MODA

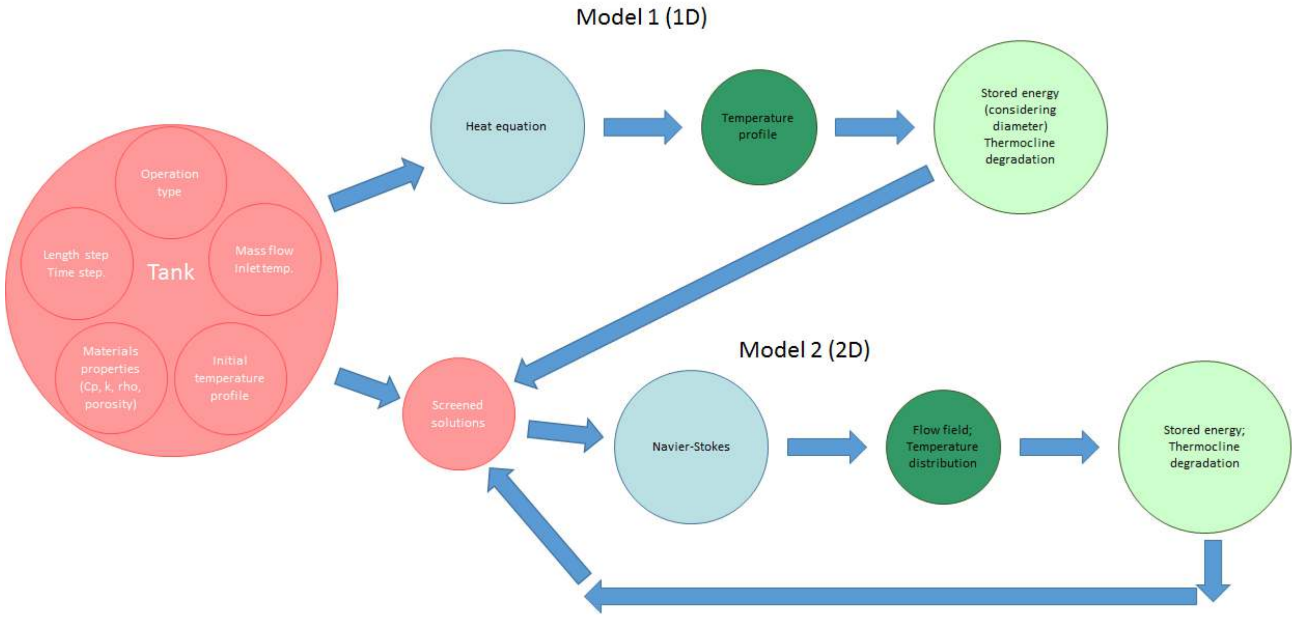
Modelling data documenting one simulation

NewSOL energy storage tank

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.

OVERVIEW of the simulation			
1	USER CASE		*In order to define the thermal storage capacity of the tank, the behaviour of a thermocline Thermal Energy Storage (TES) tank is to be described.* *Consortium will define the thermal storage capacity of the tank. 3 different height/diameter ratios will be calculated through. The stacked zones will be defined with regard to number and composition. Inlet temperature will be provided by the coordinator. The model will be prepared to work with those conditions. The results will allow further developments and adaptions.* *Several inlet and outlet mass flows (charge and discharged operations, respectively) will be screened in order to decide the best available conditions to use in the 2D model (commercial code.*
2	CHAIN OF MODELS	MODEL 1	*1D energy conservation model (tank axial dimension) to calculate the temperature along the tank height*
		MODEL 2	*2D CFD turbulence model*
		…	…
3	PUBLICATION ON THIS ONE SIMULATION		*Not available*
4	ACCESS CONDITIONS		*To be defined*
5	WORKFLOW AND ITS RATIONALE		*The thermal behaviour of the tank will be assessed in 2D model of a full CFD flow on a representation of the storage tank. This will be accomplished using a commercial software package.* *To save effort, a first screening is to be done for predefined in and outlet flows on a simplified (1D) representation of the tank along one or more charging/discharging cycles. For these situations the temperature will be calculated from which the tank performance and thermocline degradation are to be calculated. Then the details of selected cases will be simulated with a 2D CFD model.* *Considering that only fluid flow thermal phenomena occurring inside the tank are addressed, the CFD approach alone is considered to be able to provide the necessary data to optimize the tank performance considering the chosen parameters (number and composition of layers, inlet and outlet mass flows and walls heat losses) and materials. Thus, heat transfer inside the filler is not in the scope of this work.*



Workflow

Each model used in this simulation can be documented in four chapters:

