice rule depends on the choice of the generating vector. Even if we have a criterion to assess the quality of the generating vectors, there are simply too many choices to carry out an exhaustive search for large \(n\) and \(s\). And thus, computable criteria for assessing the quality of the generating vector as well as algorithms for selecting an optimal generating vector efficiently tend to be of critical importance in this field.

In order to assess the quality of the generating vector, we firstly presume that the target function has certain properties. Thus, the quality of the generating vector can be assessed by analyzing the error of the approximation of a lattice rule with respect to the worst possible function satisfying the assumed properties (Nuyens, 2014). Additionally, a fast algorithm for selecting the optimal generating vector based on the worst-case error criteria has been proposed by Nuyens and Cools (2006).
Lattice sequences

A lattice with a fixed number of \( n \) points can be generated by using the generating vector \( z \):

\[
t_k = \left\{ \frac{kz}{n} \right\}
\]  

(2)

This formula contains the parameter \( n \), which indicates that in order to generate the points, we should know \( n \) in advance. However, this is inconvenient in practice, since it is not extensible, we have to generate all of the points from scratch, in order to change the number of points. On the contrary, an extensible lattice sequence (in base 2) which allows to sequentially add points while keeping all existing points can be obtained if equation (2) is replaced by

\[
t_k = \left\{ \psi_2(k)z \right\}
\]  

(3)

here \( \psi_2(\cdot) \) is the radical inverse function in base 2: loosely speaking, if we have the index \( k = (\cdots k_2 k_1 k_0)_2 \) in binary representation, then \( \psi_2(k) = (0.k_0 k_1 k_2 \cdots)_2 \) is obtained by mirroring the bits of \( k \) around the binary point. For example, if \( k = 6 = (110)_2 \) then \( \psi_2(k) = (0.011)_2 = 0.375 \). Comparing with equation (2), it is evident that equation (3) does not contain the parameter \( n \), and hence \( n \) does not need to be known in advance. In practice, by using formula (3), more lattice points can be added to the Monte Carlo simulation until it reaches the desired accuracy.

Digital nets

“Loosely speaking, the general principle of digital nets is all about getting the same number of points in various allowable sub-divisions of the unit hypercube” (Kuo and Nuyens, 2016). This property can be generalized by introducing the \((t, m, s)\) net and the \((t, s)\) sequence (Dick and Pillichshammer, 2010). First, the sub-divisions of the \( s \)-dimensional unit hypercube in base 2 can be described by the definition of a binary box,

\[
\prod_{i=1}^{s} \left[ \frac{a_i}{2^j}, \frac{a_{i+1}}{2^j} \right).
\]  

(4)

With \( j_i \in \{0,1,\ldots\} \) and \( a_i \in \{0,1,\ldots 2^{j_i} - 1\} \). Next, let \( j = j_1 + \cdots + j_s \), where \( j_i \) are non-negative integers as mentioned before. Therefore, the \( 2^{j_i} \) binary boxes can be obtained by partitioning \([0,1]^s\) into \( 2^{j_i} \) slices of equal width along the \( i \)-th axis. And thus, the volume of a binary box is \( 1/2^{j_i} \). Moreover, for integers \( 0 \leq t \leq m \), a \((t, m, s)\) net in base 2 can be defined as a set of \( 2^m \) points in \([0,1]^s\), such that each binary box contains exactly \( 2^t \) points within the volume \( 2^{j-m} \). Furthermore, a sequence in base 2 is a \((t, s)\) sequence if for all \( m > t \), each consecutive block of \( 2^m \) points \( \{x_i: j2^m \leq i \leq (j+1)2^m\} \) is a \((t, m, s)\) net.

In addition, it is evident that, the quality of \((t, m, s)\) nets can be concluded from the parameter called “\(t\)-value”, as with smaller \( t \), each binary box will have a smaller volume. Hence, the finer we can sub-divide the unit cube the more uniformly the digital nets are distributed. Figure 4-1 shows an example of a \((0, 4, 2)\) net in base 2. The figure illustrates examples of dividing the unit cube into 16 rectangles, and each rectangle contains one point.
Digital construction

In the construction of lattice points and sequences, a set of generating vectors (one vector per dimension) is required. To construct a digital net on the other hand, a set of generating matrices $C_1, \ldots, C_s$ (one matrix per dimension) are needed.

Here, we are going to illustrate how it works in base 2. Suppose we want to obtain $2^m$ points, then the $j$th component of the $k$th point can be generated through three steps: First, we transfer $k$ in binary representation: $k=(k_{m-1}, \ldots, k_1, k_0)_2$. Next, take the $m \times m$ binary matrix $C_j$ for dimension $j$, and compute

$$
\begin{pmatrix}
  y_1 \\
  y_2 \\
  \vdots \\
  y_m
\end{pmatrix}
= C_j
\begin{pmatrix}
  k_0 \\
  k_1 \\
  \vdots \\
  k_{m-1}
\end{pmatrix}

$$

where all additions and multiplications are carried out modulo 2. At last, $P_{jk} = \psi_2(y) = (0.y_1 y_2 \cdots y_m)_2$ is taken as the $j$th component of the $k$th point. Here, $\psi_2(\cdot)$ is the radical inverse function in base 2.

Recall that the quality of a lattice rule is determined by the choice of the generating vector. The quality of a digital net is determined by the choice of generating matrices. The goal is thus to choose the generating matrices so that the corresponding $t$-value of the net is as small as possible. However, constructing good generating matrices can be a difficult task, and will hence not discuss here. We refer the reader to several explicit constructions of digital nets instead. The most well-known is the Sobol’ (1967) sequence, which is a popular example of $(t, s)$ sequences in base 2, with its $t$-value related to the dimension $s$. Alternatively, there is the Faure sequence, introduced by Faure.
(1982) and generalized by Tezuka(1995). It is a (0,s) sequence, which indicates its t-value has the best possible value. However, its base need to be at least as large as the dimension. Additionally, the Niederreiter-Xing sequence has been proposed by Xing and Niederreiter (1995). It is constructed by optimizing the asymptotic behavior of their t-value as a function of the dimension. In this report, the Sobol’ and Niederreiter-Xing sequences are applied and compared.

