Grant Agreement N°814596

SensMat Deliverable D3.4

Report on full set of MODA Sheets for the used multi-physical environmental models

WP	3	**Multi-scale and multi-physical modelling and validation**
Task	3.3	**Multi-physical environmental simulation of CH Exhibition Impacts**

Dissemination level[1]	CO
Nature[2]	R

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[1] Dissemination level: **PU** = Public, **CO** = Confidential, only for members of the consortium (including the Commision Services), **EU-RES** = Classified Information: RESTREINT UE, **EU-CON** = Classified Information: CONFIDENTIEL UE, **EU-SEC** = Classified Information: SECRET UE

[2] Type of the deliverable: **R** = Report, **ORDP** = Open Research Data Pilot, **ETHICS** = Ethics requirement, **DEM** = Demonstrator, pilot, prototype, **DEC** = Websites, patent filings, videos, etc, **O** = Other

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

Deliverable abstract

The scope of the deliverable is the definition of the multi-physical numerical models that will be used within the project to simulate different deterioration mechanisms of cultural heritage. This provides the key information for identifying the surrounding environmental conditions of museums and historical buildings. Sensitive artefacts are made from a broad range of many different materials with different levels of risk factor. For example, organic materials such as those in paintings, are very sensitive to climate, humidity, temperature, UV-light.

Due to the huge variety and complexity of environmental conditions, the materials modelling field consists of a wide number of research groups. These communities have established different terminologies, which typically focus on specific application domains and on particular types of models. As a result, a wide ranges of specific software codes are evolving. However, applications to engineering problems in advanced materials require a strong interdisciplinary approach among these fields and groups. Therefore, in order to establish a common terminology in materials modelling a standardized terminology has followed.

In this report, the information is organized according to the “materials MOdelling DAta” (MODA), the description of simulations includes user case, model, solver and post-processor.

Simulation workflows about the models, solvers and their implementation are summarized below. The MODA sheet for physics-based models is described in order to guide users towards a complete documentation of material and process simulations.

Deliverable Review

	Reviewer #1:			Reviewer #2:		
	Answer	**Comments**	**Type***	**Answer**	**Comments**	**Type***
1. Is the deliverable in accordance with						
(i) the Description of the Action?	☐ Yes ☐ No		☐ M ☐ m ☐ a	☐ Yes ☐ No		☐ M ☐ m ☐ a
(ii) the international State of the Art?	☐ Yes ☐ No		☐ M ☐ m ☐ a	☐ Yes ☐ No		☐ M ☐ m ☐ a
2. Is the quality of the deliverable in a status						
(i) that allows it to be sent to European Commission?	☐ Yes ☐ No		☐ M ☐ m ☐ a	☐ Yes ☐ No		☐ M ☐ m ☐ a
(ii) that needs improvement of the writing by the originator of the deliverable?	☐ Yes ☐ No		☐ M ☐ m ☐ a	☐ Yes ☐ No		☐ M ☐ m ☐ a
(iii) 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

Contents

1. Introduction

The objective of the deliverable is the description of the set of multi-physical numerical models. SensMat project introduces the deliverable D.3.3 to generate, for all used environmental models, corresponding MODA sheets, which will be uploaded to the EMMC cluster portal.

In the framework of the project, EnergyPlus is used by IUAV to simulate the behaviour of the HVAC system and building envelope under specified boundary conditions in terms of weather, building use, occupation density and HVAC system type and control strategy. In particular, the resulting hourly values of air and surface temperatures, as well as air humidity and HVAC system capacities are used to set the boundary conditions for concurrent CFD (Computational Fluid Dynamics) analysis developed by CETMA. In particular, three typical days will be considered in this analysis: winter design day, summer design day, typical half-season day. Consequently, the CFD simulation software will exploit the daily profile of boundary conditions provided by EnergyPlus, in order to calculate in detail air flows, stratification and consequent temperature and humidity in any place of the room, and define the boundary conditions for consequent material analyses aimed at the prediction of actual solicitations on the materials.

The goal of CETMA activities in Task 3.3 «*Multi-physical environmental Simulations of CH Exhibition Impacts*» is to analyse the impact of different elements (HVAC system operating conditions, solar radiation, building structure, visitors' presence) in terms of temperature, humidity and air velocity in every point of an indoor exhibition context. The Computational Fluid Dynamics (CFD) techniques can be properly used in order to evaluate the spatial uniformity of microclimatic parameters, such as the contaminant distribution inside indoor spaces [4] and to study the indoor airflow induced by mechanical ventilation and air-conditioning systems. In literature, there are many examples of using CFD software Ansys Fluent for simulating the airflow inside buildings [5][6] or the impact of relative humidity [7].The suitable indoors conditions are chosen according to ASHRAE indications [9]. The CFD analyses take into account the real non uniform spatial distribution of the indoor microclimatic parameters within the simulated exhibition room. It is necessary to know the main geometric and thermal characteristics of the exhibition room and the thermal–hygrometric design conditions. The best way to obtain these results is to integrate CFD simulations with Building Energy Performance Simulations (BEPS). The energy simulation program provides building heating/cooling loads and interior surface temperatures of building envelope to CFD as boundary conditions, while CFD provides convective heat transfer coefficients and detailed room air temperature distributions [5]. CFD boundary conditions, as regards the energy flux through the room walls, the volumetric airflow rate and the thermal–hygrometric conditions of the supply air are provided by the BEPS program. The results of building energy simulations will be supplied by IUAV. The numerical model is able to predict the thermal condition in every point of the analysed room and the humidity formation. So it will be possible to prevent critical conditions and avoid the damage to artworks.

TUG-IES is covering in Task 3.3 (Multi-physical environmental Simulations of CH Exhibition Impacts) the simulations of dust formation and accumulation with appropriate spatial resolution. To achieve these results, two different simulations are performed, whereby the second simulation is built on the results of the first simulation.

In the SensMat project, the modelling results are further handed over to USTUTT for usage in the micro/meso-scale deterioration models (Task 3.1). In addition, the results can be compared to the outcome of Task 7.1 (Museums characterization & Diagnosis) to get a better insight into the deposition mechanisms in different museums. The outcome of the simulations will enable the development of control strategies to minimize dust accumulation on sensitive surfaces. Due to the fact that the deposition of particulate matter reduces the value of CH objects due to interaction with the item or the requirement of frequent cleaning cycles according to [8], the results can have major impacts on further mitigation steps.

The European Material Modelling Council (EMMC) will be a target audience for networking and sharing of data and results. SENSMAT models will be placed onto the future European Material

Modelling Marketplace. This will facilitate the maintenance, support, curation of data, exchange of best-practices, sharing of trouble-shooting solutions and it will increase the visibility, accessibility and uptake of SensMat models.

2. State of the Art

Preventive Conservation (PC) today is a complex activity that involves a very wide range of multidisciplinary skills and activities. The awareness of the influence of other environmental factors on the preservation of objects has shown that it is not enough to renovate a historic building or museum or a storage area to preserve objects. Moreover, the multiplicity of criteria and their numerous interconnections for PC management make the decision process even more complicated and thus the corresponding tools are expensive. In parallel, information technologies have made huge progress (ICT, IoT, Web ...) and some innovations can be adapted for benefit of the field PC domain (i.e. energy efficiency of buildings, knowledge management and capitalization, economic aspects, agile ICT ...). Therefore, the main target of SensMat project is to increase the offer with a sustainable and cost-innovative PC solutions (tools, methods, standards…) adapted to the global context of conservation, to the EU PC market needs (regional location and rules, legislation, practices) and taking into account museum's priorities together with financial and human resources dimensions.

3. Numerical Analysis

In this task, multi-physical numerical models are developed to analyse the environment of a Culture Heritage exhibition room and the impact of external factors.
Below a description of the numerical codes, EnergyPlus, Fluent and Comsol, used by each partner and their application in the project.

<u>EnergyPlus (IUAV):</u>

EnergyPlus (https://energyplus.net/) is probably the most acknowledged and tested software for building energy simulation. It is funded by the U.S. Department of Energy's (DOE) Building Technologies Office (BTO) and managed by the National Renewable Energy Laboratory (NREL). It is developed in collaboration with NREL, various DOE National Laboratories, academic institutions, and private firms.