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

MODEL

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	*A simplified (1D) representation of the tank is to be calculated for several cases with predefined in and outlet flows. For these situations the temperature should be calculated from which the storage capacity is to be calculated.*
1.2	MATERIAL	*The thermocline tank will have cement walls.* *The interior consists of:* *Molten salt Hitec XL (42-43-15% Ca-K-Na) or other defined by the Consortium in D2.1.* *Filler preceding from S. Domingos Mines.*
1.3	GEOMETRY	*Thermal Energy Storage tank with cylindrical shape. Size to be defined. Picture not available.* *The interior of the tank will have several levels of stacked filler and molten salts (zones with no filler material and zones with filler material. Molten salts will fill the empty spaces).*
1.4	TIME LAPSE	*1 cycle for stored energy or delivered energy (respectively, charge or discharge operation. Eventually up until 7 cycles of charge and discharge for thermocline degradation along a full week). Model don't foresee stagnation periods.*
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	*Several inlet and outlet flows will be screened.* *In charging operation, the boundary conditions are the inlet mass flow and temperature of the hot stream. In discharge operation is the inlet mass flow and temperature of the cold stream.*
1.6	PUBLICATION ON THIS ONE SIMULATION	*Not available.*

2	Generic Physics Of The Model Equation		
2.0	Model type and name	*Heat equation Ch 4.3 of the RoMM.*	
2.1	Model entity	*Finite differences representing finite volumes with a single dimension.*	
2.2	Model Physics/ Chemistry equation PE	Equation	*Main equation:* $(\rho.Cp)_{eff}\frac{\partial T}{\partial t}+Cp_f\frac{\dot{m}}{A}.\frac{\partial T}{\partial z}=k_{eff}\frac{\partial^2 T}{\partial z^2}$
		Physical quantities	*Cp, Rho, k, ε (porosity), T, $\dot{m}$, z, t*
2.3	Materials relations	Relation	*values for the above coefficients will come from literature.*
		Physical quantities/ descriptors for each MR	*Not applicable.*
2.4	Simulated input	*NA*	

3	Solver and computational translation of the specifications		
3.1	Numerical Solver	*Algebraic.*	
3.2	Software tool	*In house algebraic solutions done in an Excel tool-like software (the interface in under development).*	
3.3	Time step	*5 seconds*	
3.4	Computational Representation	Physics Equation, Material Relations, Material	*1D algebraic equations for mass and energy conservation (not including radiation).*
3.5	Computational boundary conditions	*NA*	
3.6	additional Solver Parameters	*Not applicable.*	

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 circle in the workflow picture.

This output is often processed by a post processor in order to calculate values for physics variables for different entities that can be input to the next model. Or the output is homogenised for larger volumes in the form of a MR or Descriptor Rule that are the final output of the total simulation.
This will appear in your light green circle in the workflow picture and also in 2.4 of the next model.

The methodology (often including new physics) used to do this calculation is to be documented.

4	POST PROCESSING

4.1	THE PROCESSED OUTPUT	*The output (final temperature profile) allows to determine final stored energy, storage efficiency and the slope of the thermocline, which in turn will allow to determine the thermocline degradation and to foresee an operation scheme in order to improve storage efficiency and, thus, increase dispatchability.* *The optimal situation will be refined in model 2 CFD*
4.2	METHODOLOGIES	*Considering the diameter of the TES tank, the amount of energy is calculated for each length step. The integral along the height of the tank is calculated. A slope is determined between the two isothermal "volumes" of the tank. The variation of the slope along time determines the thermocline degradation.* *The spline of the final temperature profile is provided by an excel-like tool.* *Storage efficiently is calculated as the ratio between stored energy and the maximum stored energy possible.*
4.3	MARGIN OF ERROR	*During the validation procedure of the model, an error below 5% was found, considering cumulative error along the total height of the tank (to be confirmed).*

MODEL 2

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED

1.1	ASPECT OF THE USER CASE TO BE SIMULATED	*The results of model 1 will allow to define the best suitable solutions to test in 2D model of a full CFD flow on a representation of the storage tank.* *The number of layers and the distribution of filler and fluid in each layer will be tested in order to calculate the storage tank performance and thermocline degradation.*
1.2	MATERIAL	*Materials both for the bed and for the walls should be available for testing.* *The thermocline tank will have cement walls.* *The interior consists of* *Molten salt Hitec XL (42-43-15% Ca-K-Na) or other defined by the Consortium in D2.1.* *Filler preceding from S. Domingos Mines.*
1.3	GEOMETRY	*Dimensions both for the bed and for the walls should be available for testing and additional solutions provided after testing.* *Thermal Energy Storage tank with cylindrical shape. Size provided by model 1 but possible to change depending on the results. Picture not available.* *The interior of the tank will have several levels of stacked filler and molten salts (zones with no filler material and zones with filler material. Molten salts will fill the empty spaces)*
1.4	TIME LAPSE	*1 cycle for stored energy or delivered energy (respectively, charge or discharge operation. Eventually up until 7 cycles of charge and discharge for thermocline degradation along a full week).*
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	*Model 1 will provide inlet and outlet flows to be tested. Additional tests will be made dependent upon results.* *In charging operation, the boundary conditions are the inlet mass flow and temperature of the hot stream. In discharge operation is the inlet mass flow and temperature of the cold stream. The walls will also present a boundary condition. The walls dimensions and heat transfer coefficient will be represented as a heat sink in the walls.*
1.6	PUBLICATION ON THIS ONE SIMULATION	*Not available*