4.2.1.2 Randomization for error estimation

In the previous section, we have discussed that using a low-discrepancy sequence rather than pseudo-random samples can improve the sampling efficiency. Moreover, in order to terminate the simulations when sufficient accuracy has been reached, an error estimation method needs to be provided. Contrary to the standard Monte Carlo method, the conventional error estimation method based on central limit theory is not valid for the quasi-Monte Carlo method. Instead, one can randomize the initial low-discrepancy sequence by implementing related randomization techniques, and repeat the procedure r times, so that 1) each of the randomized sequence preserves the low-discrepancy property, and 2) each of the randomized sequence is independent. Resultantly, the standard error of these independent approximations can be derived:

\[
\theta = \sqrt{E[1(f) - \bar{Q}_{n,r}(f)]^2} \approx \sqrt{\frac{1}{r(r-1)} \sum_{i=1}^{r} (Q^{(i)}_n(f) - \bar{Q}_{n,r}(f))^2}
\]  

where,

\[
\bar{Q}_{n,r}(f) = \frac{1}{r} \sum_{i=1}^{r} Q^{(i)}_n(f)
\]

Here, the expectation is taken with respect to the random shifts. The mean of all the independent approximations is taken as our final approximation to the target function, see equation 7. Next, based on the Chebyshev inequality, a 75% confidence interval can be obtained by using \(\bar{Q}_{n,r}(f) \pm 2 \theta\). In the later hygrothermal case studies, we simply take \(2 \theta\) as our error indicator. Since digital nets and lattices need different kinds of randomization strategies to preserve the digital net property and lattice structure, four randomization techniques are described in detail below.

Random shift modulo 1

The following mechanism was first proposed by Cranley and Patterson (1976) for lattice rules, but it can also be implemented for other low-discrepancy point sets (Tuffin, 1996; Morohosi and Fushimi, 2000). Recall the initial lattice set is formula (2). The shifted lattice set can be obtained by adding a vector of real numbers \(\Delta = (\Delta_1, \ldots, \Delta_s)\), and here we restrict \(\Delta\) to be an s-dimensional random vector uniformly distributed over [0,1]. Thus, the shifted lattice rule becomes

\[
Q_n(f) = \frac{1}{n} \sum_{z=0}^{n-1} f\left(\left\{\frac{kz}{n} + \Delta\right\}\right)
\]
**Digital binary shift**

Contrary to Cranley-Patterson shifting for lattice rules, we need a different kind of randomization to preserve the digital net property. One strategy is to use a digital binary shift: instead of adding a vector of real numbers $\Delta$, we take the binary expansion of $\Delta$ and add it to each point of the digital net.

More specifically, let $\Delta = (\Delta_1, \ldots, \Delta_n)$ and for the $j^{th}$ dimension of the $k^{th}$ point $x_{kj}$, the randomized point is

$$\left( x_{kj} \right)_2 + \left( \Delta_j \right)_2$$

where $(\cdot)_2$ is the operator of the binary expansion.

**Scrambling**

Scrambling is originally proposed by Owen (1995), and it is a more sophisticated randomization mechanism. Besides preserving the $t$-value of a digital net, it can also improve the convergence rate of digital nets by an extra factor of $n^{-1/2}$ for sufficiently smooth functions.

Conceptually, for an $s$-dimensional digital net in base 2, let $x_{ij}$ be the $i^{th}$ point of dimension $j$. In order to scramble $x_{ij}$, we apply a permutation to each digit of its binary expansion. To make it more concrete, suppose $x_{ij}$ has a binary representation $(0, a_1 a_2 a_3 \cdots)_2$. Each coefficient $a_i$ is mapped by $\pi$ and the procedure is as follows:

$$a_1 = \pi_0(a_1),$$

$$a_2 = \pi_{a_1}(a_2),$$

$$a_3 = \pi_{a_1a_2}(a_3),$$

$$\cdots$$

$$a_k = \pi_{a_1a_2\ldots a_{k-1}}(a_k),$$

Here, $\pi$ is a random permutation which is uniformly distributed over $2!$ permutations of $[0, 1]$, and the permutations are mutually independent. More precisely, except $\pi_0$, the permutation applied to the $k^{th}$ digit depends on the first $k-1$ digits.

Owen (1995), gives the following geometrical description of scrambling, in each dimension $j=1, \ldots, s$, we divide the unit interval into two subintervals of length $1/2$, and swap them randomly. Next, we divide each subintervals into two equal parts of length $1/2^2$, taking them as two groups of two consecutive parts, and swap the two parts within each group randomly, etc. At the $k^{th}$ step, the unit interval is divided into $2^k$ equal parts, taking them as $2^{k-1}$ groups of two consecutive parts, and swap two parts within each group randomly. Therefore, an $s$-dimensional digital net can be scrambled by applying this procedure to each dimension. However, this method requires a large number of permutations and consequently increases the use of memory and expense of calculation time.
Linear permutation of digit

In order to reduce the memory storage and calculation expense, an alternative scrambling method was proposed by Matoušek (1998). Contrary to Owen scrambling, instead of mapping each digit by a permutation of \([0,1]\), the binary expansion of \(x_{ij} = (0.\bar{a}_1\bar{a}_2a_3 \cdots)_2\), can be mapped to \((0.\bar{a}_1\bar{a}_2\bar{a}_3 \cdots)_2\) by taking the form

\[
\tilde{a}_j = \sum_{i=1}^j h_{ij} a_i + g_i \mod 2
\]

Here, \(h_{ij}\) and \(g_i\) are chosen randomly, independently, and uniformly from \([0,1]\) and the \(h_{ii}\) need to be positive.

