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PROJECT FINAL REPORT

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Project website Error! Bookmark not defined. **address:** https://www.sintef.no/projectweb/nanosim/

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1 Executive Summary

NanoSim project created an efficient and cost effective multi-scale simulation platform based on free and open-source codes in the context of reactive fluid-particle flows. This platform connected models of various type (i.e., electronic, atomistic, mesoscopic, and continuum), and spanned an extremely wide range of scales. Specifically, the project achieved to connect atom-scale phenomena (i.e., chemical reactions, diffusion), and meso-scale phenomena in fluid-particle systems (e.g., clustering) with process-scale aspects such as economic feasibility or optimal process conditions. Therefore, the NanoSim project developed one offline linking, and one online coupling software tool.

The offline linking tool "Porto" is a free and open source software system for connecting multi-scale simulations. Porto allows models to be composed into automated workflows where the input and output from each scale is described semantically. This has made it possible to compose workflows consisting of both open source software and proprietary software tools, as the connection between different software packages used in the NanoSim project are realized independent of proprietary file formats and conventions.

For online coupling, the project created "COSI": a co-simulation platform based on extended versions of the popular open source LIGGGHTS® and CFDEM®coupling simulation packages. These packages implement the Discrete Element Method (DEM) to solve Newton's equation of motion, and the Finite Volume Method for classical Computational Fluid Dynamics (CFD) simulations. The combined CFD-DEM package was integrated with a newly developed simulation tool (i.e., ParScale[2]), as well as the postprocessor CPPPO[3]. COSI is in active use by industry and in research, and useful for studying heat and mass transfer problems in a large variety of industrial systems, e.g., fixed and fluidized beds.

To establish these software tools, the project performed implementation tasks, as well as developed (or improved) models and materials relations (MRs) to describe relevant phenomena. MRs were mainly developed based on simulation output at a certain scale, and were then used to close the physics equations on the next coarser scale. This scientific coupling between scales is supported by sophisticated software and data management in such a way that the actual model implementation in various software packages is fully automatic.

Reaction rate constants for methane-iron oxide systems were calculated based on electronic density functional theory (DFT) and atomistic kinetic Monte Carlo (kMC) calculations. The post-processor tool "REMARC" was developed to extract and process data from DFT and kMC output, as well as to fit the resulting reaction rate constants to Arrhenius parameters. These kinetics parameters have been supplied to a variety of continuum models. These models describe species and heat transport over a wide range of length scales: (i) within porous macroscopic particles (~ 100 µm), (ii) in reactive fluid-particle suspension flows (~100 mm), as well as (iii) within a full-scale chemical reactor (~10 m).

The modeling of reactive fluid-particle suspension flows was in the focus of NanoSim, and was concerned with dense bubbling or fixed beds, as well as circulating fluidized bed systems. The modeling consisted in the integration of new, more appropriate materials relations (using the post-processing tool, CPPPO) into formalism where the discrete form of the particles is lost, i.e., a continuum model-based description of the flow. This modeling approach was selected to tackle the industrial scale issues in terms of designing and optimizing full-scale reactors. A specific example was

[2] https://github.com/CFDEMproject/ParScale-PUBLIC
[3] https://github.com/CFDEMproject/C3PO-PUBLIC/tree/master/doc

the use of an appropriate continuum model on the device scale to quantify the process intensification advantages offered by nano-structured materials.

The NanoSim project also developed reduced (i.e., one-dimensional) continuum models for full scale fluidized bed reactors used in the chemical looping reforming (CLR) process. Such a model of the CLR reactors with the CO_2 capture process was linked with power plant simulations, i.e., a system model. Once the linking approach was established, techno-economic analysis of a gas fired power plant with CO_2 capture based on CLR has been carried out. The kinetic data for reforming reactions using nano-structured materials was used from DFT and kMC simulations.

Experimental work on lab-scale reactors supported these modeling activities: Supported nanostructured oxygen carrier materials were synthesized, both at gram and kilogram scale. Their performance under reforming conditions was evaluated using a lab-scale reactor for fluidized and packed bed experiments, built up within the project. The experimental results were used for validation of multi-scale modeling and demonstration of process intensification for syngas production from natural gas reforming.

NanoSim dissemination was successful to interact with projects under the same call (via the EMMC – European Materials Modeling Council). NanoSim also scientifically disseminated its results via 85 publications and conference presentations, successfully held 4 workshops in the frame of international conferences and released a number of software components as open source packages.

In summary, NanoSim's open source software platform and the multi-scale model linking methodology was used to facilitate the rational design of second generation gas-particle CO_2 capture technologies based on nano-structured materials with a particular focus on CLR. However, the final NanoSim platform is sufficiently generic for application to a wide range of gas-particle contacting processes. Project outcomes are therefore expected to have far-reaching positive impacts on the European and global process industry.

Contents

2 Project context and objectives of the project

The project conducted through 9 technical work packages. In WP1, SINTEF developed the core component of NanoSim: the integrated, multi-purpose and free environment for information flow and data sharing between different simulation packages, Porto. This environment supported scientific computation, data analysis, testing, validation and visualization. In WP2, DCS developed COSI, a CFD-DEM co-simulation platform and implemented novel code coupling schemes for co-simulation and ensured software quality and maintenance.

In WP3 atomistic calculations were used by UCL and SINTEF to determine fundamental thermodynamic and kinetics data of reactive materials, which were selected by SINTEF, for input into larger-scale models developed in WP4, WP5, WP6 and WP8. This was accomplished through a new post-processing tool, REMARC. REMARC was added as an extension tool to Porto for connecting the atomic scale to ParScale and the co-simulation tool COSI.

Critical closure information (e.g., for gas species and heat dispersion) for resolved simulations of fluidized bed (TUG) and fixed bed (UCOIMBRA) flows at the meso level was provided by performing direct numerical simulations (DNS) in WP4 led by TUG. The particle-scale models required for this purpose was implemented in the library PaScal, which formed an integral part of COSI. This work package received information regarding transport properties and reaction rates from the atomistic studies in WP3, as well as the experiments of SINTEF (WP7).

Development of filtered two fluid models for large scale simulation in fluidized beds was conducted in WP5 by INPT, NTNU and SINTEF. UCOIMBRA also developed models to capture multidimensional effects in fixed beds in this work package. A commercial code; ANSYS FLUENT and an in-house code; NEPTUNE_CFD, were used to accelerate the model development process. The inputs to this work package such as heat and mass transfer coefficients, effective reaction rates were provided by WP4. ANDRITZ and SINTEF tested and evaluated the filtered models regarding the practical application for full scale industrial purposes.

In WP6, UCOIMBRA, NTNU and SINTEF developed fast and user-friendly 1D phenomenological models (Phenom) especially for the purpose of industrial end-use and coupling to end user tools. ANDRITZ led this work package to keep research efforts directly in line with industrial interests.

WP3 and WP4 provided information to WP7 to guide the production of nano-materials with respect to their composition, porosity and size. The performance of the manufactured materials was subsequently tested under real CO_2 capture conditions in a pressurized gas-solid reactor constructed and operated especially for this purpose. Results from the reactor experiments were also used for model validation.

NTNU and SINTEF used the large scale filtered models and the 1D phenomenological models to design an economically optimized CO_2 capture reactor/process in WP8. The primary aim of this work package was to establish best practice guidelines for using the NanoSim platform to add maximal value to industry.

In WP9 all partners worked together towards dissemination and education based on the results of the project.

Project context and objectives specific to each work package are described in the following sections.

2.1 WP1 - Common Environment Software Platform ("Porto")

An objective of the NanoSim project is to create an efficient and cost effective multi-scale simulation platform based on free and open-source codes. This platform will connect models spanning a wide range of scales from the atomic scale through the particle and cluster scales, the industrial equipment scale and the full system scale.
The objective of WP1 Common Environment Software Platform ("Porto") has been to provide a unified environment for information flow and data sharing. Sharing is facilitated between open and proprietary software packages, independent of proprietary file formats and conventions. This is made possible by using semantically annotated data fields.
The purpose of Porto is to build workflows and connect the different software packages used in the NanoSim project. In particular, these workflows can be used to facilitate the rational design of second generation gas-particle CO2 capture technologies based on nano-structured materials with a particular focus on Chemical Looping Reforming (CLR).
The entire software platform is made available under the Lesser General Public Licence (LGPL) which will allow the software to be used in research and commercial products, while users to contribute to the platform.

2.2 WP2 - Development of Scale-Bridging Co-Simulation Software Platform ("COSI")

The objective of the NanoSim project is to create an efficient and cost effective multi-scale simulation platform based on free and open-source codes. The focus of WP2 was to create a core co-simulation platform called COSI which will be established based the existing CFDEM®coupling and LIGGGHTS® open source simulation engines (particle and continuum modeling). These 2 existing simulation engines are complemented by the new simulation code ParScale and a filtering tool (CPPPO). The development of COSI is the core of WP2 (also the integration of development of ParScale and CPPPO in WP4). COSI can then be used to perform detailed Euler-Lagrange simulations of gas-particle systems such as fluidized or packed beds. The data from these detailed simulations (each particle or parcels of particles resolved) can be filtered using CPPPO and be used for closures in Euler-Euler simulations. Thus, COSI provides the basis for the work in WP4 and WP5.

2.3 WP3 - Atomistic Modelling

Atomistic modeling allows for the detailed evaluation of chemical reaction mechanisms, and the corresponding thermodynamics and kinetics. This makes it possible to directly model the reactivity of given materials and chemicals without involving the particular flow conditions. Atomistic modeling thereby serves as a complement to the flow modeling performed in the other work packages of NanoSim as well as a tool to interpret and complement experiments. The particular focus of WP3 has been to determine rate constants for all relevant atomistic processes as well as the nanoparticle stability on support material. This also involves the development of a tool (REMARC) for post-processing and communication of reaction data from atomistic to particle scale and continuum scale, as well as between atomistic codes and communication of the obtained structural and reactivity data to the Porto database.

2.4 WP4 - Lagrangian Modelling

WP4 (Lagrangian modeling) connects to WP2 (development of the co-simulation software platform "COSI", which can be seen as the framework into which tools and results of WP4 will be integrated), as well as WP5 (this work package benefits from material relations and software developed within WP4) and WP9 (i.e., exploitation via academic education and training). Also,

WP4 has a connection to WP3 with respect to interoperability with the tool “REMARC” that produces reaction kinetic data.
WP 4 has **two main software development objectives**: i) development of a simulation tool (based on a reduced continuum model for porous particles) for predicting concentration and temperature profiles within particles, as well as ii) development of a post-processing tool for offline coupling of direct numerical (flow) simulations (DNS; based on a continuum model of fluid and particle flow) of heat and mass transfer in dense suspensions. The latter objective includes the extension of an available DNS simulator in CFDEM®. In addition, WP 4 has two **main application objectives** (i.e., heat transfer experiments and validation of flow predictions, reversibility checks, and the development of material relations), as well as **one main documentation objective** (i.e., the provision of educational resources (documentation and training material preparation to ensure future exploitation).

2.5 WP5 - Eulerian Modelling

Two approaches can be used for the numerical simulations of gas-solid flows: the Euler-Lagrange approach or the Eulerian approach. Even if the Lagrangian approach is very attractive because of the reduced number of assumptions, the colossal number of particles involved in practical application, like in chemical looping combustion, limits the Lagrangian approach to the laboratory scale. Hence, nowadays, the numerical simulation of large industrial-scale gas-particle flows can only be done by the Eulerian approach. The Eulerian modeling of dense gas-particles flows is based on the Two-Fluid Model (TFM) that is derived from the kinetic theory of granular flows. Even if the TFM approach is well established some closures laws needs to be improved for better predictability of the numerical simulations. WP5 aims to improve the TFM and especially by taking into account the effects of unresolved structures. Indeed, recently it has been highlighted that if the mesh size is too large small-scale clusters are not well predicted leading to a bad prediction of the drag force and consequently a wrong solid flow rate in a circulating fluidized bed and a wrong bed height in a dense bubbling fluidized bed. WP5 has put the focus on the reactive flows and polydisperse flows. Basically, a database of mesh-converged 2D and 3D, reactive and non-reactive periodical circulating fluidized bed has been built. A spatial filter has been applied for extracting the computational and the subgrid contribution (the missing part that requires closure) that appears when a filter is applied on the TFM. The filtered approach has been assessed by a priori and a posteriori tests. The a priori tests consist of comparing the observed values in the mesh-converged simulations to model predictions. On the other hand, a posteriori tests consist of comparing the results of coarse grid simulations using subgrid closures to resolved simulation results or to experimental data.
Although the WP5 mainly put the focus on the fluidized bed, a part has been dedicated to fixed beds. Heat and mass transfer in fixed beds have been investigated by means of Particle Resolved Direct Numerical Simulation (PR-DNS). The results of this study were subsequently used to perform simplified 1D simulations of the Packed Bed Chemical Looping Reforming (PBCLR) process. The FTFM model has also been introduced in the OpenSource platform, OpenFoam®.

2.6 WP6 - Phenomenological Modelling

1D phenomenological models are a very popular and effective framework within industry for simulation, design and optimization of reactors due to its computational efficiency and relative simplicity when compared to more complex fundamental models that are still not easily accessible by industry. The aim of the phenomenological model within NanoSim (Phenom) is to deliver results of industrial interest in a user-friendly manner and within timeframes of seconds/ minutes.
Phenom consists of an already existing transient model for fixed bed reactors developed at SINTEF that has been regularly used in industrial projects and a steady/transient model for fluidized bed reactors developed within NanoSim. The current formulation of Phenom consists of a generic 1D phenomenological model for fluidized bed reactors based on the averaging probabilistic approach

proposed by Thompson et al. (1999) that combines more than one fluidization regime and allows a smoother transition between them. Phenom's formulation includes bubbling, turbulent and fast fluidization regimes that are the most used fluidization regimes in industry and in the chemical looping reforming process. It also handles stationary and transient simulations. Other features were added to the model such as the incorporation of membranes, simulation of co-current or counter-current reactor configuration and single or a cluster of reactors.
Phenom has been applied to three different chemical looping reforming technologies: the conventional chemical looping reforming (CLR), the novel gas switching reforming (GSR) and the fuel reactor of the membrane-assisted chemical looping reforming (MA-CLR).

2.7 WP7 - Validation Experiments

There two overall objectives for NanoSim WP7 are experimental validation of:

1. Effect of nano-structured materials on the performance in chemical looping processes
2. Process intensification of chemical looping processes determined by Multiphase flow models

The effect of nano-structured materials is validated through a threefold approach:

i. Synthesis of a selected state of the art nanostructured oxygen carrier with porosity, nanoparticle distribution and fluidizable granulate size as recommended from the NanoSim platform. Inert, porous support materials of suitable shape, size and mechanical strength will be impregnated with the nanocomposite oxygen carrier material.
ii. Development of an experimental protocol based on thermogravimetric analysis data and reactor testing that will serve to validate predictions from the NanoSim model (e.g. kinetics of oxidation and reduction, mass loss and gain and thermal stability).
iii. Evaluation of the synthesis method and other relevant methods with regard to their potential for translating into industrial scalable systems.

Multiphase flow model validation is obtained through:

I. Design and construction of a lab-scale fluidized/fixed bed reactor for testing the nanostructured material under real CLR process conditions. This is applied for the demonstration of potential for process intensification through the use of nano-structured materials at high temperatures, elevated pressures and variable feed gases.
II. Data from this reactor will include instantaneous pressure, temperature and gas composition measurements over the entire reactor height. The experimental campaign will be used to verify the reactive performance and mechanical stability of the material over many cycles of CLR process operation as well as to validate the resolved reactive multiphase flow CFD models.

2.8 WP8 - Techno-Economic Assessment

The primary objective of the project NanoSim is to speed up the development of second generation CCS processes. The current work package is dedicated to techno-economic assessment in NanoSim. In line with the objectives of NanoSim, the detailed tasks of the current WP are listed below.

- Establish multiscale modeling methodology to link 1D models of reforming reactors and power plant simulations and hence reduce the time taken in design of novel CCS processes
- Process design and integration studies of pre-combustion CO_2 capture methods like chemical looping reforming (CLR) in combined cycle power plants
- Identify suitable design conditions in CLR through sensitivity studies to achieve higher net electrical efficiency and CO_2 avoidance rates
- Estimate the levelised cost of electricity for the combined cycle power plants integrated with CLR
- The overlying objective of this WP is also to contribute through scientific publications and presentations.

