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	13	Newsletters to disseminate the project progress (36)	0	DCS	R	PU	31/12/2016	02/01/2017

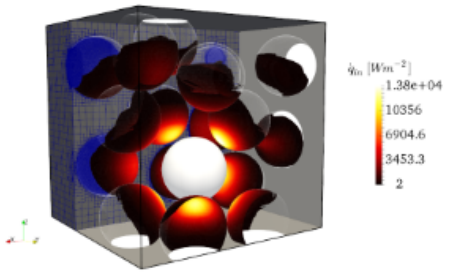
The Newsletters to disseminate the project progress (36) was assembled and successfully sent out to a group of ~130 stakeholders across Europe, including heads of laboratories and research institutes, key players in industry, as well as to members of the EMMC (European Materials Modelling Council)

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

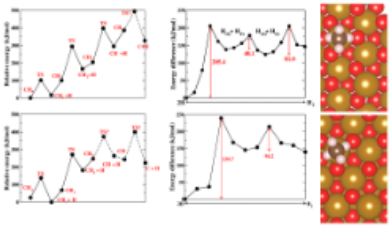
The NanoSim Project

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** is 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 is 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 is demonstrating 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 third year of research within the NanoSim projects are highlighted below. We wish you a pleasant reading.**

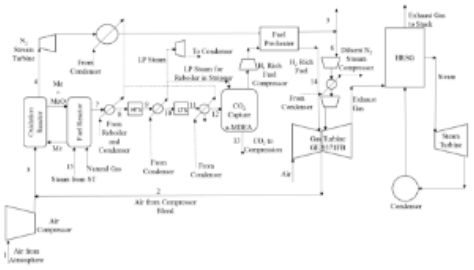


Euler-Lagrange modelling
The open source simulation code ParScale ("**Par**ticle **Scale** Models") for predicting **predict intra-particle transport processes such as heat or mass transfer and reactions** has been further developed, validated and applied this year. It can be downloaded via www.cfdem.com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

Within the last year, ParScale was applied to **wall bounded shear flow** and a corresponding publication is finished. Furthermore a lab scale experiment was set up and **validation experiments** were performed. Currently we focus on a novel and fast algorithm to **include thermal radiation** in DEM simulations which will be implemented in LIGGGHTS® (see Figure above). Also, a large array of particle-resolved direct numerical simulations has been performed with a focus on (i) bi-disperse systems, as well as (ii) wall effects. Progress of publications at conferences and workshop was satisfactory in 2016. A set of journal publication is currently in preparation.



Atomistic calculations for the design of nano-structured materials to develop fundamental insight into mechanisms
This work package involves the calculation of reaction mechanisms underlying chemical looping reforming on metal oxide surfaces. Quantum mechanical simulations were used to understand the binding and dissociation of CH4 on two metal oxides, haematite (Fe2O3) and magnetite (Fe3O4). The thermodynamics of methane dissociation on both surfaces were determined. Furthermore, kinetic barriers were determined for the first few steps of both reactions, with the finding that the barriers are very similar in magnitude (within 5 kJ/mol). Based on this, magnetite is expected to be the better CH4 reforming catalyst as the overall thermodynamics of dissociation are lower at 223.5 kJ/mol when compared to haematite at 326.6 kJ/mol. In addition, the kinetics and thermodynamics for molecular hydrogen production were also determined. Thermodynamically, both materials are very similar for H2 production, however magnetite has a higher activation barrier for H2 production. This results in kinetics of only 6.3 s−1 per site at 1000 K on magnetite in comparison to 392.4 s−1 per site for haematite. Magnetite is thus expected to be the worse H2 production catalyst. This thermodynamic and kinetic data will be used for the parameterisation of multiscale models.



Plant-Scale Modelling and 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.
The second aim is to link the 1D Phenomenological Model of CLR to the Power Plant Simulations and carry out a **techno-economic assessment**. The 1D Phenomenological Model, was linked with power plant simulations. Complete plant scale integration of pre-combustion CO2 capture method with Chemical Looping Reforming (CLR) of Natural Gas (NG), Water Gas Shift (WGS) process, CO2 capture and CO2 compression in a combined cycle power plant was carried out and the results were presented at Greenhouse Gas Control Technologies 13 (GHGT-13) conference, held between 14 – 18th November 2016 in Lausanne, Switzerland. The net electrical efficiency of the process with lower degree of heat integration was 42.5%. Studies on improvements in the process through heat integration were presented at the 4th Trondheim Gas Technology Conference 2016.

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.

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Figure 1: Newsletter (36M) to disseminate the project progress