4.3 Mathematical case study

In order to discuss what factors can influence the convergence rate of the QMC estimation and how accurate the error can be estimated by implementing randomization techniques, a mathematical case study investigates two test functions:

\[
f_1(x) = \prod_{j=1}^d (1 + (x_j^2 - x_j + \frac{1}{6}))
\]

\[
f_2(x) = \prod_{j=1}^d (1 + (x_j^6 - 3x_j^5 + \frac{5}{2}x_j^4 - \frac{1}{2}x_j^2 + \frac{1}{42}))
\]

Both of the functions integrate to 1 over \([0, 1]^d\). In order to investigate how the number of dimensions affects the convergence behavior, each function is considered in 5 and 15 dimensions. Moreover, function \(f_1(x)\) is a product of \(1 + B_2\), \(f_2(x)\) is a product of \(1 + B_6\), where \(B_2\) and \(B_6\) are degree 2 and 6 Bernoulli polynomials, respectively. From their Fourier expansions we expect 1 order of smoothness for \(f_1(x)\) and three orders of smoothness for \(f_2(x)\).

In this simple mathematical case study, besides the standard Monte Carlo (MC), three low-discrepancy sequences: Sobol' sequence (Sobol'), Good Lattice sequence (GLP) and Niederreiter-Xing sequence (NX) are studied. With respect to optimized Latin Hypercube design, since generating such design is, contrary to digital nets and Lattice sequences, a daunting task: The generation cost increasing exponentially with the size of the sampling design (Janssen, 2013). And, in this simple mathematical case study, since a large number of samples need to be evaluated, optimized Latin Hypercube design is thus not included, and it will be compared with the other quasi-Monte Carlo designs in Section 4.4. For randomization, Sobol' uses a random linear scramble combined with a random digital shift. On the other hand, the Good Lattice sequence and Niederreiter-Xing sequence are randomized by Cranley-Patterson shifting and digital shifting respectively. In this report all the digital nets and lattice sequences are randomized schemes.
4.3.1 Sampling efficiency

The sampling efficiency can be described as the number of repetitions of the core simulation required in order to reach a target accuracy. This section assesses the sampling efficiency of the four sampling schemes by comparing their exact errors. And the exact error is calculated by taking the difference between the analytical solution 1 and the (quasi) Monte Carlo approximation. Moreover, three factors are investigated: the format of the sample sizes, the order of smoothness and the number of dimensions of their integrands, all of which may affect the sampling efficiency. As mentioned in section 4.2.1.2, contrary to standard Monte Carlo, the evaluation of a single quasi-Monte Carlo sequence yields a deterministic result, and there is thus no standard error output on the estimator. Hence, multiple quasi-Monte Carlo sequences need to be created and the mean of these independent quasi-Monte Carlo evaluations, formula (7), is taken as the final approximation. Hence, the total number of function evaluations for quasi-Monte Carlo is \( r \cdot n_{\text{QMC}} \). In this mathematical case study, we take \( r = 10 \) to get a relatively robust error estimation, and \( n_{\text{QMC}} \in [2^3, \ldots, 2^{14}] \) to obtain a relatively large overview of the convergence behavior of different sampling schemes. In order to make a fair comparison with the standard Monte Carlo sampling, we should therefore take the number of samples in the standard Monte Carlo method \( n_{\text{MC}} = r \cdot n_{\text{QMC}} \), and hence \( n_{\text{MC}} \in 10 \cdot [2^3, \ldots, 2^{14}] \). On the contrary, the convergence behavior of these four sampling schemes which their sample sizes are not in the format of powers of 2 are compared. In addition, for obtaining the variances of the convergence behavior of each scheme, a box plot containing 100 independent replications is made for each of these 12 sample sizes. The comparison of the results is shown in Figure 4-2 and Figure 4-3.
Figure 4-2: Convergence behavior of all the sampling schemes (Sobol, GLP, NX, and MC sequence) for \(f_1(x)\) and \(f_2(x)\) (named smooth function, non-smooth function, respectively) in both 5 and 15 dimensions. The sample sizes of all the sampling schemes are in powers of 2.
To obtain a clear comparison of all the four schemes, the exact error in Figure 4-2 and Figure 4-3 is plotted in a range from $10^{-10}$ to $10^1$. As a result, part of the information for the Good Lattice sequence in the first graph of Figure 4-2 is missing, which demonstrated that in this figure, the exact error of the Good Lattice sequence after 512 runs is smaller than $10^{-10}$. Comparing all the sampling schemes of Figure 4-2 and Figure 4-3, it is shown that the sampling efficiency of all the sampling schemes decreases as the number of their dimensions increases and as the order of the smoothness of their integrands reduces. Moreover, Figure 4-2 and Figure 4-3 also illustrate that, the sampling efficiency of the Good Lattice sequence and Niederreiter-Xing sequence is strongly influenced by these two factors. In addition, the sampling efficiency of these two sampling strategies with sample sizes in powers of 2 is higher than their sample sizes without the format of powers of 2. However, this improvement becomes smaller for high dimension and less smooth integrands. On the other hand, for standard Monte Carlo and Sobol’ sequence, the sampling efficiency cannot be significantly improved when its integrands have higher order of smoothness or when sample sizes with the format of power 2 are used. It is also illustrated that, the sampling efficiency of Good Lattice sequence is almost always higher than standard Monte Carlo, Sobol’ sequence and Niederreiter-Xing sequence. This advantage becomes more pronounced when the samples sizes are in powers of 2.

