Wall-ACE

Deliverable

D4.8: The modelling data (MODA) template for the numerical simulations based on the Elements in materials modelling

WP	**4**	Demonstration: building validation and tools development
Task		

Dissemination level[1]	PU
Nature[2]	R

Due delivery date	31/12/2016
Actual delivery date	21/12/2016

Lead beneficiary	CEA
Contributing beneficiaries	EffinArt, Polito

Document Version	**Date**	**Author**	**Comments[3]**
0.01	30/11/2016	Mohamad Ibrahim	creation
0.02	14/12/2016	Valentina Serra	modification
0.03	15/12/2016	Mohamad Ibrahim	modification
0.04	16/12/2016	Mohamad Ibrahim	Final version (to be validated by reviewers)
Final	22/12/2016	Johann Balau	Final review

---

[1] Dissemination level: **PU** = Public, **PP** = Restricted to other programme participants (including the Commission services), **RE** = Restricted to a group specified by the consortium (including the Commission services), **CO** = Confidential, only for members of the consortium (including the Commission services)

[2] Nature of the deliverable: **R** = Report, Document, **DEM** = Demonstrator, Prototype, pilot, **DEC =** Websites, patent fillings, **O =** Other

[3] Creation, modification, final version for evaluation, revised version following evaluation, final

Deliverable abstract

This deliverable provides the MODA templates for all the modeling and simulations that will be carried out in W'ALL IN ONE. These are:

- MODA for Modeling heat and moisture transfer on a building's envelope/system scale
- MODA for Modeling heat transfer in a thermal zone (CFD)
- MODA for Modeling the dynamic thermal behavior and energy performance on a building scale

MODA for the models used for the simplified design numerical tools.

Deliverable Review

	Reviewer #1: CEA			**Reviewer #2: Johann Balau**		
	Answer	**Comments**	**Type***	**Answer**	**Comments**	**Type***
Is the deliverable in accordance with						
the Description of Action?	☒ Yes ☐ No		☐ M ☐ m ☐ a	☒ Yes ☐ No	It should be mentioned that it will exist a deviation between the MODELLING and the real results	☐ M ☐ m ☒ a
the international State of the Art?	☒ Yes ☐ No		☐ M ☐ m ☐ a	☒ Yes ☐ No		☐ M ☐ m ☐ a
Is the quality of the deliverable in a status						
that allows it to be sent to European Commission?	☒ Yes ☐ No		☐ M ☐ m ☐ a	☒ Yes ☐ No		☐ M ☐ m ☐ a
that needs improvement of the writing by the originator of the deliverable?	☐ Yes ☒ No		☐ M ☐ m ☐ a	☐ Yes ☒ No		☐ M ☐ m ☐ a
that needs further work by the Partners responsible for the deliverable?	☐ Yes ☒ No		☐ M ☐ m ☐ a	☐ Yes ☒ No		☐ M ☐ m ☐ a

* Type of comments: M = Major comment; m = minor comment; a = advice

Table of content

1. Introduction

This deliverable provides the MODA templates, based on the ***Review of Materials Modelling V***[4]**,** for all the modeling and simulations that will be carried out in W'ALL IN ONE. These are:

- MODA for Modeling heat and moisture transfer on a building's envelope/system scale

The aim is to develop numerical models and carry out simulations for the heat and moisture transfer within envelopes having the novel materials/systems. The effect of the heat losses (1 dimensional) through different envelope construction types (old and new) as well as the effect on the thermal bridge heat losses (2 dimensional) of some typical thermal bridges will be examined.

From another perspective, the humidity transfer within these envelopes will be modeled and examined to assess the risk of condensation, moisture accumulation, and mould growth.

- MODA for Modeling heat transfer in a thermal zone (CFD)

In this modeling task, a special attention is focused on the interior low-emissivity thermal coating/finishing. The application of the low-e finishing at the interior wall surfaces can change significantly the thermal behavior, especially when taking into account the thermal stratification within the zone.

Computational fluid dynamics (CFD) numerical models will be developed to simulate the temperature and velocity distribution in a single room, taking the effect of the heating device type into consideration.

The aim is to determine the effect of such coating/finishings on the radiative and convective heat losses as well as on the occupants' thermal comfort.