2.1 WP9 - Dissemination and Education

The objective of the NanoSim project is to create an efficient and cost effective multi-scale simulation platform based on free and open-source codes. This platform will connect models spanning a wide range of scales from the atomic scale through the particle and cluster scales, the industrial equipment scale and the full system scale. To support the information flow and data sharing between different simulation packages, the NanoSim project will develop an open and integrated framework for numerical design called Porto to be used and distributed in terms of the GNU Lesser General Public License (LGPL). A core co-simulation platform called COSI (also licensed as LGPL) will be established based on existing CFDEMcoupling (an open source particle and continuum modeling platform).
The goal WP9 is to foster dissemination for the NanoSim project, to disseminate tangible results over the lifetime of the project, how to interact with fellow projects under the same call.

3 Main Results of the project

3.1 WP1 - Common Environment Software Platform ("Porto")

The Porto platform

This work package developed Porto, a free and open source software system for connecting multi-scale simulations. Porto allows models to be composed into automated workflows where the input and output from each scale is described semantically.

These workflows have been demonstrated in several use cases. These use cases have demonstrated how Porto can be used for connecting the specific software packages used in NanoSim as well as demonstrating techniques and technologies used for connecting software and models of different domains, *in general*.

A key point has been to make Porto open source and freely available. Therefore, Porto is under LGPL (Lesser General Public Licence) which allows the software to be used in both research and commercial applications. The source code is available at https://github.com/NanoSim/SOFT5.

Porto is built on top of a framework called SOFT (SINTEF Open Framework and Tools), a set of tools and approaches that has been developed for working with scientific software. The structure of SOFT and Porto is illustrated in Figure 1.

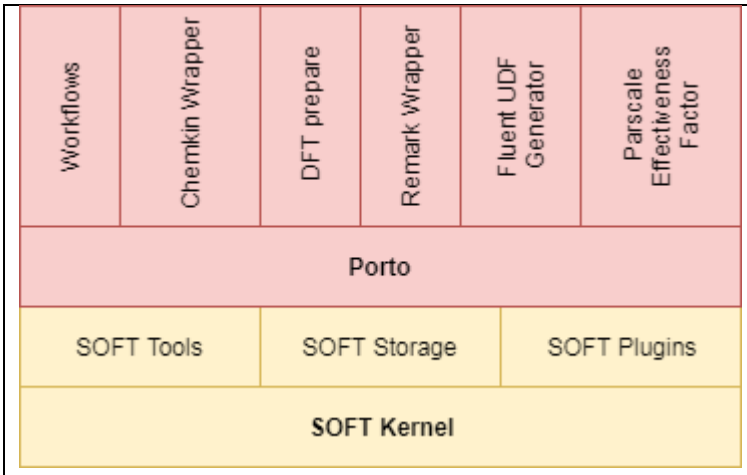


Figure 1: Structure of Porto built on top of SOFT, a set of tools and approaches used in multiple scientific software packages.

Porto has C, C++, Python and JavaScript interfaces. Porto uses MongoDB as a back-end storage database. MongoDB supports high performance storage and retrieval of large data sets. Porto also facilitates other future data storages by using a *storage plugin* architecture. For example, the HDF5 (Hierarchal Data Format) data format can be used in place of MongoDB.

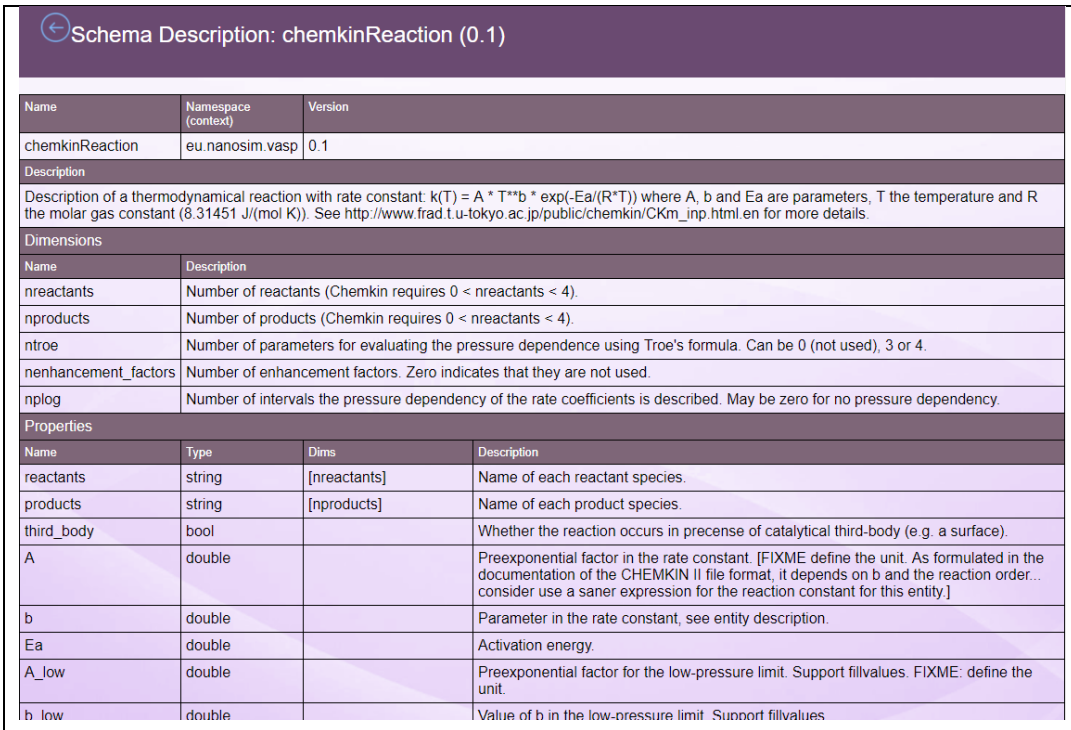
Porto builds on the needs and experiences from NanoSim as well as other use cases outside this project, combined with good software engineering practices. Making this platform publicly available can aid others with connecting scientific software across multiple scales and even across multiple domains.

In addition, the chosen software license for Porto (LGPL) ensures that any software changes to Porto that is used in proprietary software must be made public. This strongly encourages that future development and additions to Porto will be consolidated and made available to all users.

Semantic interoperability

Multi-scale modeling is the discipline of utilizing multiple models at different scales to describe a system. The data flows through the different scales, where simulations are connected steps of data transformations. The data itself does not have meaning unless it is put into a context and becomes information. The sharing and transformation of information requires that there exists information interchange mechanism.

The Porto framework encourages a focus on semantic interoperability for the offline coupling of simulators and data analysis tools. This means that Porto uses an abstract representation of data and context that does not enforce the need for syntactic standardization on file formats and protocols. This is done by describing the data on a *metadata* level by describing what kind of data should be available, not how the data is stored. For example: The property "Activation Energy" can be described by the metadata *name*, *unit*, *description* and have a value without specifying how this value is stored in a file or in a database (see Figure 2).



Schema Description: chemkinReaction (0.1)

Name	Namespace (context)	Version
chemkinReaction	eu.nanosim.vasp	0.1

Description

Description of a thermodynamical reaction with rate constant: k(T) = A * T**b * exp(-Ea/(R*T)) where A, b and Ea are parameters, T the temperature and R the molar gas constant (8.31451 J/(mol K)). See http://www.frad.t.u-tokyo.ac.jp/public/chemkin/CKm_inp.html.en for more details.

Dimensions

Name	Description
nreactants	Number of reactants (Chemkin requires 0 < nreactants < 4).
nproducts	Number of products (Chemkin requires 0 < nreactants < 4).
ntroe	Number of parameters for evaluating the pressure dependence using Troe's formula. Can be 0 (not used), 3 or 4.
nenhancement_factors	Number of enhancement factors. Zero indicates that they are not used.
nplog	Number of intervals the pressure dependency of the rate coefficients is described. May be zero for no pressure dependency.

Properties

Name	Type	Dims	Description
reactants	string	[nreactants]	Name of each reactant species.
products	string	[nproducts]	Name of each product species.
third_body	bool		Whether the reaction occurs in precense of catalytical third-body (e.g. a surface).
A	double		Preexponential factor in the rate constant. [FIXME define the unit. As formulated in the documentation of the CHEMKIN II file format, it depends on b and the reaction order... consider use a saner expression for the reaction constant for this entity.]
b	double		Parameter in the rate constant, see entity description.
Ea	double		Activation energy.
A_low	double		Preexponential factor for the low-pressure limit. Support fillvalues. FIXME: define the unit.
b_low	double		Value of b in the low-pressure limit. Support fillvalues.

Figure 2: Screenshot of an entity (chemkinReaction) described in terms of metadata, shown in the Porto entity inspection interface. Properties of entities are given names, types and a description, as well as a dimensionality for multi-dimensional properties. This information is used by Porto when connecting different software packages.

Metadata is stored in *Entities*, which describes one discrete set of data, and *Collections*, which describes the relation between entities, for example by acting as a container of multiple entities. Each software package takes one set of entities as *input* and provides one set of entities as *output*. Workflows are then composed of multiple input/output steps where entities are semantically connected. Instances of entities and collections are uniquely referred to using unique identifiers, *UUIDs*.

Using metadata to connect scales is a powerful tool. This means that if there exists a description of what goes in and out of a software, it can be connected with other software packages. In fact, this demonstrates a universal approach that can be used for general interoperability. General interoperability can be connection between different scales, between different domains and between measurement technologies.

Coupling of models in workflows

Several workflows have been realized using Porto, demonstrating that the software platform is able to automatically run multiple software packages and handle the data flow between them.

The software packages connected in these workflows can be used to facilitate the rational design of second generation gas-particle CO2 capture technologies based on nano-structured materials with a particular focus on Chemical Looping Reforming (CLR). This means that software packages from multiple scales have to be involved.

Figure 3 illustrates one such workflow component, where the three packages DFT, Remarc and ANSYS Fluent are connected.

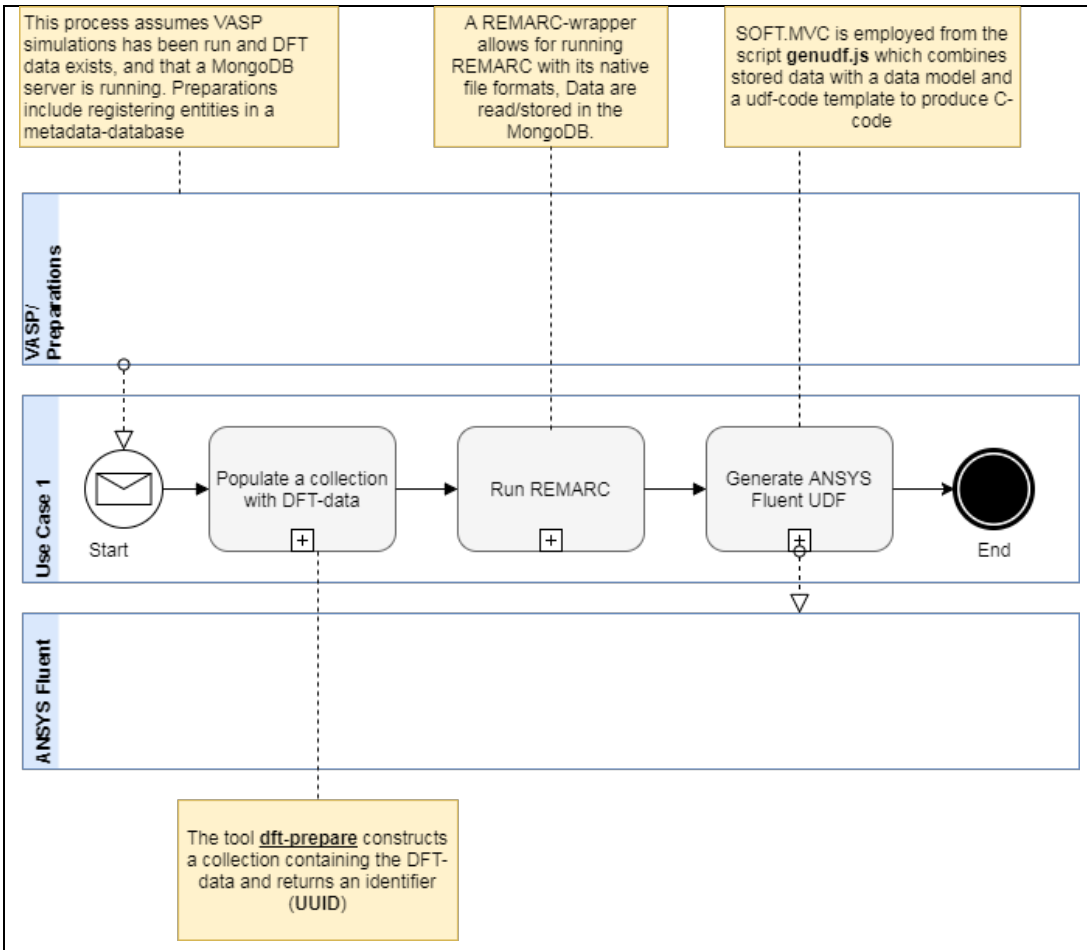


Figure 3: Schematics of one automated process using Porto. This process automates the work involved going from a DFT (Density Functional Theory) data set to the atomistic scale modeling in REMARC, to automatically generating a UDF (User Defined Function) to be used with ANSYS Fluent for CFD simulations. The entire process is executed through one user command.

These workflows allow the user to set up and run multiple scenarios without the need for manual intervention. Also, by automating the workflows, using the MongoDB database as storage and uniquely referring to simulation cases by their UUID, workflow results are also easily traceable and reproducible. This also removes some possible human errors where repeated, manual manipulation of input and output files is involved.

3.2 WP2 - Development of Scale-Bridging Co-Simulation Software Platform ("COSI")

WP 2 has achieved the following main results:

- Fully functional and operating COSI platform, culminating in a series of releases (Table 1) and outlined by a vivid user community (Figure 4).
- Substantial further development and improvement of existing LIGGGHTS® and CFDEM®coupling software (example: **Code Coupling Improvement**)
- Full integration of ParScale and CPPPO development
- Full quality control cycle established (Figure 7)

Table 1 presents and overview of the release activity of the different packages:

Table 1: Overview of the release activity of the different packages

Name	**Version(s) released (small bufgix releases omitted)**	**Date(s)**
LIGGGHTS®	3.8.0, 3.7.0, 3.6.0, 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	30/11/17, 07/07/17, 17/01/17, 19/05/16, 1 14/01/16 23/09/15, 21/07/15, 29/04/15, 18/02/15. 3 28/08/14, 12/06/14, 10/04/14, 23/01/14
CFDEM®coupling	PU: 3.8.0, 3.7.0, 3.6.0, 3.5.1, 3.4.0, 3.3.0, 2.9, 2.7.1, 2.6.1 CO:internal releases	PU: 01/12/17, 11/07/17, 18/01/1706/09/16 15/01/16, 26/02/15, 03/06/14/, 03/03/14 CO:07/10/15, 25/04/15, 24/04/15, 26/03/1 05/01/15
ParScale	PU: 1.1.1 beta, 1.0.1 beta and associated updates	27/01/17, 12/04/16, 04/02/16, 21/01/16 24/09/15, 23/08/15, 31/12/14
CPPPO	PU: 1.1, 1.0 CO: 88 commits	11/05/16, 09/05/16, 26/02/15 CO: 09/09/16 - 09/10/15

Figure 4 shows a snapshot of the user forum for the COSI components CFDEM®coupling, LIGGGHTS® and ParScale – created administered by DCS.

Forum	Topics	Posts	Last post
Contributed simulations, cases, scripts, tutorials Whenever you make something work which you think could be useful for others as well, please put it here!	14	35	By AnjanaKittu 1 week 4 days ago
ParScale - User and Developer Forum Discussions about the ParScale simulation engine go here!	23	56	By occipitalgubbins 18 hours 36 min ago
CFDEM®coupling - User Forum This is a forum dedicated to CFDEM®coupling using the LIGGGHTS® DEM code and OpenSource CFD.	757	3134	By marcelo 1 day 37 min ago
CFDEM®coupling- Developer Forum Topics related to developing with CFDEM®coupling can be discussed here: discussion about implementation details, C++, MPI and debugging tools	38	104	By zbtlfd 3 weeks 4 days ago
LIGGGHTS® - User Forum LIGGGHTS® related topics can be discussed here: discussion about models, installation, feature requests and general discussion	1756	7342	By Bruno.Brunel 2 hours 7 min ago
LIGGGHTS® - Developer Forum Topics related to developing with LIGGGHTS® can be discussed here: discussion about implementation details, C++, MPI and debugging tools	136	567	By mschramm 1 month 1 week ago
Bug Reports for CFDEM®coupling, LIGGGHTS®, and ParScale (Possible) bugs / suspicious behavior should be reported as a new thread here, not in the user forum. This should give both you and the developers a clear idea about the status of your bug report (submitted/assigned/fixed)	118	480	By arnom 1 day 6 hours ago
Post Processing Post processing of LIGGGHTS®/CFDEM®coupling/ParScale based simulations is discussed here	139	589	By richti83 3 days 21 hours ago
CFDEM®coupling, LIGGGHTS® and ParScale - Announcements from the developers Announcements from the developers go here	145	193	By aaigner 5 days 6 hours ago
CFD and DEM - General Discussion Anything that is related CFD and DEM modelling can be discussed here	47	136	By AndresMM 1 month 3 weeks ago

Figure 4: User forums (Screenshot as of 12/12/2017) available at http://www.cfdem.com/forum with 12,636 total # of forum posts

Code Coupling Improvement: In coupled simulations you have to sync two or software packages with their time steps. To date, we used a Gauss-Seidl scheme (see Figure 6) and there was an issue in case of sub time-stepping on the CFD side and major improvement was implemented in CFDEM®coupling. A drastic improvement in the consistencies of the U, voidfraction, Ksl, and force fields could be achieved.

