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6. MODAs

6.1 MODA 1 - liquid lead CFD

MODA#1

Modelling data documenting one simulation

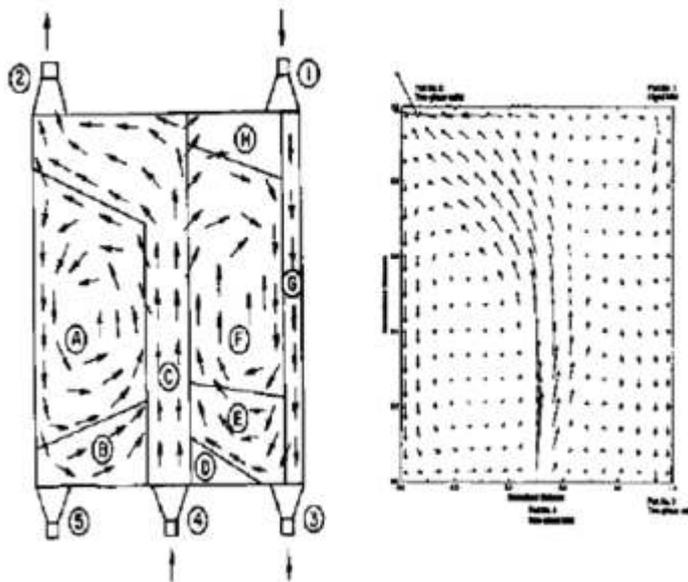
Name <NEXTOWER, TFD Analysis of SOLEAD DEMO, CFD/STH>

Metadata for these elements are to be elaborated over time

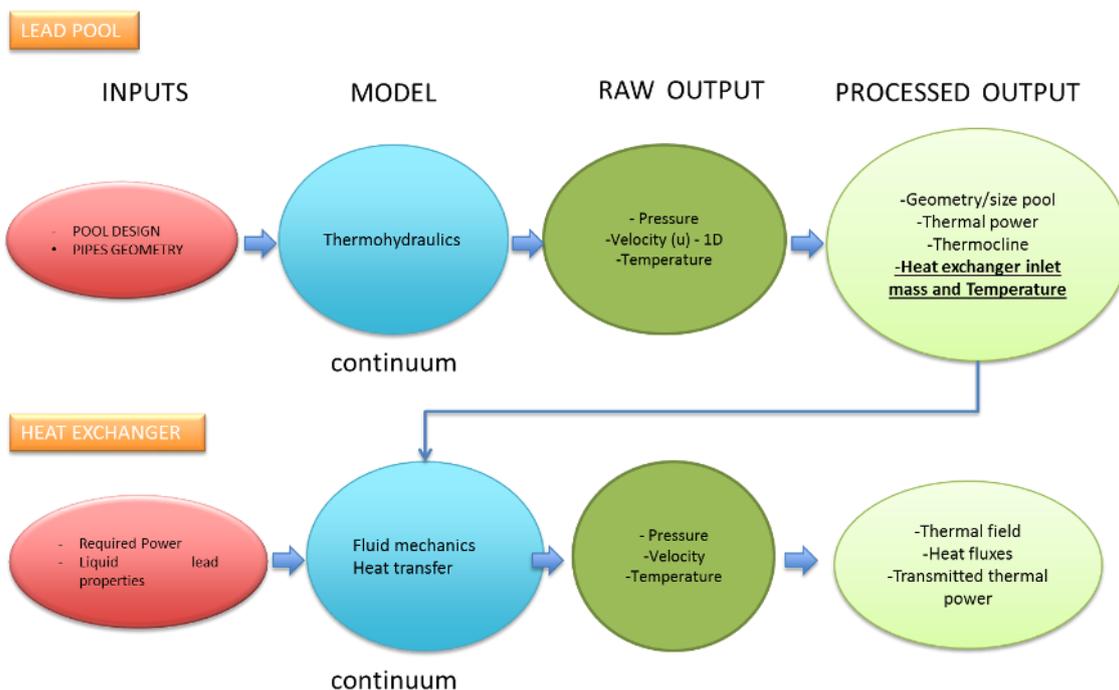
Purpose of this document:

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	<i>Thermo-fluid dynamic analysis of a lead/air heat exchanger in a high temperature thermal storage unit for concentrated solar power (called SOLEAD). The purpose of the simulation is to design correctly the geometry to assess the overall system circulation in the pool and ensure sufficient thermal power charge and storage</i>	
2	CHAIN OF MODELS	MODEL 1	<i>fluid mechanics and thermal model for analysis of the overall circulation in the lead pool of SOLEAD</i>
		MODEL 2	<i>Tightly coupled system of CFD and heat equations for analysis of the lead/air heat exchanger alone</i>
3	PUBLICATION ON THIS ONE SIMULATION	NA	
4	ACCESS CONDITIONS	<i>ANSYS available under commercial licences for parallel computing. RELAP owned by ENEA (a thermo-hydraulic code of nuclear derivation)</i>	
5	WORKFLOW AND ITS RATIONALE	<p><i>A coarse simulation will be done to determine the overall circulation of the lead pool (mass transport and natural convection) and the inlet temperature and flow rate in the heat exchanger. Then a more detailed simulation of the sole heat exchanger section will be done to refine the output and design the exchanger. Therefore:</i></p> <ul style="list-style-type: none"> <i>- MODEL 1 provides a modelling of the general circulation in the pool and its architecture.</i> <i>- MODEL 2 carries out a correct thermo-fluid dynamic design of the (primary) air/Pb Heat Exchanger alone. This point is crucial for the correct design and operations of the SOLEAD demonstrator in NEXTOWER.</i> <p><i>RELAP is a design thermohydraulic code from nuclear community and renders a general model of circulation of a reactor/storage system, like the one displayed below.</i></p>	



The CFD in MODEL 2 is just for one section of the lead pool.



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

1 ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED		
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	The overall circulation in the pool will be modelled and simulated by the System Thermal-Hydraulic code RELAP, assessing flow rate and thermal stratification in the pool.
1.2	MATERIAL	Pure liquid lead/air/AISI321 SS/ FeCrAl/KANTHAL® (the latter provided by SANDVIK)
1.3	GEOMETRY	The exact design of the heat exchange (HX) and of the position of the pool internals will be fixed by a preliminary engineering design.
1.4	TIME LAPSE	Stationary simulation
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	Adiabatic (hot air) Temperature BC (CLARIFYING NOTE: the pool is a closed hydraulic loop with fluid motion ensured by natural convection with temperature gradient coming from heat exchange in the primary and secondary heat exchanger. In the experiment, the pool will be thermo-regulated with "by cables" heating system to never go below 350°C at night. The wall are considered adiabatic in the model)
1.6	PUBLICATION ON THIS ONE SIMULATION	NA

2 GENERIC PHYSICS OF THE MODEL EQUATION			
2.0	MODEL TYPE AND NAME	Continuum models for Fluid Mechanics and energy	
2.1	MODEL ENTITY	Finite volumes	
2.2	MODEL PHYSICS/CHEMISTRY EQUATION PE	Equation	-Continuity Equation (conservation of mass) -Fluid mechanics: Momentum Equation (conservation of momentum) -Energy Equation (conservation of energy)
		Physical quantities	-Pressure -Velocity (u) – 1D -Temperature
2.3	MATERIALS RELATIONS	Relation	- For the physical properties of Lead, correlations as function for the temperature are taken from the Handbook of Liquid metals (see references); - The physical properties of air are fully known in engineering; - Physical properties for solids are provided by Sandvik - Correlations for friction factor and heat transfer in lead are taken from the Handbook (ref. Handbook [...], NEA-OECD, Science 2015, 2015)
		Physical quantities/descriptors for each MR	Physical properties of lead and air (fluids) in 300°C-700°C range: Viscosity [m^2/s] Density [kg/m^3] Specific Heat Capacity [$J/kg K$] Heat conductivity [W/mK] Physical properties of solids (AISI321 SS/FeCrAl/KANTHAL): Density [kg/m^3] Specific Heat Capacity [$J/kg K$] Heat conductivity [W/mK] Friction factor Heat transfer coefficient
2.4	SIMULATED INPUT	NA	