- MODA for Modeling the dynamic thermal behavior and energy performance on a building scale

The aim of this task is to provide a simulation-based approach to assess the impact of applying the different thermal insulation systems (at a building scale level) on the energy demands and thermal comfort for new as well as existing buildings. Different building types, construction materials of the exterior walls, roof, and ground, different window-to-wall ratios, different windows' glazing types, and different thicknesses of thermal insulation will be simulated and examined. In addition, these effects will be determined for various climates.

In what follows, we present the MODA templates following the ***Review of Materials Modelling V***.

---

[4] http://ec.europa.eu/research/industrial_technologies/modelling-materials_en.html

2. MODA templates

2.1 Modeling heat and moisture transfer on a building's envelope/system scale

OVERVIEW of the simulation			
1	**USER CASE**	Heat and moisture transfer modeling on system (wall envelope) level to assess the thermal and moisture performance of such systems in different boundary conditions. to analyze the impact of the newly developed systems on 1D heat losses, on thermal bridge (2D) heat losses, and on inner surface temperature with a condensation and mould growth risk assessment.	
2	**CHAIN OF MODELS**	**MODEL 1**	Heat transport: continuum model conservation of energy equation (1st law of thermodynamics) • Heat transfer due to conduction (diffusion) • Heat transfer due to convection • Heat transfer due to radiation • Fourier's law (conductive flow) • Newton's law of cooling (convective flow) • Stefan Boltzmann's law (radiative flow)
		MODEL 2	Moisture transport: continuum model conservation of mass (moisture transfer) • Fick's first law (vapour flow) • Darcy's law (liquid flow)
3	**PUBLICATION ON THE SIMULATION**		
4	**ACCESS CONDITIONS**	bought software license *(for WUFI or Delphin)*	

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	Analyze the impact of the newly developed systems on the heat losses, and on inner temperature with a condensation and mould growth risk assessment
1.2	MATERIAL	A wide range of materials can be found in international standards or in the database of the commercial software to be used (for e.g. WUFI database) e.g.: historical Brick with aerogel plaster at the interior surface
1.3	GEOMETRY	Cartesian (1D and 2D)
1.4	TIME LAPSE	Several years (5 years to 15 years depending on the specific simulation case)
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	External forces : heat (for e.g. solar radiation) and moisture (for e.g. rain) (the source is the weather data)
1.6	PUBLICATION ON THIS ONE SIMULATION	

<table>
<tr><th>2</th><th colspan="3">GENERIC PHYSICS OF THE MODEL EQUATION</th></tr>
<tr><td>2.0</td><td>MODEL TYPE AND NAME</td><td colspan="2">Tightly coupled equations:
- Heat transport: continuum model
- Moisture transport: continuum model</td></tr>
<tr><td>2.1</td><td>MODEL ENTITY</td><td colspan="2">finite volumes</td></tr>
<tr><td rowspan="2">2.2</td><td rowspan="2">MODEL PHYSICS/ CHEMISTRY EQUATION
PE'S</td><td>Equations</td><td>PE1: $\frac{dH}{dT}\frac{\partial T}{\partial t} = \nabla(\lambda\nabla T) + h_v\nabla(\delta_p\nabla(\varphi P_{sat}))$
PE2: $\frac{dw}{d\varphi}\frac{\partial \varphi}{\partial t} = \nabla(D_\varphi\nabla\varphi + \delta_p\nabla(\varphi P_{sat}))$</td></tr>
<tr><td>Physical quantities for each equation</td><td>PE1: Physical quantities
H=enthalpy (J)
T = temperature (K)
φ = relative humidity (-)
λ = thermal conductivity (W/(mK))
t = time (s)
δ_p = water vapour permeability (kg/(msPa))
hv = evaporation enthalpy (J/kg)
$Psat$ = water vapour saturation pressure (Pa)
PE2: Physical quantities</td></tr>
</table>

			w = water content (kg/m3) φ = relative humidity (-) D_{φ} = liquid conduction coefficient (kg/(ms)) t = time (s) δ_p = water vapour permeability (kg/(msPa)) $Psat$ = water vapour saturation pressure (Pa)
2.3.	**MATERIALS RELATIONS**	1. The material's thermal conductivity as a function of temperature (for PE1) 2. The material's thermal conductivity as a function of moisture content (for PE1) 3. The material's specific heat capacity (for PE1) 4. water vapour permeability or water vapour diffusion resistance factor (for PE1 and PE2) 5. the material's liquid conduction coefficient or liquid absorption coefficient (for PE2) 6. The sorption isotherm curve (for PE2) *(all the above are the results of experimental measurments)*	
2.4	**SIMULATED INPUT**	NA	