*Figure 4-3: Convergence behavior of all the sampling schemes (Sobol, GLP, NX, and MC sequence) for $f_1(x)$ and $f_3(x)$ (named smooth function, non-smooth function, respectively) in both 5 and 15 dimensions. The sample sizes of all the sampling schemes are not in powers of 2.*
4.3.2 Error estimation

The previous section demonstrated that the sampling efficiency of Good Lattice sequence is better than Niederreiter-Xing sequence and Sobol’ sequence. When the integrand has limited degree of smoothness and high dimensionality and the sample sizes not in powers of 2, the performance of Sobol’ sequence and Good Lattice sequence become very close (Fig 4-3). Hence, in this section, the error estimation for Good Lattice sequence and Sobol’ sequence with samples sizes not in powers of 2 are studied and compared. And in order to assess the accuracy of the error estimation method, the exact error is compared with the estimated error. In Figure 4-4 and Figure 4-5, both the exact and estimated error of Sobol’ sequence and Good Lattice sequence are evaluated for f₁(x) and f₂(x) (named non smooth function and smooth function, respectively) in both 5 and 15 dimensions. For the estimated error, we simply take the standard error of these 10 (Section 4.3.1) independent randomized quasi-Monte Carlo approximations, as the error indicator (see formula (6)). Moreover, as mentioned in section 4.3.1, the exact error is calculated by taking the difference between the analytical solution and the mean of the 10 independent randomized quasi Monte Carlo approximation, see formula (7). Furthermore, for obtaining the variances of the convergence behavior of each scheme, a box plot contains 100 independent replications is made for each of these 12 sample sizes.

![Figure 4-4: Exact and estimated error of Sobol sequence for f₁(x) and f₂(x) (named smooth function and non-smooth function, respectively) in both 5 and 15 dimensions.](image-url)
Figure 4-5: Exact and estimated error of GLP sequence for $f_1(x)$ and $f_2(x)$ (named smooth function and non-smooth function, respectively) in both 5 and 15 dimensions.

Figure 4-4 and Figure 4-5 illustrate that, the standard errors of the two sampling schemes (Sobol, and Good Lattice sequence) are very close to their exact error. Hence, we can conclude that, the use of randomization techniques for error estimation is sufficiently accurate. Moreover, it is also shown that, the estimated errors are always larger than the exact error. Therefore, it is demonstrated that the error of the two quasi-Monte Carlo methods can be quantified not only robust but also conservatively based on the error estimation method.

### 4.4 Hygrothermal case studies

#### 4.4.1 Calculation object

As mentioned in Section 3.3, the probabilistic analysis is performed for assessing the hygrothermal performance of a massive masonry wall with interior insulation. Since the reference situation prior to retrofit is commonly a massive masonry wall though, we simply adopt that configuration here as the calculation object. Moreover, in order to provide an exhaustive augmented comparison study with respect to the sampling efficiency and error estimation for different sampling schemes in different scenarios, two case studies will be performed. In the first case study, only heat transport will be taken into account and the target output is the mean and standard deviation of the
distribution of cumulated heat loss over one year. In the second case study, both heat and moisture transport will be considered. For this case, in addition to the distribution of cumulated heat loss over one year, the mean and standard deviation of the distribution of moist freeze-thaw cycles are also taken as the target outputs.

The information of boundary conditions, related input and output parameters can be found in section 3.3.1. More precisely, for the input parameters, we separate them into two categories, probabilistic and deterministic, which respectively have probability distributions and fixed values. All the details are shown in Table 3-2 and 3-3, respectively. The imposed boundary conditions corresponding to the interior room conditions are based on the European Standard (EN15026, 2007).

4.4.2 Sampling efficiency

The sampling efficiency can be described as the number of repetitions of the core deterministic simulation needed to reach a desired accuracy. Often the deviation from reference solution, the variance or root-mean-square error of the targeted outcomes are used as indicators of that accuracy. In other words, sampling strategies requiring less runs of simulations are termed ‘more efficient’. In this report, we assess the sampling efficiency of the standard Monte Carlo, uniformity-based optimized Latin Hypercube, Sobol, Niederreiter-Xing and Good Lattice, by comparing the deviations of their outcomes from a reference solution.

Similarly as in section 4.3.1, in order to obtain the standard error output on the estimator, multiple quasi-Monte Carlo sequences need to be created and the mean of these independent quasi-Monte Carlo evaluations, formula (7), will be taken as the final approximation. Hence, the total number of function evaluations for quasi-Monte Carlo is $r \cdot n_{QMC}^{QMC}$. Moreover, since the calculation time for the hygrothermal case studies is much longer than the simple mathematical case study in section 4.3, in this section, we take $r = 10$, $n_{MC}^{MC}$ and $n_{QMC}^{QMC} \in [2^3, \ldots, 2^7]$. In addition, for obtaining a robust conclusion of the convergence behavior of each sampling scheme, except for uniformity-based optimized Latin Hypercube, 10 independent replications of $r \cdot n_{QMC}^{QMC}$ quasi Monte Carlo evaluations are made at each of these five sample sizes. Since the generation cost for optimized Latin Hypercube designs is very high, no replications are generated for that particular scheme.