3 SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS		
3.1	NUMERICAL SOLVER	FINITE VOLUE ELEMENTS
3.2	SOFTWARE TOOL	RELAP (System Thermal Hydraulic code)
3.3	TIME STEP	not applicable

3.4	COMPUTATIONAL REPRESENTATION	PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL	Conservation laws integrated in volumes + correlations for friction factor and heat transfer *NB: friction about liquid lead with steel wall
3.5	COMPUTATIONAL BOUNDARY CONDITIONS	Adiabatic conditions of pool walls	
3.6	ADDITIONAL SOLVER PARAMETERS	Pure internal numerical solver details, if applicable, like <ul style="list-style-type: none"> • Specific tolerances • Cut-offs, convergence criteria: residuals 10^{-6} • Integrator options 	

4 POST PROCESSING

4.1	THE PROCESSED OUTPUT	A graphical post-proc through 1-D plot using the stripped data. Output will be given to MODEL 2 in terms of inlet temperature and flow rate in the HX.	
4.2	METHODOLOGIES	cross-sectioning of simulated domain (volume averaging to get T and v)	
4.3	MARGIN OF ERROR	NA	

MODEL 2

1 ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED

1.1	ASPECT OF THE USER CASE TO BE SIMULATED	Thermo Fluid Dynamic behaviour of (primary) air/Pb heat exchanger alone. The conjugate heat transfer in the heat exchanger and the fluid dynamics of both air and Lead will be simulated. The purpose is to determine the flux of hot atmospheric air to insure heat transfer from the solar receiver to lead-storage system.	
1.2	MATERIAL	Pure lead/air/AISI321 SS/FeCrAl/KANTHAL®	
1.3	GEOMETRY	The exact design of the HX and of the position of the pool internals will be fixed by a preliminary engineering design (a portion of overall geometry from MODEL 1)	
1.4	TIME LAPSE	Stationary calculations will be performed (static assumption)	
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	In service boundary conditions: inlet temperature, inlet mass, pressure and velocity of lead simulated by MODEL 1.	
1.6	PUBLICATION ON THIS ONE SIMULATION	NA	

2 GENERIC PHYSICS OF THE MODEL EQUATION

2.0	MODEL TYPE AND NAME	Continuum models of Fluid Mechanics (first order turbulence model) , Energy Eq	
2.1	MODEL ENTITY	Finite elements/volumes	
2.2	MODEL PHYSICS/CHEMISTRY EQUATION PE	Equation	Reynolds Averaged Navier-Stokes Equations + Turbulence model equations (2 equations) (RANS Approach) RANS Continuity Equation (conservation of mass) RANS Momentum Equation (conservation of momentum) RANS Energy Equation (conservation of energy) Closure Equation for turbulent kinetic energy 'k' Closure Equation for turbulent frequency 'omega'
		Physical quantities	Pressure Velocity components (u, v, w) Temperature

