Elements in materials modelling

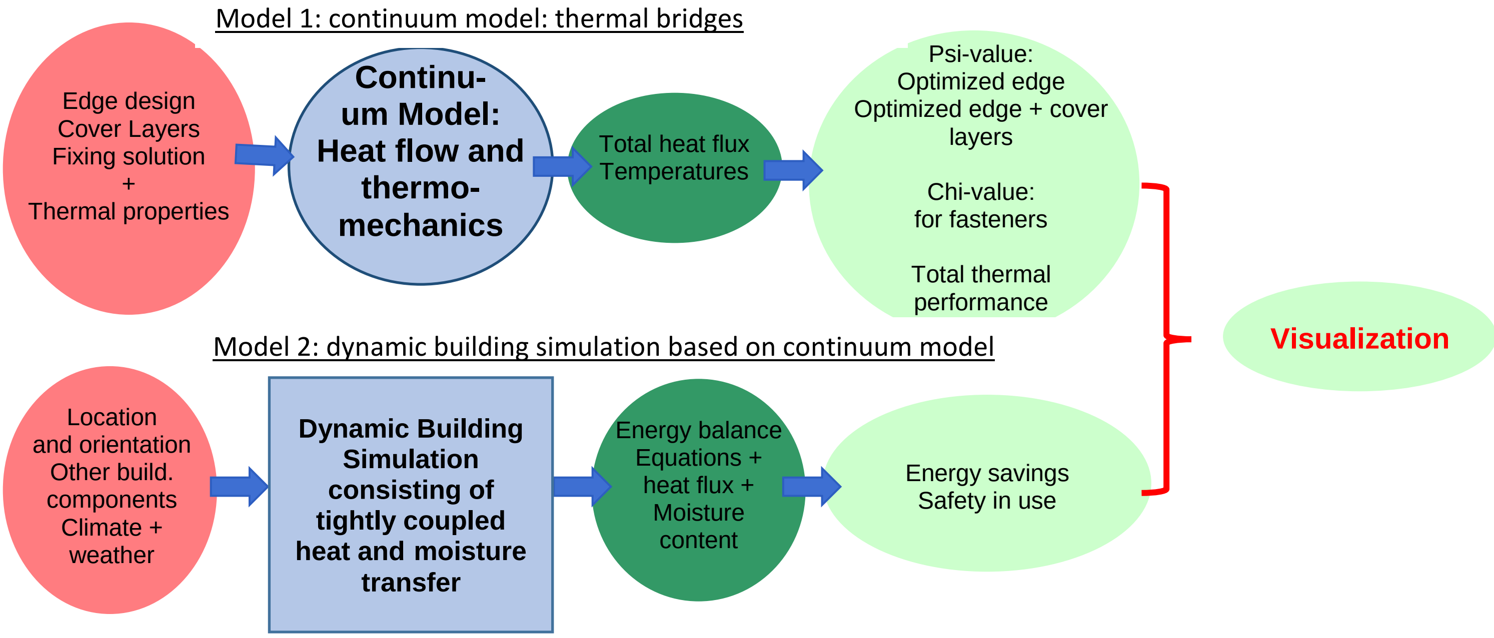
Each simulation will have its own MODA fiche.
Metadata for these elements are to be elaborated over time

Purpose of this document:
Definition of a data organisation that is applicable to ALL materials modelling simulations. The fiche should contain all elements that are needed to describe a simulation. This information spans from the end-user (manufacturer) information to the computational modelling details.

This is a combined document for MODA 1: Simulations on thermal bridges and MODA 2: dynamic building simulations with combined heat and mass transfer. MODA 1 is dealing with three applications that make use of the same heat flow equation and therefore are combined in one description.