EnergyPlus allows the user to calculate air and surface temperatures, air humidity, and heat gains/losses consequent to weather, infiltration/ventilation air flows, solar radiation rate, internal gains, walls and windows, together with the detailed action of complex HVAC (Heating, Ventilation and Air-Conditioning) systems. These calculations take into full consideration the thermal inertia of the building envelope and dynamic HVAC strategies.

The EnergyPlus program is a collection of many program modules that work together to calculate the energy required for heating and cooling a building using a variety of systems and energy sources. It does this by simulating the building and associated energy systems when they are exposed to different environmental and operating conditions. The core of the simulation is a model of the building that is based on fundamental heat balance principles.

Therefore, EnergyPlus carry out integrated simulations. This means that all three of the major parts, building, system, and plant, are solved simultaneously. During the calculations of the code with a sequential approach, the building zones, air handling systems, and central plant equipment are simulated consecutively by the internal software.

The sequential solution begins with a zone heat balance that updates the zone conditions and determines the heating/cooling loads at all time steps. This information is fed to the air handling simulation to determine the system response, but that response does not affect zone conditions. Similarly, the system information is passed to the plant simulation without feedback. This simulation technique works well when the system response is a well-defined function of the air temperature of the conditioned space.

The basis for the zone and air system integration is to formulate energy and moisture balances for the zone air and solve the resulting ordinary differential equations using a predictor-corrector approach. The formulation of the solution scheme starts with a heat balance on the zone air as detailed in the MODA sheet.

EnergyPlus provides three different solution algorithms to solve the zone air energy and moisture balance equations. These are defined in the Algorithm field in the Zone Air Heat Balance Algorithm object: the 3rd Order Backward Difference, the Euler Method and Analytical Solution. The first two methods use the finite difference approximation while the third uses an analytical result.

In building energy simulations, material properties are usually considered constant (i.e. independent of temperature, moisture content) except in the case of humid air. The main material properties that can be assigned are conductivity, density and specific heat. In addition, in EnergyPlus exists the internal database of materials and constructions, from ASHRAE and DOE-2 software, that can be assigned to the building surface.

Boundary conditions are expressed in terms of weather parameters, occupants' habits and HVAC control parameters, by means of schedules, typically with 1-hour time step scheduling

<u>Ansys Fluent (CETMA):</u>

ANSYS Fluent is a powerful and flexible general-purpose computational fluid dynamics software package used to model flow, turbulence, heat transfer, and reactions for industrial applications. The physical models allow accurate Computational Fluid Dynamics (CFD) analysis for a wide range of fluids problems, ranging from airflow over an aircraft wing to combustion in a furnace, from bubble columns to oil platforms, from blood flow to semiconductor manufacturing, and from cleanroom design to wastewater treatment plants.

Navier-Stokes equations are the governing equations of Computational Fluid Dynamics. It is based on the conservation law of physical properties of fluid.

For all flows, ANSYS Fluent solves conservation equations for mass and momentum. For flows involving heat transfer or compressibility, an additional equation for energy conservation is solved. For flows involving species mixing or reactions, conservation equations for the mixture fraction and its variance are solved. Additional transport equations are also considered when the flow is turbulent.

The CFD tool, ANSYS-Fluent, uses the Finite Volume Method (FVM) to solve the following conservation equations:

- The equation for conservation of mass, or continuity equation, it can be written as follows:

$$\frac{\delta\rho}{\delta t} + \nabla\cdot(\rho\vec{v}) = S_m$$

It is valid for incompressible as well as compressible flows.

The symbols in the equation are: ρ the density, t the time, v the overall velocity vector, S_m the source, it is the mass added to the continuous phase from the dispersed second phase (for example, due to vaporization of liquid droplets) and any user-defined sources.

- The equation for conservation of momentum in an inertial (non-accelerating) reference frame is described:

$$\frac{\delta}{\delta t}(\rho\vec{v}) + \nabla\cdot(\rho\vec{v}\vec{v}) = -\nabla p + \nabla(\bar{\bar{\tau}}) + \rho\vec{g} + \vec{F}$$

where p is the static pressure, $\bar{\bar{\tau}}$ is the stress tensor, and $\rho\vec{g}$ and $\vec{F}$ are the gravitational body force and external body forces (for example, that arise from interaction with the dispersed phase), respectively. $\vec{F}$ also contains other model-dependent source terms such as porous-media and user-defined sources.

The stress tensor $\bar{\bar{\tau}}$ is given by:

$$\bar{\bar{\tau}} = \mu\left[(\nabla\vec{v} + \nabla\vec{v}^T) - \frac{2}{3}\nabla\cdot\vec{v}I\right]$$

where μ is the molecular viscosity, I is the unit tensor, and the second term on the right-hand side is the effect of volume dilation.

- The equation for conservation of Energy

$$\frac{\delta}{\delta t}(\rho E) + \nabla\cdot\big(\vec{v}(\rho E + p)\big) = -\nabla\cdot\left(k_{eff}\nabla T - \sum\nolimits_j h_j\vec{J_j} + (\bar{\bar{\tau}}_{eff}\cdot\vec{v})\right) + S_h$$

where k_{eff} is the effective conductivity, and $\vec{J_j}$ is the diffusion flux of species j. The first three terms on the right-hand side of Equation represent energy transfer due to conduction, species diffusion, and viscous dissipation, respectively. S_h includes the heat of chemical reaction, and any other volumetric heat sources defined.

In the equation, the term E is:

$$E = h - \frac{p}{\rho} + \frac{v^2}{2}$$

where sensible enthalpy h is defined for ideal gases as:

$$h = \sum_j Y_j h_j$$

and for incompressible flows as:

$$h = \sum_j Y_j h_j + \frac{p}{\rho}$$

where the Y_j and h_j are respectively the mass fraction and the enthalpy of species j.

Resolving the differential equations described, it is possible to obtain the temperature, pressure and velocity fields inside the analysed ambient.

In a museum environment and historical building, the temporal stability and the spatial uniformity of the indoor microclimatic parameters are necessary, primarily for the correct artwork conservation and then for the occupant thermal comfort.

Thus, an air-conditioning system, working during all the year and characterized by high performances, is necessary: an optimal control is required as regards the indoor microclimatic parameter values [1], [2] that have to be stable over time and space; moderate energy costs are desirable too. Testing the Heating, Ventilation and Air-Conditioning systems (HVAC) performances becomes a fundamental practice inside the designing activity [3], [4], and using the numerical analyses is very convenient in order to predict the ability of the proposed system in maintaining the design data.

Comsol (TUG-IES):

TUG-IES is covering in Task 3.3 (Multi-physical environmental Simulations of CH Exhibition Impacts) the simulations of dust formation and accumulation with appropriate spatial resolution. To achieve these results, two different simulations are conducted, whereby the second simulation is built on the results of the first simulation. First, a computational fluid dynamic (CFD) simulation is performed on the basis of the IUAV model results and experimental sensor data from particulate matter (PM10, PM2.5), temperature and humidity sensors. The CFD simulations are based on the well-known Navier-Stokes equations. Second, particle tracing simulations are performed on the basis of the prior results of the CFD simulations. The particle tracing is based on Newton's law of motion. The simulations are accomplished in COMSOL Multiphysics 5.4 (COMSOL Multiphysics GmbH) which is built on the finite element method (FEM), where the computations of the whole domain are split into smaller, simpler steps. COMSOL enables the possibility to either couple different physical models or perform successive physical simulations based on the prior results. This facilitates the modelling of particle movement and accumulation on previous fluid dynamic simulations. From a geometrical point of view, the simulations are performed for a case study museums room provided by IUAV. Here, the openings (doors, windows), HVAC system or possible visitors are particle sources and have a major impact on the simulation. The boundary conditions are the walls and openings, temperature and humidity. Both simulations are conducted in air. The time scale of the simulations will be in the range of minutes for daily particle formation. The particle simulations take into account solid particles consisting of soot, mineral dust and other organic sources. COMSOL implements different numerical solvers for a variety of simulations/applications, whereby either a proper solver is chosen from the program or can be set from the user.

