Grant Agreement No.: 604656

Project acronym: NanoSim

Project title: A Multiscale Simulation-Based Design Platform for Cost-Effective CO_2 Capture Processes using Nano-Structured Materials (NanoSim)

Funding scheme: Collaborative Project

Thematic Priority: NMP

THEME: [NMP.2013.1.4-1] Development of an integrated multi-scale modelling environment for nanomaterials and systems by design

Starting date of project: 1st of January , 2014

Duration: 48 months

WP N°	Del. N°	Title	Version	Lead beneficiary	Nature	Dissemin. level	Delivery date from Annex I	Actual delivery date dd/mm/yyyy
9	12	Newsletters to disseminate the project progress (24)	0	DCS	R	PU	31/12/2015	05/01/2016

The Newsletters to disseminate the project progress (12) was assembled and successfully sent out to a group of ~130 stakeholders across Europe, including heads of laboratories and research institutes, key players in industry, as well as to members of the EMMC (European Materials Modelling Council)

A professional (yet free) newsletter service provider was used to each recipient can unsubscribe if desired. The list of recipients is stored and can be extended over time. Figure 1 shows a snapshot of the newsletter.

NanoSim

NanoSim - A Multi-scale Simulation-Based Design Platform for Cost-Effective CO2 Capture Processes using Nano-Structured Materials

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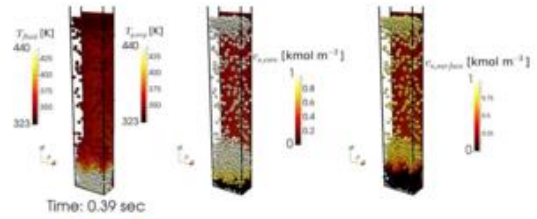
The NanoSim Project

The objective of the NanoSim project is to **create an efficient and cost-effective multi-scale simulation platform based on free and open-source software.** 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 develops an open and integrated framework for numerical design called **Porto** under the GNU Lesser General Public License (LGPL). An open source core co-simulation platform called **COSI** will be established based on the existing CFD-DEM and DEM software **LIGGGHTS®** and **CFDEM®coupling** and the new **ParScale** and **CPPPO** codes. The resulting open source software platform will 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 NanoSim project will demonstrate the capabilities of this multi-scale software platform to custom design an industrial scale reactor/process in a way that most effectively leverages the superior reactivity and tailored selectivity of any specific nano-structured material. **Some snapshots from the second year of research within the NanoSim projects are highlighted below. We wish you a pleasant reading.**

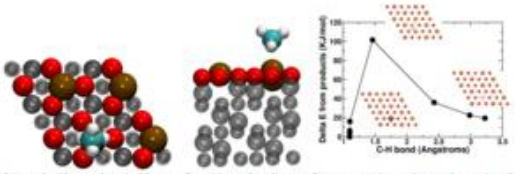


parScale

Euler-Lagrange modelling

The open source simulation code ParScale ("**Par**ticle **Scale** Models") for predicting **predict intra-particle transport processes such as heat or mass transfer and reactions** has been further developed, validated and applied this year. It can be downloaded via www.cfdem.com and github.

Furthermore, **Direct Numerical Simulation (DNS) are used to develop so-called closure models**, which are then used in unresolved modelling approaches (such as CFD-DEM). DNS are simulations which are solving for all the degrees of freedom required to correctly picture the physical behaviour of a flow system. The existing DNS solver implemented in CFDEM®coupling has been improved at TU Graz to produce accurate results for particle beds in fully periodic boxes. The solver has been proven accurate and efficient since, in order to represent the particle surface, it requires a lower grid resolution compared to the original algorithm present in the CFDEM®coupling package. Furthermore, first parametric studies involving unresolved CFD-DEM simulations accounting for intra-particle effects (e.g., heat conduction, heterogeneous reactions, or diffusion) have been completed.



Atomistic calculations for the design of nano-structured materials to develop fundamental insight into mechanisms

This work involves the calculation of reaction mechanisms underlying chemical looping reforming on metal oxide surfaces, which requires the usage of quantum mechanical simulations to understand the binding and dissociation of methane on metal oxide surfaces. Specifically this is the (0001) surface of haematite. We have determined the kinetics for the first few elementary steps of the decomposition reaction ($CH_4 \rightarrow CH_3 \rightarrow CH_2 \rightarrow CH$). In particular, we have found that the activation barrier for the first two steps of the dissociation barrier are relatively high, at 102 and 193 kJ/mol respectively. The activation barriers suggest that chemical kinetics are slow, with the kinetics for the first dissociation being 1.5×10^7 s-1 at an operating temperature of 870 K. Heightened temperatures are essential for looping reforming reactions. This thermodynamic and kinetic data is useful for parameterisation of multiscale models.

ANDRITZ DCS TU Graz INP NTNU SINTEF UCL

The consortium: The NanoSim consortium consists of SINTEF (coordinator: **Shahriar Amini**, Shahriar.Amini@sintef.no), TU Graz, DCS Computing, UC London, NTNU, Andritz, INP Toulouse and University of Coimbra.

Phenomenological Modelling & Techno-Economic Assessment

The successful research on the small scale must be translated into process scale simulation. Naturally, any new process development must be supported by a techno-economic assessment to evaluate its economic usefulness.

Phenom is a 1D phenomenological model for a single FB reactor that can operate under the three most common fluidization regimes in industry, bubbling, turbulent and fast fluidization. It consists of a heterogeneous model based on the two-zone theory with axial dispersion effects to model the dense zone and a dispersion plug flow model for the lean zone. A Finite Volume method with low order schemes is used to solve the system of equations (continuity, mass, energy and pressure) that constitute the model. The generality of Phenom is achieved through an averaging probabilistic approach. It requires a library of closures that describe the reactor hydrodynamics for the three mentioned fluidization regimes which has been already implemented into the code. Furthermore, the heterogeneous reactions used for a first version of Phenom consider Nickel oxide as the active material. **Phenom is then linked to the Power Plant Simulations and for carrying out a techno-economic assessment.** Firstly, a thermodynamic comparison on the basis of exergy destruction was done between CLR and conventional partial oxidation process. The results were presented at TCCS-8 conference. A first version of the Phenom 1D Phenomenological Model was linked with power plant simulations on Thermoflow Suite using Microsoft Excel for data exchange. First cut efficiencies of the combined cycle power plant with CLR and CO2 Capture were estimated. With simple heat integration, the efficiency of the process is 48.15%, whereas the efficiency of the standard combined cycle power plant with post combustion MEA absorption CO2 capture process is 49.9%. Process integration and optimization will now be carried out followed by economic assessment of the process.

Validation Experiments

All modelling needs to be supported by experimental verification in order to ensure its validity. **Different nano-structures of thermally stable oxygen carrier materials on suitable inert, mechanically strong support materials are synthesised and characterized.** Significantly different nanostructured iron oxide active particles are used (commercial nano-rods as well as synthesized nanoparticles of iron oxide oxygen carrier). The effects of nano-structuring will be studied using a newly developed **lab-scale fluidized/fixed bed reactor**. The reactor will be operated under real CLR process conditions at high temperatures and elevated pressures, and will be used to demonstrate the potential for process intensification through the use of nano-structured materials in the CLR process.

SEVENTH FRAMEWORK PROGRAMME

The NanoSim project is running from January 2014 to December 2017. NanoSim is funded from the **European Union's Seventh Framework Programme for research, technological development and demonstration** under grant agreement no. 604656.

Figure 1: Newsletter (24M) to disseminate the project progress