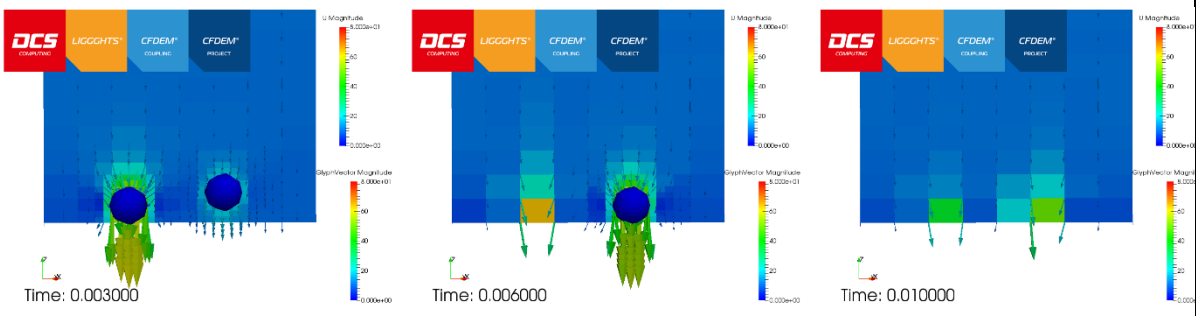


Figure 5: Stability improvement for unresolved CFD-DEM by improvement of volume fraction calculation: Volume fraction calculated by CFDEM®coupling versions 3.4.0 and 3.5.1.

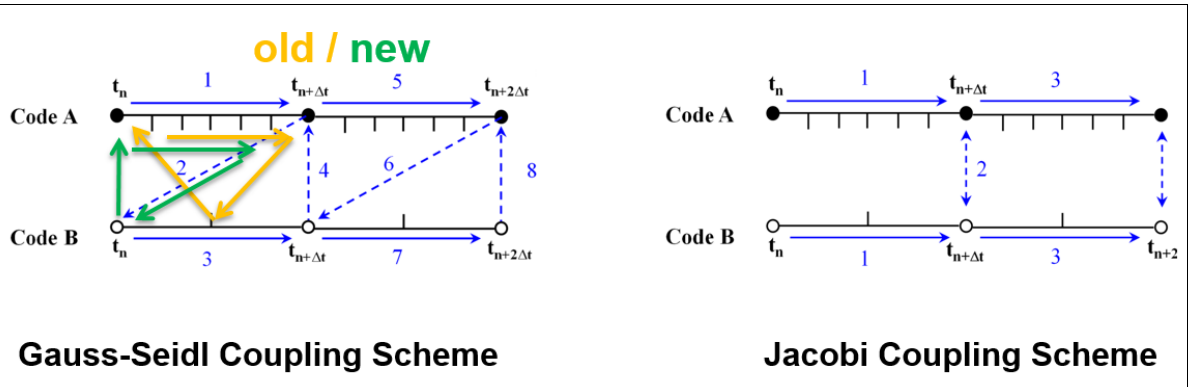


Figure 6: Code coupling schemes

Full quality control cycle established: A new test server has been set up at DCS Computing, because the existing one reached the end of its lifetime (operating system was outdated), and an existing customized test system (based on the backbone of the Jenkins CI system) has been validated, further developed, improved and adapted to encompass all COSI components. The system is now comprised of more than 1000 tests (only a small portion of the tests shown in Figure 7), and extends to different combinations of the COSI components as well as OpenFOAM®. The system tests compilation as well as several unit tests and larger simulations, the quality critera can be defined on a per-testcase basis, but usually include #particles, energies, pressure probes and similar data.

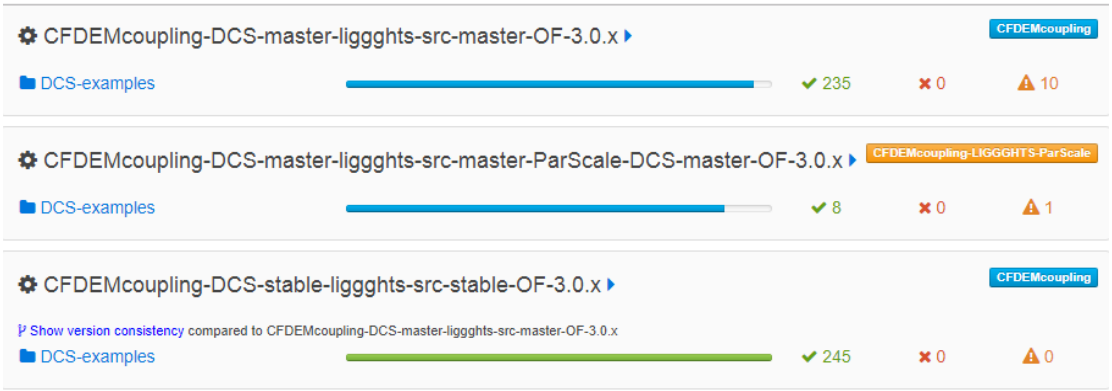


Figure 7: Coverage of testing system for different COSI components in the automated test routine

3.3 WP3 - Atomistic Modelling

The main results of WP3 are:

- The REMARC (REaction Mechanism And Rate Calculator) set of scripts developed in Python for the extraction and postprocessing of data calculated by Density Functional Theory (DFT) codes to provide kinetic and thermodynamic data for kinetic modeling in a semi-automatic way. The raw and processed results from the atomistic calculations were described semantically using Porto and, via its Python interface, distributed to the other WPs.
- Reaction mechanisms for methane, hydrogen, water vapour, carbon monoxide and carbon dioxide reacting at iron oxide (haematite Fe_2O_3 and magnetite Fe_3O_4) surfaces calculated by DFT (see example in Figure 8). The choice of materials and reactants was made in discussion with WP7.
- Rate constants for the above reactions extracted from kinetic Monte Carlo (kMC) calculations that in turn were based on DFT energies and fitted by REMARC to Arrhenius expressions to describe temperature dependence. These kinetics parameters were distributed for use in kinetic modeling in the form of CHEMKIN-II files or equivalent data for User Defined Functions (UDFs) used in modeling in WP4, WP6, and WP8. The calculated rate constants depend on the size, shape and composition of the reactive particles (see Figure 9). This has been the main activity of WP3 during the last 12 months of the project and it will therefore be described in more detail below.
- The oxygen transport kinetics of the iron oxide materials, Fe_2O_3, Fe_3O_4, and FeO were studied by molecular dynamics (MD) simulations. Oxygen diffusion constants were obtained for the three materials for various temperatures. These data are crucial for the modeling of the redistribution of oxygen in the oxides during reaction.
- Fe interstitial defect formation energies for differing silicate and hexaaluminate materials calculated by DFT calculations. These data were used to investigate different barrier materials resistance to iron inclusion as a support to experimental activities in WP7, specifically the stability of the different combinations of iron oxide nanomaterials and support materials.

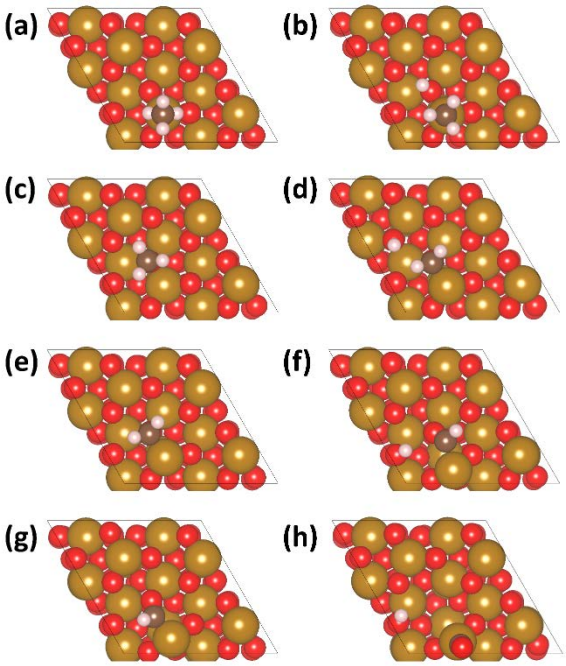


Figure 8: Thermodynamically stable structures for CH4 adsorption and molecular fragments produced upon reforming on the Fe2O3-(0001) surface (left) and Fe3O4(110) surface (right). (a) is CH4, (b) is CH3+H, (c) is CH3, (d) is CH2+H, (e) is CH2, (f) is CH+H, (g) is CH, and (h) is C+H. Iron is represented by large brown sphere, oxygen by small red sphere, carbon by small dark brown sphere, and hydrogen by small blue sphere.

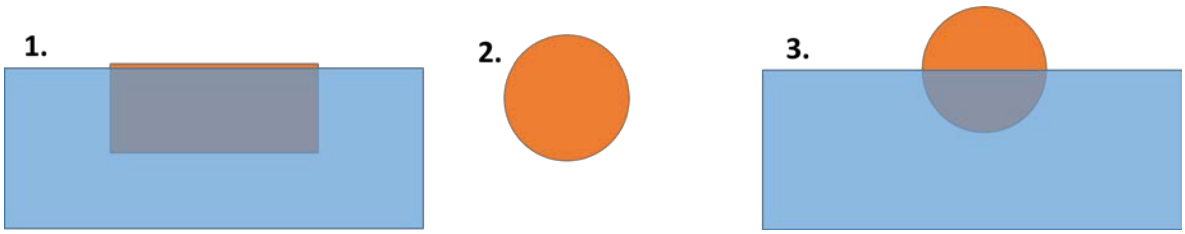


Figure 9: The three cases of reactive particle considered: 1. Embedded square block with only flat surface exposed, 2. Spherical particle with whole surface exposed, and 3. Embedded spherical particles (half surface exposed).

Kinetic Monte Carlo Modelling of gas-surface reactions at Fe_3O_4 surface

Rate constants for methane-iron oxide systems have been calculated based on DFT and kinetic Monte Carlo (kMC). The focus has been on in particular methane interacting with Fe_2O_3 and Fe_3O_4 surfaces. Also, CO and H_2 oxidation reactions and CO_2 and H_2O reduction reactions have been considered. The latter was concluded to be more relevant to chemical looping reforming applications.

The kMC method allows for the kinetics of a system to be studied with greater accuracy than traditional microkinetic rate equation models. In particular, it allows for resolving a complex reactive system in *molecular detail* including individual sites and atoms and molecules. At the same time, there is no need to describe the system in *atomistic details*, including molecular structures and interactions, such as for molecular dynamics or electronic structure calculations, allowing for fast simulations. In a *lattice kMC* model one only needs to specify a number of

connected sites, populations of atoms and molecules at these sites, and the rates of reaction and transition (e.g., diffusion or adsorption/desorption). Subsequently, a stochastic simulation of the motion and reaction of the species can be carried out, where one process at a time occurs. The time scale of the simulation is determined by the sum of the individual rates for the processes.

The kMC output are given in the form of turnover-frequencies (TOFs), i.e, reaction rate per site, for the production (or consumption) of given species. These TOFs have been converted to reaction rate constants that are dependent on the size, shape and composition of the reacting particles. Subsequently, rate constants calculated at a range of temperatures, typically 700-1100°C, are fitted to Arrhenius parameters that describe the temperature dependence of the rate constants

Kinetic Monte Carlo simulations have been performed using the *kmos* framework. The (1x1) surface unit cells of Fe_2O_3 and Fe_3O_4 are used to model the gas-surface reactions. A (20x20) unit cell with periodic boundary conditions has been employed for all simulations (see Fig. 35 for an example of the visual interface of *kmos* during simulation). The simulations have been performed based on DFT data as input for different adsorption, desorption, diffusion and reaction processes.

The calculation of rate constants is system-specific. We have considered three specific cases as reactive particles(Figure 9):

1. Square block with only flat surface exposed
2. Spherical particle with whole surface exposed
3. Embedded spherical particles (half surface exposed)

Rate constants are calculated from TOFs for specific processes and are therefore calculated as effective rate constants for simplified overall reactions based on the complex reaction network of elementary reactions as calculated by DFT. Rate constants calculated in the temperature range 700-1100°C have been fitted to Arrhenius expressions for describing their temperature dependence.

The kinetics parameters have been supplied to WP4, WP6, and WP8 in suitable formats, e.g., CHEMKIN-II (see Figure 10) or native formats used in, for instance, user defined functions (UDFs).

Rate constant expression (Arrhenius):

$$\boldsymbol{k(T) = AT^{\beta} exp(-E_a/RT)}$$

```
 CHEMKIN II file produced by REMARC for T =  973.00 - 1373.00 K
and P =   1.00 atm
! This is the case of an embedded 10nm nanoparticle
! Rate constant units are: s, cm, moles, kJ/mole
   ELEMENTS C H FE O
   END
   SPECIES
   CH4    CO    CO2    H2    H2O
   Fe12O18   CFe12O18   H2Fe12O18
   Fe2O3   Fe3O4    Fe3O3
   END

   REACTIONS  KJOULES/MOLE  MOLES
   CH4+Fe12O18=>CFe12O18+2H2Fe12O18     1.810E+06 0.000 18.535
   CFe12O18=>CO+3Fe2O3+2Fe3O4           3.192E+12 0.000 18.381
   CFe12O18=>CO2+4Fe3O4                 6.808E+12 0.000 85.315
   H2Fe12O18=>H2+6Fe2O3                 6.244E+12 0.000 34.317
   H2Fe12O18=>H2O+3Fe2O3+2Fe3O4         3.756E+12 0.000 15.021
   CH4+Fe3O4=>CO+2H2+Fe3O3              1.169E+11 0.000 132.368
   H2+Fe3O4=>H2O+Fe3O3                  2.647E+15 0.000 233.538
   CO+Fe3O4=>CO2+Fe3O3                  1.545E+18 -3.381 0.000
   CO2+Fe3O3=>CO+Fe3O4                   3.101E+20 -4.804 0.000
   H2O+Fe3O3=>H2+Fe3O4                   1.069E+23 0.000 375.990
   END
```

```
! CHEMKIN II file produced by REMARC for T =  973.00 - 1373.00
K and P =   1.00 atm
! This is the case of a 1 micron particle
! Rate constant units are: s, cm, moles, kJ/mole
   ELEMENTS C H FE O
   END
   SPECIES
   CH4    CO    CO2    H2    H2O
   Fe12O18   CFe12O18   H2Fe12O18
   Fe2O3   Fe3O4   Fe3O3
   END

   REACTIONS  KJOULES/MOLE  MOLES
   CH4+Fe12O18=>CFe12O18+2H2Fe12O18     3.621E+04 0.000 18.535
   CFe12O18=>CO+3Fe2O3+2Fe3O4           3.192E+12 0.000 18.381
   CFe12O18=>CO2+4Fe3O4                 6.808E+12 0.000 85.315
   H2Fe12O18=>H2+6Fe2O3                 6.244E+12 0.000 34.317
   H2Fe12O18=>H2O+3Fe2O3+2Fe3O4         3.756E+12 0.000 15.021
   CH4+Fe3O4=>CO+2H2+Fe3O3             2.338E+09 0.000 132.368
   H2+Fe3O4=>H2O+Fe3O3                 5.294E+13 0.000 233.538
   CO+Fe3O4=>CO2+Fe3O3                 3.090E+16 -3.381 0.000
   CO2+Fe3O3=>CO+Fe3O4                  6.202E+18 -4.804 0.000
   H2O+Fe3O3=>H2+Fe3O4                  2.138E+21 0.000 375.990
   END
```

Figure 10. CHEMKIN-II files for reactions at Fe_2O_3 and Fe_3O_4 surfaces for the cases embedded 10 nm spherical particle (left) and 1 µm spherical particle (right)

3.4 WP4 - Lagrangian Modelling

1) **New Software for implanting Material Models into Device and Process Models: ParScale**
ParScale was established as a unique simulation tool that can act both as a stand-alone simulator, as well as a sub-module on the "COSI" platform. The software architecture features interface capabilities to any C/C++-based simulator (via packaging in a library). Most important, ParScale has specialized data containers that allow fast and efficient processor-to-processor communication – this enables an efficient coupling of ParScale to any simulator of mesoscopic models (e.g., granular dynamics simulators such as LIGGGHTS®). With respect to models, ParScale features a general modular approach (i.e., multiple model equations can be added via a simple input script, and material relations can be plugged in as needed). This makes ParScale easy to be applied to a large variety of problems that can be described with a **reduced continuum approach** (ParScale is currently limited to one spatial coordinate). The **expected results** with respect to the ability to model complex reaction-diffusion problems **was clearly exceeded**: ParScale is in fact able to describe different types of diffusion (i.e., classical continuum and Knudsen diffusion), is able to describe a three-phase system (i.e., liquid-gas-solid phases within each particle), and has an interface to the widely-used "CHEMKIN II" file format to describe chemical reactions. This is of outmost importance, since it allows **implanting material models (e.g., that describe chemical reaction rates) into a device model** (e.g., that predicts flow in a bed of particles) **or even a process model** (e.g., that predict the performance of a chemical reactor).
The **quality of this result** is demonstrated by (i) **4 forks (i.e., adaptations) of the "ParScale" software tool** by users outside of NanoSim, (ii) **numerous publications** that have used ParScale (see, e.g., Forgber and Radl[4] and references therein), and (iii) **documented usage** of "ParScale" outside of NanoSim (i.e., already 55 forum posts on that are related to ParScale).
This results was produced within Task 4.1 and 4.2 (see Description of Work, DoW) in close collaboration between TU Graz and DCS Computing.

