The European Materials Modelling Council

In Power: Design and simulation of thermal storage materials for innovative Thermal storage systems in different type of power block in CSP plant.

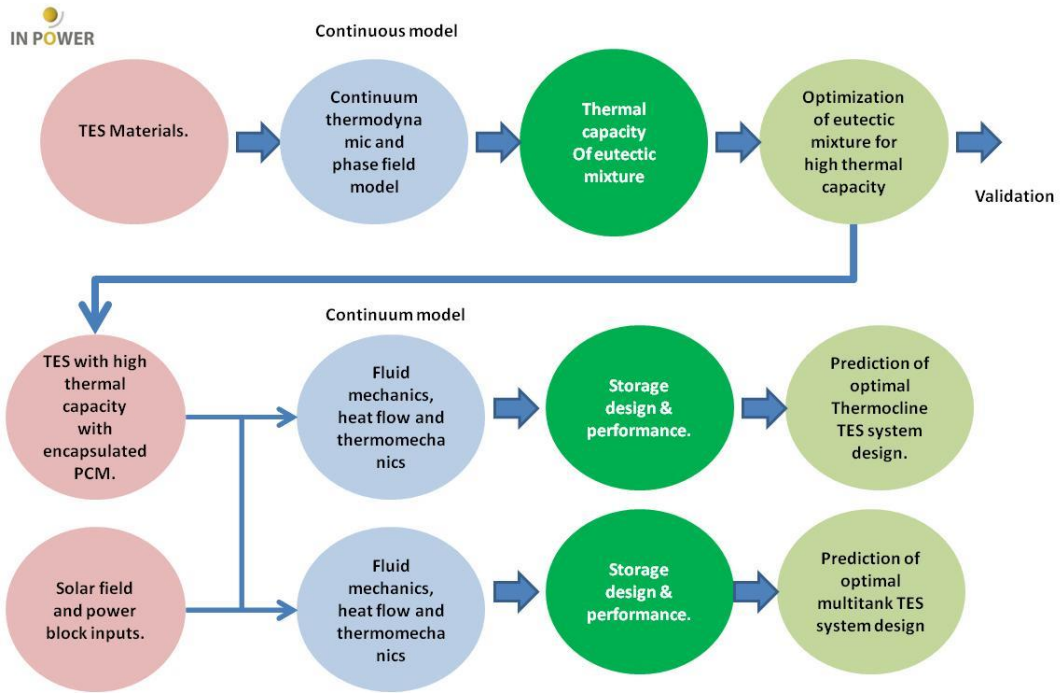
2016.10.19

Purpose of this document:
Definition of a data organization 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**	*Design and simulation of thermal storage materials for innovative Thermal storage (TES) systems in different type of power block in CSP plant. The materials eutectic mixtures and Phase Change Material are selected.*	
2	**CHAIN OF MODELS #2**	**MODEL 1**	*Continuum model. Continuum thermodynamic and phase field model (model 4.4 from ROMM). The model 1 is dedicated to find the optimal TES eutectic mixture material in order to have high thermal capacity, three times respect state of the art.*
		MODEL 2	*Continuum model. Fluid mechanics, heat flow and thermomechanics (4.2 and 4.3 models from ROMM). The model 2 is related to simulate performance of new thermocline TES system geometry, for high temperature storage systems with oil or salts as HTF.*
		MODEL 3	*Continuum model. Fluid mechanics, heat flow and thermomechanics (4.2 and 4.3 models from ROMM). The model 3 is related to simulate performance of new multitank TES system, for Direct Steam Generation power plants.*
3	**PUBLICATION**	*Not available*	
4	**ACCESS CONDITIONS**	*Scilab: free software from Scilab Enterprises* *Dymola: commercial modeling and simulation environment based on the open Modelica modeling language from Dassault Systèmes AB.* *FactSage Version 6.4. FACT Pure Substances Database, FACT Solutions Database. Licensed.*	

Each model used in a simulation is documented in four chapters:
1-Aspect of the User Case/ system simulated with the model
2-Model
3-Computation
4-Post-Processing. In some cases between two simulations the post/preprocessing takes place. This processes the output (or part of the output) of one simulation into input for next simulation.

Workflow for models needed for In Power, Chain 2.