4. Conclusion

In this Workpage CETMA, USTUTT, IUAV, TUG, TTI, are currently collaborating for the integration of the numerical codes in order to simulate the effect of multi-physical environmental conditions on CH exhibitions. The different numerical models are linked to each other.

Using the software Energy Plus, IUAV can simulate the behaviour of a building envelope under specified boundary conditions in terms of weather, building use, occupation density and HVAC system type and control strategy.

The results have been the building heating/cooling loads, the average interior surface temperatures, the energy flux through the room walls, the volumetric airflow rate and the thermal–hygrometric conditions of the supply air.

These results have been used by CETMA as input data to carry out fluid-dynamic simulations. In particular, starting from the building energy simulation results, CETMA has realized a preliminary CFD model able to calculate the temperature, the humidity and the air velocity in every point of an exhibition room.

Unlike IUAV model which provides only average spatial values of the thermodynamic variables, CETMA numerical model is able to predict the thermal conditions in every point of the analysed room. In this way, it will be possible to prevent critical conditions and avoid the damage of artworks. The CH materials defined in the task 3.1 will be considered.

In the end, these CFD results will be provided to USTUTT for the micro/meso-scale deterioration modelling. Likewise, building energy and CFD results will be provided to TUG for the simulation of dust formation.

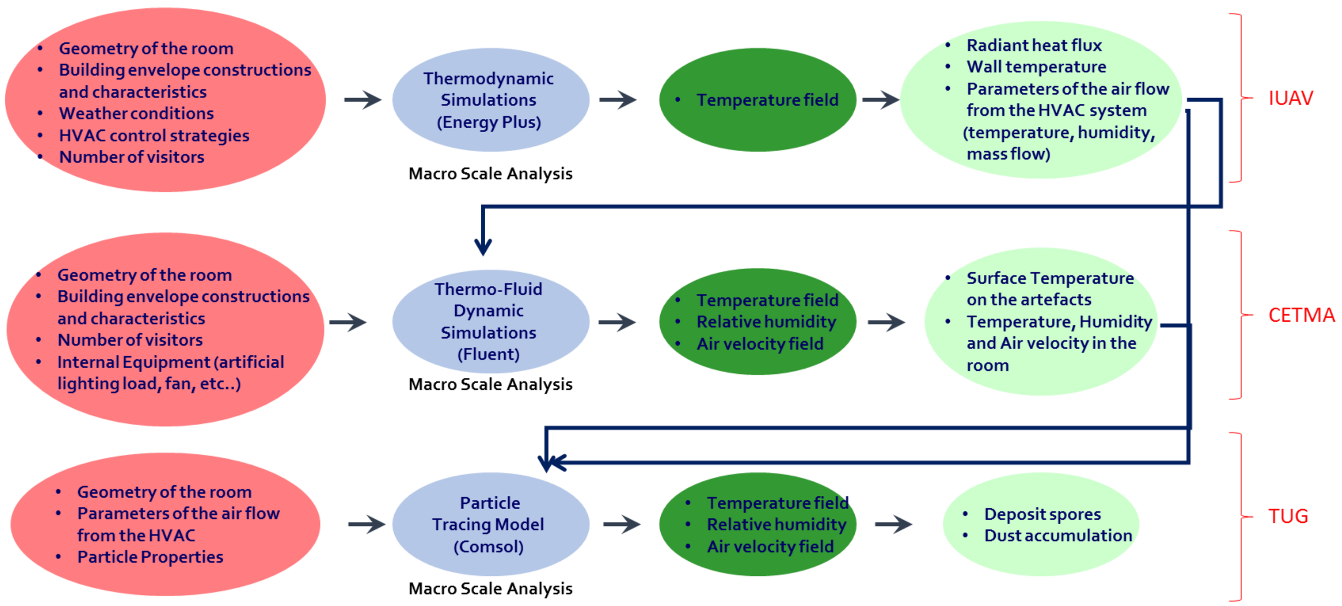
Using the software Comsol, TUG has developed a multi-physical model to simulate dust formation and accumulation. The boundary conditions for these simulationsare provided by the energy and CFD analyses.

Therefore, in this phase, the partners are testing the model and data exchange (input-output) among codes to settle the data of interest. In order to draw up a complete documentation of material models and simulations, this deliverable D.3.3 is a definition and organization of the multi-physical models to simulate different deterioration mechanisms of CH. The information are organized according to the “materials MOdelling DAta” (MODA), the description of simulations includes user case, model, solver and post-processor. Simulation workflows of the models, solvers and their implementation are also included in the MODA sheet.

5. Annex

Summary of the 3 Models (IUAV, CETMA, TUG)

1	USER CASE	Multi-physical environmental Simulations of CH Exhibition Impacts	
2	CHAIN OF MODELS	MODEL 1 (IUAV)	Thermal models based on well-established building energy software EnergyPlus.
		MODEL 2 (CETMA)	Impact of different elements (HVAC system operating conditions, solar radiation, building structure, visitors' presence) in terms of temperature, humidity and air velocity in every point of an indoor exhibition context by computational fluid-dynamic (CFD) analyses.
		MODEL 3A, 3B (TUG)	Aerosol formation as well as aerosol transport (diffusion, thermophoresis, and gravity) based on different numerical multi-physical models including dispersion and computational fluid dynamic (Particle Tracing and CFD).
3	PUBLICATION PEER-REVIEWING THE DATA		
4	ACCESS CONDITIONS		
5	WORKFLOW AND ITS RATIONALE		



MODEL 1 (IUAV)

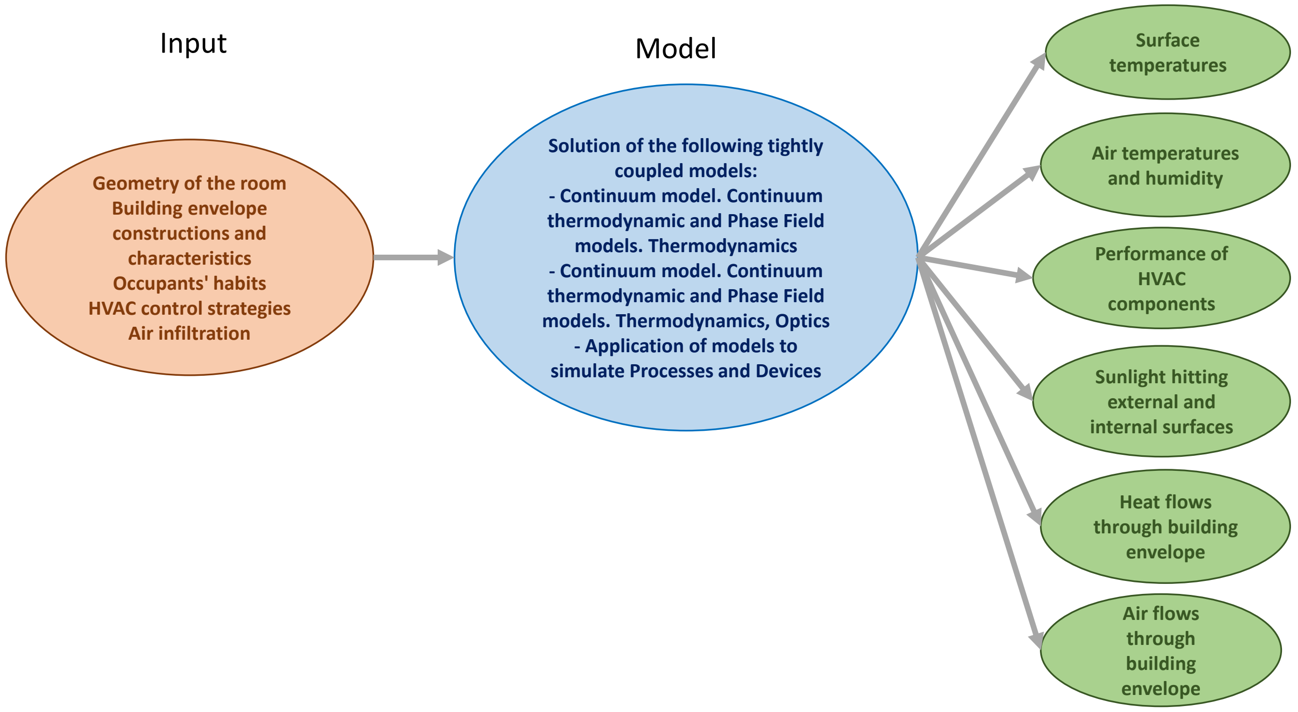
MOdelling DAta providing a description
for Building Energy Simulations
in project *SENSMAT*