2) **New Software that lifts the Development of New Material Relations to the Next Level: CPPPO**
CPPPO is a "first of its kind" tool for the development of material relations to be used in continuum (or hybrid continuum/mesoscopic) models for flow predictions. While CPPPO is "only" a post-processing tool, it has shown to have a large impact on the **quality of material relations** developed by researchers: due to its unique modular approach, CPPPO allows the screening of potentially-useful correlations between quantities to be modeled (in the context of NanoSim, this would be a material relations for the rate of momentum exchange, for example) and "markers" (i.e., properties of flow field that are known, e.g., difference in the average speed of particles and fluid). Two outstanding demonstrations of this fact are (i) the seminal work of J.H. Cloete[5] performed at SINTEF (work done as part of WP5), as well as (ii) of Municchi[6] performed at TU Graz as part of WP4.
The **quality of this result** is demonstrated by (i) **a wide** application of CPPPO within the NanoSim project (e.g., by SINTEF in WP5), and (ii) **numerous publications** that have used

[4] T Forgber, S Radl. 2018. A novel approach to calculate radiative thermal exchange in coupled particle simulations, Powder Technology 323, 24-44.
[5] JH Cloete. 2018. Development of Anisotropic Filtered Two Fluid Model Closures, PhD Thesis, NTNU, Norway.
[6] F Municchi. 2017. Coarse Grained models for momentum, heat and mass transfer in dense gas-particle suspensions from Particle-Resolved Direct Numerical Simulation, PhD Thesis, TU Graz, Austria.

ParScale (see, e.g., Municchi and Radl,[7] or that of Cloete[8] and co-workers; see for a typical result see Figure 11).

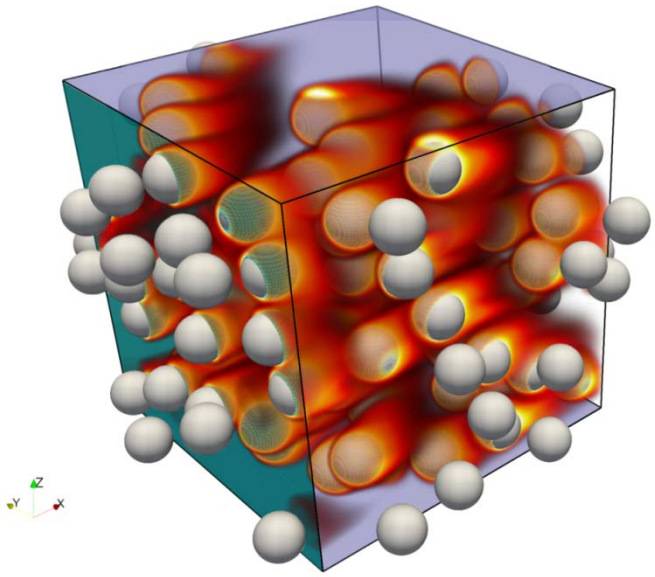


Figure 11: Temperature distribution in a gas-particle suspension confined by walls in z-direction (particles are held at fixed temperature and are cooled by the gas).

This result was produced within Task 4.3 of the DoW in close collaboration between TU Graz and DCS Computing. CPPPO was heavily applied by SINTEF in WP5 as well.

3) Application to Heat Transfer and Impregnation Problems brings New Insight

It is key to also check whether the developed simulation tools are able to predict real-world phenomena. Figure 12 illustrates an example result, specifically the cooling of a particle bed via cool air. Also, more complex systems were studied, most important the distribution of salt within impregnated porous particles. The **quality of this result** is demonstrated by the publication of Dahl et al.[9] For example, it could be show that drying temperature needs to significantly altered to produce useful catalyst particles for a reforming reaction.

[7] F Municchi, S Radl. 2018. Momentum, heat and mass transfer simulations of bounded dense mono-dispersed gas-particle systems, International Journal of Heat and Mass Transfer 120, 1146-1161.

[8] JH Cloete, S Cloete, F Municchi, S Radl, S Amini. 2017. The sensitivity of filtered Two Fluid Model to the underlying resolved simulation setup, Powder Technology 316, 265-277.

[9] PI Dahl, S Radl, A Zaabout, JR Tolchard, S Amini. 2017. Impregnation and Cycling Studies of an Iron-based Oxygen Carrier for CLR Processes. Poster presented at the WCCE 2017, Barcelona, Spain.

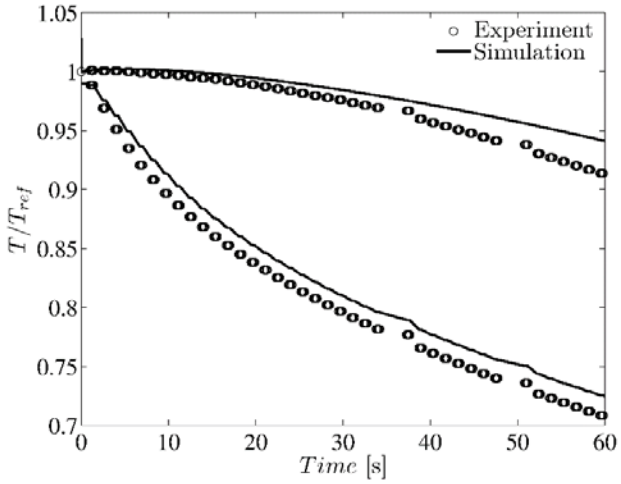


Figure 12: Validation study of cooling behaviour of packed bed.

This result was produced within Task 4.4, 4.5 and 4.6 of the DoW in close collaboration between TU Graz and SINTEF.

4) Application to Fixed Beds results in Improved Material Relations

Another key result are new material closures for heat and mass transfer in fixed beds produced by UCOIMBRA and SINTEF. Most important, computationally extremely demanding computations were performed, including both spherical and non-spherical particles, exceeding the expectations outlined in the DoW. A demonstration of the quality of work performed in WP4 is the publication of Singhal et al.[10] in **the highly regarded "Chemical Engineering Journal"**, as well as follow-up work on cylindrical particles (see Figure 13).

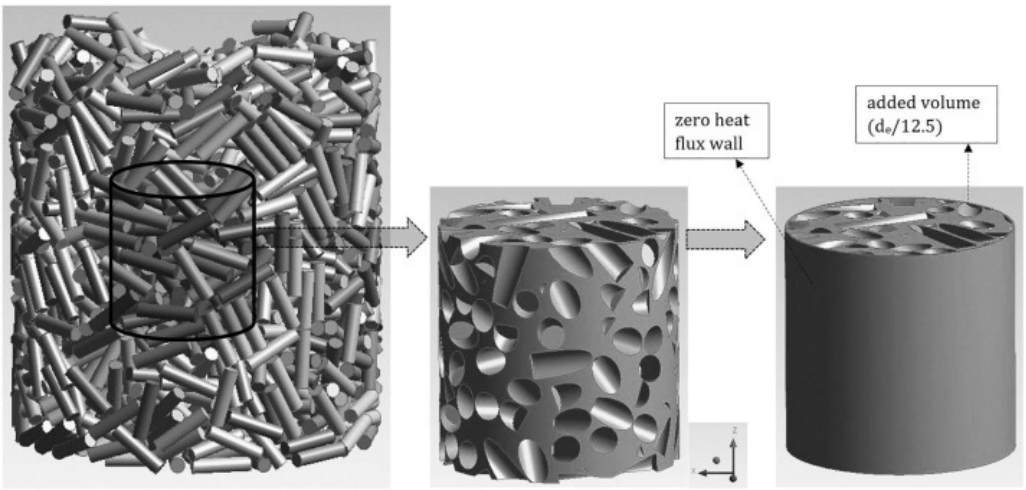


Figure 13: Illustration of the approach used to study heat transfer in fixed beds.[11]

This result was produced within Task 4.7 and 4.8 of the DoW in close collaboration between UCOIMBRA and SINTEF. TU Graz supported this task with advice and review of manuscripts.

5) Educational Resources stimulate Uptake by Users

The developed educational resources[12] were used during training provided by DCS Computing, as well as in academic courses held by TU Graz. While the impact of these

resources cannot be directly quantified at the moment, it is clear that such resources are of **outmost importance for the uptake** of software tools by the community.
This result was produced within Task 4.9 of the DoW with the main contributor being TU Graz. The framework for the documentation was provided by DCS Computing.

[10] A Singhal, S Cloete, S Radl, R Quinta-Ferreira, S Amini. 2016. Heat transfer to a gas from densely packed beds of monodisperse spherical particles, Chemical Engineering Journal 314, 27-37.
[11] A Singhal, S Cloete, S Radl, R Quinta-Ferreira, S Amini. Heat transfer to a gas from densely packed beds of cylindrical particles, Chemical Engineering Science 172, 1-12.
[12] https://www.tugraz.at/institute/ippt/downloads-software/

3.5 WP5 - Eulerian Modelling

Recent works have shown that the Two-Fluid Model (TFM) predictions may be very sensitive to the size of the mesh used for the numerical simulation. Basically, when the size of the mesh is too large the small-scale solid structures (small clusters) are not correctly predicted. That leads to a bad prediction of the solid flow rate in circulating fluidized beds and a wrong prediction of the bed height in dense bubbling fluidized beds. From those findings a new approach called Filtered Two-Fluid Model (FTFM) has been developed. Following that approach a spatial filter is applied on the standard TFM set of equations. That filtering operation exhibits new terms, called subgrid terms (SGS), requiring closure models. For modeling these terms mesh-converged, also called resolved, numerical simulation of gas-particle dense flows is performed based on the TFM. From these numerical simulations a spatial filter – like for the development of the FTFM – is applied on the solutions for measuring the filtered and the SGS contributions.

Such a methodology is commonly used for deriving filtered closures for drag, kinetic stresses, heat transfer, scalar transport and reactions. However, these works have been accomplished by several research groups in the world using different closures for TFM. Hence a question arises about the uncertainties on the developed filtered models with respect to the TFM closures. In WP5, NTNU faces such a question by investigating the effect of TFM closures on the filtered quantities (Task 5.2). The analysis has been done for drag law, inclusion or not of a frictional pressure model, the value of the particle-particle restitution coefficient used, and the choice of closure for the radial distribution function in the TFM. The main result is that the change in filtered correlations with different resolved TFM closures is small (up to 12% for all factors excluding the drag) meaning that the FTFM approach is not very sensitive to the choice of TFM closures (except for the drag) used in the resolved simulations from which the filtered models are derived. A larger effect was observed for the drag model (~20% average deviation) that is questionable because there is not yet consensus in the literature regarding the most relevant choice of drag model. The results of this study have been published in Cloete et al., Powder Technology (2017). That paper gives the recommended TFM closures for the development of the FTFM approach and probably will unify the way to perform the mesh-converged numerical simulation.

Still for evaluating the standard TFM closures, NTNU has also investigated the effect of the boundary condition on the numerical predictions of the gas-solid flow in a riser. It has been shown that the new boundary conditions proposed by Schneiderbauer (2012) improve the predictions in the near-wall region of the riser compare to the widely used Johnson & Jackson (1987) boundary condition (see Cloete et al., Powder Technology 2016).

In parallel of such a work, INPT has extended the FTFM for polydisperse flows. Mesh-converged numerical simulations of a three-dimensional periodical circulating fluidized bed with two particle classes have been performed. When investigating polydisperse flows the number of degrees of freedom increases largely because in addition to the basic parameters (particle diameter, average particle volume fraction) the ratio between the two particle diameters and the one between the two solid volume fractions vary as well. Building such a database of mesh-converged numerical simulation was a part of the Task 5.1. The analysis of these numerical simulations by following the FTFM methodology allowed INPT to investigate the effect of the filtering on the gas-particle and particle-particle momentum transfers in polydisperse flows. The effect of the drag has been found similar to the one in monodisperse case. A monodisperse model from the literature - previously developed by INPT - has been used with the whole local solid volume fraction and not the local particle volume fraction of each particle class (Task 5.4). A very important result has been found in

this study. Basically, the model for the subgrid drag contribution is modelled by two functions: one taking into account the effect of the local particle volume fraction and a second function taking into the effect of the filter width. In the literature the models based on this decomposition proposed quiet complex function for the effect of the filter width. In WP5, INPT has shown that a linear approximation for the dependence of the SGS drag contribution is enough if the dynamic model developed by INPT is used.

In polydisperse flows, inter-particle collisions lead to additional terms in momentum and particle agitation equations. As shown by Figure 14, the analysis by filtering of the mesh-converged solutions has shown that the subgrid inter-particle momentum transfer may be of the same order of the drag contribution highlighting the need of a model (Chevrier, ICMF, 2016).

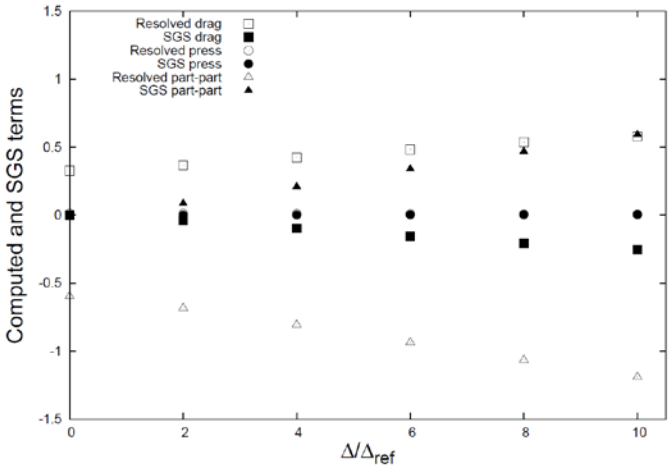


Figure 14: Resolved and sub-grid contributions in the particle momentum filtered transport equation for $d_p = 150\mu m$ for various filter widths Δ (normalized by $\widetilde{\alpha_q}\rho_q g_z$)

The development of a subgrid model for the inter-particle momentum transfers is more tricky because the correlation analysis have shown that it depends on the solid volume fractions of the two-particle classes, and on the mean inter-particle relative velocity. A first proposition has been done based on an analogy with the subgrid drag contribution. A priori tests (Task 5.4) have been realized showing that the proposed model gives the main trend (better than without any model) but needs to be improved. Indeed, the analogy with the subgrid drag contribution has a limitation because the inter-particle collision terms depend on the collision frequency that is a function of the particle agitations. Hence, INPT made the filtering analysis of the particle kinetic energy in polydisperse flows (Task 5.2). This analysis has shown how the filtering affects each contribution, but the main result is that the production of particle agitation by the gradients of the mean particle velocity is decreasing for increasing the filter width. Such a dependency was unexpected and currently no model has been derived for such a contribution.