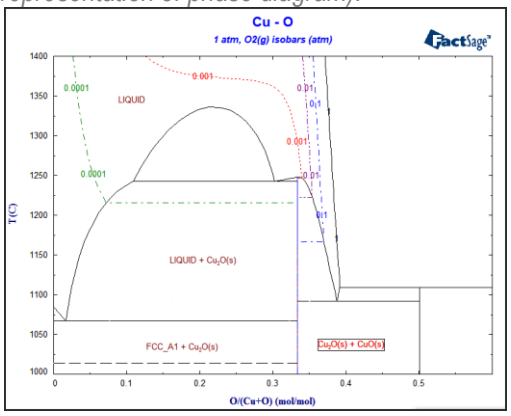


1. Model 1: Selection and optimization of TES materials [WP5:Task 5.1]

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	*Evaluation of eutectic point from simulated phase diagram and the liquidus surface of quaternary X-Y-NO3 (X = K, Na, Li and Y=Sr) system. Definition of new eutectic mixture with high thermal capacity, looking for three times thermal capacity respect to state of the art.*
1.2	MATERIAL	*Eutectic X-Y-NO3 (X = K, Na, Li and Y=Sr) mixtures*
1.3	GEOMETRY	*atoms*
1.4	TIME LAPSE	*static*
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	*Melting behaviour of selected compositions used in different TES systems.*
1.6	PUBLICATION ON THIS ONE SIMULATION	*H.L. Lukas, S.G. Fries, B. Sundman, Computational Thermodynamics – The Calphad method. Cambridge University Press (2007).* *Christian Robelin, Patrice Chartrand, Arthur D. Pelton, "Thermodynamic evaluation and optimization of the (NaNO3 + KNO3 + Na2SO4 + K2SO4) system", Chem.Thermodynamics 83 (2015) 12–26.*

2	GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	*Continuum model. Continuum thermodynamic and phase field model (model 4.4 from ROMM)*	
2.1	MODEL ENTITY	*Thermodynamic description of condensed phases*	
2.2	MODEL PHYSICS/ CHEMISTRY	**Equation**	*Gibbs equation* $G = (n_A g^0_A + n_B g^0_B) - T\Delta S^{config} + (n_{AB}/2)\,\Delta g_{AB}$

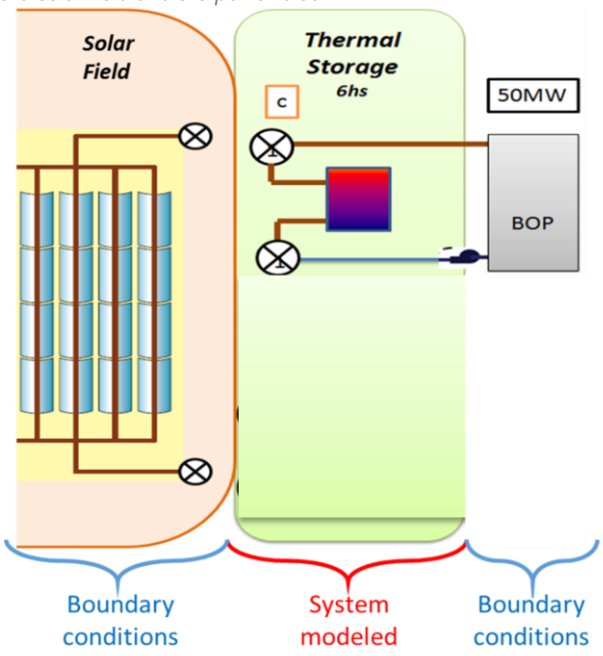
	EQUATION PE	Physical quantities	*A and B system components, G is Gibbs free energy, g0A and g0B are molar Gibbs energies of the pure components, ΔSconfig is the configurational entropy of mixing.*
2.3	MATERIALS RELATIONS	Relation	$\Delta g_{AB} = \sum_{i+j\geq 0} g_{AB}^{ij} Y_A^i Y_B^j, \quad i \geq 0, j \geq 0,$ $= \sum_{k\geq 0} g_k \ Y_b^k$
		Physical quantities/ descriptors for each MR	*gk and Ykb are free parameters to be determined from experimental data.*
2.4	SIMULATED INPUT	*Not applicable*	