OVERVIEW of the simulation			
1	**User Case**		MODA 1: Determine heat-transfer through material, building components and systems MODA 2: Determine dynamic building behavior and the energy savings associated with the technical solutions and to transfer the INNOVIP idea to other climatic zones and different buildings. Check for moisture accumulation and drying of the components. VIPs are a total barrier for water vapour in building constructions – except at their panel to panel joints. Moisture accumulation in the component or drying out of water used for mortar and plaster can only occur at these joints.
2	**Chain of Models**	**Model 1 MODA 1**	Continuum model Heat flow equation used on the three aspects of the user case
		model 2 MODA 2	Dynamic building simulation modelling using the heat flow equation with radiative term for solar heat gain (RoMM Ch 4.3) but also CFD (Chapter 4.2) for the mass (moisture) transfer through the building components as Extra terms are added to the heat flow equation used in MODA 1 to model hygrothermal effect like phase change etc (see below). The simulations will be done with different material relations (MR).
3	**Publication on the simulation**		*Please give the publication which documents **the simulation** to indicate peer review and quality of the simulated data.*
4	**Access conditions**		All MR will be treated as "confidential" The software-tools for the PE are all commercial – except "Therm" for 2-dim Heat Transfer. Therm is available for free at LBNL (Lawrence Berkeley National Laboratory) https://windows.lbl.gov/software/therm/therm.html

Workflow



First the components are modelled as a static situation. The heatfluxes will be used to optimise the design. For this optimised design a dynamic building simulation will be done.The building will be modelled in a dynamic situation to catch transient behaviour;

Each model used in a simulation can be documented in three chapters:

1. Aspect of the User Case or System simulated with this model
2. Model
3. Computation
4. Post processing

This processes the output of one simulation into input for the next simulation.

Please use the following four tables to document each "simulation with one model".
Coupled models can be written up collectively in one set of four tables.

MODA 1: Heat-transfer through material, building components and systems making use of:

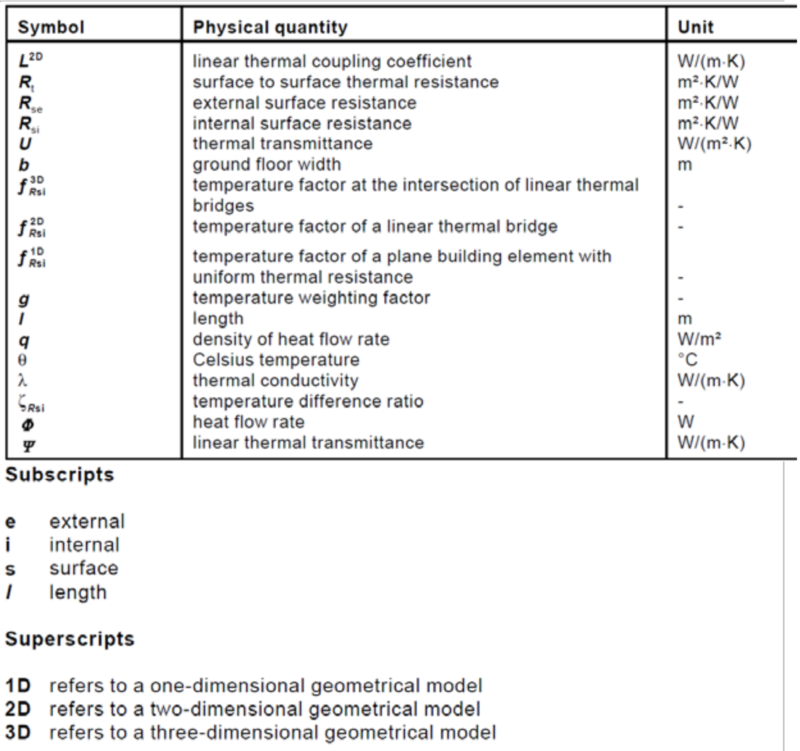
MODEL 1: Continuum Model for Heat-flow and thermo-mechanics