NTNU in WP5 has also developed a sub-grid closure for first-order, solids catalyzed reactions. It has been found that the predictive capability of the closure can be improved compared to those in literature by adding the slip velocity magnitude, which serves as a measure of the inhomogeneity of the flow, as independent variable in the closure equation. The importance of incorporating the effect of anisotropy in FTFM closures was also investigated. The behavior of fluidization is highly anisotropic due to the gravity force in the vertical direction. Indeed, it has been shown that the standard isotropic approaches common in literature will substantially overpredict the drag in the lateral directions and mispredict the deviatoric component of the stresses resulting from sub-grid solids velocity fluctuations. A new set of anisotropic closures have subsequently been proposed for

the filtered drag and stresses and it has been shown that this leads to a significant improvement in the capability of the models to predict the sub-grid corrections observed in the highly resolved simulations. Verification against large-scale 2D resolved simulations have shown that the proposed models can very accurately predict both the hydrodynamics and reactions on much coarser grids than what is required for the resolved simulations, resulting in several orders of magnitude speed up (Cloete et al., AIChE Annual meeting, 2017). The anisotropic stress closure, especially, was found to be important for accurate predictions (see Figure 15).

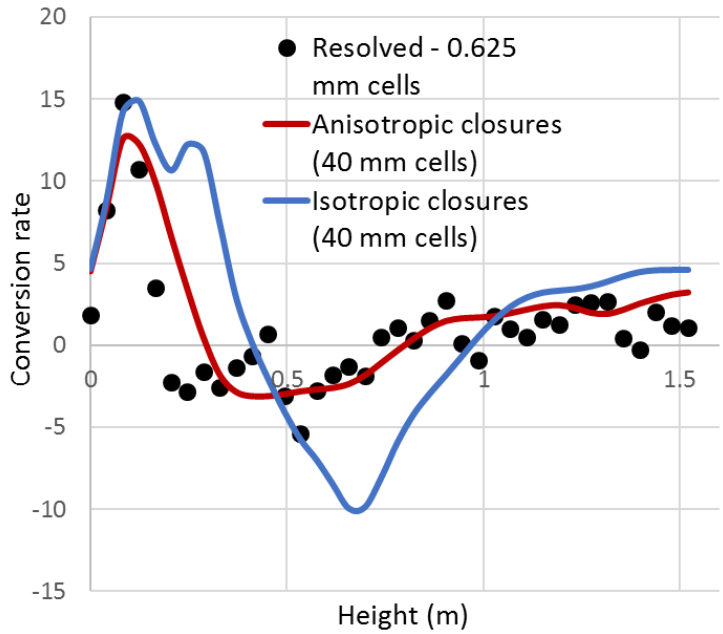


Figure 15: The time-averaged profiles of the conversion rate, $\frac{d(-log(X_A))}{dy}$, along a vertical line in a fluidized bed. The comparison of coarse grid simulation results to the resolved simulation results highlight the important of accounting for anisotropy in the hydrodynamic closures in order to accurately predict the reactive behaviour on coarse grids.

Furthermore, closures developed in this work has been successfully validated against hydrodynamic experimental data from literature. The experimental data included laboratory scale experiments, where the influence of the reactor walls is large, as well as experiments on a pilot scale. It has also been found that these closures perform significantly better than two benchmark models (Igci and Sundaresan, 2011 and Sarkar et al., 2016) from literature.

INPT has performed three-dimensional numerical simulations of reactive periodical circulating fluidized bed. The model for the reaction was very simple. Basically, a heterogeneous reaction was mimicked by a reaction terms proportional to the local solid volume fraction, the local mass fraction of methane and parameterized by an ad hoc reaction characteristic timescale. That parameter was set in the range between 1s to 0.001s. The resolved simulations have shown that for short reaction timescale a correlation between the solid volume fraction and methane reaction rate exists and by applying a spatial filter, the presence of a subgrid contribution of the reaction rate has been highlighted. For long reaction timescale the subgrid contribution has not been found, however it can be imagined that the correlation requires more physical time than the one numerically simulated. A correlation analysis showed that the subgrid reaction term is correlated with the computed variables. This study drops the basis for the development of subgrid reaction terms.

The FTFM has been evaluated on an industrial scale boiler of ANDRITZ (Task 5.5). Such an exercise pushed the model far outside of its comfort zone. Indeed, the very large cells that had to be used in

this simulation required the use of filter sizes that were much larger than those used in the model derivation process. This required a large amount of extrapolation of the model, which always introduces significant uncertainty. The particle and fluid properties in the industrial scale reactor were very different from those used in the derivation of the filtered model and therefore required the tuning of some model parameters. Using this approach a similar pressure drop profile to the experiments could be obtained. However, it must be kept in mind that this test was more a proof of concept than a validation.

Concerning the fixed bed reactor, the aim was to develop large scale reactor models through multiscale modeling approach (Task 5.3). Firstly, the computationally costly particle resolved direct numerical simulations (PR-DNS) were used to develop closure models in WP4, following which the reduced scale models (specifically 2D and 1D) were developed and verified against the PR-DNS results in WP5. For the verification purposes (Task 5.4), the first test of the large-scale reactor model using closures developed from PR-DNS was done for a simple first order hypothetical catalytic reaction: *A (g) + B (s) → C (g) + B (s).* The work involved verification over a range of different mass transfer (Thiele modulus) and heat transfer (Prandtl number) resistances as well as a number of different reaction enthalpies. This ensured that the generality of the 1D large-scale reactor model was stringently evaluated. The second test involved complex steam methane reforming reactions, which implicate several levels of complexities in terms of 1) multiple reactions, 2) multiple reactants and products per reaction and 3) gas volume generation during the reaction. 1D model with suitable improvements to address the aforementioned complexities was able to perform well in comparison to the PR-DNS. The verified 1D model was then used to simulate a reforming stage of a large scale packed bed chemical looping reforming reactor (PBCLR) (10m in length). The PBCLR process works in a similar manner as the gas switching reforming (GSR) process that utilizes a fluidized bed instead of a packed bed. In practice, the PBCLR process (because of the plug-flow nature of the packed bed) helps it to operate at lower temperatures or higher pressures, while achieving similar performance to the GSR concept. Typical results can be found in Singhal et al, CFD (2017) and in Singhal et al. Energy Procedia (2017) and in Figure 16.

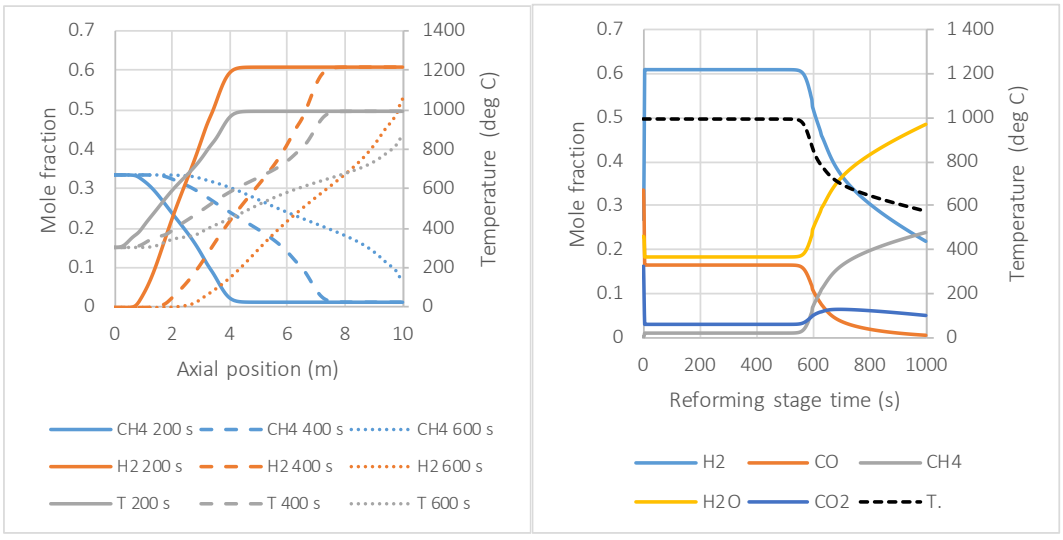


Figure 16: Axial species and temperature profiles along the bed at different times (left) and outlet species and temperature profiles during the reforming stage of the PBCLR process (right).

Similarly, for the thorough verification of 2D models similar reforming stage (as explained above) was simulated with a 2D-axisymmetrical simulation (in addition with 2.5m bed radius) that included direct modeling of the heat losses through surrounding refractory lining. The redundancy check

revealed that the 1D models were sufficient to describe the packed bed reactor running chemical looping reforming reactions.

3.6 WP6 - Phenomenological Modelling

The model foundation for fluidized bed reactors has been completed and consists on a generic 1-D phenomenological model based on the averaging probabilistic approach developed by Thompson et al. (1999) [1] that allows a smooth transition between the different fluidization regimes. One key benefit of this approach is that discontinuities can be avoided when individual models for different regimes are implemented. Phenom takes into account three fluidization regimes, bubbling, turbulent and fast fluidization which flow patterns are described through a library of state-of-the-art closures from literature. The averaging probabilistic approach is used to interface between the models for different regimes and, consequently, for the estimation of the model hydrodynamic parameters. Figure 17 represents a sketch of the developed program.

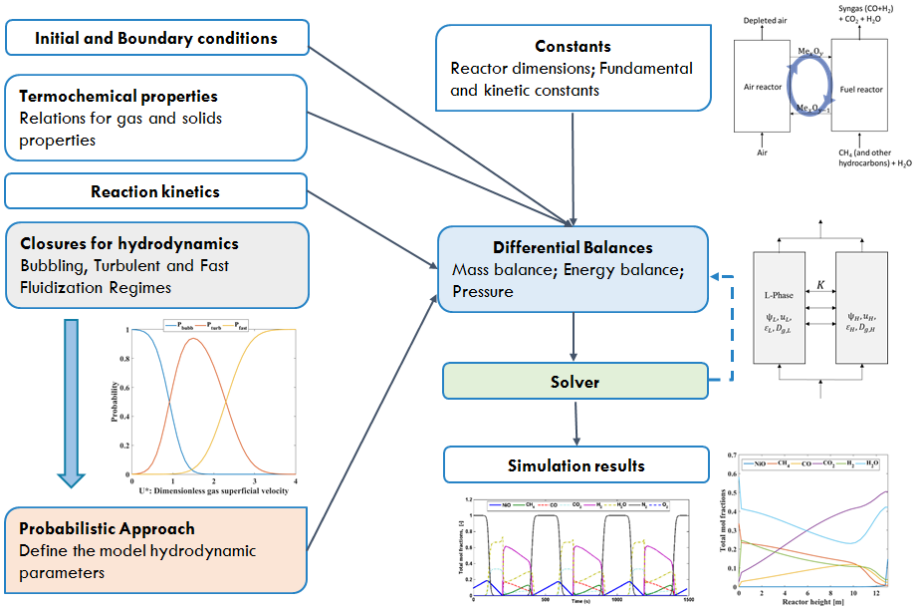


Figure 17: Sketch of the Phenom's framework

Figure 17 shows that Phenom's framework involves an accurate coupling of several phenomena. The model structure consists of a set of consistent differential equations (Differential Balances in Figure 17) that define the axial profiles of the state variables (*e.g.* gas and solids composition, temperature, pressure). These balances are then coupled with relations with different degrees of complexity that give information regarding the thermo-chemical properties, geometry, physics and hydrodynamics of the system. The system of differential equations together with the multiple relations describing the system behaviour are solved simultaneously. Phenom handles stationary and transient simulations and can be applied to single or cluster of fluidized bed reactors.

The developed phenomenological model relies on the following major assumptions: (i) it is a 1D model therefore only resolves the axial direction; (ii) the reactor is assumed a cylinder with constant cross-section area over the axial direction; (iii) the system is assumed adiabatic; (iv) all the gases are considered ideal; (v) dynamic model; (vi) each reactor is divided into two phases, a low-dense phase (L-phase) and a high-dense phase (H-phase); (vii) temperature is uniform therefore H- and L-phases are at the same temperature; (viii) both phases are modelled as an axially dispersed plug flow; (ix) model parameters are determined along the height of the reactor based on the closure laws; (x) the model is heterogeneous and (xi) the gas-solid interphase gradients are neglected due to the intense mixing characteristic from fluidized beds. Energy and mass conservation tests in cold flow and reactive flow have been performed to ensure the proper functioning of Phenom. Thus, by ensuring

the conservation of mass and energy and using closure laws validated in literature, Phenom is suitable for conceptual design purposes.

Phenom has been applied to three different chemical looping reforming technologies: the conventional chemical looping reforming (CLR), the novel gas switching reforming (GSR) and the fuel reactor of the membrane-assisted chemical looping reforming (MA-CLR). The generic approach of Phenom allows for comparison of different reactor concepts operating in different fluidization regimes using a single modeling framework. Thus, its full capabilities where used to compare the conventional CLR technology against the novel GSR concept. The conventional CLR technology consists of a cluster of two interconnected reactors operating under stationary conditions and under turbulent/fast fluidization (according to the assumed dual circulating fluidized bed configuration [2]) whereas the novel GSR consists of a single fluidized bed operating under bubbling/turbulent fluidization regime in a transient fashion. Phenom was used to estimate the performance of each configuration, which was evaluated in terms of CH_4 conversion, H_2 conversion and CO selectivity for different oxygen carrier utilizations. The axial profiles for the CLR using 40% utilization of oxygen carrier obtained from these simulations for the fuel and air reactors are represented in Figure 18 and Figure 19, respectively.

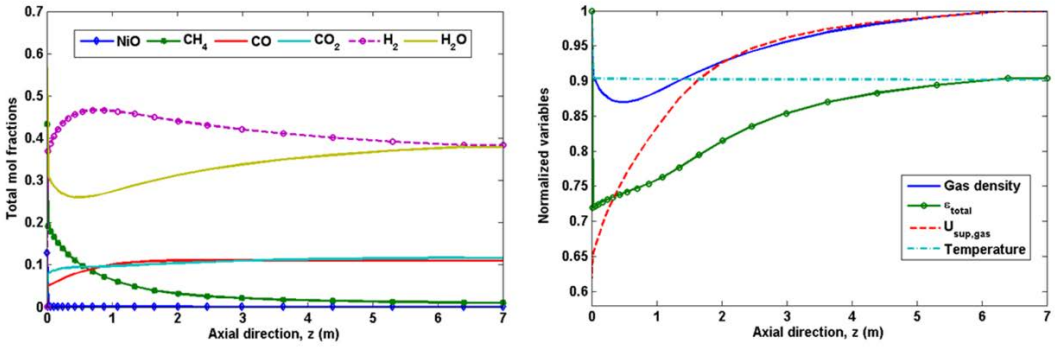


Figure 18: Axial profiles in the fuel reactor using 40% utilization of the oxygen carrier. Left: Gas composition profile. Right: Profiles for four important variables normalized by the following maximum values: 2.94 kg/m³ for the gas density, 1 for the void fraction, 2.4 m/s for the superficial velocity and 989 °C for the temperature.

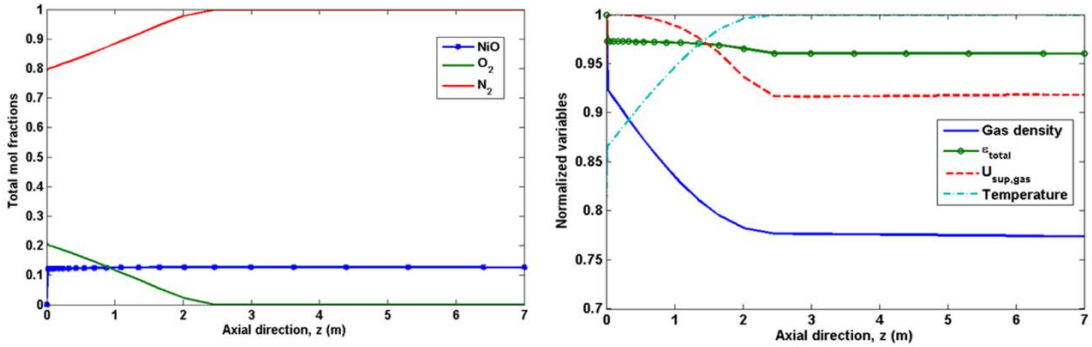


Figure 19: Profiles in the air reactor using 40% utilization of oxygen carrier. Left: Gas composition profile. Right: Profiles for four important variables normalized by the following maximum values: 5.49 kg/m³ for the gas density, 1 for the void fraction, 2.45 m/s for the superficial velocity and 1100 °C for the temperature.

In Figure 18 (left side) for the fuel reactor, it is verified that initially, at the bottom of the reactor, the reforming reactions are favoured with the production of H_2. After this, the system reaches equilibrium and the heterogeneous reaction dominate. Regarding the hydrodynamic and physical properties (on the right), the additional gas volume production by the reforming and oxidation of

methane leads to an increase in the total void fraction and gas superficial velocity along the reactor bed. The reactor temperature is almost constant due to the good axial mixing. In Figure 19 (left side) for the air reactor, it is verified that the oxidation reaction is very fast and all oxygen is consumed within the first 2.5 m. Regarding the hydrodynamic and physical properties (on the right), the gas density decreases along the reactor height due to the significant temperature increase from the highly exothermic oxidation reaction and the reactor operates under high void fraction mostly due to the fast regime of fluidization. The gas velocity decreases as the oxygen is consumed despite the gas density reduction caused by the rising temperature.