			<i>Turbulent kinetic energy Turbulent Frequency</i>
2.3	MATERIALS RELATIONS	Relation	<ul style="list-style-type: none"> - For the physical properties of the lead pool, correlations as function for the temperature are taken from the Handbook of Liquid metals (see references); - The physical properties of air are fully known in engineering; - Physical properties for solids are provided by Sandvik - Correlations for friction factor and heat transfer in lead are taken from the Handbook (ref. Handbook [..], NEA-OECD, Science 2015), which includes - Kinematic Eddy Viscosity and Closure Coefficients and Auxiliary Relation for the turbulent kinetic energy K in the k-ω approach.
		Physical quantities/ descriptors for each MR	<i>Physical properties of lead and air (fluids) in 300°C-700°C range:</i> <i>Viscosity [m²/s]</i> <i>Density [kg/m³]</i> <i>Specific Heat Capacity [J/kg K]</i> <i>Heat conductivity [W/mK]</i> <i>Physical properties of solids (AISI321 SS/FeCrAl/KANTHAL):</i> <i>Density [kg/m³]</i> <i>Specific Heat Capacity [J/kg K]</i> <i>Heat conductivity [W/mK]</i>
2.4	SIMULATED INPUT	<i>Mass flow rate and inlet temperature in the HX component from MODEL 1.</i>	

3 SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS			
3.1	NUMERICAL SOLVER	<i>ANSYS CFX</i>	
3.2	SOFTWARE TOOL	<i>CFX (Computational Fluid Dynamic module of the ANSYS code)</i>	
3.3	TIME STEP	<i>not applicable</i>	
3.4	COMPUTATIONAL REPRESENTATION	PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL	<i>Reynolds Averaged Navier-Stokes equations + k-omega SST (Menter) turbulence model. The discretization of the equation is finite element/finite volume</i>
3.5	COMPUTATIONAL BOUNDARY CONDITIONS	<i>NA</i>	
3.6	ADDITIONAL SOLVER PARAMETERS	<i>Pure internal numerical solver details, like</i> <ul style="list-style-type: none"> • <i>Specific tolerances on geometry to resolve mesh problems (as needed)</i> • <i>Cut-offs, convergence criteria: residuals 10⁻⁶</i> • <i>Integrator options</i> • <i>Mesh density</i> 	

4 POST PROCESSING			
4.1	THE PROCESSED OUTPUT	<i>The output will be post-processed to determine heat fluxes and air mass transport</i>	
4.2	METHODOLOGIES	<i>cross-sectioning of simulated domain for visualization, volume averaging</i>	
4.3	MARGIN OF ERROR		

6.2 MODA 2 - ceramic receiver

MODA#2

Modelling data documenting one simulation

Name <NEXTOWER, FEMME MODEL OF THERMOSTRUCTURAL BEHAVIOR OF SOLAR RECEIVER>

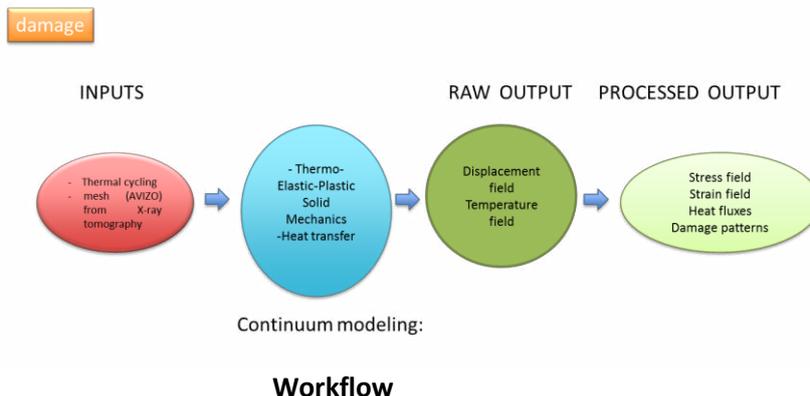
IMPORTANT: FEMME here is not to be mistaken for the FEMME code used in electromagnetism that is already in the ECMM database