4.4.2.1 Case study 1- Heat transport

For case study 1, the reference solutions are 194.0888 kWh and 45.3854 kWh for respectively the mean and the standard deviation of the resulting heat loss distribution. It is obtained via 10 replications of a $2^{15}$-run randomized good lattice sequence and its generating vector is optimized for up to $2^{20}$ points (Cools et al, 2006). To assess the accuracy of the reference solution for case study 1, the standard errors of these 10 replications are calculated, which is 0.0017 for the mean and 0.0105 for the standard deviation, respectively. Figure 4-6 compares the sampling efficiency for the mean and standard deviation of the cumulated heat loss distribution of standard Monte Carlo, uniformity-based optimized Latin Hypercube, Sobol, Niederreiter-Xing and Good Lattice.
Figure 4-6: the sampling efficiency of standard Monte Carlo (MC), uniformity-based optimized Latin hypercube (Uniform), Sobol (Sobol), Niederreiter-Xing (NX) and Good Lattice (GLP), with respect to the mean (left figure) and standard deviation (right figure) of the cumulated heat loss

In Figure 4-6, it can be seen that all the quasi-Monte Carlo sampling strategies outperform the standard Monte Carlo method for both the mean and standard deviation. It is also clear that the uniformity-based optimized Latin Hypercube scheme has a similar sampling efficiency as the other three quasi-Monte Carlo sequences. It can also be noticed that the convergence rate of Good Lattice sampling is slightly slower than Sobol and Niederreiter-Xing, and the performance of quasi-Monte Carlo methods is better for quantifying the mean than the standard deviation of the distribution of cumulated heat loss.

4.4.2.2 Case study 2 – Heat and moisture transport

Heat loss
For case study 2, the reference solutions of heat loss are 206.7787 kWh and 46.4312 kWh for respectively the mean and the standard deviation of the resulting heat loss distribution. Since the computational cost for case study 2 is relatively high, its reference is derived by 10 replications of a $2^{12}$-run randomized good lattice sequence and its generating vector is optimized for up to $2^{20}$ points (Cools et al, 2006). To assess the accuracy of the reference solution for the heat loss of case study 2, the standard errors of these 10 replications are calculated, which is 0.0062 for the mean and 0.0387 for the standard deviation, respectively. The sampling efficiency of standard Monte Carlo, uniformity-based optimized Latin Hypercube, Sobol, Niederreiter-Xing and Good Lattice, for the mean and standard deviation of the cumulated heat loss distribution, are shown in Figure 4-7.
In Figure 4-7 (left), it can be seen that for the mean, all the quasi-Monte Carlo sampling strategies outperform the standard Monte Carlo method. However, for the standard deviation, the outperformance of quasi-Monte Carlo methods becomes less obvious. One possible reason is due to the accuracy of the reference solution. Since for the standard deviation, the standard error for the reference solution is only 0.0387, using the deviation from the reference to represent the exact error may lead to a bias. Similar to case study 1, the sampling efficiency of uniformity-based optimized Latin Hypercube scheme is close to the other three quasi-Monte Carlo sequences. In addition, it is also shown that, for quantifying the mean, among all the quasi-Monte Carlo methods, the convergence speed of Niederreiter-Xing is slower than the Sobol and Good lattice sequence, and hence not be preferred.

**Freeze-thaw cycles**

In order to evaluate the risk of frost damage, the number of moist freeze-thaw cycles per year at 0.5 cm from the exterior brick surface is taken as the risk indicator (Vereecken et al, 2015). The reference solutions are 0.62 and 0.03, for respectively the mean and the standard deviation of the distribution of the resulting moist freeze-thaw cycles. To assess the accuracy of the reference solution, the standard errors of these 10 replications are calculated, which is 0.0053 for the mean and 0.0153 for the standard deviation, respectively. The sampling efficiency of standard Monte Carlo, uniformity-based optimized Latin Hypercube, Sobol, Niederreiter-Xing and Good Lattice, for the mean and standard deviation of the distribution of the moist freeze-thaw cycles is shown in Figure 4-8.
Figure 4-8 illustrates that, contrast to the cumulated heat loss (Fig 4-6 and 4-7), there is no significant superiority of quasi-Monte Carlo sampling strategies over the standard Monte Carlo method with respect to quantifying mean and standard deviation of the distribution of amount of moist freeze-thaw cycle. The reason of degrading the performance of quasi-Monte Carlo methods will be investigated in the following section.

### 4.4.3 Smoothness and effective parameters of the HAM model

Quasi-Monte Carlo method uses low-discrepancy sequences to approximate the target function and have a convergence rate $O((\log n)^d/n^1)$ in dimension $d$ for functions having sufficient smoothness, in contrast to $O(n^{1/2})$ for Monte Carlo which uses pseudo random samples. However, one restriction for quasi-Monte Carlo to converge at a rate $O((\log n)^d/n^1)$ is that the partial mixed derivatives of the target function need to exist and to be square-integrable (Dick, 2007). On the other hand, in the cases where the target functions are discontinuous or lack smoothness, the convergence rate of quasi-Monte Carlo method may degrade to $O(n^{1/2})$ (Moskowitz and Caflisch, 1996), examples of which can be found in (Moskowitz and Caflisch, 1995) and in the results of section 4.4.2.2 of this report. In building physical applications, some discrete parameters such as different materials and climates are often involved in the analysis, and these discrete parameters may bring discontinuity to the target function.

A second limitation occurs when the target function has a large number of dimensions. In this case, in order to let $O((\log n)^d/n^1)$ substantially smaller than $O(n^{-1/2})$, $n$ needs to be huge. However, in many high-dimensional problems, quasi-Monte Carlo method has been shown to be superior to standard Monte Carlo. And the concept of effective dimension has been proposed by (Wang and Fang, 2003). It is shown that, even though a lot of parameters are involved in the analysis, the efficiency of quasi-Monte Carlo method is mainly determined by the parameters which have dominant influence on the function. And thus, for the high-dimensional problems, we can still expect the superiority of quasi-Monte Carlo over standard Monte Carlo, if the number of effective dimensions is relatively small. In many building physical engineering applications, (Van Gelder et al, 2014) has shown that, even though the total number of input parameters may be large, the number of effective parameters is usually fairly small.
For getting a deeper understanding of our calculation object and illustrating the potential reasons of the contradictory results shown in section 4.4.2.2, a Gaussian kernel smoother estimation is implemented in this section to estimate the form of our target functions, with respect to each input parameters. After that, since the smoothness of a continuous function is determined by the order of its derivatives, and the derivative of a function can be viewed as its slope. Hence, the smoothness of our target function with respect to each parameters can be roughly estimated by analyzing their slopes. In addition, the effectiveness of each input parameters can be roughly observed from the variation of its respect output.