3	SPECIFIC COMPUTATIONAL MODELLING METADATA		
3.1	NUMERICAL SOLVER	*Included in FactSage Software.*	
3.2	SOFTWARE TOOL	*FactSage Version 6.4. FACT Pure Substances Database, FACT Solutions Database.*	
3.3	TIME STEP	*Not aplicable*	
3.4	COMPUTATIONAL REPRESENTATION *Refers to how your computational solver represents the material, properties, equation variables,*	PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL	*Gibbs free energy of the phases of the system (example of visual representation of phase diagram).*  *Written up for the entity in the model.*
		BOUNDARY CONDITIONS	*Not applicable.*
		ADDITIONAL SOLVER PARAMETERS	*To be defined.*
3.5	PUBLICATION	*http://www.IPSEpro.com*	

4	POST PROCESSING	
4.1	THE PROCESSED OUTPUT IS CALCULATED FOR	*The Phase equilibrium diagram will let to decide the best liquid TES materials to be applied in the TES systems. The TES material with highest thermal capacity will be used for model 2 and 3.*
4.2	METHODOLOGIES	*Simulation/calculation of phase diagram and liquidus surface from calculated Gibbs free energy functions of the phases will let to establish the invariant points of system (eutectic, peritectic…) as well as heat capacity of the liquid phase. Formulation of new compositions and optimal working conditions are done in terms of the simulated phase diagrams and liquidus surfaces.*

		For this, phase diagram, thermodynamic properties of the liquid phase and finally invariant (eutectic, peritectic…) points of binary to multicomponent system are established. The invariant points will be evaluated from minimization of the Gibbs free energy of condensed phases in multicomponent systems. *Molten salt phase: Modified quasichemical model.* *Solid solution phases: Compound Energy Formalism.* *Multicomponent properties: Generalized Kohler-Toop technique.*
4.3	MARGIN OF ERROR	*Temperature 5%. Composition 10%*

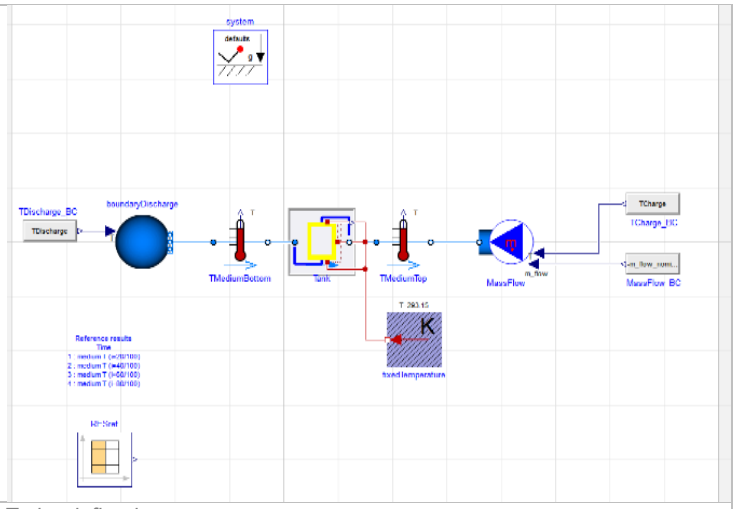
2. Model 2: Thermocline TES system for high temperature storage. [WP5: Task 5.3].

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	*The model will be used to design and size high temperature thermocline storage for commercial scale CSP plants with oil or molten salts as heat transfer fluid (HTF).*
1.2	MATERIAL	*HTF: a eutectic molten salt mixture coming from model 1; and encapsulated PCM (aluminium alloys).*
1.3	GEOMETRY	*Geometry will take into account a unique tank in connexion with (boundary conditions) the solar field and the power block.* 
1.4	TIME LAPSE	*One charge-discharge cycle (approximately 24 hours)*
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	*In service conditions: Several operating strategies will be simulated (selection of the optimum operating temperature range, best combination of HTF and filler material to meet a specific storage requirement, etc.)*
1.6	PUBLICATION ON THIS ONE SIMULATION	*The corresponding model will be developed during the project, thus there are no publications yet documenting this ONE simulation.*

2	GENERIC PHYSICS OF THE MODEL EQUATION	
2.0	MODEL TYPE AND NAME	*Continuum model. Fluid mechanics, heat flow and thermomechanics (4.2 and 4.3 models from ROMM).*
2.1	MODEL	*Continuum model of dual-media thermocline systems with the additional use of top and/or*