The transient profile for the gas composition along the different stages of GSR using 40% oxygen carrier utilization is represented in Figure 20.

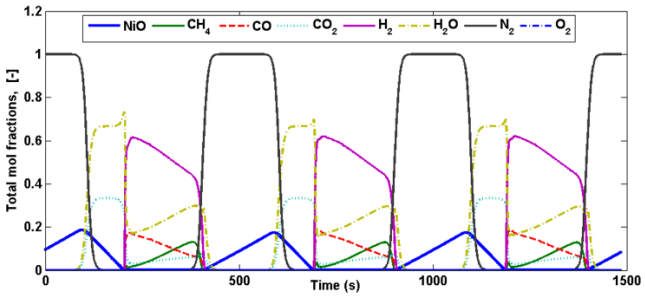


Figure 20: Species molar fractions profile over 3 complete GSR cycles using the 40% oxygen carrier utilization case

Figure 20 shows that O_2 is completely consumed in the oxidation stage and the NiO is completely reduced by methane to metallic Ni used in the reforming stage to catalyse the reforming reactions. It is also verified that undesired nitrogen is mixed with the produced syngas and CO_2 during the transition between the reforming and oxidation stages and between oxidation and reduction, respectively. By comparing these two technologies, it was verified that the CO selectivity and H_2 productivity are higher in GSR whereas methane conversion is higher in CLR. With this analysis, it was concluded that CLR process is best suited to thermal power production with pre-combustion CO_2 capture, while the GSR process is best suited to pure hydrogen production. The reduction stage of the GSR process presents the opportunity to efficiently utilize the off-gas fuel from a PSA unit for high purity pressurized hydrogen production, while ensuring inherent CO_2 separation.

Phenom has also been extended to incorporate membranes and used to simulate the fuel reactor of the MA-CLR technology. Unlike the previous configurations, the fuel reactor of MA-CLR was simulated considering counter-current configuration of the fuel reactor to enhance its performance. The results from this simulation were validated against data from literature and the effect of non-isothermal conditions on the performance of the MA-CLR were quantified. Although most of the models for MA-CLR reactors assume constant temperature due to the intense gas-solid mixing inherent to this reactors. It was verified that neglecting the axial temperature gradient developing inside the reactor can enforce a ~10% lower gas throughput than predicted by isothermal reactor modeling which can lead to an improper design of the system.

In addition to these applications, Phenom simulations of the conventional CLR have been linked to the plant simulations in WP8 and used for techno-economic assessment of the process. Thus, Phenom can be used as a common simulation framework for any chemical looping process or fluidized bed for conceptual design proposes which benefits from the utilization of a single generic model structure.

1. Thompson, M.L., H. Bi, and J.R. Grace, *A generalized bubbling / turbulent fuidized-bed reactor model.* Chemical Engineering Science, 1999. **54**: p. 3-10.
2. Kolbitsch, P., et al., *Design of a Chemical Looping Combustor using a Dual Circulating Fluidized Bed (DCFB) Reactor System.* Chemical Engineering & Technology, 2009. **32**(3): p. 398-403.

3.7 WP7 - Validation Experiments

Nanomaterial synthesis and characterization

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

1) Large scale (kg batches) wet impregnation of commercial support materials generating nanostructures, defined by the pore size/structure.
2) Small-scale (10 gram batches) synthesis of nanoparticles embedded in a support obtained through three different methods, of which one was selected for upscaling to ~300 grams.

The most promising, scalable method generating nanoparticles (10-20 nm) directly during synthesis follows a two-phase gel procedure. High temperature XRD demonstrates the effect of atmosphere during heat treatment, for the development of the active nanoparticles, which are shown in the SEM image to the right. A comparable route was applied to obtain iron based active particles in the 0.5-1 µm range. Thermogravimetric analysis and micro reactor tests on the nanostructured oxygen carriers were not too conclusive, and limited kinetics data were extracted. However, significant conversion of methane was indeed obtained at 900°C.

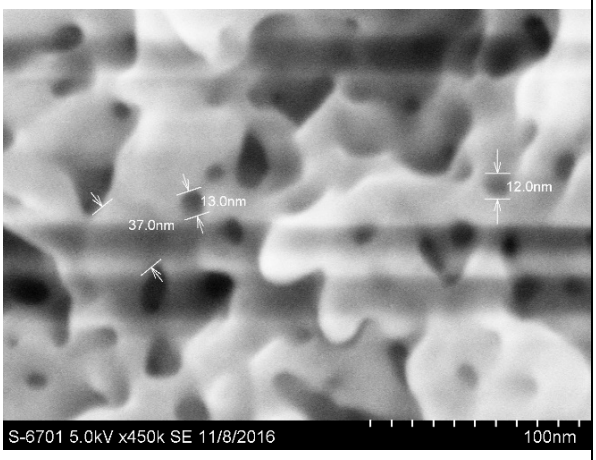


Figure 21: Active, iron based nanoparticles (dark spots) on porous support material.

In order to meet the mass/volume requirements of the lab scale pilot reactor constructed and applied within the project, the above-mentioned synthesis routes were scaled up to ~300 grams. IN addition the active material was impregnated into commercially available porous supports by wet impregnation, on a kg scale. The impregnation process was optimized in collaboration with modeling of WP4 to improve the penetration of solution into the support particle bulk. Uniform distribution of the iron based materials throughout the mesoporous supports were obtained, while maintaining high surface area (>100 m^2/g) and pore volume (~1 mL/g). A total loading of 10-35 wt% active material was obtained. Cold attrition tests indicate good mechanical stability of the particles.

Construction of reactor and methane reforming tests

A lab scale fluidized bed was used to test the prepared iron-based oxygen carriers, as well as ilmenite ($FeTiO_3$) under the Gas Switching water-splitting process. This process produces hydrogen by splitting water on a reaction with FeO to form Fe_3O_4, which is further oxidized to Fe_2O_3 to generate the heat needed for the oxygen carrier regeneration in the endothermic reaction with fuel. The working principle of the Gas Switching water splitting process is illustrated in Figure 22-left. In the looping configuration, this 3-step process is completed in 3 reactors with the iron-based oxygen carrier circulating between them. In the Gas Switching reactor, the 3 steps are completed in the same reactor by alternating gas feeds into the reactor (Figure 22-right), thereby facilitating operation under pressurized conditions and maximizing process efficiency.

A typical performance representing the reactor outlet gas composition under steam methane reforming of the nano- and coarse iron based oxygen carrier is shown in the graph of Figure 23. A

good conversion of methane was achieved for the nano-structured oxygen carrier combined with a high hydrogen yield in comparison to the micro-structured ones.

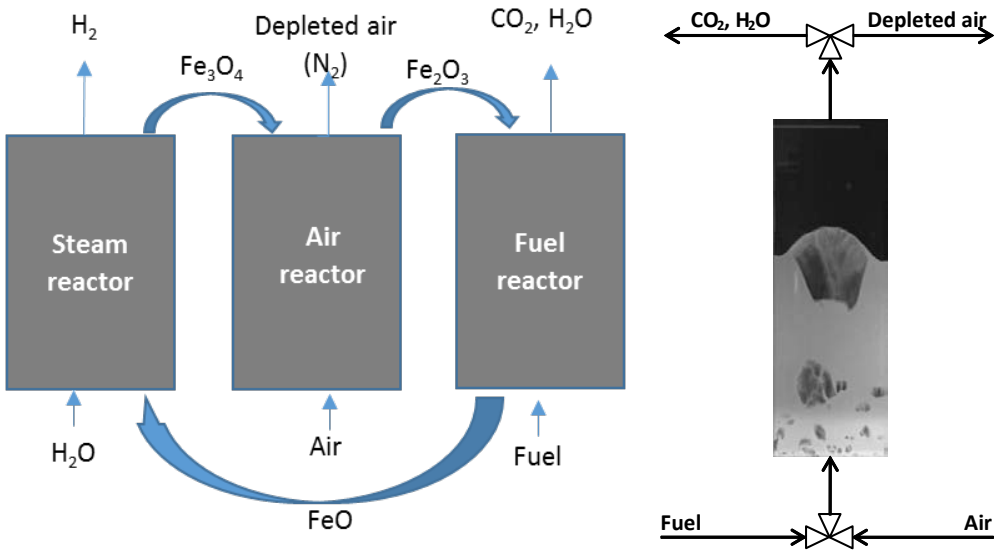


Figure 22: Left: a simplified scheme of the water-splitting process completed following the chemical looping route. Right: Gas switching technology applied combustion, GSC.

The good performance found for the nano material is due to the larger amounts (10 wt%) of magnetite (Fe_3O_4) as compared the coarse particles (2 wt%). There could be an effect of particle size on the reduction of the material. Smaller particles of hematite (Fe_2O_3) will be more prone to be reduced to magnetite, Fe_3O_4, through the bulk. In the coarser particles, the kinetics for reducing the bulk is limiting resulting in a reduced layer.

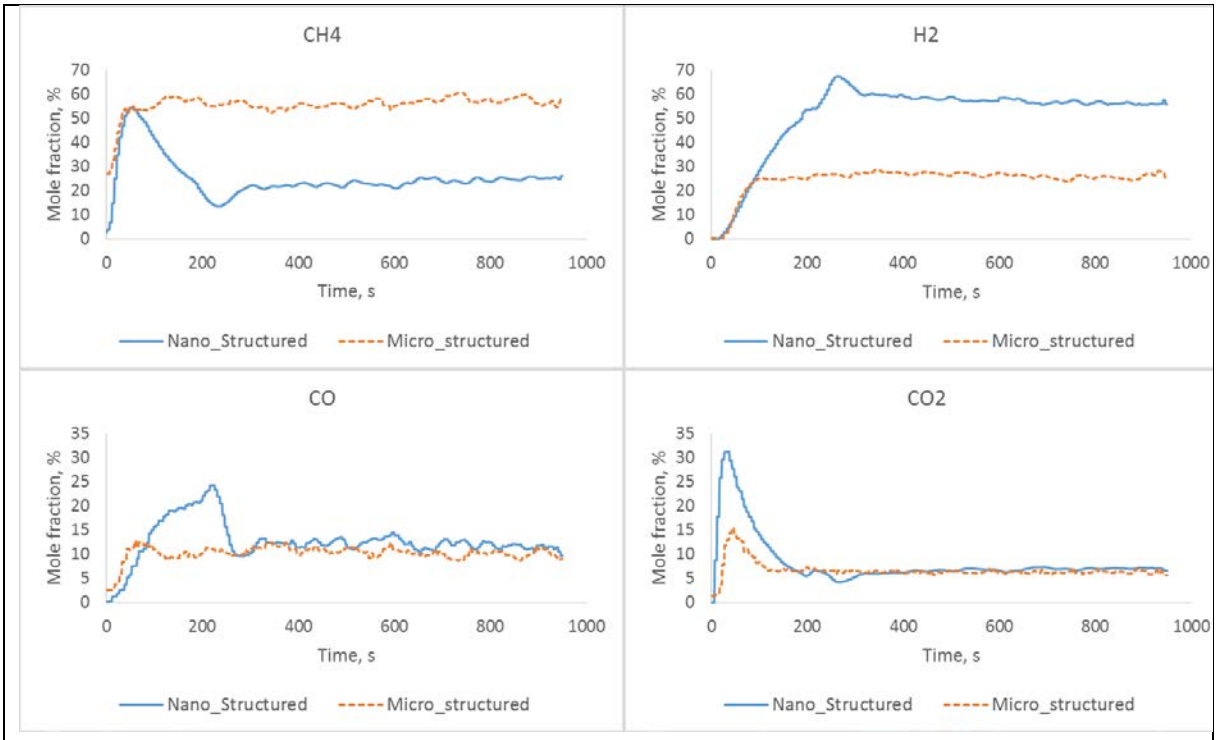


Figure 23: Steam methane reforming using the nano and micro structured iron-based oxygen carriers. Operating temperature was 800 °C and inlet gas composition was CH4:H2O=1:2. CH4 feed rate is 0.8 Nl/min. An initial mass of 70g of each oxygen carrier was put in the reactor.

Validation of resolved reactive multiphase flow models

Modeling of reactive flows in fluidized beds requires accurate description of two primary rate-limiting steps: gas-to-particle mass transfer and particle-scale reaction rate. Reactive multiphase flow models directly resolve the former rate limiting step, whereas the latter must be incorporated as a closure model derived from experiments or sub-particle scale modeling.

The validation study completed in the NanoSim project showed that the reactor performance prediction of resolved reactive multiphase flow models is highly sensitive to the reaction rate closure employed. The gas-to-particle mass transfer limitation that is directly resolved by the reactive multiphase flow model was shown to involve a much lower degree of uncertainty.

Specifically, the comparisons to experiments concerning the reduction of Ilmenite with CO showed that factors influencing the gas-to-particle mass transfer limitation only had a minor influence on the results, increasing confidence in the multiphase flow model. However, a significant change to the reaction rate closure was required to achieve a reasonable match to experimental observations.

Process intensification of reactors through multi-scale modeling

The process intensification study in NanoSim illustrated the potential of highly reactive nano-structured oxygen carriers to reduce the size of the reactor used in a chemical looping reforming process. Three modeling scales were considered in this multiscale modeling exercise: 1) the reaction rate is determined through atomistic modeling, 2) intra-particle diffusion resistances are accounted for by a particle-scale mass transfer model, and 3) mass transfer resistances imposed by the mesoscale clustering behaviour of fluidized beds are modelled by a filtering approach. The final filtered model allowed for computationally affordable 3D simulations of large reactors.

The study found that, for the partial oxidation of methane over magnetite, the use of a highly reactive nano-structured oxygen carrier could reduce the required reactor diameter by a factor of 2.2 (4.7x smaller reactor volume), and reduce the required amount of oxygen carrier by a factor of 11.3. Figure 24 shows how good methane conversion (low CH4 slip) can be achieved at much higher fuel feed rates for the nano-structured oxygen carrier compared to a normal oxygen carrier. Even though the nano-structured oxygen carrier would be significantly more expensive than a standard oxygen carrier, these large process intensification advantages are likely to result in significant cost savings.

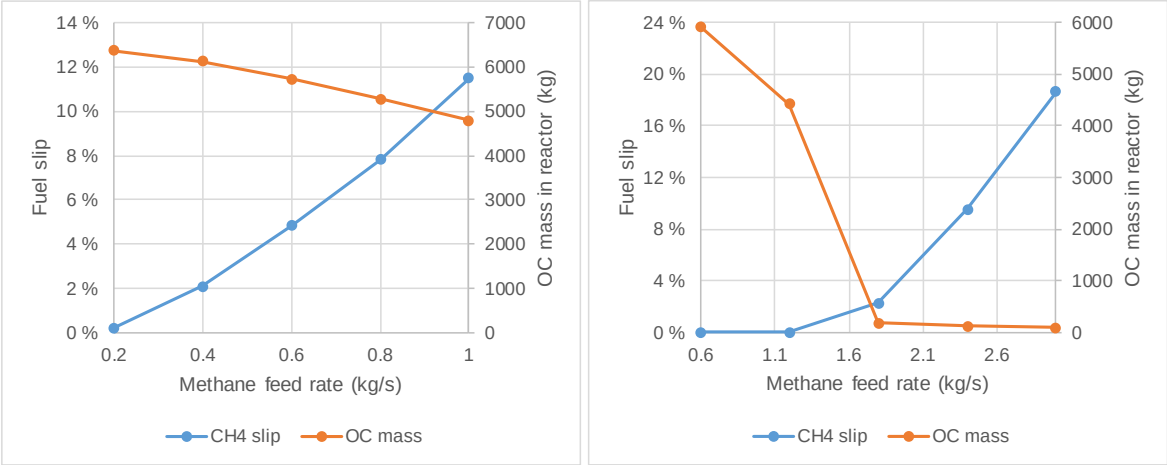


Figure 24: Reactor performance with the normal (left) and nano-structured (right) oxygen carriers (OC).