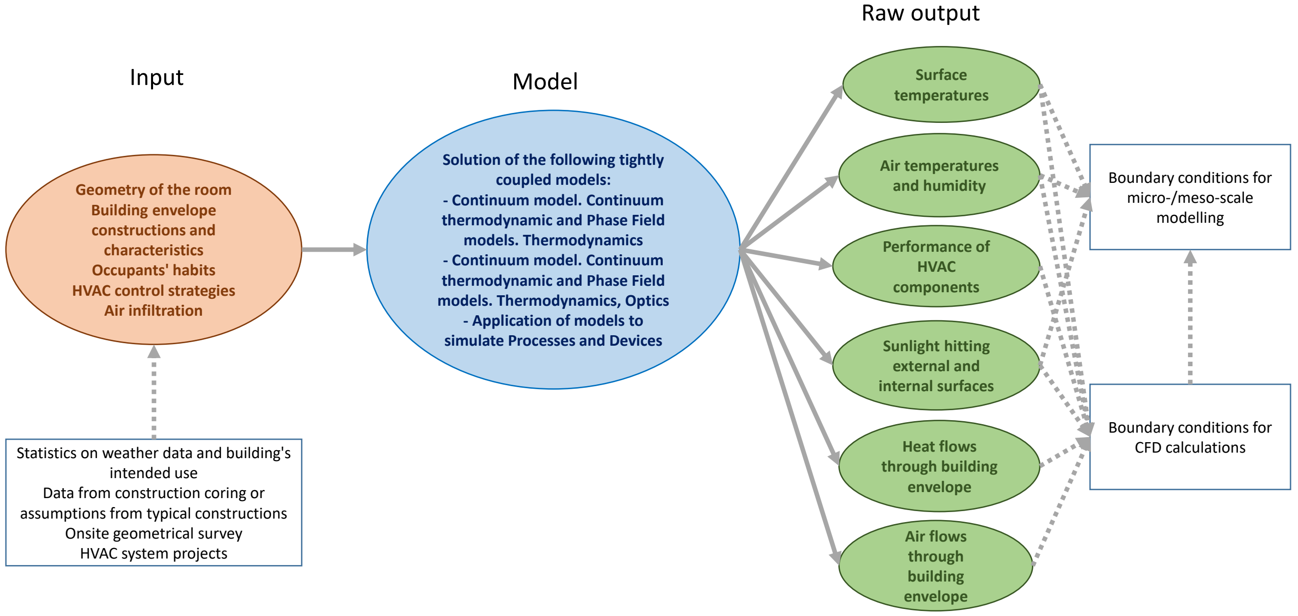
Data Owner [Massimiliano Scarpa, *IUAV*,
mscarpa@iuav.it]

OVERVIEW of the SIMULATION			
1	USER CASE	Building Energy Simulation for the prediction of room air and surface temperatures, as well as thermal and air flows in the room, depending on variable boundary conditions and complex HVAC (Heating, Ventilation and Air Conditioning) system components and control strategies. The object of the simulations is a room in the historical Palazzo Ducale, in Venice. This kind of simulations is usually performed by means of simulation engines discretizing the building envelope into large and homogeneous surfaces and include the simulation of HVAC systems and the action of weather and occupants on the heat, air and humidity balance of the room.	
2	CHAIN OF MODELS[4]	MODEL 1 (HEAT AND MOISTURE TRANSPORT + SOLAR RADIATION AND LIGHT + HVAC SYSTEM OPERATION)	The model consists of the simultaneous solution of the following models: - Continuum model. Continuum thermodynamic and Phase Change models. Thermodynamics. - Continuum model. Electromagnetism. Optics. - Application of models to simulate Processes and Devices.
		DATA MINING METHODOLOGY	The models may take advantage of data-based curves/correlations expressing the performance of materials and HVAC components.
3	PUBLICATION PEER-REVIEWING THE DATA	-	
4	ACCESS CONDITIONS	Software EnergyPlus (https://energyplus.net/) for building energy simulation, which is free and open-source software. EnergyPlus is funded by the U.S. Department of Energy's (DOE) Building Technologies Office (BTO) and managed by the National Renewable Energy Laboratory (NREL). EnergyPlus is developed in collaboration with NREL, various DOE National Laboratories, academic institutions, and private firms.	
5	WORKFLOW AND ITS RATIONALE	When coming to the calculation of the effects of weather conditions, occupants' behaviour and HVAC systems on the room heat- and humidity-balance, hence on temperature and humidity prediction, building energy simulation engines must be used. In fact, they consider the simulation dominium as a set of large and homogeneous surfaces and fictitious air and water nodes which allow to summarize the behaviour of such large spaces, constructions and equipments by means of large ensembles of material layers and devices, thus reducing calculation variables and time, compared to simulation software based on microscopic continuum models. Moreover, the node-based models characterizing many parts of building	

		energy simulation engines make it possible to include the simulation of HVAC devices acting on the indoor environment by means of real performance tables and HVAC system management algorithms. All of these features allow the user to assess indoor environment (i.e. inside the rooms) characteristics, such as temperature, humidity and air flows, even along the whole year, with a fine time discretization (typically, 10 minutes per calculation timestep) and considering various boundary conditions (in terms of weather conditions and occupants' behaviour), HVAC system layouts and system management strategies. Thus, building enegy simulation tools are meant to link the macro-scale world with the micro-/meso-scale. In this field, EnergyPlus is a well-acknowledged and validated software, used as a reference in building energy simulation at an International level.

Workflow picture





MODEL 1 (IUAV)

1 ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED

1.1 ASPECT OF THE USER CASE TO BE SIMULATED

Boundary conditions such as weather data, programmed HVAC operation and internal heat gains greatly affect energy simulation results. They are summarized below:

- *Weather conditions:*

Type of reference day	Ref. calendar day	Outdoor air dry bulb temperature [°C]		Outdoor air wet-bulb temperature [°C]	Sky clearness
		Max	Min		
Mid-season	21^{st} of April	16.2	9.7	8.0	0.7
Winter design day	21^{st} of December	-4.0	-4.0	-4.0	0.0
Summer design day	21^{st} of July	31.1	22.3	23.5	1.0

- *Internal heat gains*

Category	Nominal value	Daily scheduling	
		Time [hh:mm→hh:mm]	Fraction [%]
People	5 people	00:00→08:00	0%
		08:00→20:00	100%
		20:00→24:00	0%
Lights	10 W/m^2	00:00→08:00	0%
		08:00→20:00	100%
		20:00→24:00	0%

- *Indoor environment control temperatures*

Scope	Daily scheduling	
	Time	Control temperature [°C]
Heating	00:00→08:00	18
	08:00→20:00	21
	20:00→24:00	18
Cooling	00:00→08:00	28
	08:00→20:00	26
	20:00→24:00	28

- *Indoor environment control humidity levels:*

Scope	Value [%]
Humidification	40
Dehumidification	55

- *Infiltration air flow rate: 0.4 air changes per hour*

1.2 **MATERIAL**

Construction and relevant materials were hypothesized based on typical historical buildings in Venice.