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED AND HOW IT FORMS A PART OF THE TOTAL USER CASE	Application 1: Determine the thermal bridging effects "psi-value" and total heat flux caused by the metallized layers of the foil-envelopes of the VIP and the additional materials placed at the edges to form the new "edge design" of the INNOVIP product. Application 2: Determine the thermal bridging effects if additional cover layers on the panels are used. Depending on the thermal conductivity of the cover layer material, these layers can function as a remarkable additional thermal resistance reducing the thermal bridging effect at the panel edge or in an opposite way as a collector for heat from the undisturbed part of the panel towards the edge. We will determine a range for the total heat flux that is optimized for the desired function and for thermal performance of the insulation construction. Application 3: Determine the additional effect of penetrating fasteners and fixing solutions on the heat transfer (point thermal transmittance of fasteners). Some of the optimized combinations of Application 1 and Application 2 will be simulated to determine the additional thermal bridging effect that is caused by fasteners and penetrating fixing solutions (point thermal transmittance: "chi-value")
1.2	MATERIAL	A wide range of materials for which thermal performance values can be found with tabulated values in international standards, such as ISO 10456 and ISO 10077-2. For stationary heat-transfer modelling, only thermal conductivity values (ideally: temperature dependent) are needed. Relevant temperature dependent properties are taken into account (e.g. temperature dependent thermal conductivity, temperature dependent heat capacity, moisture content etc.). Properties taken from databases or measured values. Temperature dependent properties will be used if necessary. Isotropic material properties will be used mostly. Anisotropic properties only if needed for the correct definition of the heat transfer of the simulated component (e.g. equivalent thermal conductivity of air-gaps or anisotropic thermal conductivity behavior of some building materials (baked clay)).
1.3	GEOMETRY	The size of the model will be "real" size, measured in m or mm.
1.4	TIME LAPSE	Stationary situation
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	Simulations for thermal performance can be carried out for standard conditions given in CEN or ISO standards (e.g. 20°C inside the building and -5°C or -10°C for the exterior climate). The warm side surface Resistance is (due to slow air speed from natural convection): Rsi

		= 0.13 m²*K/W and the cold side resistance usually 0.04 m²*K/W (higher wind-speeds on the outside surface). Heat-transfer simulations are carried out on non-deformed systems, omitting bending forces, external pressure or dilatation as a result of temperature increase or decrease.
1.6	**PUBLICATION ON THIS ONE SIMULATION**	*Publication documenting **the simulation** with this single model (if available and if not included in the overall publication).*

2	**GENERIC PHYSICS OF THE MODEL EQUATION**		
2.0	**MODEL TYPE AND NAME**	Continuum Model: 4.3 Heat flow and thermo mechanics	
2.1	**MODEL ENTITY**	Flat (2d) elements and volumetric (3d) elements.	
2.2	**MODEL PHYSICS/ CHEMISTRY EQUATION PE'S**	**Equations**	When modelling heat-transfer in (and through) building parts and components, the PE has three terms of heat transfer: - Heat-Conduction in the solid material and conduction in liquids and gases (Fourier's law) - Convection (various descriptions bases on Newton's law of cooling) - Radiation (Stephan-Boltzmann's law) $\dot{q} = K\Delta T \begin{cases} \text{conduction} & \vec{q} = -k\nabla T \\ \text{convection} & \dot{q} \equiv h\left(T_{\mathrm{w}} - T_{\infty}\right) \\ \text{radiation} & \dot{q} = \varepsilon\sigma\left(T_{\mathrm{w}}^4 - T_{\infty}^4\right) \end{cases}$
		Physical quantities for each equation	$\dot{q}$ heat-flux density in W/m² K (in building systems usually called thermal transmittance "U-value") in W/(m²*K) Delta T is the temperature difference at the system's boundaries in K k Thermal conductivity (usually λ is used for building materials) in W/(m*K) T absolute Temperature in K ∇T: Temperature Gradient/ Temperature Difference on a specific layer in K h (convective) heat transfer coefficient ε emissivity of surfaces σ Stephan-Boltzmann constant
MATERIALS RELATIONS		**MR Equations**	$\Phi_l = L^{2D}\,(\theta_i - \theta_e)$ $\Psi = L^{2D} - \sum_{j=1}^{N} U_j\, l_j$ χ = L3D – U*A U = 1/(Rsi+Σdi/λi+Rse)

	Physical quantities/ descriptors for each MR	(see below)