	ENTITY	*bottom PCM layers, with heat flow calculations.*	
2.2	**MODEL PHYSICS/ CHEMISTRY EQUATION PE**	**Equation**	*Mass and energy conservation in storage fluid, PCM and filler material.* *Conservation of mass* $$\frac{\partial \rho}{\partial t} = \nabla . (\rho \, \vec{u})$$ *Conservation of momentum,* $$\int_V \left(\frac{\partial (\rho \vec{u})}{\partial t} + \nabla \cdot (\rho \vec{u} \vec{u}) \right) dv = \oint_S \vec{n} \cdot \vec{\vec{\sigma}} ds + \int_V \rho \vec{f} dv$$ *Conservation of energy* $$\frac{\partial}{\partial t}\left(\frac{\rho}{2}\left|\vec{u}\right|^2 + \rho\varepsilon \right) + \frac{\partial}{\partial x_k}\left[\frac{\rho}{2}\left|\vec{u}\right|^2 u_k + u_l (P\delta_{lk} - \pi_{lk}) + \rho\varepsilon u_k + F_k \right] = -\rho u_k \frac{\partial \Phi}{\partial x_k}$$ *Heat flow is derived from the energy conservation law. Heat due to conduction or convection will be modelled.*
		Physical quantities	*u: velocity vector* *σ: stress matrix* *F:external forces (like gravity)* *ε: energy density* *P: pressure* *F_k: conductive flux* *Also: Temperatures / enthalpies and mass flows of storage fluid.Temperatures / enthalpies and masses of PCM and filler material.*
2.3	**MATERIALS RELATIONS**	**Relation**	*Closure relations or materials relations will take into account, giving thermal and physical properties of the materials, such as densisty (ρ), viscosity, thermal conductivity, density, specific heat,etc. All these relations, as functions of the temperature (for solid and monophasic fluids) or of pressure and enthalpy (for PCM and diphasic fluids).Materials are considered isotropic and at macroscopic scale. Constitutive equations are the Fourier's law for conductive heat flow, and Newton's law of cooling for convective heat flow.*
		Physical quantities/ descriptors for each MR	*Thermal and physical properties of the materials.*
2.4	**SIMULATED INPUT**	*Mass and energy flows of the HTF, from model 1, at the inlet of the storage system.*	

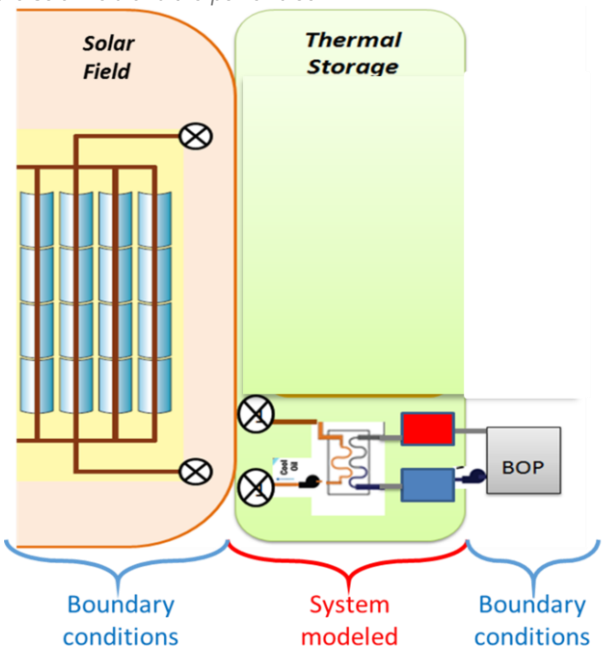
3	**SPECIFIC COMPUTATIONAL MODELLING METADATA**		
3.1	**NUMERICAL SOLVER**	*To be defined*	
3.2	**SOFTWARE TOOL**	*Two simulation software tools are considered at this point: either Scilab or Dymola*	
3.3	**TIME STEP**	*From 1 s to 5 min.*	
3.4	**COMPUTATIONAL REPRESENTATION** *Refers to how your computational*	**PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL**	*Written up for elementary volumes with 1D discretization*.

	solver represents the material, properties, equation variables,		
		BOUNDARY CONDITIONS	*To be defined*
		ADDITIONAL SOLVER PARAMETERS	*To be defined.*
3.5	**PUBLICATION**		