2	GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	*Navier-Stokes equations*	
2.1	MODEL ENTITY	*Finite volumes in 2D*	
2.2	MODEL PHYSICS/ CHEMISTRY EQUATION	Equation	*Continuity equation:* $\frac{\partial \rho}{\partial t}+\nabla\cdot(\rho\vec{v})=S_m$ *Momentum conservation equations*

	PE		$$\frac{\partial}{\partial t}(\rho\vec{v})+\nabla\cdot(\rho\vec{v}\,\vec{v})=-\nabla p+\nabla\cdot(\overline{\overline{\tau}})+\rho\vec{g}+\vec{F}$$ *with* $$\overline{\overline{\tau}}=\mu\left[\left(\nabla\vec{v}+\nabla\vec{v}^{T}\right)-\frac{2}{3}\nabla\cdot\vec{v}I\right]$$ *Transport equations for the Standard k-w model. This model is envisaged in a first approach and uses the Boussinesq hypothesis for Reynolds stresses modelling.* $$\frac{\partial}{\partial t}(\rho k)+\frac{\partial}{\partial x_i}(\rho k u_i)=\frac{\partial}{\partial x_j}\left(\Gamma_k\frac{\partial k}{\partial x_j}\right)+G_k-Y_k+S_k$$ and $$\frac{\partial}{\partial t}(\rho\omega)+\frac{\partial}{\partial x_i}(\rho\omega u_i)=\frac{\partial}{\partial x_j}\left(\Gamma_\omega\frac{\partial\omega}{\partial x_j}\right)+G_\omega-Y_\omega+S_\omega$$ *Energy equation* $$\frac{\partial}{\partial t}(\rho E)+\nabla\cdot(\vec{v}(\rho E+p))=\nabla\cdot\left(k_{eff}\nabla T-\sum_j h_j\vec{J}_j+\left(\overline{\overline{\tau}}_{eff}\cdot\vec{v}\right)\right)+S_h$$ *Depending on the verified flow pattern, other models can be used.*
		Physical quantities	*For the turbulence model:* *k: turbulence kinetic energy* *w: specific dissipation rate;* *rho: density;* *u: velocity;* *x: cell length;* *Gk: generation of turbulence kinetic energy due to mean velocity gradients;* *Gw: generation of w;* *Yk and Yw: dissipation of k and w due to turbulence;* *Sk and Sw: not used (user-defined terms);* *x and y: directions (dimensions).*
2.3	**MATERIALS RELATIONS**	**Relation**	*values for materials coefficients will come from literature and from partners*
		Physical quantities/ descriptors for each MR	*Not applicable*
2.4	**SIMULATED INPUT**	*Please document the simulated input and with which model it is calculated.*	

3	**SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS**		
3.1	**NUMERICAL SOLVER**	*Finite volumes solver Pressure-based*	
3.2	**SOFTWARE TOOL**	*Ansys Fluent (commercial application)*	
3.3	**TIME STEP**	*5 seconds (depending on results other values may be tested in order to allow the modelling of all phenomena and decrease the computational time)*	
3.4	**COMPUTATIONAL REPRESENTATION**	**PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL**	*1 equation for continuity* *1 equation momentum* *2 equation for viscous model (turbulence)* *1 equation for energy* *Radiation is not considered.*
3.5	**COMPUTATIONAL BOUNDARY CONDITIONS**	*Inlet, outlet and walls*	
3.6	**ADDITIONAL SOLVER**	*Not applicable*	

	PARAMETERS	

4	POST PROCESSING	
4.1	THE PROCESSED OUTPUT	*The output (final temperature profile) allows to determine final stored energy, storage efficiency and the slope of the thermocline, which in turn will allow to determine the thermocline degradation and to foresee an operation scheme in order to improve storage efficiency and, thus, increase dispatchability.* *Tank performance can decrease due to heat transfer along the walls. Flow pattern near walls will also be an output for minimization of recirculation in the flow.*
4.2	METHODOLOGIES	*Considering the diameter of the TES tank, the amount of energy is calculated for each length step. The integral along the height of the tank is calculated. A slope is determined between the two isothermal "volumes" of the tank. The variation of the slope along time determines the thermocline degradation.* *The spline of the final temperature profile is provided by an excel-like tool.* *Storage efficiently is calculated as the ratio between stored energy and the maximum stored energy possible.* *Tank performance can decrease due to heat transfer along the walls. Flow pattern near walls will also be analysed for minimization of recirculation in the flow.*
4.3	MARGIN OF ERROR	*Not yet available*