3	**SPECIFIC COMPUTATIONAL MODELLING METADATA**		
3.1	**NUMERICAL SOLVER**	Finite volume in 1D and 2D • Fully implicit for the discretization in time • Iterative solver (the solver is part of the software used) • Iterative coupling of heat and mass transfer	
3.2	**SOFTWARE TOOL**	WUFI or Delphine (https://wufi.de/en/ ; http://bauklimatik dresden.de/delphin/index.php?aLa=en)	
3.3	**TIME STEP**	Variable (1h or less) depending ion convergence failure	
3.4	**COMPUTATIONAL REPRESENTATION**	**PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL**	written up for finite volumes
		BOUNDARY CONDITIONS	The physics boundary conditions are written up for the faces of the outer finite volumes
		ADDITIONAL SOLVER PARAMETERS	convergence criteria: • node temperatures (or heat flux density) difference from one iteration step to another is less than a predefined tolerance value (for e.g. 0.00001°C for temperatures / 0.001 W/m² for heat flux)) • finer meshes will be used at specific areas

4	**POST PROCESSING**	
4.1	**THE PROCESSED OUTPUT IS CALCULATED FOR**	Temperatures will be used to estimate the thermal losses/gains throughout the envelope Relative humidity will be used to estimate the moisture risks (such as condensation)
4.2	**METHODOLOGIES**	physics definition for loss and gain literature relations for condensations and mould as function of temperature and humidity
4.3	**MARGIN OF ERROR**	For the heat flow, the simulation program is validated according the procedure of ISO 10211 and the error is within 1%. However, this error is for fixed boundary conditions and steady state conditions. When considering real applications, the margin of error is strongly depending on the quality of the model and on some limitations and assumptions of the program, and it is expected to be 10% to 15%

2.2 *Modeling heat transfer in a thermal zone (CFD)*

OVERVIEW of the simulation			
1	**USER CASE**	The effect of the low-e thermal interior coating-finishing on the convective and radiative heat transfer in a stratified thermal zone taking into consideration the heating system type	
2	**CHAIN OF MODELS**	**MODEL 1**	Continuum, CFD model
3	**PUBLICATION ON THE SIMULATION**		
4	**ACCESS CONDITIONS**	bought software license *(ANSYS-fluent)*	

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**	fluid flow and temperature profiles in a stratified thermal zone taking into consideration the heating system type and the different envelope characteristics
1.2	**MATERIAL**	• A wide range of envelope materials can be found in international standards or databases • The properties of newly developed materials will be supplied from experimental measurements
1.3	**GEOMETRY**	3D real size single room
1.4	**TIME LAPSE**	Steady-state simulations
1.5	**MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS**	External forces : heat (for e.g. solar radiation, temperature difference) and external pressure (the source can be the weather data)

<table>
<tr><td>1.6</td><td>PUBLICATION ON THIS ONE SIMULATION</td><td></td></tr>
</table>