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	<i>Stress analysis of solar receiver subject to microstructural damage The purpose of the simulation is to design correctly the solar receiver and provide insight about durability and damage trends (cliff edges in stress/gradients distributions). The goal is damage evolution and patterns following field operations and accelerated thermal cycling in furnace testing</i>	
2	CHAIN OF MODELS	MODEL 1	<i>micromechanics model for stress field tightly coupled to a heat transport equation. No MR is entered for damage, because microcracks patterns in the microstructure and at the interfaces/joints between SiSiC and SiC pieces are given as element removal in the mesh and the overall loss of stiffness measured from compaison of elastic simulations before and after damage.</i>
3	PUBLICATION ON THIS ONE SIMULATION	NA	
4	ACCESS CONDITIONS	<i>For AVIZO, ENEA has licence for parallel computing. For FEMME, UOXF is proprietary and will make it available to ICCRAM and ENEA.</i>	
5	WORKFLOW AND ITS RATIONALE		



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

5. Aspect of the User Case or System simulated with this model
6. Model
7. Computational aspects
8. Post processing

MODEL 1

1 ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED		
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	<p>Comparison of damaged and pristine solar receiver subject under static and cyclic load to assess damage evolution and produce data to estimate degradation rates and patterns, as well as lifetime of component in service</p> <p>Conditions chosen to match accelerated testing in solar furnace</p> <p>mechanical constraints + imposed heat fluxes and temperature gradient cycling associated to solar receiver and support (CIEMAT design, including air recirculator) .</p>
1.2	MATERIAL	SiSiC and SiC ceramics (linked to the two receivers foreseen in the NEXTOWER)
1.3	GEOMETRY	<p>Geometry corresponding to the prototype and smaller samples produced by ENGICER-LIQTECH after CIEMAT design of the receiver</p> <p>geometry from x-ray tomography (rendered by AVIZO software)</p> <p>The x-ray tomography of pristine and aged ceramic receivers will be fed as an input mesh for the finite element simulation of damage</p>
1.4	TIME LAPSE	6-12 months of thermal cycling
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	<p>Static load</p> <p>Mechanical constraint (constrained expansion from connection of receiver to metal support)</p>
1.6	PUBLICATION ON THIS ONE SIMULATION	N/A

2 GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	Continuum models of thermostructural mechanics. Tightly coupled system of solid mechanics and energy equation
2.1	MODEL ENTITY	Finite volumes and finite elements of full size receiver pieces. Not unit cell or RVE but actual replica of foam- cellular solid microstructure/geometry/porosity
2.2	MODEL PHYSICS/CHEMISTRY EQUATION PE	<p>Equation</p> <p>Equations of solid mechanics</p> <ul style="list-style-type: none"> - Conservation of linear momentum (Cauchy's equation) - Conservation of angular momentum (with imposed symmetry of stress tensor) <p>Laplace equation for heat transfer</p>
		<p>Physical quantities</p> <ul style="list-style-type: none"> - Cauchy stress tensor - Small strain Tensor - Temperature - Heat flux
2.3	MATERIALS RELATIONS	<p>Relation</p> <ol style="list-style-type: none"> 1. Elastic properties of SiSiC and SiC + joining (as determined by POLITO) 2. Yield behaviour 3. Coefficient of thermal expansion (CTE) of receiver components 4. Constitutive relations for finite strain thermo-elastic and plastic)

		Physical quantities/ descriptors for each MR	<ol style="list-style-type: none"> 1. Young's modulus and Poisson ration as $f(T)$ 2. Temperature (T) and heat fluxes 3. CTE of materials 4. densities
2.4	SIMULATED INPUT	N/A (there is no earlier model)	

3 SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS			
3.1	NUMERICAL SOLVER	ANSYS solvers	
3.2	SOFTWARE TOOL	ANSYS	
3.3	TIME STEP	none	
3.4	COMPUTATIONAL REPRESENTATION	PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL	Solid represented by Finite Elements, Microcracks inserted in the mesh by "element removal procedure"
3.5	COMPUTATIONAL BOUNDARY CONDITIONS	N/A	
3.6	ADDITIONAL SOLVER PARAMETERS	Mesh control (e.g. density, shape, order of elements)	