4	**POST PROCESSING**	
4.1	**THE PROCESSED OUTPUT IS CALCULATED FOR**	*The evaluation of Thermal capacity of the system and cost-performance model to determine the unit cost of storage capacity (€/KWh) for a given operating temperature range and storage materials combination will be done..*
4.2	**METHODOLOGIES**	*Thermocline storages are using a combination of HTF and filler material to meet a specific storage requirement. Optimal HTF, coming from model 1, is a eutectic molten salt mixture with optimized low melting point, stable, affordable and non-toxic salt formulation. To increase the utilization rate of the storage system, the use of encapsulated PCM (aluminium alloys) layer at the top of the tank is considered.* *Thermal capacity will be evaluated, under the boundary conditions (solar field and power block inputs). Mass, energy and momentum balances, in differential form and at any direction where gradients are expected (along and across the flow) will be considered using ordinary differential equations (ODEs) or partial differential equations (PDEs), under the hypotheses of Newtonian fluids and incompressible flow. Two phases (solid and liquid) will be considered for PCM. Changes in mechanical properties will be considered as a function of the temperature. Then, energy balances will be assessed through integration of heat flows.* *Cost performance: Mass of storage fluid, filler materials, and containers will be deduced from the TES optimized design in order to calculate the global cost of the system (in €); This cost will be compared to the simulated storage capacity (in kWh) to determine the unit cost in €/kWh. Material costs will be found in the literature. All the methodology will follow definition of storage key features following standards from SolarPaces and IEC.*
4.3	**MARGIN OF ERROR**	*To be determined*

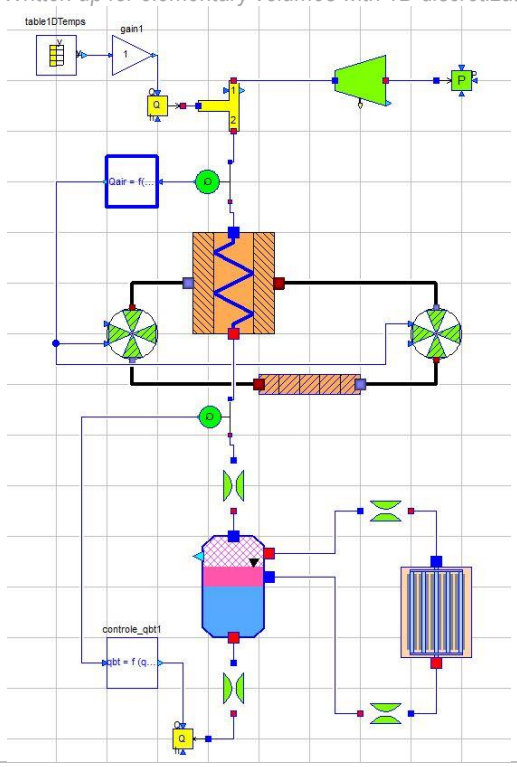
3. Model 3: Two tanks TES system for Direct Steam Generation CSP plants. (WP5: Task 5.4)

1	**ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED**	
1.1	**ASPECT OF THE USER CASE TO BE SIMULATED**	*The model will be used to design and size high temperature multi-stage storage for commercial scale DSG CSP plants.*

1.2	**MATERIAL**	*Eutectic mixture from model 1, as high temperature sensible storage; and sodium nitrate PCM for latent heat storage.*
1.3	**GEOMETRY**	*Geometry will take into account two tanks (cold and hot) in connexion with (boundary conditions) the solar field and the power block.* 
1.4	**TIME LAPSE**	*One charge-discharge cycle (approximately 24 hours)*
1.5	**MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS**	*In service conditions. Several operating strategies will be simulated (selection of the optimum operating temperature and pressure range, water level control, etc.)*
1.6	**PUBLICATION ON THIS ONE SIMULATION**	*The corresponding model will be developed during the project, thus there are no publications yet documenting this ONE simulation.*

