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	11	Newsletters to disseminate the project progress (12)	0	DCS	R	PU	31/12/2014	12/01/2015

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. An online version of the newsletter can be viewed here:

http://75500.seu1.cleverreach.com/m/6084941/523090-9601c7219d8a7d3672fe90109f3acdb2

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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NanoSim

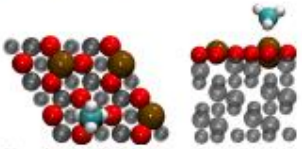
NanoSim - A Multi-scale Simulation-Based Design Platform for Cost-Effective CO2 Capture Processes using Nano-Structured Materials

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 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 develops 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 the existing CFD-DEM and DEM codes LIGGGHTS® and CFDEM®coupling. 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)**. However, the final **NanoSim platform will be sufficiently generic for application in a wide range of gas-particle contacting processes**.
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 first year of research within the NanoSim projects are highlighted below. We wish you a pleasant reading. Feel free to contact us!

parScale

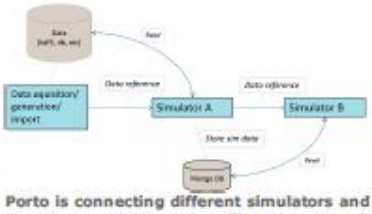
A new open source simulation engine is born: ParScale stands for "**Par**ticle **Scale** Models". ParScale is a new, **stand-alone simulation engine**, and can **predict intra-particle transport processes such as heat or mass transfer and reactions**. It will be publicly available in December 2015 via www.cfdem.com and its github account.
ParScale can currently be **coupled to** the soft-sphere DEM simulation engine **LIGGGHTS®**, and a coupling to the CFD-DEM engine **CFDEM®coupling** will be available soon. This will then allow full handling of reactions in gas-solid systems: For example, the rate of oxidation of porous metal particles suspended by a hot gas stream can be predicted directly by ParScale. ParScale is the last tool that completes the multi-physics co-simulation platform "COSI" within the NanoSim project. COSI is the first open-source simulation platform that is able to perform fully-coupled parallel simulations of reactive fluid-particles systems with sophisticated intra-particle transport models



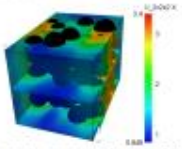
Atomistic calculations for the design of nano-structured materials: UCL is performing calculations on the reaction mechanisms underlying chemical looping reforming on metal oxide surfaces. Advanced quantum mechanical simulations, using Density Functional Theory to treat atoms explicitly, are being used to understand the binding and dissociation of CH4 molecules in order to determine the thermodynamics and kinetics of the reaction. In the Figure, the binding geometry of methane to the (0001) surface of haematite iron oxide is shown. Furthermore the change in electronic density, reflecting the formation of chemical bonds, shows that there is a significant charge transfer to the methane. This data is useful for parameterisation and optimisation of materials and multiscale models

ANDRITZ DCS TU Graz INP NTNU SINTEF UCL

The consortium: The NanoSim consortium consists of SINTEF (coordinator), TU Graz, DCS Computing, UC London, NTNU, Andritz, INP Toulouse and University of Coimbra.



Porto is connecting different simulators and scales. The novelty of the Porto framework lies in the **offline data-centric code-coupling strategy**. Due to the complexity of (correctly, safely and maintainable) sharing data between multiple in-house and commercial tools (proprietary and open) the new approach to the problem is building a database of meta-data that describes the data (and models) in terms of entities and relationships. This meta-data can be used for various things such as validating type correctness (avoid confusion about types, units, dimensions etc), automatic configuration of generic file import/export filters, it can be used for code generation (metaprogramming of classes and structures) and even generation of source code that can be used to extend software such as OpenFOAM, Octave/MatLab and ANSYS Fluent. The Porto framework is made available for download here with a brief tutorial that teaches the key features of the scripting environment



A new post-processing tool for particle simulations is born: CPPPO stands for "**C**ompilation for Fluid-**P**article Data **P**ost **PrO**cessing", and will be publicly available by December 2015 here . CPPPO is designed as a **generic tool for the post-processing - especially filtering - of flow data**, as well as heat and concentration data from parallel multiphase CFD simulations. An application is the extraction of velocity and force statistics to characterize two-phase flows. For example, CPPPO is able to compute a filtered (i.e., spatially-averaged) fluid velocity field during a simulation run (i.e., "on the fly"), as well as derive meaningful statistics from this data. An example of a filtered velocity field is shown in Figure 1, in which the filtered fluid velocity from a test case (i.e., flow through an array of particles) is compared with the original fluid velocity.

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 to disseminate the project progress