4.4.3.1 Kernel smoother

A kernel smoother is a non-parametric statistical technique for estimating a real valued function $f(x)$ by using its noisy observation. A detailed introduction of this method can be found in (Hastie et al, 2001). Unlike the traditional parametric estimations which require prior assumptions about the form of $f(x)$, the non-parametric approach can estimate $f(x)$ directly from the data. As a result, the set of irregular observations is represented as a smooth curve or surface. The idea is that, in order to estimate the value of a target point $x_0$, we mainly use those observations which are close to this point. This can be achieved by implementing a kernel function $K_\lambda(x_0, x_i)$, so that a weight can be assigned to $x_i$ based on its distance from $x_0$. Here $\lambda$ is called the bandwidth, which determines the width of the considered neighborhood, and data points that are closer to $x_0$ will be assigned higher weights. Hence, the value of $x_0$ can be estimated based on the Nadaraya-Watson kernel-weighted average:

$$\hat{f}(x_0) = \frac{\sum_{i=1}^{N} K_\lambda(x_0, x_i) y_i}{\sum_{i=1}^{N} K_\lambda(x_0, x_i)}$$

(13)

Here, $N$ is the number of observed points, $y_i$ represent the observations at $x_i$ points. $K$ is the related kernel.

4.4.3.2 Gaussian kernel

As we mentioned before, a kernel is a weighting function and different kernels represent different shapes of the weighting function. There are many kernels can be taken as the weighting function. And in this report, a Gaussian kernel is used in the analysis. A Gaussian kernel with the bandwidth $\lambda$ is expressed as below:

$$K_\lambda(x, x_i) = \frac{1}{\sqrt{2\pi}} e^{-\frac{(x-x_i)^2}{2\lambda^2}}$$

(14)

Here, the bandwidth parameter $\lambda$ need to be determined. Big $\lambda$ implies lower variance which may lead under smoothing to the target function. On the other hand, small $\lambda$ indicates higher variance and it may yield an estimation curve which is too noisy to interpret. Therefore, how to find an optimal bandwidth that minimizes the error between the estimated function and the real function becomes a key component of the kernel smoother method. A review of different bandwidth selection method has been proposed by Berwin and Turlach (1993). In this report, we take $\lambda = 0.9A n^{-0.2}$, where $A = \min(\sigma IQR^{1/3}, 1)$. Here, IQR is the interquartile difference, the difference between the 75th and the 25th percentile, $\sigma$ is the standard deviation of the observations. More details with respect to this bandwidth can be found in (Silverman, 1986) and (Hardle, 1991).
4.4.3.3 Gaussian kernel smoother analysis for case study 2

In this section, a Gaussian kernel smoother analysis for case study 2 is proposed. In this study, the results based on heat loss and number of moist freeze-thaw cycles, which are calculated by a 12800-run standard Monte Carlo analysis, are taken as observations. And the output of our Gaussian kernel smoother analysis is shown in Figure 4-9 and Figure 4-10, respectively.

Figure 4-9: Gaussian kernel smoother analysis of the total heat loss as a function of each continuous parameter.
Figure 4-10: Gaussian kernel smoother analysis of the number of moist freeze-thaw cycles as a function of each continuous parameter.

In Figure 4-9, the estimated function curves with respect to thickness of the wall, solar absorption coefficient and scale factor catch ratio have no gaps and do not contain any nasty angles. Therefore, we can roughly regard them as smooth functions. In addition, for convective heat transfer coefficient and wall orientation, only few angles are shown in the fitted function curves. Thus, we can simply conclude that all curves are relatively smooth, but the target function with respect to thickness of the wall, solar absorption coefficient and scale factor catch ratio are smoother than convective heat transfer coefficient and wall orientation. Moreover, it is shown that the thickness of the wall and the convective heat transfer coefficient are the most two effective parameters, illustrated by the slope of the curves.

For the number of moist freeze-thaw cycles, the estimated function curves become more oscillatory, with respect to each continuous parameter. Therefore, we can simply conclude that the function of freeze-thaw cycle is less smooth than the function of the cumulative heat loss. Further it is shown in Figure 4-10 that, except for the solar absorption coefficient, all the parameters are significant, and thus, comparing with cumulative heat loss, the number of moist freeze-thaw cycles are dominated by more parameters.

4.4.3.4 The true effect of discontinuous parameters

As we mentioned before, the convergence rate of quasi-Monte Carlo may degrade to O(n^{-1/2}), if the target function is discontinuous. However, this is contradictory to our simulation result in section 4.4.2.1, since we found that, for the heat loss analysis, even though 2 discrete parameters (types of climates and bricks) are involved in the calculation, the superiority of quasi-Monte Carlo over standard Monte Carlo is still significant. As inspired by the idea of effective parameters, we suppose that, even though the target functions contains discrete parameters, as long as they are not
dominant, we can still expect a higher convergence rate than $O(n^{-1/2})$ for the quasi-Monte Carlo method. In order to evaluate the effect of the two discontinuous parameters, the box plots in Figure 4-11 and Figure 4-12 contain the result of the heat losses and freeze-thaw cycle, with respect to the types of climates and bricks.

**Figure 4-11:** Boxplot of the total heat loss as a function of each different climate and each different brick type.

**Figure 4-12:** Boxplot of the frost thaw cycle as a function of each different climate and each different brick type.
It is shown in Figure 4-11 that, the result of the heat losses are fairly close for all the types of climates and bricks. This indicates that for the heat loss, both of these discrete parameters are not effective parameters. Figure 4-12 presents a different scenario; a significantly larger amount of moist freeze-thaw cycles was reached with Munich climate than found for Bremerhaven and Essen. Furthermore, a significantly smaller amount of moist freeze-thaw cycles was the result when using brick type 2 compared to brick type 1 and 3. Therefore, comparing with heat loss, for freeze-thaw cycles, both discrete parameters are effective parameters.