<table>
<tr><td>2</td><td colspan="3">GENERIC PHYSICS OF THE MODEL EQUATION</td></tr>
<tr><td>2.0</td><td>MODEL TYPE AND NAME</td><td colspan="2">Continuum fluid mechanics
• Navier-Stokes equations coupled with energy balance equation (Tightly coupled equations)</td></tr>
<tr><td>2.1</td><td>MODEL ENTITY</td><td colspan="2">finite volume</td></tr>
<tr><td rowspan="2">2.2</td><td rowspan="2">MODEL PHYSICS/ CHEMISTRY EQUATION
PE’S</td><td>Equations</td><td>• PE1 (conservation of mass): $\frac{\partial\rho}{\partial t}+\nabla(\rho.\vec{v})=0$
• PE2 (conservation of momentum):
$\frac{\partial}{\partial t}(\rho.\vec{v})+\nabla(\rho.\vec{v}\vec{v})=-\nabla p+\nabla(\bar{\bar{\tau}})+f$
with
$\bar{\bar{\tau}}=\mu\left[(\nabla\vec{v}+\nabla\vec{v}^{T})-\frac{2}{3}\nabla.\vec{v}I\right]$
• PE3 (conservation of energy):
$\frac{\partial}{\partial t}(\rho.E)+\nabla\big(\rho.\vec{v}(\rho.E+P)\big)=\nabla\lambda(\nabla T)+\nabla(\bar{\bar{\tau}}.\vec{v})+S_h$
For turbulent flows, two equations several schemes exist, such as the standard $k-\varepsilon$ equations representing the turbulent kinetic energy and its rate of dissipation.</td></tr>
<tr><td>Physical quantities for each equation</td><td>Physical quantities
ρ= density (kg/m3)
T = temperature (K)
$\vec{v}$ = velocity vector (m/s)
λ = thermal conductivity (W/(mK))
t = time (s)
f = external body force
E = total energy (J)
P = pressure (Pa)
I = identity tensor
μ= dynamic viscosity (kg/(m.s))</td></tr>
<tr><td colspan="2">2.3. MATERIALS RELATIONS</td><td colspan="2">Since the assumption of the incompressible and Newtonian Fluid, the viscosity and density are just properties (constants).
For the the buoyancy-driven flows, the Boussinesq model is employed for the body force which assumes that density can be treated as a constant except in the buoyancy force term. The approximation is only valid when temperature differences are small so that density variations are very small.
$\rho_0-\rho=\rho\beta(T-T_0)$</td></tr>
</table>

		β= coefficient of thermal expansion (K^{-1}) T_0 = reference temperature (K) ρ_0 = reference density (kg/m3)
2.4	**SIMULATED INPUT**	NA

3	**SPECIFIC COMPUTATIONAL MODELLING METADATA**		
3.1	**NUMERICAL SOLVER**	Finite volume (3D) Different schemes can be assigned for e.g.: • The pressure-based solver that employs the projection method • The semi-implicit method for pressure-linked equations (SIMPLE) to solve pressure-velocity coupling	
3.2	**SOFTWARE TOOL**	ANSYS-Fluent (http://www.ansys.com/Products/Fluids/ANSYS-Fluent)	
3.3	**TIME STEP**	Steady state simulations	
3.4	**COMPUTATIONAL REPRESENTATION**	**PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL**	The computational domain is discretized on structured or unstructured mesh. Each mesh element has cell centres and 6 faces. The integral form of the PEs from is written up for a finite volume mesh. Cell centres and faces have the following properties: Cells contain the temperature, velocity, and the pressure and fields. Faces contain the flux field.
		BOUNDARY CONDITIONS	Specific boundary conditions are specified to translate the physics boundary conditions and process conditions for the walls and the inlet and outlet. a. on walls: no-slip boundary condition b. on inlet (if exist): pressure inlet velocity, as pressure is fixed and known at inlet, the velocity is evaluated from the flux normal to the inlet c. on outlet: pressure outlet
		ADDITIONAL SOLVER PARAMETERS	convergence criteria: • Temperatures, pressures, velocities differences from one iteration to the next iteration do not exceed a tolerance value • Flux equilibrium • Stability of the physical variables • finer meshes will be used at specific areas

4	**POST PROCESSING**	
4.1	**THE PROCESSED OUTPUT IS CALCULATED FOR**	Temperatures and fluxes will be used to estimate the thermal losses/gains throughout the envelope Temperatures and velocities will estimate the level of thermal comfort in the zone
4.2	**METHODOLOGIES**	physics definition for loss and gain literature concepts and definitions for thermal comfort such as the PMV index
4.3	**MARGIN OF ERROR**	The margin of error is strongly depending on the quality of the model

2.3 Modeling the dynamic thermal behavior and energy performance on a building scale

OVERVIEW of the simulation			
1	**User Case**	Assess the impact of applying the developed systems for new houses or to retrofit old houses on the energy demands and thermal comfort.	
2	**Chain of Models**	**Model 1**	Heat transport: continuum model conservation of energy equation (1st law of thermodynamics) • Heat transfer due to conduction (diffusion) • Heat transfer due to convection • Heat transfer due to radiation • Fourier's law (conductive flow) • Newton's law of cooling (convective flow) • Stefan Boltzmann’s law (radiative flow)
3	**Publication on the simulation**		
4	**Access conditions**	Free software *(for EnergyPlus)*	

