1 Public summary - WP1

The Porto platform has been developed as a tool for industrial technologies in Europe. Current needs for the materials modelling development involves complex workflows and interoperability between numerous expert tools and systems. With a focus on metadata, interoperability and workflows, the Porto platform is now one of the most promising technologies to take on this challenge.

WP1 has mainly been a software development project, where the initial tasks involved requirements engineering in terms of defining test systems, use cases, software development platforms etc. The consortium was involved in a series of workshops to define the connections between the scales, and to define the data that should be shared. Figure 1 illustrates one such workflow that was included in the MODA for WP4. Enabling a common scripting platform with a set of storage back-ends (MongoDB) and defined interfaces was the next step. The Qt5 Framework (The Qt Company Ltd) was employed as the main development framework as it has a rich feature set and is very cross platform portable. Qt5 also have support for an integrated ECMAScript engine (JavaScript) that was suitable to use as the main scripting engine with a few custom extensions.

Enabling a database backend for Porto was necessary for us to have a common meta-data storage as well as a scalable common storage for different types of simulation data (inputs, configurations, results and other types of relevant information).

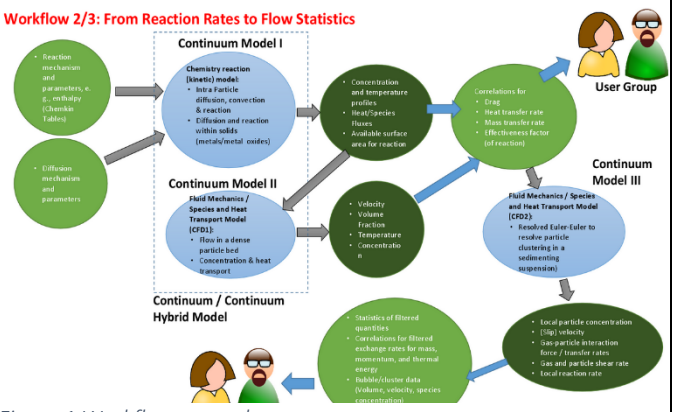

Figure 1 Workflow example

The first software preview was made available on GitHub with a tutorial such that the community could start playing with some of the key concepts and ideas. Further work was the development of the workflow runner, which is able to run tests as well as production workflows.
The final work done on the Porto platform was to enable custom back-ends to serve as specialized readers and writers to/from proprietary file formats. By taking this out from the simulation tools and into the platform, the platform is now able to deliver proprietary I/O capabilities in software that was never written for handling these kinds of formats. Since they only have to consider custom what the data is, the Porto platform will take care of the syntactic layer and the operations on how the data is handled.

2 Public summary – WP2

The COSI open source simulation software platform is composed of three core components:

- LIGGGHTS®, a DEM software for the simulation of flow of granular particles
- CFDEM®coupling, a CFD-DEM software for the simulation of flow of gases or liquids in conjunction with granular particles
- ParScale, a novel simulator for modelling intra-particle transport processes such as heat transfer or chemical reactions

The existing LIGGGHTS® and CFDEM®coupling packages are based on two other established open source packages, LAMMPS and OpenFOAM®. Both packages were successfully extended, enhanced and maintained to the benefit of NanoSim

Moreover, the newly developed ParScale simulator could be successfully integrated with LIGGGHTS® and CFDEM®coupling, and quality control mechanisms were developed, extended and applied to all three packages.

In M1-M36, the following results have been achieved:

- several software releases for the COSI platform (D2.4), namely via LIGGGHTS® versions 3.5.0, 3.4.1, 3.4.0, 3.3.1, 3.3.0, 3.2.1, 3.2, 3.1, 3.0.4, 3.0.4, 3.0.2, 3.0.1, 3.0.0, CFDEMcoupling releases 3.5.1, 3.4.0, 3.3.0, 2.9, 2.7.1, 2.6.1, ParScale releases 1.1.1 beta, 1.0.1 beta and associated updates and CPPPO releases 1.1, 1.0
- smooth start of collaborative software development (D2.1),
- establishing core functionality for COSI for parallel scalability (D2.2)
- first version of software testing system for COSI testing (D2.3)

The following detailed sub-goals could be achieved:

- adding support for multiple OpenFOAM versions (most recently: 3.X) to the COSI simulation eco-system
- adding support for multiple OpenFOAM branches (Weller, extend)) to the COSI simulation eco-system and in the software testing system
- other improvement of the testing coverage for the COSI system (LIGGGHTS, CFDEMcoupling, ParScale)
- improvement of the flux consistency in unresolved CFD-DEM capabilities in CFDEMcoupling
- successive improvements of the Many2Many code coupling scheme, including performance improvement by, introducing an error-tolerant scheme to avoid any allreduce communication
- stability improvement for unresolved CFD-DEM by improvement of volume fraction calculation
- stability improvement for unresolved CFD-DEM by exchange term smoothing
- improvement of various capabilities, canalized in a new release of LIGGGHTS and CFDEMcoupling

3 Public summary – WP3

3.1

WP3.1

Over the last 18 month period we have performed DFT simulations on the methane reforming and hydrogen production thermodynamics and kinetics of two materials, haematite Fe_2O_3, and magnetite Fe_3O_4.