### 4.4.3.5 Conclusion

Compared with the result of freeze-thaw cycles, it is demonstrated that the function of heat loss is relatively smooth. It is also illustrated that the function of heat loss contains less effective parameters and the dominance of the discrete parameters is relatively smaller. Whereas, compared to the mathematical functions (11) and (12) which have respectively one and three orders of smoothness, several slightly non-smooth behaviors with respect to the heat loss transport function can be observed. All in all, because of the relatively smooth property of the heat loss transport function, the sampling efficiency of the quasi-Monte Carlo method should be higher than the standard Monte Carlo method. And it has been confirmed by the results in section 4.4.2.1 and section 4.4.2.2. On the other hand, due to these slightly non-smoothness behaviors, these quasi-Monte Carlo sampling strategies should converge slower for quantifying distribution of the heat loss than for integrating the mathematical functions (11) and (12).

On the contrary, Figure 4-10 and Figure 4-12 illustrate that, for the function of freeze-thaw cycle, it turns to be less smooth and contains more effective parameters. In addition, since the dominance of the discrete parameters is relatively large for the freeze-thaw cycle, the function of freeze-thaw cycle may even be regarded as discontinuous function. As a consequence, section 4.4.2.2 illustrates that, for quantifying the distribution of the freeze-thaw cycle, the convergence rate of quasi-Monte Carlo methods degrade to $O(n^{-1/2})$, which confirms the statements of (Moskowitz and Caflisch, 1996) and (Moskowitz and Caflisch, 1995).

### 4.4.4 Error estimation

As mentioned in Section 4.2.1.2, quasi-Monte Carlo method makes use of the standard error of all the independent replications to quantify the error of its approximation. In this report, two times the standard error is chosen as error indicator. In order to evaluate the accuracy and convergence speed of the error indicator, the ratio of the error indicators of each sampling schemes to their exact errors, as well as the convergence behavior of these error indicators, for both the means and standard deviations of all the target outputs are shown in this section.

#### 4.4.4.1 Case study 1 – Heat transport

For case study 1, the ratio of error indicators of each sampling schemes to their exact errors (deviation from the reference solution) and the convergence behavior of these error indicators, for the mean and standard deviation of the distribution of cumulated heat loss are shown in Figure 4-13 and Figure 4-14.
Figure 4-13: The ratio of the error indicator of each sampling scheme to their exact error (left) and the convergence behavior of error indicators (right), with respect to the mean of the cumulated heat loss distribution.

Figure 4-14: The ratio of the error indicator of each sampling scheme to their exact error (left) and the convergence behavior of error indicators (right), with respect to the standard deviation of the cumulated heat loss distribution.

It is shown in Figure 4-13 (left) and Figure 4-14 (left) that, except for the uniformity-based optimized Latin Hypercube scheme, the ratio of the error indicators of the sampling schemes to the deviations of their respective quasi-Monte Carlo approximations from the reference solution are almost always bigger than 1 and often smaller than 10, which implies that their error indicators are always larger than their exact errors and usually within the difference of one magnitude. Hence, the error of the three quasi-Monte Carlo methods can be quantified robustly and conservatively based on the error estimation method. On the other hand, for the uniformity-based optimized Latin Hypercube design, their error indicators are however always smaller than their exact errors. The reason has been mentioned before: because there is no randomization technique for optimized Latin Hypercube design, correlations may exist between the smaller subdesigns and thus, an error indicator derived by the standard error of these smaller subdesigns may lead to a too optimistic error estimation.

In addition, it is shown in Figure 4-13 (right) and Figure 4-14 (right) that the error indicator of all the sampling strategies decrease as the number of the evaluations increase, with respect to the mean of the cumulated heat loss, and it is also shown that this indicator decreases faster for quasi-Monte Carlo approximations.
Carlo methods than standard Monte Carlo method. Moreover, it is also demonstrated that this indicator declines faster for the Sobol and Niederreiter-Xing sequences than for the Good Lattice sequence.

Finally it is illustrated that, the error indicators of quasi-Monte Carlo methods converge faster for the mean than for the standard deviation of the distribution of heat loss.

4.4.4.2 Case study 2 – Heat and moisture transport

Heat Loss

For case study 2, the ratio of error indicators to the deviation from the reference solution and the convergence behavior of these error indicators, for the mean and standard deviation of the cumulated heat loss distribution are shown in Figure 4-15 and Figure 4-16.

Figure 4-15: The ratio of the error indicators of each sampling schemes to their exact errors (left) and the convergence behavior of error indicators (right), with respect to the mean of the cumulated heat loss distribution

Figure 4-16: The ratio of the error indicators of each sampling schemes to their exact errors (left) and the convergence behavior of error indicators (right), with respect to the standard deviation of the cumulated heat loss distribution
As in case study 1, the ratio of the error indicators of the four sampling schemes to the deviations of their respective quasi-Monte Carlo approximations from the reference solution are almost always bigger than 1 and often smaller than 10. Hence, the error of the three quasi-Monte Carlo methods can be quantified robustly and conservatively based on the error estimation method. In addition, it is shown in Figure 4-15 (right) and Figure 4-16 (right), the error indicators of all the sampling strategies decrease as the number of the evaluations increase, with respect to both the mean and the standard deviation of the cumulated heat loss, and it is also shown that these indicators decreases faster for quasi-Monte Carlo methods than standard Monte Carlo method. It is also illustrated that, among all the quasi-Monte Carlo methods, the performance of Sobol sequence is most robust, with respect to the convergence of its error indicators for both mean and standard deviation of heat loss distribution.