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**	Assess the impact of applying the developed systems for new houses or to retrofit old houses on the heating/cooling demands and thermal comfort. • Dynamic thermal behaviour • Energy performance and energy savings for different climates • Thermal comfort analysis (especially for summer overheating risks)
1.2	**Material**	e.g.: an old brick house with aerogel plaster layer at the interior wall surfaces
1.3	**Geometry**	Real size buildings and building components
1.4	**Time Lapse**	1 year
1.5	**Manufacturing process or in-service conditions**	Statistical weather conditions
1.6	**Publication** **on this one simulation**	

2	**Generic Physics Of The Model Equation**		
2.0	**Model type and name**	Heat transport: continuum model	
2.1	**Model entity**	Finite volume	
2.2	**Model Physics/ Chemistry equation** **PE's**	**Equations**	PE1: $\rho cp \frac{\partial T}{\partial t} = \nabla(\lambda\nabla T)$
		Physical quantities for each equation	PE1: Physical quantities T = temperature (K) λ = thermal conductivity (W/(mK)) t = time (s) ρ = density (kg/m3) cp = specific heat (J/(kg.K))
2.3. Materials relations		1. The material's thermal conductivity (for PE1) 2. The material's specific heat capacity and density (for PE1) *(all the above are the results of experimental measurements)*	
2.4	**Simulated input**	*NA*	

3	**Specific Computational Modelling Metadata**		
3.1	**Numerical Solver**	Energy balance equations solved using Finite difference method • Difference scheme: FullyImplicitFirstOrder • Iterative solver	
3.2	**Software tool**	EnergyPlus (https://energyplus.net/)	
3.3	**Time step**	1h or less	
3.4	**Computational Representation**	**Physics Equation, Material Relations, Material**	All physical equations are written up for finite difference control volumes
		Boundary Conditions	Weather data (temperature, radiation, …) The physics b.c. are written up for the faces of the outer control volumes
		additional Solver Parameters	Inside face temperature convergence criteria: <0.0001

4	POST PROCESSING	
4.1	THE PROCESSED OUTPUT IS CALCULATED FOR	Temperatures and heat fluxes will be used to estimate heating/cooling loads for a specific climate Energy savings compared to the state-of-the-art solutions
4.2	METHODOLOGIES	physics definition for loss and gain
4.3	MARGIN OF ERROR	

2.4 Simplified design numerical tools

OVERVIEW of the simulation			
1	USER CASE	Simplified numerical tools able to aid designers in assessing the thermo hygrometric behavior of the proposed systems under actual working conditions. Heat and moisture simplified transfer modeling of systems (wall envelopes) in different boundary conditions.	
2	CHAIN OF MODELS	MODEL 1	Heat transport: continuum model (dynamic regime) conservation of energy equation (1st law of thermodynamics) • Heat transfer due to conduction (diffusion) • Heat transfer due to convection + radiation (surface heat transfer coefficients) • Fourier's law (conductive flow) • Newton's law of cooling (convective flow) • Linearized radiative heat flux And/Or Inverse modeling based on experimental data (provided by Task 4.4, 4.5, 4.6)
		MODEL 2	Moisture transport: continuum model (steady state) conservation of mass (moisture transfer) • Fick’s first law (vapour flow)
3	PUBLICATION ON THE SIMULATION		
4	ACCESS CONDITIONS	Free. The models will be developed in MATLAB/SIMULINK environment and/or Macro Excel (the final user must have a licensed version of these software in order to be able to use these models).	

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**	Analyze the impact of the newly developed systems on: the heat losses, inner surface temperature and energy storage capabilities.
1.2	**Material**	A wide range of solutions will be modeled based on the outcomes of the laboratory results, as far as the new developed layers are concerned
1.3	**Geometry**	Cartesian (1D)
1.4	**Time Lapse**	From 24 hours to 1 year
1.5	**Manufacturing process or in-service conditions**	For the external boundary conditions the source is the weather data, for the indoor boundary conditions the source is typical indoor environment conditions in buildings.
1.6	**Publication** **on this one simulation**	*Possible publication on Scientific Conferences and/or journals*