The following constructions, with related material layers, were used:

Construction	Layer	Description	Thickness [m]	Th. conductivity [W/(m·K)]	Density [kg/m³]	Specific heat [J/(kg·K)]	R [m²·K/W]	Total th. conductance [W/(m²·K)]
Floor	01 (Ext)	Plaster	0.03	0.6	2200	900		0.80
	02	Wood	0.20	0.17	700	2000		
	03 (Int)	Marble	0.05	2.5	2700	880		
External wall	01 (Ext)	Bricks	0.36	1.31	2200	900		1.66
	02	Plaster	0.03	0.6	2200	900		
	03	Air	0.2				0.16	
	04 (Int)	Wood	0.02	0.17	700	2000		
Ceiling	01 (Ext)	Marble	0.05	2.5	2700	880		0.80
	02	Wood	0.20	0.17	700	2000		
	03 (Int)	Plaster	0.03	0.6	2200	900		
Internal wall	01 (Ext)	Plaster	0.03	0.6	2200	900		0.96
	02	Bricks	0.12	1.31	2200	900		
	03	Plaster	0.03	0.6	2200	900		
	04	Air	0.2				0.16	
	05 (Int)	Wood	0.02	0.17	700	2000		

1.3 **GEOMETRY**

A room (ref.: Figure 1) of Palazzo Ducale (ref.: Figure 2) of the following sizes is considered:

- Width: 9 m
- Length: 8 m
- Height: 6 m

Actually, in the current (and simulated) layout, the room has no accessible window. In fact, the external wall is covered by an opaque double wall hampering sunlight to hit art masterpieces and reserving space to a temporary air-conditioning system.

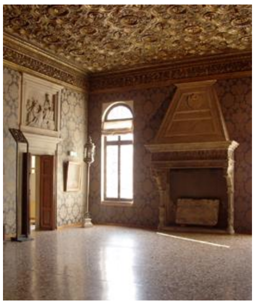


Figure 1 – View of the simulated room.

		 *Figure 2 – External view of Palazzo Ducale (Venice).*
1.4	**TIME LAPSE**	The simulations may cover a time period spanning from 1 day to several years. However, in the present case, 3 days are considered: - Winter design day - Summer design day - Typical day of intermediate season
1.5	**MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS**	The following main sets of boundary conditions are considered: - Weather, derived from actual measurements in the same area where the building is sited. - Occupants' habits and HVAC system control strategies, which may be derived after statistical analysis.
1.6	**PUBLICATION ON THIS DATA**	-

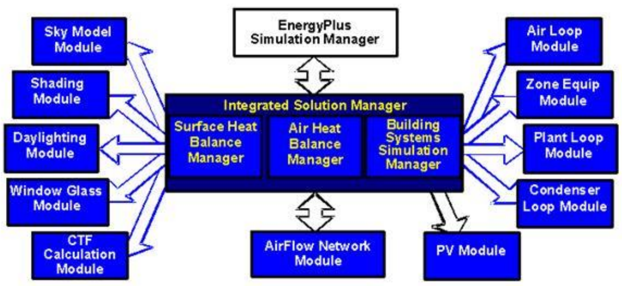
2	**GENERIC PHYSICS OF THE MODEL EQUATION**		
2.1	**MODEL TYPE AND NAME**	Solution of the following tightly coupled models: - Continuum model. Continuum thermodynamic and Phase Change models. Thermodynamics. - Continuum model. Electromagnetism. Optics. - Application of models to simulate Processes and Devices	
2.2	**MODEL ENTITY**	Finite volumes	
2.3	**MODEL PHYSICS/ CHEMISTRY EQUATION** **PE**	**Equation**	From the documentation of EnergyPlus (Engineering Reference): << The basis for the zone and air system integration is to formulate energy and moisture balances for the zone air and solve the resulting ordinary differential equations using a predictor-corrector approach. The formulation of the solution scheme starts with a heat balance on the zone air. $$C_z\frac{dT_z}{dt}=\sum_{i=1}^{N_{sl}}\dot{Q}_i+\sum_{i=1}^{N_{surfaces}}h_iA_i\left(T_{si}-T_z\right)+\sum_{i=1}^{N_{zones}}\dot{m}_iC_p\left(T_{zi}-T_z\right)+\dot{m}_{\inf}C_p\left(T_{\infty}-T_z\right)+\dot{Q}_{sys}$$ If the air capacitance is neglected, the steady-state system output must be: $$-\dot{Q}_{sys}=\sum_{i=1}^{N_{sl}}\dot{Q}_i+\sum_{i=1}^{N_{surfaces}}h_iA_i\left(T_{si}-T_z\right)+\sum_{i=1}^{N_{zones}}\dot{m}_iC_p\left(T_{zi}-T_z\right)+\dot{m}_{\inf}C_p\left(T_{\infty}-T_z\right)$$ >>

		Physical quantities	From the documentation of EnergyPlus (Engineering Reference): << $\sum_{i=1}^{N_{sl}} \dot{Q}_i$ = sum of the convective internal loads $\sum_{i=1}^{N_{surfaces}} h_i A_i (T_{si} - T_z)$ = convective heat transfer from the zone surfaces $\dot{m}_{\text{inf}} C_p (T_\infty - T_z)$ = heat transfer due to infiltration of outside air $\sum_{i=1}^{N_{zones}} \dot{m}_i C_p (T_{zi} - T_z)$ = heat transfer due to interzone air mixing $\dot{Q}_{sys}$ = air systems output $C_z \frac{dT_z}{dt}$ = energy stored in zone air $C_z = \rho_{air} C_p C_T$ ρ_{air} = zone air density C_p = zone air specific heat C_T = sensible heat capacity multiplier (Detailed description is provided below) >>

2.4	**MATERIALS RELATIONS**	**Relation**	In building energy simulations, material properties are usually considered constant (i.e. independent of temperature, moisture content, …), except in the case of: - Humid air. In the case of humid air, the fundamental property in heat exchange and energy balances is enthalpy, which depends on humidity ratio as follows: $h_{\text{Humid Air}} = h_{\text{Dry Air}} + x \cdot h_{\text{Water Vapour}} = c_{\text{p,Dry Air}} \cdot \theta + (r + c_{\text{p,Water Vapour}} \cdot \theta)$, where: ○ h = enthalpy ○ x = humidity ratio ○ c_p = specific heat ○ θ = temperature ○ r = evaporation heat Moreover, humidity may affect heat transmission and that can be taken into consideration via the HAMT (combined Heat and Moisture Transfer) finite solution algorithm. It is a completely coupled, one-dimensional, finite element, heat and moisture transfer model, which simulates the movement and storage of heat and moisture in surfaces simultaneously from/to the rooms and the outdoor environment. The theoretical model which consistutes the base for the HAMT model is based on the following equation: $\frac{\partial H}{\partial T}\frac{\partial T}{\partial \tau} = \frac{\partial}{\partial x}\left(k^w \frac{\partial T}{\partial x}\right) + h_v \frac{\partial}{\partial x}\left(\frac{\delta}{\mu}\frac{\partial T}{\partial x}\right)$, where: ○ ∂H/∂T = Moisture dependent heat storage capacity ○ T = Temperature ○ τ = Time ○ x = Distance between cell centers ○ k^w = Moisture dependent thermal conductivity ○ h_v = Evaporation enthalpy of water ○ δ = Vapor diffusion coefficient in air ○ μ = Moisture dependent vapor diffusion resistance factor The three terms in the equation describe the storage, transport and generation of heat respectively. - Thermochromic glasses. In thermocromic glasses, optical properties greatly vary with temperature. In fact, they absorb sunlight and turn the sunlight energy into heat, which warms up the glass and special films that decrease their own optical transmission properties when the temperature increases. This behaviour can be simulated in EnergyPlus, by means of a series of sets of optical coefficients. Each set of optical coefficients is associated to a reference temperature. The EnergyPlus calculation engine, at each simulation time-step (for instance, every 10 minutes in a 1 year-long simulation), calculates the temperature of the glass (based on current weather conditions and solar shading devices operation) and finds the most appropriate set of optical coefficients, which are then used in the calculation of the sunlight absorption in the glasses, in order to better calculate the actual temperature of the glass, in an iterative process. This approach makes it possible to use data coming from typical catalogues of thermocromic glasses. - Phase-Change Materials (PCM). In the building energy design, PCM are materials changing their phase (from solid to liquid and viceversa) at temperatures in the range of comfort conditions. For instance, during a summer day with sun shining and internal heat gains in the room, the phase