4 POST PROCESSING			
4.1	THE PROCESSED OUTPUT	<p>Damage parameters defined as %loss of effective stiffness :</p> <p>The output will be post-processed by a standard post-processor for FE simulations (ParafEM parafem.org.uk/) for peak stress identification by analysis of stress and strain fields distribution over the volume. Damage evaluation will proceed from microcrack patterns distribution and from the relative loss of stiffness from pristine conditions</p>	
4.2	METHODOLOGIES	visualization tool for strain mapping and damage pattern recognition	
4.3	MARGIN OF ERROR	N/A ¹	

¹ Associated to spurious stresses on free boundaries and mesh dependence of stress field in thin walled elements (of solar receiver)

6.3 MODA 3 - atomistic scale

MODA#3

Modelling data documenting one simulation

Name <NEXTOWER, Molecular dynamics modelling of the Fe/Pb interface>

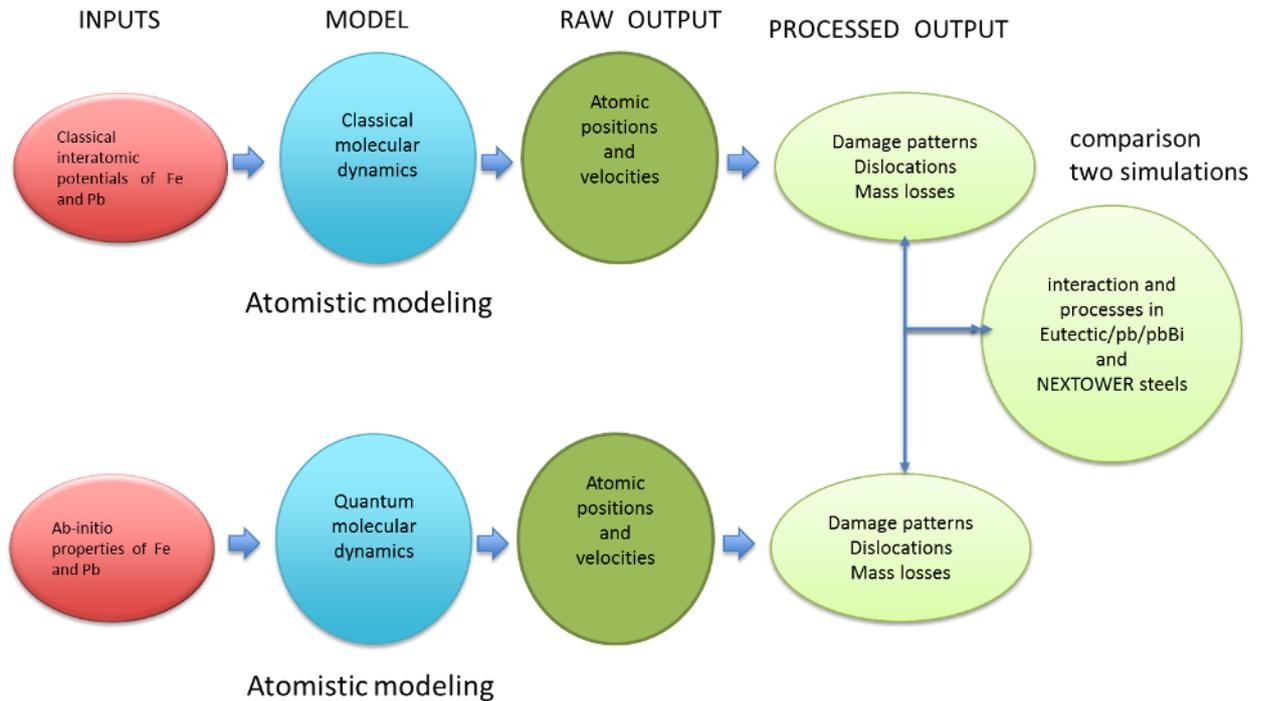
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OVERVIEW of the simulation		
1	USER CASE	<p><i>Simulation of the Fe/Pb interface in a model pipe within a demo loop. Emulating loop (plant demo) operation conditions at the atomic level for varying exposure temperatures</i></p> <p><i>The purpose of the simulation is to understand correctly the steel-eutectic (Fe/Pb) interface and to study the corrosion effects of high-temperature Pb fluid over the Fe surface, giving an exact description at the atomic level of all the steel and eutectic components.</i></p>
2	CHAIN OF MODELS	<p>MODEL 1 <i>Classical molecular dynamics of modelling of a Fe/Pb interface (Ch 2.3;1)</i></p>
		<p>MODEL 2 <i>Quantum molecular dynamics of modelling of the Fe/Pb interface (Ch 2.3.2)</i></p>
3	PUBLICATION ON THIS ONE SIMULATION	NA
4	ACCESS CONDITIONS	<i>LAMMPS is an open source code. CPMD is an open source code.</i>
5	WORKFLOW AND ITS RATIONALE	<p><i>Two approaches that are not interlinked giving complementary information (i.e. two separate Models):</i></p> <p><i>Model 1 has a reduced representation of the materials at the atomic scale</i></p> <p><i>Model 2 without a reduced representation, materials are described in an exact manner at a finer scale.</i></p> <p><i>The models run in parallel with NO interoperability.</i> <i>The models will be examined and benchmarked together in the post-processing, establishing what performs better vs. experimental results</i></p>

