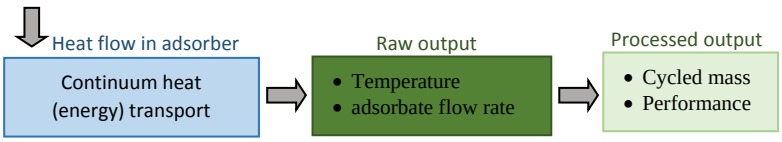
Elements in materials modelling

Each simulation will have its own 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.

THE SIMULATION GENERAL DESCRIPTION			
1	USER CASE	Heat flow in an absorber	
2	CHAIN OF MODELS	MODEL 1	*Modelling projects consist of a chain of models, (workflow). All models should be identified as electronic, atomistic, mesoscopic or continuum and the related chapter in Review of Materials Modelling IV available on http://ec.europa.eu/research/industrial_technologies/e-library.cfm) should be given.* Continuum heat (energy) transport equation
		MODEL 2	none
		...	...
3	PUBLICATION	*Please give the publication which documents the work flow if available*	
4	ACCESS CONDITIONS	*Please list whether the model and/or data are free, commercial or open source.* *Please list the owner and the name of the software or database (including web link if available)*	

Inputs



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

Between each two simulations or models, some post/pre-processing may take place. This processes the output of one simulation into input for the next simulation.

Elements in the simulation with one single materials model from the chain

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	Cycled mass and performance of an adsorber due to heat flow.
1.2	MATERIAL	The fluid is water
1.3	GEOMETRY	The picture below shows a typical geometry of an adsorber dedicated to cold production sorption system. The adsorber is based on fin and tube heat exchanger which gaps are filled with adsorbent material (pellets, beads, etc.). Cooling/heating fluid can flow in the tubes allowing to perform a temperature swing of the adsorber. 
1.4	TIME LAPSE	Minutes. The cycle time of this system (i.e. the time necessary for an adsorber to go through the various steps (pre-heating, desorption, pre-cooling and adsorption) is usually about a few tens of minutes depending of thermophysical properties, adsorption equilibrium and adsorber size.
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	The boundary conditions will consist on three thermal sources: high, medium and low temperature as sorption cooling system are 3-temperature thermodynamic heat pumps. The choice of the temperature of the sources will be directly linked to the type of sought application. For example for solar cooling, typical temperature for the heat sources would be respectively: 90, 35 and 10 °C
1.6	PUBLICATION	*n.a.*

<table>
<tr><td>2</td><td colspan="4">GENERIC PHYSICS OF THE MODEL EQUATION</td></tr>
<tr><td>2.0</td><td>MODEL TYPE AND NAME</td><td colspan="3">Heat equation applied to describe the dynamic behaviour of an adsorber</td></tr>
<tr><td>2.1</td><td>MODEL ENTITY</td><td colspan="3">continuum</td></tr>
<tr><td rowspan="2">2.2</td><td rowspan="2">MODEL PHYSICS/ CHEMISTRY EQUATION PE'S</td><td>Equations</td><td colspan="2">1. Energy balance during the desorption step
$\frac{d}{dt}\left\{\left(MC_{a,M}+MC_{ac}+M_{ac}q_dC_{p,MeOH}\right)T_d\right\}=\Delta h\cdot M_{ac}\frac{dq_d}{dt}+\dot{m}_{HW}C_{p,HW}\left(T_{HW,out}-T_{HW,in}\right)$
2. Energy balance during the adsorption step
$\frac{d}{dt}\left\{\left(MC_{d,M}+MC_{ac}+M_{ac}q_ac_{pl,MeOH}\right)T_a\right\}=$
$\Delta h\cdot M_{ac}\frac{dq_a}{dt}+MC_{ac}c_{pv,MeOH}\frac{dq_a}{dt}\left(T_{ev}-T_a\right)+\dot{m}_{MW}c_{p,MW}\left(T_{MW,in}-T_{MW,out}\right)$</td></tr>
<tr><td>Physical quantities for each equation</td><td colspan="2">In the energy balance equations the following quantites appear:
• Temperature: desorber (Td), adsorber (Ta), heating/cooling fluid (T_{MW}, T_{HW}, in and out)
• The adsorption capacity: desorber (q_d) and adsorber (q_a). It is a function of the temperature and the pressure inside the adsorber. The pressure will be given by that at the evaporator or the condenser (saturation pressure of the refrigerant at Tev or Tcond which are boundary conditions)
• The heat capacity (thermal inertia) of the adsorbent, metal and adsorbate ($MC_{ac,}$ MC_M and Mqc, respectively)
• The heat of adsorption ΔH
• The secondary fluid flow rate and specific heat capacity (m_{MW} and c_p)</td></tr>
<tr><td colspan="2" rowspan="2">MATERIALS RELATIONS</td><td>Equations</td><td colspan="2">• to describe the heat transfer inside the adsorber (one example hereafter)
$T_{out}=T+(T_{in}-T)\cdot\exp(-UA/\dot{m}C_p)$
• to describe the adsorption equilibrium (various model from the litterature can be used to describe the experimental data: Langmuir familiy, Dubinin family, etc. (one example hereafter with Dubinin-Astakov equation)
$q=q_0\cdot\rho_l(T)\cdot\exp\left(-D\left[T\cdot\ln\left(\frac{P_{sat}}{P}\right)\right]^n\right)$
• state equation for the adsorbate (working fluid)</td></tr>
<tr><td>Physical quantities/ descriptors for each MR</td><td colspan="2">n.a.</td></tr>
<tr><td>2.4</td><td>SIMULATED INPUT</td><td colspan="3">n.a.</td></tr>
<tr><td>2.5</td><td>PUBLICATION</td><td colspan="3">Clausse M., Meunier F., Coulié J., Herail E., 2009, Comparison of adsorption systems using natural gas fired fuel cell as heat source, for residential air conditioning, Int. J. Refrig., 32(4), 712-719.
Clausse, M., Alam, K.C.A., Meunier, F., 2008, Residential air conditioning and heating by means of enhanced solar collectors coupled to an adsorption system, Sol. Energy, 82(10), 885-892</td></tr>
</table>