3.8 WP8 - Techno-Economic Assessment

Task 8.1: Link Phenom to the full plant simulation tool

The 1D phenomenological model of the CLR was linked with the process models for CO_2 capture and power plant. The 1D model for CLR was developed using MATLAB and comprises of kinetics and hydrodynamics of the reactions inside the CLR, and hence the model is dynamic in nature. The water-gas shift and CO_2 capture and compression were modeled in Aspen Hysys V8.6 since Aspen Hysys contains the Acid Gas thermodynamic model which has the property data for amines used in CO_2 capture section. The power plant was modeled using the Thermoflex component of the Thermoflow suite V26 since Thermoflow contains a database of standard commercial gas turbine systems. The process models in Aspen Hysys V8.6 and Thermoflow suite V26 are steady state models whereas the 1D model for CLR is a dynamic model. A multi-scale modeling methodology established to link the dynamic 1D model with the steady state process models developed in commercial software tools. The different process models in the respective software tools were linked on a Microsoft Excel platform. The Aspen Simulation Workbook and the Thermoflow E-Link plug-ins help in establishing the linking of software tools in Excel.

This task required a close collaboration between WP6 and WP8, since the 1D model was developed as a part of WP6 whereas the steady state process models were developed as a part of WP8.

Task 8.2 Design economically optimized reactors

This task is directly linked with the task related to techno-economics of the process, since an optimal design of reactors effects the techno-economic performance of the overall process. The process under study is a natural gas fired combined cycle power plant with pre-combustion CO_2 capture and CLR. The process is denoted as CLR-CC. A sensitivity study was carried out for different design conditions in CLR and the effect on the net electrical efficiency, CO_2 avoidance rates and levelised cost of electricity of the CLR-CC process. The size of both the oxidation and fuel reactor of CLR was considered to be 6 m height and 6 m diameter. The assumption of the size of the reactor is based on the velocity regimes and conversion profiles inside the oxidation and fuel reactor. The oxidation reactor should operate mainly in the fast fluidization regime whereas the fuel reactor should operate in the turbulent/fast fluidization regimes. In addition, the height of the reactor is considered in such a way that it allows maximum conversion of natural gas in the fuel reactor. The assumed size of the reactor was found to be optimal for the cases studied. The weight of the reactor is estimated using the methodology specified in the Peters and Timmerhaus (1991). The reference cost of the reactor per weight is assumed similar to the cost of Fluidized Catalytic Cracker (Spallina et al. 2016) since the cost of CLR is not available in the literature . The capital cost of the CLR accounts to 8% of the capital cost of the overall CLR-CC process. The main results for the techno-economic analysis are shown in the results in Task 8.3 of this project.

The task was initially linked with developments in WP5, but it was decided to use the 1D model developed as a part of WP6 to design the economically optimized reactor configuration. The results from the 1D model were analysed as a part of WP6 whereas the inputs to the 1D models and the analysis of the overall process was carried out as a part of WP8.

Task 8.3 Carry out the techno-economic evaluation

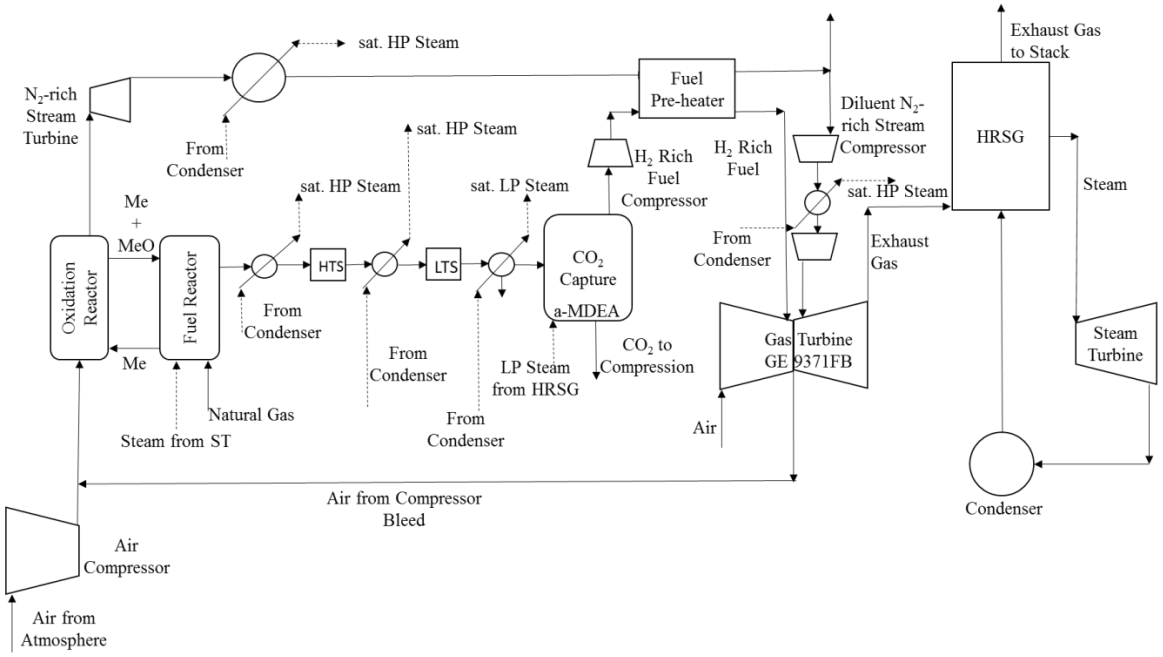


Figure 25: Schematic of the CLR-CC process

The CLR-CC process integrates CLR, WGS, CO_2 capture and compression in a gas-fired combined cycle power plant. The schematic of the CLR-CC process is shown in Figure 25. The net electrical efficiency of the CLR-CC process, which involves all the heat recovery from the high temperature process streams to prepare LP steam that is further expanded in a ST to produce power and for the process when the design pressure in CLR is 18 bar, is 42.5%. The net electrical efficiency for such a cycle is 16%-points less than the reference case NGCC plant without CO_2 capture. Apart from the inherent efficiency penalty due to reforming and WGS reactions, the heat recovery and additional components due to CLR and pre-combustion capture in the CLR-CC process cause higher efficiency penalty. Producing HP steam to recover heat from the process streams in the CLR-CC process can improve the net electrical efficiency to 46.5 %. Anyhow, operational challenges like metal dusting might limit the improvement in efficiency from different heat integration options. The design pressure of the CLR-CC cycle is an important parameter to make decisions on process design and it affects the net electrical efficiency of the CLR-CC process. The higher the design pressure of the CLR-CC cycle, the higher is the net electrical efficiency of the process. Anyhow, when the CLR is designed for pressures higher than the GT system's compressor bleed discharge pressure (~18 bar), an additional air compressor to compress the air bleed from GT is needed in the process.

A sensitivity analysis was carried out to study the effect of three other process parameters on the performance of the CLR-CC process: 1) The air flowrate to the oxidation reactor, 2) steam/carbon ratio in the fuel reactor and 3) oxidation reactor outlet temperature. These parameters were varied in 12 cases. The net electrical efficiency of the CLR-CC was calculated to be between 40 - 44% for CO_2 avoidance rates between 68 - 86%. For the same cases, an economic analysis was carried out to estimate the levelised cost of electricity (LCOE). The LCOE is highly sensitive to the natural gas price and the process contingency costs (additional capital costs accounting for level of maturity of the process). A sensitivity study to see the effect of natural gas price (between 4.5 and 10.2 $/GJ-LHV) and process contingency (between 10 and 50% of the bare erected costs) on LCOE was also carried out. The LCOE of the CLR-CC process lies between 75-145 $/MWh.

This task was done in close collaboration with partners in WP6. The 1D phenomenological model for CLR developed as a part of WP6 was linked with the process models for CO_2 capture and power plant to carry out a techno-economics analysis of the CLR-CC process. The techno-economic analysis of the overall process was carried out as a part of WP8 based on the inputs related to CLR from partners in WP6.

The techno-economic performance of the CLR-CC process was also studied using nano-structured oxygen carrier in the CLR. The rate of the reforming reactions using nano-structured materials is 50 times more when compared to the oxygen carrier of particle size 1 micron. The amount of oxygen carrier circulating between the oxidation and fuel reactor of the CLR is less when nano-structured oxygen carrier is used. The conversion of natural gas in the fuel reactor of the CLR is also higher. Hence, the net electrical efficiency of the CLR-CC process with nano-structured oxygen carriers is more than the CLR-CC process with higher sized (1 micron) oxygen carriers in CLR. Similarly, the levelised cost of electricity for the CLR-CC process is lower because the specific natural gas consumption is low. Partners in WP3 provided the kinetic data for the reforming reactions using nano-structured oxygen carriers. Partners in WP6 used the kinetic data in the 1D model of the CLR. The results from the WP6 were used by partners in WP8 to carry out techno-economic analysis of the overall process.

Task 8.4: Establish best practice guidelines

The best practice guidelines to use the multi-scale model linking approach have been established, presented and reported on scientific platforms through conference presentations and journal articles. The following list of articles in scientific journals gives a detailed explanation into the methodology of model linking and results from the techno-economic analysis of CLR-CC process.

Paper I

Nazir, S. M., Bolland, O., Amini, S., *Full Plant Scale Analysis of Natural Gas Fired Power Plants with Pre-Combustion CO_2 Capture and Chemical Looping Reforming (CLR)*. Energy Procedia 2017, 114, 2146-2155.

Paper II

Nazir, S., Bolland, O., Amini, S., *Analysis of Combined Cycle Power Plants with Chemical Looping Reforming of Natural Gas and Pre-Combustion CO_2 Capture*. Energies 2018, 11 (1), 147.

Paper III

Nazir S.M., Morgado J.F., Bolland O., Quinta-Ferreira R., Amini S., *Techno-economic assessment of chemical looping reforming of Natural Gas for Hydrogen production and power generation with integrated CO_2 capture*. International Journal of Greenhouse Gas Control (2017). (Under Review).

3.9 WP9 - Dissemination and Education

The following main results were obtained:

- A total of **85 publications** were created out of the project. Table 2 shows an overview over the metrics. A full list is available at https://www.sintef.no/projectweb/nanosim/publications/
- **4 official NanoSim workshops were successfully held** (in the frame of Particles 2015 conference, Particles 2017 conference, CFDEMconference 2017 and CFD 2017 conference). Table 3, Table 4 and Figure 26 show impressions from these workshops
- the NanoSim consortium has been represented at a number major international conferences, including keynote lectures at major international conferences and events, such as the CFDEM®user conference and workshop 2016 in Linz and CFDEM®conference 2017 (Austria, both > 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 was set up following the Exploitation Strategy Seminar (ESS) in Brussels
- Cluster activity performed in the frame of the EMMC (European Materials Modeling Council) in the frame of several meetings with the goal to work towards closer integration of Materials Modeling
- 4 official newsletters were sent out
- A number of software releases were performed via WP1 and WP2 as open source software
- A strong user community and usage could be achieved for the COSI platform (WP2). Figure 28 shows a screenshot of the forum activity.

Table 2: Overview of NanoSim related publications, full list available at https://www.sintef.no/projectweb/nanosim/publications/

Contribution to conference (meeting, congress, workshop) proceedings	Lecture or presentation	Journal papers submitted
47	15	23

Table 3: Programme of the NanoSim consortium workshop at the Particles 2015 conference, with NanoSim consortium member contributions being highlighted

IS-Multi-Scale Modeling of Reactive Particle-Based Processes **Invited Session organized by Christoph Kloss, Stefan Radl, Christoph Goniva, Thomas Hagelien and Shahriar Amini**	**WeE02** **Room: VS217** **Chair: Christoph Kloss** **Co-Chair: Christoph Goniva and Stefan Radl**
Application-driven development of CFD-DEM modeling for particle-based processes *C. Goniva*, B. Blais and C. Kloss*	
ParScale - An open-source library for the simulation of intra particle heat and mass transport processes in coupled simulations *S. Radl, T. Forgber*, A. Aigner and C. Kloss*	
Design and validation of a robust CFD-DEM model for the investigation of viscous solid-liquid mixing in agitated vessels *B. Blais*, M. Lassaigne, C. Goniva, L. Fradette and F. Bertrand*	

Application-driven development of Discrete Element Method modeling for reactive particle-based processes
C. Kloss, S. Radl and C. Goniva*

Optimal particle parameters for CLC and CLR processes – predictions by intra-particle transport models and experimental validation
*T. Forgber, J.R. Tolchard, A. Zaabout, P.I. Dahl and S. Radl**

DEM particle characterization by artificial neural networks and macroscopic experiments
L. Benvenuti, C. Kloss and S. Pirker*

Numerical simulation of reactive flow in granular media using a LBM approach. Application to the study of biomass torrefaction
S. Martin and O. Bonnefoy*

*Figure 26: **Group photo of CFDEM®conference 2017***

Table 4: NanoSim-related presentations at 12th International Conference on Computational Fluid Dynamics In the Oil & Gas, Metallurgical and Process Industries

Session	Title
Euler-Lagrange	13: Implementing the Kinetic Theory of Granular Flows into the Lagrangian Dense Discrete Phase Model , S.Cloete & Amini
Packed bed	50: Comparison of particle-resolved direct numerical simulation and 1D modeling of catalytic reactions in a packed bed , Singhal, S.Cloete, Radl, Quinta-Ferreira & Amini
Packed bed	67: A multi-domain 1D particle-reactor model for packed bed reactor applications , Tabib, S.Cloete, Morud, Lysberg & Amini
Fluidized bed 3	92: Verification of filtered two fluid models for reactive gas-solid flows , J.H.Cloete, S. Cloete, Radl & Amini

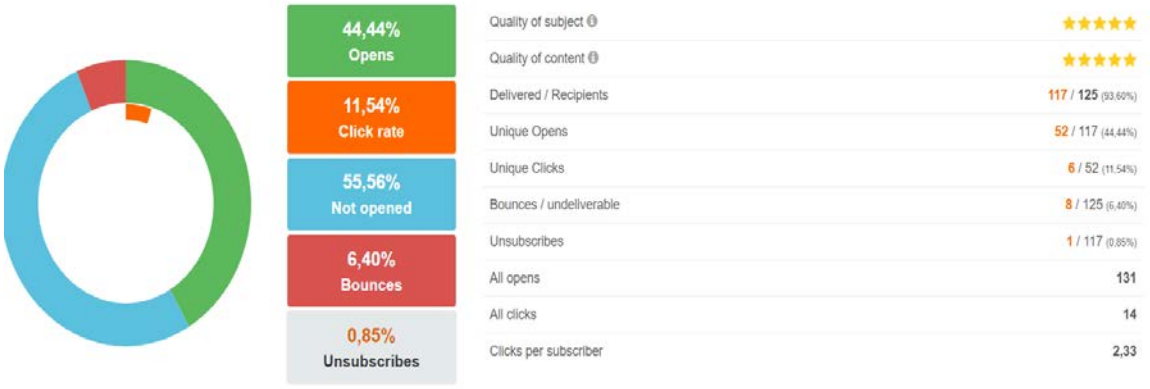


Figure 27: Quality assessment for the 36M newsletter

Forum	Topics	Posts	Last post
Contributed simulations, cases, scripts, tutorials Whenever you make something work which you think could be useful for others as well, please put it here!	14	35	By AnjanaKittu 1 week 4 days ago
ParScale - User and Developer Forum Discussions about the ParScale simulation engine go here!	23	56	By occipitalgubbins 18 hours 36 min ago
CFDEM®coupling - User Forum This is a forum dedicated to CFDEM®coupling using the LIGGGHTS® DEM code and OpenSource CFD.	757	3134	By marcelo 1 day 37 min ago
CFDEM®coupling- Developer Forum Topics related to developing with CFDEM®coupling can be discussed here: discussion about implementation details, C++, MPI and debugging tools	38	104	By zbtlfd 3 weeks 4 days ago
LIGGGHTS® - User Forum LIGGGHTS® related topics can be discussed here: discussion about models, installation, feature requests and general discussion	1756	7342	By Bruno.Brunel 2 hours 7 min ago
LIGGGHTS® - Developer Forum Topics related to developing with LIGGGHTS® can be discussed here: discussion about implementation details, C++, MPI and debugging tools	136	567	By mschramm 1 month 1 week ago
Bug Reports for CFDEM®coupling, LIGGGHTS®, and ParScale (Possible) bugs / suspicious behavior should be reported as a new thread here, not in the user forum. This should give both you and the developers a clear idea about the status of your bug report (submitted/assigned/fixed)	118	480	By arnom 1 day 6 hours ago
Post Processing Post processing of LIGGGHTS®/CFDEM®coupling/ParScale based simulations is discussed here	139	589	By richti83 3 days 21 hours ago
CFDEM®coupling, LIGGGHTS® and ParScale - Announcements from the developers Announcements from the developers go here	145	193	By aaigner 5 days 6 hours ago
CFD and DEM - General Discussion Anything that is related CFD and DEM modelling can be discussed here	47	136	By AndresMM 1 month 3 weeks ago

*Figure 28: User forums (Screenshot as of 12/12/2017) available at **http://www.cfdem.com/forum** with 12,636 total # of forum posts*

4 Use and dissemination of foreground

The consortium explains the exploitable foreground, in particular:

•Its purpose

•How the foreground might be exploited, when and by whom

• IPR exploitable measures taken or intended

• Further research necessary, if any

• Potential/expected impact

4.1 Porto

The exploitable foreground is the Porto framework. The source code of Porto is freely available under a LGPL license, which allows anyone to use, extend and modify the code and use it for academic and commercial purposes. In particular the workflows demonstrated in this project can be freely exploited. This means that these workflows can be used, extended, adapted or reduced to fit academic and commercial activities.