Fe/Pb interface



Workflow

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

- 9. Aspect of the User Case or System simulated with this model
- 10. Model
- 11. Computational aspects
- 12. Post processing

MODEL 1

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	Classical molecular dynamics of modelling of the Fe/Pb interface.
1.2	MATERIAL	Fe/Pb (reduced representation of FeCrAl/KANTHAL®)
1.3	GEOMETRY	Model interface with PBC at atomic level
1.4	TIME LAPSE	1-10 ns
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	Emulating loop (plant demo) operation conditions at the atomic level. Temperature range 500C – 700C
1.6	PUBLICATION ON THIS ONE SIMULATION	

2 GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	<i>Classical MD.</i>
2.1	MODEL ENTITY	<i>The entity in this materials model is atoms</i>
2.2	MODEL PHYSICS/CHEMISTRY EQUATION PE	Equation <i>Newton's equation of motion Chapter 2.3.1</i>
		Physical quantities <i>Atomic positions, Atomic velocities, Interatomic forces</i>
2.3	MATERIALS RELATIONS	Relation <i>Interatomic potentials</i>
		Physical quantities/ descriptors for each MR <i>form of force field for Fe/Pb,</i>
2.4	SIMULATED INPUT	NA

3 SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS		
3.1	NUMERICAL SOLVER	<i>Verlet Algorithm for integration.</i>
3.2	SOFTWARE TOOL	<i>LAMMPS</i>
3.3	TIME STEP	<i>Femtoseconds</i>
3.4	COMPUTATIONAL REPRESENTATION	PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL
3.5	COMPUTATIONAL BOUNDARY CONDITIONS	<i>Periodic Boundary Conditions (PBC) to model particle flow at the interface</i>
3.6	ADDITIONAL SOLVER PARAMETERS	<i>Pure internal numerical solver details, If applicable, like</i> <ul style="list-style-type: none"> <i>Specific tolerances</i> <i>Cut-offs, convergence criteria: residuals 10^{-6}</i> <i>Integrator options</i>

4 POST PROCESSING		
4.1	THE PROCESSED OUTPUT	<i>Damage patterns, exchanges of compounds at the surface and within the liquid metal flow. Dislocations, defects (and propagation) and mass losses of Fe.</i>
4.2	METHODOLOGIES	<i>Dislocation analysis (via Burger's vector), defect analysis (Wigner Seitz method) and Centro Symetry parameter. Everything will be done via opensource software as OVITO(http://ovito.org/) and self developed code (from EU-FP7-RADINTERFACES) RADAMAT-FOAM®. RADIATION DAMAGE IN MATERIALS FOR OPENFOAM. Ekhi Arroyo, Jordi Fradera, Santiago Cuesta, Universidad de Burgos. BU-59-13. 03/05/2013.</i>
4.3	MARGIN OF ERROR	<i>Depending on truncation error, system size and thresholding for convergence</i>