Symbol	Physical quantity	Unit
L^{2D}	linear thermal coupling coefficient	W/(m·K)
R_t	surface to surface thermal resistance	m²·K/W
R_{se}	external surface resistance	m²·K/W
R_{si}	internal surface resistance	m²·K/W
U	thermal transmittance	W/(m²·K)
b	ground floor width	m
f^{3D}_{Rsi}	temperature factor at the intersection of linear thermal bridges	-
f^{2D}_{Rsi}	temperature factor of a linear thermal bridge	-
f^{1D}_{Rsi}	temperature factor of a plane building element with uniform thermal resistance	-
g	temperature weighting factor	-
l	length	m
q	density of heat flow rate	W/m²
θ	Celsius temperature	°C
λ	thermal conductivity	W/(m·K)
ζ_{Rsi}	temperature difference ratio	-
Φ	heat flow rate	W
Ψ	linear thermal transmittance	W/(m·K)

Subscripts

e	external
i	internal
s	surface
l	length

Superscripts

1D	refers to a one-dimensional geometrical model
2D	refers to a two-dimensional geometrical model
3D	refers to a three-dimensional geometrical model

L3d thermal coupling coefficient from three-dimensional calculation
U U-value
A Area
Rsi internal surface resistance
d thickness of layer
λ thermal conductivity
Rse external surface resisstance

χ point thermal transmittance in W/K

2.4	**SIMULATED INPUT**	No simulated input used.

This part is similar to the description on input files to simulation software and requires understanding of the underlying architecture of the data in certain class of solvers for the models.

3	**SPECIFIC COMPUTATIONAL MODELLING METADATA**		
3.1	**NUMERICAL SOLVER**	Finite-Difference (FD) or Finite-Element (FE) in 2-dim and 3-dim will be used. The solver is part of the software tool used. Iterative Solvers can be used if the dimensions of neighboring elements don't differ too much. FD is strongly recommended for the very thin layers of the foils at the edges of VIPs.	
3.2	**SOFTWARE TOOL**	Therm; Heat 2d; Heat 3d; Nastran; COMSOL	
3.3	**TIME STEP**	Not applicable for stationary heat transfer	
3.4	**COMPUTATIONAL REPRESENTATION** *Refers to how your computational solver represents the material, properties, equation variables,*	**PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL**	Material properties and all other physics variables are written up for the entity in the model.
		COMPUTATIONAL BOUNDARY CONDITIONS	
		ADDITIONAL SOLVER	<u>Stop criteria on convergence:</u> *Heat-flux density:* 0.001 to 0.0001 W/m² from simulation step to

		PARAMETERS	simulation step. *Temperature:* Usually around 0.00001 to 0.000001 K from step to step. A finer mesh will be used at specific areas. Symmetric planes will be used to limit the number of nodes and elements and to increase the speed of the solver. For stationary heat-transfer modelling (until equilibrium is reached for constant boundary conditions on the warm and the cold side of the model) the time lapse is not relevant, as the simulation will be carried out until a stop criterion is reached. As stop criterion the deviation of temperature or total-heat flux from one simulation step to the next step is limited to a certain value. The simulation is faster if it is carried out without heat-capacity properties of the materials.

Post processing

> *The "raw output" calculated by the model is per definition the physics variable in the PE(s).*
> *This is already specified in the entry 2.2 and will appear in your dark green circles in the workflow picture.*
> *This output is processed by a post processor in order to calculate values for physics variables for larger entities that can be input to the next model or that are the final output of the total simulation.*
> *The physics used to do this calculation is to be documented.*

4	**POST PROCESSING**	
4.1	**THE PROCESSED OUTPUT IS CALCULATED FOR**	Simulated output is usually the total heat flux for the given model or the heat-flux density or temperature. The processed output is not used as input for model 2. INNOVIP will use the ouput to optimise the design.
4.2	**METHODOLOGIES**	The total heat flux or the heat flux density is calculated by volume averaging. (by calculating the effective R- or U-value of the simulated system with all influencing factors). This is used to derive the thermal performance of the construction directly The total heat flux or the heat flux density is further used to define the linear thermal transmittance (Psi-value) for the optimized edge and for the optimized edge when using cover layers: $\Phi_l = L^{2D}(\theta_i - \theta_e)$ $\Psi = L^{2D} - \sum_{j=1}^{N} U_j l_j$ The processed output from the 3-dim Simulation of the fasteners will be used to derive the point thermal transmittance (Chi-value) for fasteners. χ = L3D – U*A
4.3	**MARGIN OF ERROR**	For the heat flow from the simulation the program validation procedure in ISO 10211 is carried out and all programs should be within 1 % of the total heat flow. The total margin of Error is strongly depending on the quality of the model and on some limitations of the program in comparison to the real building component (e.g.