4.2 COSI platform

D2.2 Novel co-simulation code-coupling scheme („Many2Many")

- Its purpose

The purpose is to have a coupled CFD-DEM simulation with different domain decomposition running efficiently on MPI-based HPC supercomputing architecture.

- How the foreground might be exploited, when and by whom

the foreground will, after revisions and improvements be exploited by DCS – DCS will provide it to some of its lead customers.

- IPR exploitable measures taken or intended

DCS will only make this available to selected lead customers,

- Further research necessary, if any

The routine is currently being reviewed and extended to incorporate advanced physics which require different data structures for communication, such as the multi-sphere approach

- Potential/expected impact (quantify where possible)

The incorporation of this functionality into CFDEMcoupling is significantly pushing the computational boundaries and load-balancing of CFD-DEM

D2.3 Test-harness up and running

- Its purpose

The purpose of the test harness system is to perform software developments in a sustainable, quality controlled way by regularly executing a set of automated software tests, which are tailored to the scientific needs of COSI

- How the foreground might be exploited, when and by whom

The testing system is used internally at DCS for any software development

- IPR exploitable measures taken or intended

The testing system is used only internally at DCS, so no specific IPR protection measures are forseen

- Further research necessary, if any

Further R&D is being performed internally at DCS to improve the system as necessary

- Potential/expected impact (quantify where possible)

For the whole software development at DCS profits from this; the testing system allows to flexibly monitor difference development branches of different components of the COSI platform.

It is therefore of utmost importance and a core tool for DCS

D2.4 Release of code coupling, new EL functionality, improvements, bug-fixes

- Its purpose

The purpose of D2.4 is to create a monolithic, quality-controlled platform which includes featues and functionalities from

- How the foreground might be exploited, when and by whom

Forground is being exploited by DCS. Main route is to offer Premium functionalities on top of the Public release version.

- IPR exploitable measures taken or intended

DCS has recently decided to delay releasing further developments (those made outside the NanoSim project) to the open public for a certain period of time (e.g. one year), to be able to protect the IP and business model of DCS

- Further research necessary, if any

further development of the COSI platform is necessary and already ongoing (bi-lateral contracts, other funded projects via national Austrian funding as well as H2020)

- Potential/expected impact (quantify where possible)

Having a maintainable core co-simulation platform is the main business asset of DCS – most of the projects DCS is currently operating are building on it!

4.3 Reactor modelling

The filtered Two Fluid Model (fTFM) closures, which enable large-scale fluidized bed simulations within feasible computational times, have been improved compared to the state of the art. The focus has been on developing approaches to account for anisotropy in the closures, polydisperse flows and reactive flows. Verification and validation exercises have shown that the models developed in the framework of NANOSIM will lead to more accurate and more reliable predictions of industrial scale fluidized bed behavior by means of coarse grid simulations. Consequently, the progress within this work package brings the fTFM closer to being used in industry as a reliable predictive tool. More some

models developed in the framework of WP5 have been implemented in an OpenSource code in order to free-of-using by the researcher community as well as companies.

However, a substantial amount of further research remains to close the remaining knowledge gaps. Potential topics for future research includes: 1) Scaling of closures to different fluid/particle configurations, 2) Development of closures from large scale 3D simulations, 3) Development of transport equations for the sub-grid heterogeneity and 4) the development of reactive closures for a wide range of reaction rates and reaction types. Such research is underway in follow-up projects.

Provided the fTFM becomes a more mature simulation tool based on further research, it may become widely used within industry for process design and optimization on an industrial scale. This might decrease the number of pilot plant studies required for industrializing new reactor concepts, thereby decreasing the time and cost associated with scale up. Furthermore, the same multi-scale model development procedure used for fTFMs may be applied to different multiphase flow problems. Consequently, similar progress for industrial scale simulation can be achieved for other reactors than fluidized beds.

4.4 System modelling

The 1D model for chemical looping reforming (CLR) was linked with the steady state power plant simulations to perform a techno-economic assessment of a gas-fired combined cycle power plant integrated with reforming and CO_2 capture. The reforming method studied in this project is CLR. The linking methodology can now be exploited to speed up the assessment and help in carrying out techno-economic analysis of second generation CCS processes. This helps in understanding the techno-economic potential and viability of the novel process technologies for CCS. The results for the techno-economic analysis for the integrated power plant has been published in scientific articles.

The model linking methodology developed can be exploited by the R&D community to develop novel CCS processes. The results from WP8 not only adds on the advancement to the scientific knowledge, but also acts as standards for further analysis. The processes studied within WP8 can be further optimized as a part of future work. The results give a deeper know how of the process technology and various sensitivity studies carried out will help in process design decisions. The methodologies developed and the results presented will have a direct impact on speeding up the process development of CCS processes.

4.5 Production of Nano-structured materials

A novel synthesis route for supported nanoparticles was developed within the NanoSim project. As opposed to most synthesis methods for nanomaterials reported in the literature, this synthesis route is scalable and could hence be of commercial interest. SINTEF will exploit this foreground from NanoSim by evaluating the potential use of such nanomaterials in other application beside chemical looping technologies, e.g. Fischer-Tropsch, fuel cell technologies and other catalyst-based processes where one relies on supported catalyst nanoparticles. Based on potential application areas, patent possibilities will be considered and if not found relevant the work will be published. Further research is required to investigate how generic the synthesis method is by e.g. applying the method for different material systems. Furthermore, the effect of the supported nanoparticles for specific applications will have to be studied. SINTEF aim to realize new projects to drive the research forward, with the intention of triggering the interest of industries. A potential impact for the end user could be a significant cost reduction in the material production costs, which would directly reduce the CapEx for the catalytic processes in question.

4.6 Dissemination

- A total of **85 publications** were created out of the project. Table 2 shows an overview over the metrics. A full list is available at https://www.sintef.no/projectweb/nanosim/publications/
- **4 official NanoSim workshops were successfully held** (in the frame of Particles 2015 conference, Particles 2017 conference, CFDEMconference 2017 and CFD 2017 conference). Table 3, Table 4 and Figure 26 show impressions from these workshops
- the NanoSim consortium has been represented at a number major international conferences, including keynote lectures at major international conferences and events, such as the CFDEM®user conference and workshop 2016 in Linz and CFDEM®conference 2017 (Austria, both > 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 was set up following the Exploitation Strategy Seminar (ESS) in Brussels
- Cluster activity performed in the frame of the EMMC (European Materials Modeling Council) in the frame of several meetings with the goal to work towards closer integration of Materials Modeling
- 4 official newsletters were sent out
- A number of software releases were performed via WP1 and WP2 as open source software
- A strong user community and usage could be achieved for the COSI platform (WP2). Figure 28 shows a screenshot of the forum activity.

5 Report on societal implications

General Information

C Workforce Statistics

3. Workforce statistics for the project: Please indicate in the table below the number of people who worked on the project (on a headcount basis).

Type of Position	Number of Women	Number of Men
Scientific Coordinator	1	6
Work package leaders		9
Experienced researchers (i.e. PhD holders)	4	9
PhD Students	2	3
Other		3

4. How many additional researchers (in companies and universities) were recruited specifically for this project?	**6**
Of which, indicate the number of men:	5

D Gender Aspects

5. Did you carry out specific Gender Equality Actions under the project?

○ Yes
◉ No

6. Which of the following actions did you carry out and how effective were they?

	Not at all effective				Very effective
❑ Design and implement an equal opportunity policy	○	○	○	◉	○
❑ Set targets to achieve a gender balance in the workforce	○	○	◉	○	○
❑ Organise conferences and workshops on gender	○	○	○	○	○
❑ Actions to improve work-life balance	○	○	○	○	◉

○ Other:

7. Was there a gender dimension associated with the research content – i.e. wherever people were the focus of the research as, for example, consumers, users, patients or in trials, was the issue of gender considered and addressed?

○ Yes- please specify

◉ No

E Synergies with Science Education

8. Did your project involve working with students and/or school pupils (e.g. open days, participation in science festivals and events, prizes/competitions or joint projects)?

○ Yes- please specify : Class room teaching at the university level specific for the NanoSim project. TU Graz hosts open days ("long night of research") that raises general awareness related to engineering, and specifically modelling

◉ No

9. Did the project generate any science education material (e.g. kits, websites, explanatory booklets, DVDs)?

◉ Yes- please specify : documentation and screencasts (https://github.com/CFDEMprojec, as well as https://www.tugraz.at/institute/ippt/downloads-software/)

○ No

F Interdisciplinarity

10. Which disciplines (see list below) are involved in your project?

◉ Main discipline[13]: 2.3

◉ Associated discipline[13]:1.1 ○ Associated discipline[13]:

G Engaging with Civil society and policy makers

11a Did your project engage with societal actors beyond the research community? *(if 'No', go to Question 14)*

○ Yes
◉ No

11b If yes, did you engage with citizens (citizens' panels / juries) or organised civil society (NGOs, patients' groups etc.)?

○ No

○ Yes- in determining what research should be performed

○ Yes - in implementing the research

○ Yes, in communicating /disseminating / using the results of the project		
11c In doing so, did your project involve actors whose role is mainly to organise the dialogue with citizens and organised civil society (e.g. professional mediator; communication company, science museums)?	○ ○	Yes No

12. Did you engage with government / public bodies or policy makers (including international organisations)

- ○ No
- ○ Yes- in framing the research agenda
- ○ Yes - in implementing the research agenda
- ◉ Yes, in communicating /disseminating / using the results of the project

13a Will the project generate outputs (expertise or scientific advice) which could be used by policy makers?

- ○ Yes – as a **primary** objective (please indicate areas below- multiple answers possible)
- ○ Yes – as a **secondary** objective (please indicate areas below - multiple answer possible)
- ○ No

13b If Yes, in which fields?

Agriculture		Energy		Human rights	
Audiovisual and Media		Enlargement		Information Society	
Budget		Enterprise		Institutional affairs	
Competition		Environment		Internal Market	
Consumers		External Relations		Justice, freedom and security	
Culture		External Trade		Public Health	
Customs		Fisheries and Maritime Affairs		Regional Policy	
Development Economic and Monetary Affairs		Food Safety		Research and Innovation	
		Foreign and Security Policy		Space	
Education, Training, Youth		Fraud		Taxation	
Employment and Social Affairs		Humanitarian aid		Transport	

[13] Insert number from list below (Frascati Manual).

13c If Yes, at which level?

- ○ Local / regional levels
- ○ National level
- ○ European level
- ○ International level

H Use and dissemination

14. How many Articles were published/accepted for publication in peer-reviewed journals?	**18**
To how many of these is open access[14] provided?	**13**
How many of these are published in open access journals?	**4**
How many of these are published in open repositories?	**14**
To how many of these is open access not provided?	**6**
Please check all applicable reasons for not providing open access:	
❑ publisher's licensing agreement would not permit publishing in a repository ❑ no suitable repository available ❑ no suitable open access journal available ❑ no funds available to publish in an open access journal ❑ lack of time and resources ❑ lack of information on open access ❑ other[15]: ……	

15. How many new patent applications ('priority filings') have been made? *("Technologically unique": multiple applications for the same invention in different jurisdictions should be counted as just one application of grant).*		
16. Indicate how many of the following Intellectual Property Rights were applied for (give number in each box).	Trademark	
	Registered design	
	Other	**2**
17. How many spin-off companies were created / are planned as a direct result of the project?		
Indicate the approximate number of additional jobs in these companies:		

18. Please indicate whether your project has a potential impact on employment, in comparison with the situation before your project:

❑	Increase in employment, or	❑	In small & medium-sized enterprises
❑	Safeguard employment, or	❑	In large companies
❑	Decrease in employment,	☒	None of the above / not relevant to the project
❑	Difficult to estimate / not possible to quantify		

19. For your project partnership please estimate the employment effect resulting directly from your participation in Full Time Equivalent (*FTE = one person working fulltime for a year*) jobs:	*Indicate figure:* *10.5*
Difficult to estimate / not possible to quantify	❑

I Media and Communication to the general public

20. As part of the project, were any of the beneficiaries professionals in communication or media relations?

○ Yes ⊙ No

21. As part of the project, have any beneficiaries received professional media / communication training / advice to improve communication with the general public?

○ Yes ⊙ No

22 Which of the following have been used to communicate information about your project to the general public, or have resulted from your project?

❑	Press Release	❑	Coverage in specialist press
❑	Media briefing	❑	Coverage in general (non-specialist) press
❑	TV coverage / report	❑	Coverage in national press
❑	Radio coverage / report	❑	Coverage in international press
❑	Brochures /posters / flyers	☒	Website for the general public / internet
❑	DVD /Film /Multimedia	❑	Event targeting general public (festival, conference, exhibition, science café)

23 In which languages are the information products for the general public produced?

❑	Language of the coordinator	☒	English
❑	Other language(s)		

***Question F-10*:** Classification of Scientific Disciplines according to the Frascati Manual 2002 (Proposed Standard Practice for Surveys on Research and Experimental Development, OECD 2002):

FIELDS OF SCIENCE AND TECHNOLOGY

1. NATURAL SCIENCES

1.1 Mathematics and computer sciences [mathematics and other allied fields: computer sciences and other allied subjects (software development only; hardware development should be classified in the engineering fields)]

1.2 Physical sciences (astronomy and space sciences, physics and other allied subjects)

1.3 Chemical sciences (chemistry, other allied subjects)

1.4 Earth and related environmental sciences (geology, geophysics, mineralogy, physical geography and other geosciences, meteorology and other atmospheric sciences including climatic research, oceanography, vulcanology, palaeoecology, other allied sciences)

1.5 Biological sciences (biology, botany, bacteriology, microbiology, zoology, entomology, genetics, biochemistry, biophysics, other allied sciences, excluding clinical and veterinary sciences)

2 ENGINEERING AND TECHNOLOGY

2.1 Civil engineering (architecture engineering, building science and engineering, construction engineering, municipal and structural engineering and other allied subjects)

2.2 Electrical engineering, electronics [electrical engineering, electronics, communication engineering and systems, computer engineering (hardware only) and other allied subjects]

2.3. Other engineering sciences (such as chemical, aeronautical and space, mechanical, metallurgical and materials engineering, and their specialised subdivisions; forest products; applied sciences such as geodesy, industrial chemistry, etc.; the science and technology of food production; specialised

[14] Open Access is defined as free of charge access for anyone via Internet.

[15] For instance: classification for security project.

technologies of interdisciplinary fields, e.g. systems analysis, metallurgy, mining, textile technology and other applied subjects)

3. MEDICAL SCIENCES

3.1 Basic medicine (anatomy, cytology, physiology, genetics, pharmacy, pharmacology, toxicology, immunology and immunohaematology, clinical chemistry, clinical microbiology, pathology)

3.2 Clinical medicine (anaesthesiology, paediatrics, obstetrics and gynaecology, internal medicine, surgery, dentistry, neurology, psychiatry, radiology, therapeutics, otorhinolaryngology, ophthalmology)

3.3 Health sciences (public health services, social medicine, hygiene, nursing, epidemiology)

4. AGRICULTURAL SCIENCES

4.1 Agriculture, forestry, fisheries and allied sciences (agronomy, animal husbandry, fisheries, forestry, horticulture, other allied subjects)

4.2 Veterinary medicine

5. SOCIAL SCIENCES

5.1 Psychology

5.2 Economics

5.3 Educational sciences (education and training and other allied subjects)

5.4 Other social sciences [anthropology (social and cultural) and ethnology, demography, geography (human, economic and social), town and country planning, management, law, linguistics, political sciences, sociology, organisation and methods, miscellaneous social sciences and interdisciplinary , methodological and historical S1T activities relating to subjects in this group. Physical anthropology, physical geography and psychophysiology should normally be classified with the natural sciences].

6. HUMANITIES

6.1 History (history, prehistory and history, together with auxiliary historical disciplines such as archaeology, numismatics, palaeography, genealogy, etc.)

6.2 Languages and literature (ancient and modern)

6.3 Other humanities [philosophy (including the history of science and technology) arts, history of art, art criticism, painting, sculpture, musicology, dramatic art excluding artistic "research" of any kind, religion, theology, other fields and subjects pertaining to the humanities, methodological, historical and other S1T activities relating to the subjects in this group]