2	**GENERIC PHYSICS OF THE MODEL EQUATION**		
2.0	**MODEL TYPE AND NAME**	*Continuum model. Fluid mechanics, heat flow and thermomechanics (4.2 and 4.3 models from ROMM)*	
2.1	**MODEL ENTITY**	*Continuum thermodynamics and phase field model, with heat flow calculations.*	
2.2	**MODEL PHYSICS/ CHEMISTRY EQUATION PE**	**Equation**	*Mass and energy conservation in HTF (water-steam) and storage media (eutectic molten salts and PCM).* *Conservation of mass* $$\frac{\partial \rho}{\partial t} = \nabla.(\rho\,\vec{u})$$ *Conservation of momentum,* $$\int_V \left(\frac{\partial(\rho\vec{u})}{\partial t} + \nabla\cdot(\rho\vec{u}\vec{u})\right)dv = \oint_S \vec{n}\cdot\vec{\sigma}ds + \int_V \rho\vec{f}\,dv$$ *Conservation of energy* $$\frac{\partial}{\partial t}\left(\frac{\rho}{2}|\vec{u}|^2+\rho\varepsilon\right)+\frac{\partial}{\partial x_k}\left[\frac{\rho}{2}|\vec{u}|^2 u_k + u_i(P\delta_{ik}-\pi_{ik})+\rho\varepsilon u_k + F_k\right] = -\rho u_k\frac{\partial\Phi}{\partial x_k}$$ *Heat flow is derived from the energy conservation law. Heat due to conduction or convection will be modelled.*

		Physical quantities	*ρ: density* *u: velocity vector* *σ: stress matrix* *F:external forces (like gravity)* *ε: energy density* *P: pressure* *F_K: conductive flux* *Also: (1) enthalpies, pressures and mass flows of HTF (water-steam). (2) Temperatures / enthalpies and masses of storage media (eutectic molten salts and PCM).*
2.3	**MATERIALS RELATIONS**	**Relation**	*Closure relations or materials relations are the formulas giving thermal and physical properties of the materials (viscosity, thermal conductivity, density, specific heat,…) as functions of the temperature (for solid and monophasic fluids) or of pressure and enthalpy (for water / steam).* *Materials are considered isotropic and at macroscopic scale.* *Constitutive equations are the Fourier's law for conductive heat flow, and Newton's law of cooling for convective heat flow.*
		Physical quantities/ descriptors for each MR	*Thermal and physical properties of the materials.*
2.4	**SIMULATED INPUT**	*Mass and energy flows of the HTF at the inlet of the storage system.*	

3	**Solver and Computational translation of the specifications**		
3.1	**NUMERICAL SOLVER**	*To be defined.*	
3.2	**SOFTWARE TOOL**	*Two simulation software tools are considered at this point: either Scilab or Dymola*	
3.3	**TIME STEP**	From 1 s to 5 min.	
3.4	**COMPUTATIONAL REPRESENTATION** ,	**PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL**	*Written up for elementary volumes with 1D discretization*. 
3.5	**COMPUTATIONAL BOUNDARY CONDITIONS**	*To be defined.*	

3.6	ADDITIONAL SOLVER PARAMETERS	*To be defined*.

4	POST PROCESSING	
4.1	THE PROCESSED OUTPUT	*The modelling let predict the optimal, in terms of thermal storage capacity and costs, of multitank system design. The evaluation of Thermal capacity of the system and cost-performance model to determine the unit cost of storage capacity (€/KWh) for a given operating temperature range and storage materials combination will be done. Thermodynamic variables of the storage material and heat transfer fuid (HTF) as temperature, pressure, mass flow, specific enthalpy. Mass of storage fluid, filler materials, and containers will be deduced from the TES optimized design in order to calculate the global cost of the system (in €); This cost will be compared to the simulated storage capacity (in kWh) to determine the unit cost in €/kWh.*
4.2	METHODOLOGIES	*Parametric studies will be performed to optimize geometry (for example the tank shape will be adjusted to minimize the thermal gradient across the height of the tank, and the insulation thickness will also be determined to minimize the heat loss to the surroundings) and the operating strategies through performance predictions and experimental validation.* *Thermal storage capacity: Mass, energy and momentum balances, in differential form and at any direction where gradients are expected (along and across the flow) will be considered using ordinary differential equations (ODEs) or partial differential equations (PDEs), under the hypotheses of Newtonian fluids. Two phases (solid and liquid) will be considered for PCM. Changes in mechanical properties will be considered as a function of the temperature. A two-phase flow (liquid and vapour) is also considered for the HTF (water / steam).* *Energy balances, storage levels, and storage efficiencies will be evaluated.* *Cost performance: Energy balances will be assessed through integration of heat flows. Mass of storage fluid, filler materials, and containers will be deduced from the TES optimized design in order to calculate the global cost of the system (in €); This cost will be compared to the simulated storage capacity (in kWh) to determine the unit cost in €/kWh. Material costs will be found in the literature. All the modelling will follow definition of storage key features following standards from SolarPaces and IEC.*
4.3	MARGIN OF ERROR	*To be defined.*