For the former materials we have continued our exploration of the surface chemistry, determining the thermodynamics for the full set of reforming reactions and H_2 production steps. We have improved our understanding of the kinetics of the reforming reaction, and determined the kinetics for H_2 production. Only determination of the CH→C+H activation energy is required for a complete understanding of the kinetics of the reforming reaction.

We have also started exploring the surface chemistry of the Fe-oxide phase produced upon Fe_2O_3 reduction, magnetite Fe_3O_4. We determined the complete kinetics and thermodynamics for H_2 production on this material. We have also completed a complete thermodynamic assessment of the reforming reaction on this surface, and obtained activation energies for the first two steps. Only determination of the CH_2→CH+H and CH→C+H activation energies are required for a complete understanding of the kinetics of the reforming reaction.

WP3.2

Over the last 18 months we have completed our work on the determination of oxygen transport kinetics of the Fe-oxide materials, Fe_2O_3, Fe_3O_4, and FeO. This work was performed using classical pair potentials. We obtained oxygen diffusion constants for the three materials for various temperatures, and reported these in a deliverable report (D3.4). Our data will be transferred to WP4 for multiscale modelling.

WP3.3

In order to facilitate transfer of rate constants to WP4, REMARC was further developed and connected to Porto. Relevant meta-data were defined for the parameters to be transferred in collaboration with WP1. This will be a part of deliverable 3.5.

To further process the elementary reaction kinetics parameters obtained from WP3.1, Kinetic Monte Carlo (kMC) simulations are underway and will be analyzed to provide overall rates for effective reactions for WP4. In the course of the work it was found that SPPARKS, the originally intended kMC software, was inadequate for these purposes, and replaced by the kmos software instead. A first simple kMC model has been established, demonstrating CH_4 reacting with an iron oxide surface. This model will be further refined and the simulations will be analyzed to provide the necessary rate data. A simple reaction scheme has been implemented and will be populated with rate data for WP4. This will also be a part of deliverable 3.5.

WP3.4

Over the last 18 months we used DFT simulations to investigate different barrier materials resistance to Fe inclusion. We obtained Fe interstitial defect formation energies for differing silicate and hexaaluminate materials, and reported these in a deliverable report (D3.3).

WP3.5

A first version of the REMARC set of scripts was developed and documented, as reported in deliverable report D3.2.

4 Publishable summary – WP4

This work package is in the stage of refining and employing the produced open-source software tools for the simulation of reactive particulate flows. Specifically, model development and verification studies regarding thermal radiation were finished, and a new mesh-less model is currently applied to a sheared box setup to evaluate the relative importance of radiation (see Figure 1 for a typical result). Also, the developed immersed boundary method for particle-resolved direct numerical simulation of suspension flow has been extended. Furthermore, the formulation for the forcing term in the momentum equation has been improved to enhance stability and accuracy. A number of publications has been accepted in, or submitted to, renowned international journals to effectively disseminate the results of the work package.

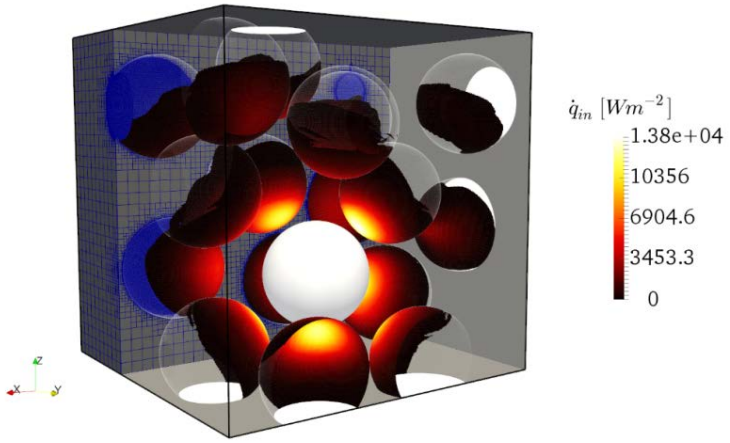

Figure 2: Intristic thermal radiative flux in a paced bed using a finite volume discrete ordinate method.