MODEL 2

1 ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED		
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	Quantum molecular dynamics modelling of the Fe/Pb interface. Interface will be designed precisely without a reduced representation.
1.2	MATERIAL	Fe/Pb (FeCrAl/KANTHAL®) introducing proper atoms for a more precise description of the eutectic (Pb-Bi) and the steel
1.3	GEOMETRY	Model interface with PBC at atomic level
1.4	TIME LAPSE	1 ns (simulation scale) but directly induced acceleration of damage conditions will be tested
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	Emulating loop (plant demo) operation conditions at the atomic level. Temperature range 500C – 700C
1.6	PUBLICATION ON THIS ONE SIMULATION	NA

2 GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	Ab initio Molecular Dynamics (Car-Parrinello Molecular Dynamics). Chapter 2.3.2
2.1	MODEL ENTITY	The entity in this materials model is atoms
2.2	MODEL PHYSICS/CHEMISTRY EQUATION PE	Equation <i>classical equations of motion for the nuclei</i> <i>(They are integrated using the sum of the interatomic potential and the forces derived from the electron potential energy surface. At each time step, the ground-state electronic potential surface can be calculated using standard quantum mechanical methods (Born-Oppenheimer Molecular Dynamics) or introducing fictitious dynamics for the electrons which follow adiabatically the nuclei and are subjected to small readjustments "on the fly" during the nuclei evolution to keep them close to the ground state potential surface (Car-Parrinello Molecular Dynamics). (Chapter 2.3.2)</i>
		Physical quantities <i>Atomic positions, velocities and interatomic forces</i>
2.3	MATERIALS RELATIONS	Relation <i>Forces derived from Interatomic potentials and the electron potential energy surface</i>
		Physical quantities/ descriptors for each MR <i>Positions (atomic arrangement at the interface)</i> <i>Electric charge</i> <i>Mass</i>
2.4	SIMULATED INPUT	Fe/Pb Bi (FeCrAl/KANTHAL®)



3		SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS	
3.1	NUMERICAL SOLVER	Verlet / rattle algorithm	
3.2	SOFTWARE TOOL	CPMD (public)	
3.3	TIME STEP	It will be adjusted during simulation process (1 fs – 10 ⁻³ fs)	
3.4	COMPUTATIONAL REPRESENTATION	PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL	
3.5	COMPUTATIONAL BOUNDARY CONDITIONS	Periodic Boundary Conditions (PBC) to model particle flow at the interface	
3.6	ADDITIONAL SOLVER PARAMETERS	Pure internal numerical solver details, If applicable, like <ul style="list-style-type: none"> • Specific tolerances • Cut-offs, convergence criteria: residuals 10⁻⁶ • Integrator options 	



4		POST PROCESSING	
4.1	THE PROCESSED OUTPUT	Damage patterns, exchanges of compounds at the surface and within the liquid metal flow. Dislocations, defects (and propagation) and mass losses of Fe. In addition to the above information, common to the classic approach – MODA 1, we will be able to infer forces and deduce changes mechanical properties.	
4.2	METHODOLOGIES	Dislocation analysis (via Burger's vector), defect analysis (Wigner Seitz method) and Centro Symetry parameter. Everything will be done via opensource software as OVITO(http://ovito.org/) and self developed code (from EU-FP7-RADINTERFACES) RADAMAT-FOAM®. RADIATION DAMAGE IN MATERIALS FOR OPENFOAM. Ekhi Arroyo, Jordi Fradera, Santiago Cuesta, Universidad de Burgos. BU-59-13. 03/05/2013.	
4.3	MARGIN OF ERROR	Depending on truncation error, system size and thresholding for convergence	