		cracks in wall constructions influencing the thermal conduction in the material; measurement tolerances in the building sector usually exceed some mm). In addition to that thermal modelling of building components strongly depend on the quality of the input data – especially for thermal conductivity of the material. Therefore the total margin of error (based on the heat flux) can only be estimated to be in between ±1% (for the programs with fixed input values) and ±10 % (for program plus dimensions plus measured values of thermal conductivity plus insufficient drying etc….). For heat transport simulation in wet materials the margin of error is estimated even higher around ±15%).

MODA 2: Dynamic building behavior making use of:

MODEL 2: Dynamic building simulation with Continuum Model for Heat-flow and thermo-mechani

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED AND HOW IT FORMS A PART OF THE TOTAL USER CASE	Dynamic building behaviour. Determination of thermal performance in use Energy savings in different climates Building physical aspects of the use of the INNOVIP elements in constructions.
1.2	MATERIAL	Thermal: see Model 1 For simulating the combined heat and mass transfer, additional properties are needed, such as capillary effects in the material, water absorption, water intake, pore sizes, temperature and moisture dependent sorption isotherms etc.
1.3	GEOMETRY	Simulation on real size building components (m).
1.4	TIME LAPSE	For instationary heat-transfer (e.g. for non-constant boundary conditions on the warm and on the cold side of the model) the time lapse is usually set by the given climatic data. For short time simulations, minute or 5-minute values are used – for long term simulations usually hourly, daily or monthly-values are used.
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	Hygrothermic simulations are carried out on non-deformed systems, omitting bending forces, external pressure or dilatation as a result of temperature increase or decrease. Standard Conditions given by climatic data for various climatic regions of the world. Hygrothermal: Typical Meteorological Data is used (standard reference years with additional data on the amount and the duration of rain). This is processed climatic data, but not a simulated input.
1.6	PUBLICATION ON THIS ONE SIMULATION	*Publication documenting **the simulation** with this single model (if available and if not included in the overall publication).*

2	GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	Dynamic simulation with combined heat and mass transfer - making use of a Continuum Model: Heat flow and CFD	
2.1	MODEL ENTITY	1-dim and 2-dim Elements, 3-dim Volumes	
2.2	MODEL PHYSICS/ CHEMISTRY EQUATION PE's	**Equations**	When modelling heat-transfer in (and through) building parts and components, the PE has three terms of heat transfer: - Heat-Conduction in the solid material and conduction in liquids and gases (Fourier's law) - Convection (various descriptions bases on Newton's law of cooling) - Radiation (Stephan-Boltzmann's law) $\dot{q} = K\Delta T \begin{cases} \text{conduction} & \vec{q} = -k\nabla T \\ \text{convection} & \dot{q} \equiv h\left(T_{w} - T_{\infty}\right) \\ \text{radiation} & \dot{q} = \varepsilon\sigma\left(T_{w}^{4} - T_{\infty}^{4}\right) \end{cases}$ In this simulation of hygrothermal behavior, many additional effects are taken into account nl phase change of water (ice – water – water vapour), latent heat transported by warm water moving through the component, additional effects on solid conduction (reduced coupling resistances and higher conductivity due to absorbed water):

Phase change between liquid and vapour, i.e. the release of latent heat, is considered as part of the convective heat flow through the structure.

Conservation of mass can be used to determine the air flow rate. If buoyancy can be neglected the air flow rate is calculated from the total pressure difference over the construction.

$$g_{\mathrm{a}} = \rho_{\mathrm{a}}\, C\, \Delta P_{\mathrm{a}}{}^{\mathrm{n}}$$

The increase of the moisture content of a control volume is determined by the net inflow of moisture. The moisture flow rate equals the sum of the vapour flow rate and the flow rate of liquid water.

$$\frac{\partial w}{\partial t} = -\frac{\partial g}{\partial x}$$

$$g = g_{\mathrm{v}} + g_{\mathrm{l}}$$

The liquid phase of water inside a building material can be described by the moisture content mass by volume. Due to the capillary forces the pressure inside the water is different from the pressure of the surrounding air. The difference is called suction.