5 Public summary – WP5

Modelling of dense gas-particle flows, using the Two Fluid Model (TFM) approach closed by the Kinetic Theory of Granular Flows (KTGF) is well established. However, recently, it has been shown that the numerical simulations using a too coarse mesh may fail to predict the behavior of the solid phase by the bad prediction of the solid clusters. The development of a filtered approach and subgrid models allows to take into account the effect of the unpredicted solid cluster on the large-scale behavior of the solid phase.

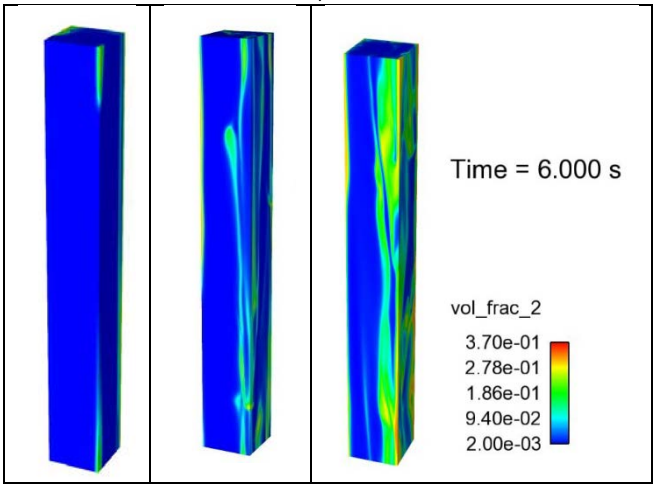

Figure 3 - Effect of the mesh refinement on the distribution of the solid phase in circulating fluidized bed (from left to right the mesh is finer).

This work package focus primarily on circulating fluidized beds. Highly resolved mono- and bi-disperse, reactive and non-reactive, numerical simulations are performed for different particle material properties. A spatial filter is applied on the results from highly resolved numerical simulations. This approach allows separating the exact filtered terms and the computed terms obtain in simulation with a coarse mesh. The difference between these two contributions, called subgrid (SGS) contribution, has to be modeled. The budget analysis of the TFM set of equation identifies that the gas-particle interaction term is dominant even in binary mixture. New SGS models are developed in WP5 even some based on the local velocity gradients.

6 Public summary – WP6

The WP6, Phenom, within NanoSim consists of a platform with 1-D generic phenomenological models for both fixed bed and fluidized bed reactors. The fluidized bed model consists on a steady-state model based on the two-phase/zone fluidization concept proposed by Toomey and Johnstone (1954). The generality of Phenom is related to the probabilistic approach developed by Abba et al. (2003) used to describe the reactor hydrodynamics. The current model is able to complete full scale reactor simulations within reasonable timeframes and can be run under both regimes, stationary and transient. Phenom is also the primary link to the system-scale simulations carried out in WP8.

7 Publishable summary – WP7

The synthesis work has followed a two-pronged approach, with nanostructured oxygen carrier materials produced and tested on two different scales:

1) Small-scale (10 gram batches) synthesis of nanoparticles embedded in a support obtained through three different methods.
2) Large scale (kg batches) wet impregnation of commercial support materials generating nanostructures, defined by the pore size/structure.

The synthesis of several 10 gram batches of nanostructured oxygen carriers embedded in inert support material was realized using three different approaches;

i. Gelling of support material commercial irregular shaped (10x50-100 nm) nanoparticles.
ii. Gelling of support material with small (<10 nm), pre-synthesized nanoparticles.
iii. "Two phase gel" method generating nanoparticles (10-20 nm) directly during synthesis.

The oxygen carrying capacity of the prepared oxygen carrier materials was investigated using thermo-gravimetric analysis (TGA). After cycling between reducing and oxidizing atmospheres at temperatures up to 700°C, some degree of reaction between the carrier and matrix materials is observed from XRD analysis, however, the oxygen capacity remains stable over time. Micro reactor tests on several of these nanostructured oxygen carriers indicates some (however limited) activity towards methane reforming at 700°C. Applying an activation step and increasing the temperature to 900°C proved a ~30% conversion of methane for one of the materials. The obtained CO/H2 ratio from this experiment indicated the presence of combustion which is also confirmed by the presence of significant amounts of CO_2 produced. Some further optimization of the micro reactor experiments is needed for better understanding of reaction mechanisms. A comparable analysis of nano- and non-nanostructured oxygen carrier materials is still to be performed.