			change taking place in a PCM at, for instance, 25°C makes it possible to store very much heat before the temperature of the wall gets increasing again. This way, overheating in the room has lower occurrences. EnergyPlus can take into consideration this behavior. For this purpose, constructions including PCMs are simulated by means of a finite difference approach, solved via a Crank-Nicholson or a fully implicit algorithm: ○ In the case of a Crank-Nicholson approach, the base equation is (ref.: EnergyPlus Documentation – Engineering Reference): $$C_p\rho\Delta x\frac{T_i^{j+1}-T_i^j}{\Delta t}=\frac{1}{2}\left(k_W\frac{T_{i+1}^{j+1}-T_i^{j+1}}{\Delta x}+k_E\frac{T_{i-1}^{j+1}-T_i^{j+1}}{\Delta x}+k_W\frac{T_{i+1}^{j}-T_i^{j}}{\Delta x}+k_E\frac{T_{i-1}^{j}-T_i^{j}}{\Delta x}\right),$$ where: ▪ T = node temperature ▪ Δt = calculation time step ▪ Δx = finite difference layer thickness ▪ C_p = specific heat of material ▪ k_W = thermal conductivity for interface between node i and node i + 1 ▪ k_E = thermal conductivity for interface between node i and node i − 1 ▪ ρ = density of material ▪ i = node being modeled ▪ i + 1 = adjacent node to interior of construction ▪ i − 1 = adjacent node to exterior of construction ▪ j + 1 = new time step ▪ j = previous time step Then, the correspondance between temperature and enthalpy is verified by means of the next equation: $$h_i=\mathrm{HTF}\left(T_i\right),$$ where: ▪ HTF is an enthalpy-temperature function using user input data for the specific PCM. ○ In case of fully implicit algorithm, the following base equation is applied: $$C_p\rho\Delta x\frac{T_i^{j+1}-T_i^j}{\Delta t}=\left(k_W\frac{T_{i+1}^{j+1}-T_i^{j+1}}{\Delta x}+k_E\frac{T_{i-1}^{j+1}-T_i^{j+1}}{\Delta x}\right),$$ with the same symbols as in the case of the Crank-Nicholson algorithm.
		Physical quantities/ descriptors for each MR	Main material properties: - Thermal conductivity - Density - Specific heat
2.5	**PHYSICS FORMULATION OF THE CONDITIONS**	Boundary conditions are expressed in terms of weather parameters, occupants' habits and HVAC control parameters, by means of schedules, typically with 1-hour time step scheduling.	

2.6	**SIMULATED INPUT**	The input data is not simulated and it is a result of:
		- Measurements about:
		  ○ Geometry and shape of the room
		- Assumptions (where possible, based on interviews with staff members) about:
		  ○ Constructions
		  ○ Occupation schedule
		  ○ Operation of the HVAC system
		  ○ Weather conditions, also based on standards and statistical analyses

3	**SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS**		
3.1	**NUMERICAL SOLVER**	The solver is based on simultaneous solution of heat and mass (air and water vapour) transfer equations, by an iterative algorithm. The heat transfer through surfaces is usually based on conduction transfer functions, but conduction finite-difference calculation scheme is available as well.	
3.2	**SOFTWARE TOOL**	Software EnergyPlus (https://energyplus.net/) for building energy simulation, which is free and open-source software. EnergyPlus is funded by the U.S. Department of Energy's (DOE) Building Technologies Office (BTO) and managed by the National Renewable Energy Laboratory (NREL). EnergyPlus is developed in collaboration with NREL, various DOE National Laboratories, academic institutions, and private firms.	
3.3	**TIME STEP**	The time step for the solution of the energy balance for the whole building may vary from 1 minute to 1 hour, in terms of (integer) number of time steps per hour.	
3.4	**COMPUTATIONAL REPRESENTATION**	**PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL**	Calculations based on discrete representations of surfaces, air nodes, HVAC system nodes and HVAC system components. The scheme of EnergyPlus calculations is given below.  *Source: https://energyplus.net/*
3.5	**COMPUTATIONAL BOUNDARY CONDITIONS**	Boundary conditions relate to: - Weather - Occupants' behaviour, including the use of electrical devices, lights, hot water,… as well as thermostat and humidistat settings - Ventilation requirements - HVAC control strategies - Presence of particular environments adjacent to the simulated ones, such as ground, adiabatic surfaces or surfaces adjacent to rooms with imposed temperature.	

3.6	**ADDITIONAL SOLVER PARAMETERS**	The main additional solver parameters consist of:
		- Loads Convergence Tolerance Value [%]:
		  ○ Min: 0.0001
		  ○ Max: 0.5
		- Temperature Convergence Tolerance Value [K]:
		  ○ Min: 0.0001	

		○ Max: 0.5 - Minimum Number of Warmup Days [days]: ○ Min: 25 - Maximum Number of Warmup Days [days]: ○ Min: 6 - Shadow Calculation – Calculation Frequency [days]: ○ Min: 1 ○ Max: 31 - Minimum System Timestep [1/h]: ○ Min: 0 ○ Max: 60 - Maximum HVAC Iterations [min]: ○ Min: 1 - Minimum Plant Iterations [min]: ○ Min: 1 - Maximum Plant Iterations [-]: ○ Min: 2 In addition, more parameters are considered for specific elements or HVAC components.

4	POST PROCESSING	
4.1	THE PROCESSED OUTPUT	No post-processing procedure is currently considered.
4.2	METHODOLOGIES	No post-processing procedure is currently considered.
4.3	MARGIN OF ERROR	No post-processing procedure is currently considered.

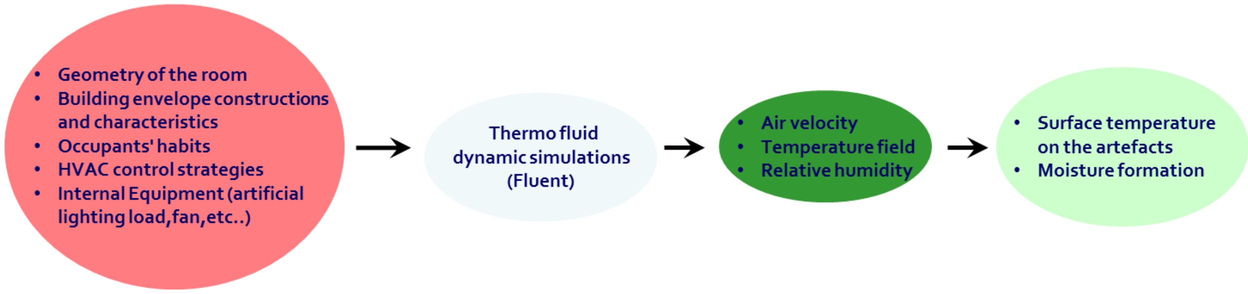
MODEL 2 (CETMA)

MOdelling DAta providing a description
for CFD Simulations of an indoor exhibition context
in project SENSMAT

Data Owner [Antonio Gerardi, CETMA,
antonio.gerardi @cetma.it]

OVERVIEW of the SIMULATION			
1	USER CASE	Impact of different elements (HVAC system operating conditions, solar radiation, building structure, visitors' presence) in terms of temperature, humidity and air velocity in every point of an indoor exhibition context by computational fluid-dynamic (CFD) analyses.	
2	CHAIN OF MODELS[5]	MODEL 1	The model represents the flow in an indoor museum environment. It' a mixture of two phases (air and water vapor) with energy transport and possible phase change (condensation).
		DATA MINING METHODOLOGY	The models may take advantage of data-based curves/correlations expressing the performance of materials.
3	PUBLICATION PEER-REVIEWING THE DATA	– Cătălin-George Popovicia, Valeriu Sebastian Hudi·teanua, "Numerical simulation of HVAC system functionality in a sociocultural building", Procedia Technology 22 (2016) 535 – 542 – Pietro Mazzei, Alfonso Capozzoli, Francesco Minichiello, Daniele Palma, "HVAC SYSTEMS TO CONTROL MICROCLIMATE IN THE MUSEUMS". Delia D'Agostino, Paolo Maria Congedoa, Rosella Cataldo, "Ventilation control using computational fluid-dynamics (CFD) modelling for cultural buildings conservation", Procedia Chemistry 8 (2013) 83 – 91	
4	ACCESS CONDITIONS	Simulation of CFD models carried out with commercial software Ansys Fluent (https://www.ansys.com) Input data: proprietary of the CAD models from the museums or scanner	
5	WORKFLOW AND ITS RATIONALE	The selected model to describe the indoor exhibition environment is the Continuum model: the fluid domain is a mixture of two phases (air and water vapor) with energy transport and possible phase change (condensation). The results from IUAV studies provide the boundary conditions, like the building heating/cooling loads, the average interior surface temperatures, the energy flux through the room walls, the volumetric airflow rate and the thermal–hygrometric conditions of the supply air. The thermo fluid-dynamic analyses allow to evaluate of the spatial uniformity of microclimatic parameters, such as the contaminant distribution inside indoor spaces and to study the indoor airflow induced by mechanical ventilation and air-conditioning systems.	