$$s = P_{\mathrm{a}} - P_{\mathrm{l}}$$

The suction of the pore water is related to the relative humidity of the surrounding air by the Kelvin equation:

$$s = -\rho_{\mathrm{l}}\, R_{\mathrm{H2O}}\, T \ln \varphi$$

The heat transport through heat conduction is calculated with Fourier's law and includes all processes where the transport of heat is closely correlated to the temperature gradient. The second heat flow term accounts for the effects of both air flow and moisture flow, including sensible and latent heat:

$$q_{\mathrm{cd}} = -\lambda(w,T)\cdot\frac{\partial T}{\partial x}$$

$$q_{\mathrm{cv}} = c_{\mathrm{p,a}}\cdot\left(T - T_{\mathrm{ref}}\right)\cdot g_{\mathrm{a}} + c_{\mathrm{p,l}}\cdot\left(T - T_{\mathrm{ref}}\right)\cdot g_{\mathrm{l}} + h_{\mathrm{e}}\cdot g_{\mathrm{v}}$$

Air (and liquid moisture) flow into the construction:

$$q = h_{\mathrm{eff}}\cdot\left(T_{\mathrm{eq}} - T_{\mathrm{surf}}\right) + g_{\mathrm{air}}\cdot c_{\mathrm{p,air}}\cdot\left(T_{\mathrm{air}} - T_{\mathrm{ref}}\right) + g_{\mathrm{l}}\cdot c_{\mathrm{p,l}}\cdot\left(T_{\mathrm{air}} - T_{\mathrm{ref}}\right) + h_{\mathrm{e}}\cdot g_{\mathrm{v}}$$

Physical quantities for each equation

$\dot{q}$ heat-flux density in W/m²

K (in building systems usually called thermal transmittance "U-value") in W/(m²*K)

Delta T is the temperature difference at the system's boundaries in K

k Thermal conductivity (usually λ is used for building materials) in W/(m*K)

T absolute Temperature in K

∇T: Temperature Gradient/ Temperature Difference on a specific layer in K

			h (convective) heat transfer coefficient ε emissivity of surfaces σ Stephan-Boltzmann constant **Symbol Quantity Unit – hygrothermal simulations** C flow coefficient per unit area $\mathrm{m^3/(m^2\ s\ Pa_n)}$ D_l liquid diffusivity $\mathrm{m^2/s}$ I_{sol} total flux of incident solar radiation W/m$_2$ P_a pressure of the surrounding air Pa $\otimes P_a$ total air pressure difference Pa P_l water pressure inside pores Pa R_{H2O} gas constant of water vapour J/(kg K) R_l liquid moisture flow resistance of interface, m/s T thermodynamic temperature K T_a air temperature of the surrounding environment K T_{eq} equivalent temperature of the surrounding environment K T_r mean radiation temperature of the surrounding environment K T_{ref} arbitrary reference temperature K T_s surface temperature K $c_{p,a}$ specific heat capacity at constant pressure of air J/(kg K) $c_{p,l}$ specific heat capacity at constant pressure of liquid water J/(kg K) $c_{p,s}$ specific heat capacity at constant pressure of solid matrix J/(kg K) d_l thickness of the layer I m g density of moisture flow rate $\mathrm{kg/(m^2\ s)}$ g_r density of air mass flow rate $\mathrm{kg/(m^2\ s)}$ g_l density of liquid moisture flow rate $\mathrm{kg/(m^2\ s)}$ g_p available water due from to precipitation $\mathrm{kg/(m^2\ s)}$ g_v density of vapour flow rate $\mathrm{kg/(m^2\ s)}$ h_c convective heat transfer coefficient W/(m$_2$⊕K) h_e specific enthalpy of liquid-vapour phase change J/kg h_{eff} effective heat transfer coefficient W/(m$_2$⊕K) h_r radiative heat transfer coefficient W/(m$_2$⊕K) n flow exponent - p_v partial vapour pressure, Pa $p_{v,sat}$ saturated vapour pressure Pa q density of heat flow rate W/m$_2$ q_{cond} density of conduction heat flow rate W/m$_2$ q_{conv} density of convection heat flow rate W/m$_2$ s suction Pa $\otimes s$ suction difference across interface Pa s mean suction at interface Pa s_d equivalent vapour diffusion thickness m v wind speed m/s w moisture content kg/m$_3$ w_l water content kg/m$_3$ α_{sol} solar absorptance – δ_0 permeability of vapour in air kg/m s Pa ε long-wave emissivity of the external surface - λ thermal conductivity W/(m⊕K) $\lambda_{m,l}$ moisture conductivity for capillary water transport s φ relative humidity - μ diffusion resistance factor – ρ_l liquid water density $\mathrm{kg/m^3}$ ρ_a density of air $\mathrm{kg/m^3}$ ρ_s density of solid matrix $\mathrm{kg/m^3}$
MATERIALS RELATIONS		**MR Equations**	Effective heat transfer coefficient and the equivalent temperature:

			$h = h_c + h_r$ $T_{eq} = T_a + \frac{1}{h}(I_{sol}\,\alpha_{sol} + (T_r - T_a)h_r)$
		Physical quantities/ descriptors for each MR	See List above…
2.4	**SIMULATED INPUT**	NA	

This part is similar to the description on input files to simulation software and requires understanding of the underlying architecture of the data in certain class of solvers for the models.

3	**SPECIFIC COMPUTATIONAL MODELLING METADATA**		
3.1	**NUMERICAL SOLVER**	Finite volume based solver Coupled Heat and Mass transfer equations on components: implicite, iterative finite-volume solver with adaptive time steps - with iterative coupling of heat and mass transfer. Building simulation between zones: energy balance equations with implicit and iterative solver with adaptive time steps or explicit solver with short time steps (auto-adjusted) depending on the sub-models used	
3.2	**SOFTWARE TOOL**	WUFI + (combined hygrothermal simulation and dynamic building simulation program)	
3.3	**TIME STEP**	Hygrothermal: Time step dependent on climatic data (real time – 5 min or hourly values)	
3.4	**COMPUTATIONAL REPRESENTATION** *Refers to how your computational solver represents the material, properties, equation variables,*	**PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL**	All physical vlaues are written up for finite volumes
		COMPUTATIONAL BOUNDARY CONDITIONS	The physics b.c. are written up for the faces of theouter finite volumes.
		ADDITIONAL SOLVER PARAMETERS	<u>Stop criteria on convergence:</u> *Heat-flux density:* 0.001 to 0.0001 W/m² from simulation step to simulation step. *Temperature:* Usually around 0.00001 to 0.000001 K from step to step. A finer mesh will be used at specific areas. Symmetric planes will be used to limit the number of nodes and elements and to increase the speed of the solver.

Post processing

The "raw output" calculated by the model is per definition the physics variable in the PE(s).
This is already specified in the entry 2.2 and will appear in your dark green circles in the workflow picture.
This output is processed by a post processor in order to calculate values for physics variables for larger entities that can be input to the next model or that are the final output of the total simulation.
The physics used to do this calculation is to be documented.

4	**POST PROCESSING**	
4.1	**THE PROCESSED OUTPUT IS CALCULATED FOR**	Hygrothermal: simulated output is the temperature, the heat-flux and the local water

		content. From these, the risk for mould growth or the moisture accumulation within the component will be derived. Dynamic building simulation: the output is the performance of the building in the specific climatic zone. The output is calculated to provide building data and building component data directly to the End-User. The user needs information about the safety in use (regarding to moisture problems) and about the overall thermal performance in relation to the original state before refurbishment with the INNOVIP solution (energy savings). Safety in use: Moisture content of the material in a certain position over time and the equivalent temperature. Energy Savings compared to the state before refurbishment: Effective heat transfer coefficient
4.2	**METHODOLOGIES**	$h = h_c + h_r$ $T_{eq} = T_a + \frac{1}{h}\left(I_{sol}\,\alpha_{sol} + (T_r - T_a)h_r\right)$
4.3	**MARGIN OF ERROR**	For heat transport simulation in wet materials the margin of error is estimated around ±15%).