In order to meet the mass/volume requirements of the lab scale pilot reactor constructed and applied within the project, the active material was impregnated into commercially available porous supports by wet impregnation, on a kg scale. The impregnation process is still to be optimized to improve penetration into the support particle bulk and reduce the surface coating of the support particles. This is necessary to minimize the generation of fines, expected from fluidization of the particles at high temperatures (> 800°C). This work is in progress with the support of modelling activities on the wet impregnation drying procedures.

The lab scale fluidized/fixed bed reactor designed and constructed in 2015 is commissioned and currently being operated under real CLC and CLR process conditions and at elevated pressures. Initial experiments performed using the nanostructured materials made via wet impregnation into commercial supports indicate poor activity towards reforming. This will be evaluated further and new materials tested. Other tests were completed with ilmenite and Mn-based oxygen carriers running the CLC process under pressurized conditions. The data will be used for CFD model verifications.

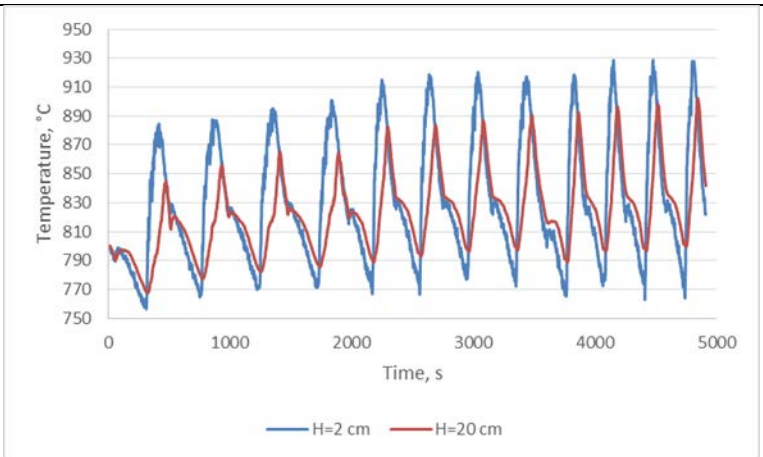

Figure 4: Transient temperature of autothermal operation of the GSC reactor under operating pressures of 3, 4 and 5 bar (4 redox cycles were completed for each operating pressure). The gas feed was increased with the same proportion as the pressure in order to maintain equal superficial gas velocity in the reactor. Ilmenite was used as oxygen carrier and CO as fuel gas

8 Publishable summary – WP8

The aim of the Work Package 8 is to link the 1D Phenomenological Model of Chemical Looping Reforming (CLR) to the Power Plant Simulations and carry out a techno-economic assessment. Firstly, a thermodynamic comparison on the basis of exergy destruction was carried out for CLR and conventional partial oxidation process. CLR proves to be a better process when the conditions in the reactor are near adiabatic. 1D Phenomenological Model, developed as a part of WP6, was linked with Water Gas Shift (WGS) & CO_2 capture process simulation on Aspen Hysys and power plant simulations on Thermoflow Suite. The linking was established using the Microsoft Excel platform for data exchange. This fulfilled the Task 8.1 of the WP8, and the respective deliverable report has been published. As a part of Task 8.3 to carry out the techno-economic assessment of the entire process, full plant scale analysis were carried out. Net efficiency of the process was estimated by integrating the CLR, WGS, CO_2 capture & compressions and power plant process. The results were presented at GHGT-13 and a paper has also been submitted. Studies on process improvement through heat integration were presented at TGTC-4. The net electrical efficiency of the process after heat integration is 45%.

9 Public summary – WP9

WP 9 has achieved the following tangible results so far:

- one official NanoSim workshop was successfully held (in the frame of Particles 2015 conference)
- two more official workshops are planned and confirmed for 2018
- the NanoSim consortium has been represented at a number major international conferences
- keynotes were held at major international conferences and events, such as the CFDEM®user conference and workshop 2016 in Linz (Austria, > 100 participants), at the 7th International Conference on Discrete Element Methods in Dalian (China, > 300 participants), the China-UK High Level Cooperation and Advanced Materials Forum as well as the PRACE autumn school and workshop 2016 in Hagenberg (Austria, > 50 participants)
- the exploitation strategy set up following the Exploitation Strategy Seminar (ESS) in Brussels
- Cluster activity performed
- 3 official newsletters were sent out
- a project website as well as an interactive user forum are in operations and are both continuously used and updated
- A total research output (papers + conference contributions) of 25 in the reporting period (M19-M36)