Workflow picture



MODEL 2 (CETMA)

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	Study of the indoor microclimatic parameter values (temperature, humidity, and air velocity) in the exhibition room, varying different elements (HVAC system operating conditions, solar radiation, building structure, visitors' presence). The case study is a selected room of Palazzo Ducale, in Venice. The goal is to predict the thermodynamical condition in every point of the analysed room and the humidity formation. So it will be possible to prevent critical conditions and avoid the damage to artworks
1.2	MATERIAL	Air and water vapor Walls materials: marble, wood, bricks, plaster Artworks material
1.3	GEOMETRY	Simulated room as provided by IUAV.
1.4	TIME LAPSE	The simulations conditions cover all the year, so three rappresentative days are considered: - Winter design day, - Summer design day, - Typical day of intermediate season.
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	CFD boundary conditions as regards the energy flux through the room walls and the thermal–hygrometric conditions of the supply air, are provided by using the BEPS program.
1.6	PUBLICATION ON THIS DATA	Fabrizio Ascione, Laura Bellia, Alfonso Capozzoli, "A coupled numerical approach on museum air conditioning: Energy and fluid-dynamic analysis", Applied Energy 103 (2013) 416–427

2	GENERIC PHYSICS OF THE MODEL EQUATION		
2.1	MODEL TYPE AND NAME	Continuum model: the flux is a mixture of two phases (air and water vapor) with energy transport and possible phase change (condensation).	
2.2	MODEL ENTITY	Continuum volume entity	
2.3	MODEL PHYSICS/ CHEMISTRY EQUATION PE	**Equation**	Balance equations of mass: $\frac{\delta \rho}{\delta t} + \nabla \cdot (\rho \vec{v}) = S_m$ Balance equations of momentum: $\frac{\delta}{\delta t}(\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla(\bar{\bar{\tau}}) + \rho \vec{g} + \vec{F}$ Balance equations of energy: $\frac{\delta}{\delta t}(\rho E) + \nabla \cdot (\vec{v}(\rho E + p)) = -\nabla \cdot \left(k_{eff} \nabla T - \sum_j h_j \vec{J_j} + (\bar{\bar{\tau}}_{eff} \cdot \vec{v})\right) + S_h$
		Physical quantities	Density, pressure, temperature, velocity, conductivity
2.4	MATERIALS RELATIONS	**Relation**	For air and water vapour: Ideal Gas Law: $\rho = \frac{p}{\frac{R}{M_w} T}$
		Physical quantities/ descriptors for each MR	Density, pressure, temperature, molar mass.
2.5	PHYSICS FORMULATION OF THE CONDITIONS		
2.6	SIMULATED INPUT	The input data provided by the museum are: – Geometry and shape of the room, walls structures, – Conditions (temperature, humidity, mass flow) of the air flow from the HVAC system, (provided by BEPS analysis); – Number of persons, – Position of electrical equipment, – Wall's temperature (provided by BEPS analysis).	

3	SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS		
3.1	NUMERICAL SOLVER	Finite volume - Pressure-based solver	
3.2	SOFTWARE TOOL	Ansys Fluent	
3.3	TIME STEP	From one hour to one day.	
3.4	COMPUTATIONAL REPRESENTATION	PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL	The pressure-based solver employs an algorithm which belongs to a general class of methods called the projection method. In the projection method, wherein the constraint of mass conservation (continuity) of the velocity field is achieved by solving a pressure (or pressure correction) equation. The pressure equation is derived from the continuity and the momentum equations in such away that the velocity field, corrected by the pressure, satisfies the continuity. Since the governing equations are nonlinear and coupled to one another, the solution process involves iterations wherein the entire set of governing equations is solved repeatedly until the solution converges.
3.5	COMPUTATIONAL BOUNDARY CONDITIONS	The external wall conditions provided by BEPS are considered as an energy flux through the walls. The internal walls are considered adiabatic. The occupants in the room and the electrical equipment are considered as thermal loads.	
3.6	ADDITIONAL SOLVER PARAMETERS		

4	POST PROCESSING	
4.1	THE PROCESSED OUTPUT	The main results are: – temperature, humidity and air velocity in every point of the museum room, – surface temperature and humidity on the artefacts.
4.2	METHODOLOGIES	In the post-processing of the simulation results additional operations as averaging, filtering, interpolation, deriving and differentiating can support and detail the analysis.
4.3	MARGIN OF ERROR	The deviation among experimental and numerical results must be < 5%

MODEL 3 (TUG)

MOdelling DAta providing a description

for Simulation of dust formation and dust accumulation

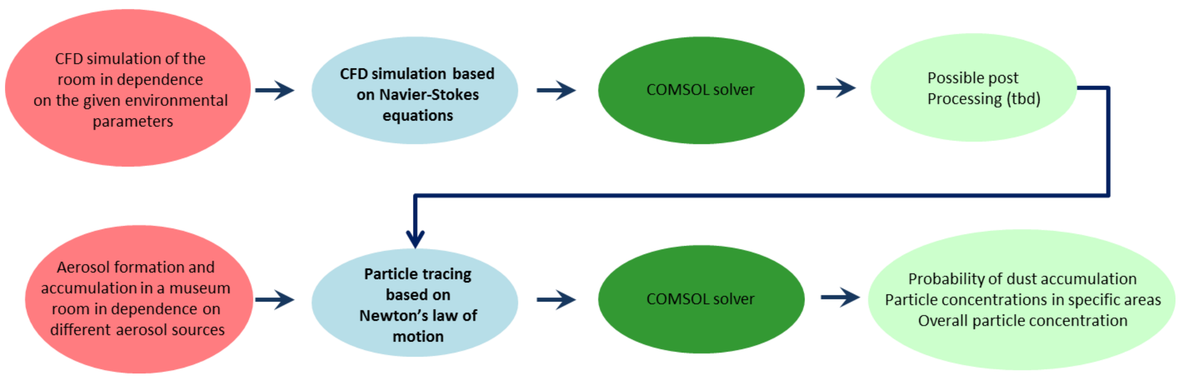
in project SENSMAT

Data Owner [Markus Knoll, *TUG*,

markus.knoll@tugraz.at]

OVERVIEW of the SIMULATION			
1	USER CASE	Simulation of dust formation and dust accumulation with appropriate spatial resolution on basis of the prior simulation results of IUAV (room geometries, doors, HVAC system, temperature field) and CETMA (flow field). Particle simulations are carried out for different particle sizes, inlet velocities and locations of doors and HVAC system.	
2	CHAIN OF MODELS	MODEL A	Computation Fluid Dynamics (CFD) simulation based on boundary conditions provided by IUAV.
		MODEL B	Particle Tracing (using Newton's law of motion) based on the prior simulated flow field of the CFD simulation.
		DATA MINING METHODOLOGY	-
3	PUBLICATION PEER-REVIEWING THE DATA	-	
4	ACCESS CONDITIONS	COMSOL Multiphysics 5.4, COMSOL Inc., Proprietary EULA license, https://www.comsol.com/	
5	WORKFLOW AND ITS RATIONALE	CFD simulation in combination with particle tracing is an appropriate method for simulating particle behaviour (formation and accumulation) in dependence of temperature, air flow (HVAC system, doors), particle size and number, etc. in micro and macro sized geometrical conditions.	