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 forthe models.

3	SPECIFIC COMPUTATIONAL MODELLING METADATA		
3.1	NUMERICAL SOLVER	Differential Algebraic Equation solver	
3.2	SOFTWARE TOOL	DASPK (Fortran package for DAEs solving)	
3.3	TIME STEP	n.a.	
3.4	COMPUTATIONAL REPRESENTATION Refers to how your computational solver represents the material, properties, equation variables,	PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL	The DDASPK solver uses the backward differentiation formulas of orders one through five to solve a system of the form G(t,y,y') = 0 for y = Y and y' = YPRIME. Values for Y and YPRIME at the initial time must be given as input. These values should be consistent, that is, if T, Y, YPRIME are the given initial values, they should satisfy G(T,Y,YPRIME) = 0. In our case, Y will content the values id the temperature and the adsorbed quantities of each adsorber while YPRIME will content their derivative as a function of time. source : http://www.engineering.ucsb.edu/~cse/software.html
		BOUNDARY CONDITIONS	Boundary conditions are scalars linked to the heat source temperatures. They can be directly the temperature or the saturation pressure for this temperature.
		ADDITIONAL SOLVER PARAMETERS	*n.a.*
3.5	PUBLICATION	*n.a.*	

Post processing

The “raw output” calculated by the model for the model entities is contained in the metadata above (physics quantity in the PE) . This output is processed by a post processor in order to calculate values for physics variables for larger entities.
When this post-processed output is used in a next model, a pre-processor might be used.

4	POST PROCESSING	
4.1	THE PROCESSED OUTPUT IS CALCULATED FOR	*the performance: cooling capacity and COP (Coefficient of Performance).*
4.2	METHODOLOGIES	*The cyclic average cooling capacity (CACC) can be evaluated by the following expressions:* $$CACC = \frac{\int_{\text{begin of adsorption step}}^{\text{end of adsorption step}} \dot{m}_{adsorbate} \Delta h_{lv} dt}{\text{Cycle time}}$$ *The cycle COP (Coefficient of Performance) can be calculated by the following equation:* $$COP_{cycle} = \frac{\int_{\text{begin of adsorption step}}^{\text{end of adsorption step}} \dot{m}_{adsorbate} \Delta h_{lv} dt}{\int_{\text{begin of cycle time}}^{\text{end of cycle time}} \dot{m}_{HW} c_{HW} (T_{HW,in} - T_{HW,out}) dt}$$
4.3	MARGIN OF ERROR	*n.a.*