<table>
<tr><th>2</th><th colspan="3">Generic Physics Of The Model Equation</th></tr>
<tr><td>2.0</td><td>Model type and name</td><td colspan="2">- Heat transport: continuum model
- Moisture transport: continuum model, Fick’s law</td></tr>
<tr><td>2.1</td><td>Model entity</td><td colspan="2">Finite difference for direct modeling and/or ARX, ARMAX, PEM, … black-box models</td></tr>
<tr><td>2.2</td><td>Model Physics/ Chemistry equation
PE’s</td><td>Equations</td><td>Direct modelling:
Eq. 1 :
$$\frac{\partial}{\partial x}\left(\lambda_x \frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(\lambda_y \frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(\lambda_z \frac{\partial T}{\partial z}\right)+q_i=\rho c\cdot\frac{\partial T}{\partial t}$$
Eq. 2 :
$$\frac{\dot{m}}{A}=-D\,\frac{\mu}{R\,T}\,\frac{\partial p}{\partial x}=-\delta\,\frac{\partial p}{\partial x}$$
Inverse modelling:
General form of the equations :
$$A(q)\cdot y(t)=\frac{B(q)}{F(q)}\cdot u(t-nk)+\frac{C(q)}{D(q)}\cdot e(t)$$
Where:
$$A(q)=1+a_1\cdot q^{-1}+.........+a_{na}\cdot q^{-na},$$
$$B(q)=b_1+b_2\cdot q^{-1}+.........+b_{nb}\cdot q^{-nb+1}$$</td></tr>
</table>

			$C(q) = 1 + c_1 \cdot q^{-1} + ... + c_{nc} \cdot q^{-nc}$, $D(q) = 1 + d_1 \cdot q^{-1} + ... + d_{nd} \cdot q^{-nd}$ $F(q) = 1 + f_1 \cdot q^{-1} + ... + f_{nf} \cdot q^{-nf}$. Being : na, nb, nc, nd ed nf positive integers which represent the order of the polynomials. nk is the “number of fixed delays” between the inputs ui(t) and the outputs yj(t) (as a multiple of the sampling interval, T). Outputs and inputs are, in our case, surface temperatures and/or heat fluxes
		Physical quantities for each equation	Direct modelling: Eq. 1: Physical quantities T = temperature (K) λ = thermal conductivity (W/(mK)) t = time (s) ρ = density [kg/m3] c = specific heat [J/(kgK)] Eq. 2: Physical quantities μ = Molecular mass D = Diffusivity (m2/s) T = temperature (K) T = temperature (K) R = perfect gas constant [J/(kgK)] t = time (s) δ = water vapour permeability (kg/(msPa)) p = water vapour pressure (Pa) Inverse modelling: u(t), y(t) = time series of surface temperatures and specific heat fluxes
2.3. MATERIALS RELATIONS			1. The material’s thermal conductivity, eventually, as a function of temperature (for PE1) 2. The material’s specific heat capacity (for PE1) 3. The material’s density (for PE1) 4. water vapour permeability or water vapour diffusion resistance factor (PE2) 5. Measured time history of Temperatures and heat fluxes for inverse (black-box) models *(all the above are the results of experimental measurments)*
2.4	**SIMULATED INPUT**	NA	

3	**SPECIFIC COMPUTATIONAL MODELLING METADATA**	
3.1	**NUMERICAL SOLVER**	Direct modeling - Finite difference in 1D • Fully implicit for the discretization in time • Iterative solver (the solver is part of the software used) • Iterative coupling of heat and mass transfer Inverse modeling : • Built-in Simulink solver (Black-box model toolbox)

3.2	**SOFTWARE TOOL**	MATLAB/SIMULINK, Excell	
3.3	**TIME STEP**	Variable (1h or less) depending on numerical convergence criteria	
3.4	**COMPUTATIONAL REPRESENTATION**	**PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL**	written up for finite differences
		BOUNDARY CONDITIONS	The physics boundary conditions are written up for the faces of the outer surfaces of the system
		ADDITIONAL SOLVER PARAMETERS	convergence criteria: • Built – In Simulink/Excel solvers

4	**POST PROCESSING**	
4.1	**THE PROCESSED OUTPUT IS CALCULATED FOR**	Temperatures will be used to estimate the thermal losses/gains throughout the envelope Relative humidity will be used to estimate the moisture risks (such as condensation)
4.2	**METHODOLOGIES**	physics definition for loss and gain
4.3	**MARGIN OF ERROR**	*Expected accuracy within ± 10%*

3. Conclusion

The MODA templates are presented in this document based on the Review of Materials Modelling V. These templates will form the basis for all the modelling and simulation to be carried out within the project. These templates maybe evolved or updated during the project’s lifetime.