Workflow picture



MODEL 3A (TUG) Computation Fluid Dynamics (CFD)

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	A CFD simulation of the exhibition room (geometries provided by IUAV) is carried out on the basis of the preceding simulation results and in dependence of the given environmental parameters: • Air flow (HVAC system, doors) • Temperature • Humidity Additionally, simulations are carried out for modified geometries which include windows in the room to model different real life aspects on the impacts of the resulting velocity field.
1.2	MATERIAL	Air
1.3	GEOMETRY	Exhibition room as provided by IUAV Additional simulations for adapted geometries including windows.
1.4	TIME LAPSE	Time scale provided by IUAV. In macro scale, for three different cases: • Winter season day • Summer season day • Intermediate season day
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	Boundary conditions • Openings (doors, windows, HVAC system) • Walls • Temperature (Openings, walls, room) Global conditions • Temperature • Humidity
1.6	PUBLICATION ON THIS DATA	

<table>
<tr><th>2</th><th colspan="3">GENERIC PHYSICS OF THE MODEL EQUATION</th></tr>
<tr><td>2.1</td><td>MODEL TYPE AND NAME</td><td colspan="2">Single phase flow based on the well-known Navier-Stokes (RANS) equations. As interface a turbulent flow, k-ε model is used. The flow near to walls is modelled using wall functions.</td></tr>
<tr><td>2.2</td><td>MODEL ENTITY</td><td colspan="2">Finite volumes</td></tr>
<tr><td rowspan="2">2.3</td><td rowspan="2">MODEL PHYSICS/ CHEMISTRY EQUATION
PE</td><td>Equation</td><td>Turbulent flow theory, based on Navier-Stokes equations (CFD simulation):
For a incompressible and Newtonian fluid it is assumed:
$$\rho\frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot[-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)] + \mathbf{F}$$
$$\rho\nabla\cdot\mathbf{u} = 0$$
The k-ε model introduces two additional transport equations. The turbulent viscosity is defined as
$$\mu_T = \rho C_\mu\frac{k^2}{\varepsilon}$$
, further is the turbulent kinetic energy, k, given as
$$\rho\frac{\partial k}{\partial t} + \rho\mathbf{u}\cdot\nabla k = \nabla\cdot\left(\left(\mu + \frac{\mu_T}{\sigma_k}\right)\nabla k\right) + P_k - \rho\varepsilon$$
, and the turbulent dissipation rate, ε, is defined as follows:
$$\rho\frac{\partial \varepsilon}{\partial t} + \rho\mathbf{u}\cdot\nabla\varepsilon = \nabla\cdot\left(\left(\mu + \frac{\mu_T}{\sigma_\varepsilon}\right)\nabla\varepsilon\right) + C_{\varepsilon 1}\frac{\varepsilon}{k}P_k - C_{\varepsilon 2}\rho\frac{\varepsilon^2}{k}$$
(Equations from COMSOL user guides)</td></tr>
<tr><td>Physical quantities</td><td>Involved physical quantities:
• Velocity field (u)
• Pressure (p)
• Turbulent kinetic energy (k)
• Turbulent dissipation rate (ε)</td></tr>
<tr><td rowspan="2">2.4</td><td rowspan="2">MATERIALS RELATIONS</td><td>Relation</td><td>For air, the ideal gas law is given as:
$$\rho = \frac{pM}{RT}$$</td></tr>
<tr><td>Physical quantities/
descriptors for each MR</td><td>Involved physical quantities:
• Densitiy of the gas (ρ)
• Pressure (p)
• Universal gas constant (R)
• Molecular weight of the gas (M)
• Temperature (T)</td></tr>
<tr><td>2.5</td><td>PHYSICS FORMULATION OF THE CONDITIONS</td><td colspan="2"></td></tr>
</table>

2.6	**SIMULATED INPUT**	The simulated input is provided by IUAV and the exhibition museum room: • Geometries (room) • Interfaces (doors, windows, HVAC system) • Conditions (temperature, humidity)

3	SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS		
3.1	NUMERICAL SOLVER	Stationary COMSOL Solver	
3.2	SOFTWARE TOOL	COMSOL Multiphysics 5.4	
3.3	TIME STEP		
3.4	COMPUTATIONAL REPRESENTATION	PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL	
3.5	COMPUTATIONAL BOUNDARY CONDITIONS		
3.6	ADDITIONAL SOLVER PARAMETERS	Solver: Smoothed aggregatic	

4	POST PROCESSING	
4.1	THE PROCESSED OUTPUT	• Pressure • Temperature • Velocity field
4.2	METHODOLOGIES	Statistical evaluation of the measurement results
4.3	MARGIN OF ERROR	To be evaluated

MODEL 3B (TUG) particle tracking

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	Aerosol formation and accumulation in the provided exhibition museum room in dependence on different aerosol sources • Visitors (human) • Openings (doors, windows, HVAC system) • Ambient air quality in real world museum rooms (measured concentrations) • Etc. and on the basis of the previous EnergyPlus (IUAV) and CFD simulation (velocity field). The simulations are applied in macro scale (formation, accumulation) and micro scale (accumulation on different surfaces, materials)
1.2	MATERIAL	Aerosol formation and accumulation are simulated in air. The simulation takes into account solid particles only consisting of soot, mineral dust and other organic sources.
1.3	GEOMETRY	Simulated room as provided by IUAV Additional simulations for adapted geometries including windows.
1.4	TIME LAPSE	Time scale provided by IUAV. In macro scale, for three different cases: • Winter season day • Summer season day • Intermediate season day
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	Boundary conditions from previous CFD simulation
1.6	PUBLICATION ON THIS DATA	

2	GENERIC PHYSICS OF THE MODEL EQUATION		
2.1	MODEL TYPE AND NAME	Particle tracing based on Newton's law of motion.	
2.2	MODEL ENTITY	Finite volumes, particles	
2.3	MODEL PHYSICS/ CHEMISTRY EQUATION **PE**	**Equation**	*Newton's second law (Particle tracing):* $\frac{d}{dt}(m_p \mathbf{v}) = \mathbf{F}_D + \mathbf{F}_g + \mathbf{F}_{\text{ext}}$ *(Equations from COMSOL user guides)*
		Physical quantities	Involved physical quantities: • Particle mass (m_p) • Velocitiy field (v) • Drag force (F_D) • Gravity force (F_g) • External forces (F_{ext})
2.4	MATERIALS RELATIONS	**Relation**	Material properties of the particulates are assumed to be constant for the simulation time. Simulations are performed in air. For air, the ideal gas law is given as: $\rho = \frac{pM}{RT}$
		Physical quantities/ **descriptors for each MR**	Material properties of the surrounding gas: Air Material properties of the particulates: • Density (ρ=2250 kg/m³) • Size (for different particle diameters between 100 nm and 10µm) • Shape (a spherical shape is assumed) For the ideal gas law: • Densitiy of the gas (ρ) • Pressure (p) • Universal gas constant (R) • Molecular weight of the gas (M) • Temperature (T)
2.5	PHYSICS FORMULATION OF THE CONDITIONS		
2.6	SIMULATED INPUT	• Simulation result of previous CFD simulation • Measured air quality in real world museum rooms • The simulated input from the previous CFD simulations (see above)	

3	SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS		
3.1	NUMERICAL SOLVER	Time-Dependent COMSOL Solver	
3.2	SOFTWARE TOOL	COMSOL Multiphysics 5.4	
3.3	TIME STEP	Time steps may vary dependent if a short term or long term dust formation and accumulation is simulated. Timesteps are in the range of seconds.	
3.4	COMPUTATIONAL REPRESENTATION	PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL	
3.5	COMPUTATIONAL BOUNDARY CONDITIONS		
3.6	ADDITIONAL SOLVER PARAMETERS	Nonlinear method: Constant (Newton)	

4	POST PROCESSING	
4.1	THE PROCESSED OUTPUT	• Probability of dust accumulation in specific areas of the room • Particle concentrations in specific room areas • Overall particle concentration in the room
4.2	METHODOLOGIES	• Statistical evaluation of the measurement results • Volume averaging • Dust accumulation • Post CFD particle agglomeration calculation
4.3	MARGIN OF ERROR	To be evaluated

6. Reference

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