**Freeze-thaw cycle**

The ratio of error indicators to the deviation from the reference solution and the convergence behavior of these error indicators, for the mean and standard deviation of the freeze-thaw cycles are shown in Figure 4-17 and Figure 4-18.

*Figure 4-17: The ratio of the error indicators of each sampling schemes to their exact errors (left) and the convergence behavior of error indicators (right), with respect to the mean of freeze-thaw cycle*

*Figure 4-18: The ratio of the error indicators of each sampling schemes to their exact errors (left) and the convergence behavior of error indicators (right), with respect to the standard deviation of freeze-thaw cycle*
It is shown in Figure 4-17 and Figure 4-18 that, the error of quasi-Monte Carlo methods can be quantified robustly and conservatively based on the error estimation method. However, in contrast to the cumulated heat loss, there is no significant superiority of quasi-Monte Carlo sampling strategies over the standard Monte Carlo method with respect to the convergence speed of their error indicators. The potential reasons for this have been mentioned in section 4.4.3.

### 4.5 Conclusion

In this section, the potential use of quasi-Monte Carlo methods for uncertainty propagation has been assessed, via one mathematical and two hygrothermal case studies. Four quasi-Monte Carlo sampling strategies – Optimized Latin Hypercube, Sobol sequence, Niederreiter-Xing sequence, Good Lattice sequence – were applied and compared. The outcomes show that, in most of the scenarios, the quasi-Monte Carlo methods outperform the standard Monte Carlo method, and from the QMC methods the Sobol’ sequence tends to be the best. Furthermore, it is also shown that the error of the quasi-Monte Carlo methods can be quantified robustly and conservatively with the standard error. However, it was also demonstrated that the superiority of quasi-Monte Carlo methods over the standard Monte Carlo may degrade if the target function has strong discontinuities, a large number of effective parameters and/or a highly non-smooth behavior.

All in all though, the superior sampling efficiency of the Sobol sequence for probabilistic assessments of hygrothermal performances has been established. Application of randomised Sobol sequences as sampling scheme in combination with the standard error as error indicator will hence be integrated in the overall methodology put forward in Section 3. Doing so will make the methodology as efficient as possible, which will benefit the proficient execution of all necessary simulations in RIBuild’s WP6.

### 4.6 References


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5 Summary and conclusions

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This report presents the first of two deliverables related to RIBuild’s WP 4 ‘Probabilistic assessment of interior insulation solutions’. The key objective of WP4 is the development of an efficient strategy for the probabilistic hygrothermal assessment of interior insulation solutions. That strategy involves Monte-Carlo-based repetitions of hygrothermal simulations, and hence requires an efficient deterministic hygrothermal simulator and an efficient probabilistic assessment approach. Prior to the initiation of the RIBuild project, both a deterministic simulator and a probabilistic methodology were already available. Their joint application to interior insulation solutions does however require further developments, primarily in relation to their numerical efficiency.

The various tasks in WP4 hence focus on efficiency improvements of both the deterministic simulator and the probabilistic methodology. Tasks 4.1 and 4.2 target the efficient one-, two- and three-dimensional simulation of heat, air and moisture transfer in building components, Tasks 4.3 and 4.4 aim for the efficient probabilistic assessment of hygrothermal performances based on these simulations. In the final Task 4.5, the developments of Tasks 4.1 to 4.4 are to be brought together in a final application example. This deliverable reports on the results from the general developments in WP4 (Section 3), and from the specific activities within Task 4.1 (Section 2) and Task 4.3 (Section 4). The future D4.2 is then to report on the outcomes of Task 4.2 and Task 4.4.

Section 2 details the further developments with respect to the deterministic hygrothermal assessment of interior insulation solutions, which was the prime target of Task 4.1. Within that Task, the Delphin hygrothermal simulation program has been significantly extended, concerning both effectiveness and efficiency. In relation to the former, the program has been extended to three-dimensional geometries, anisotropic material properties, and inclusion of air flow, each of which are important for the reliable hygrothermal assessment of internal insulation solutions. With respect to the latter, a modular solver framework, including iterative solver methods, has been implemented, greatly reducing the computational cost of the hygrothermal simulations.

Section 3 embeds that deterministic simulator into the probabilistic framework. To that end, a Matlab master code has been implemented, handling both preprocessing (assignment uncertain parameters, manipulation Delphin input files, execution hygrothermal simulations) and postprocessing (collection and quantification of output variables). Subsequently, the developed technique has been used in order to investigate a simplified balance model to integrate interior environment simulation in hygrothermal simulation models. Finally, the developed technique has been employed to study the performance of interior insulation solutions, both via one- and two-dimensional simulations. In relation to the latter, it was shown that both approaches yield different findings.

Section 4 finally focuses on the core of the probabilistic methodology, in particular efficient sequential Monte-Carlo sampling. In relation to this, the sampling efficiency of different low-discrepancy-based sampling schemes has been investigated, on the basis of simple mathematical functions as well as hygrothermal case studies. These revealed the Sobol series as the most dependable approach. In a subsequent study, approximate error quantification has been evaluated, based on randomized replications in combination with a standard-error-based estimator. It was
shown that this estimator gives a reliable and conservative error quantification, which allows halting the simulations when a sufficient level of accuracy is reached.

The combination of the approaches presented in Sections 2, 3 and 4 will pave the way for the massive simulation campaign in RIBuild’s WP6, having drastically augmented the efficiency of probabilistic hygrothermal assessment of interior insulation solutions. RIBuild’s WP6 should however also heed the evaluation of damage criteria: it has been shown that the applied models also result in predictions of damage for the uninsulated reference construction, implying that a relative rather than an absolute damage criteria evaluation is required. Finally, RIBuild’s WP6 should also pay attention to the effect of the multi-dimensional behavior, which has been shown to affect the hygrothermal conditions and damage evaluation.