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	2	Outcome of workshops (18)	0	DCS	R	PU	30/06/2015	08/10/2015

The first NanoSim workshop was held as an "Invited Symposium" (IS) in the frame of the IV International Conference on Particle-based Methods - PARTICLES 2015 (Particles 2015) conference organized by CIMNE, held in Barcelona , 28-30 September 2015, with ~400 attendants (http://congress.cimne.com/particles2015). The change to month 22 was approved by the project officer. DCS has advertised the workshop on its web platform cfdem.com which has a high visibility in the particle modelling area. In Table 1, the program of the workshop, entitled "Multi-Scale Modelling of Reactive Particle-Based Processes" is shown. Presentations by NanoSim Consortium members have been highlighted.

IS-Multi-Scale Modelling 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 modelling for particle-based processes *C. Goniva*, B. Blais and C. Kloss*	
***ParScale* - An open-source library for the simulation of ìntra 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 modelling 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*	

Table 1: Programme of the NanoSim consortium workshop at the Particles 2015 conference

The audience of the invited symposium was about 100 listeners from different fields. The NanoSim consortium had lots of interesting discussions with modelers and engineers, including colleagues from Univ. Grenoble, JKU Linz, TU Braunschweig, Twente University, Univ. Edinburgh, Univ. Leeds, Univ. Manchester, CIMNE, DEM Solutions, Nestle, John Deere, Procter & Gamble, ArcelorMittal, Johnson Matthey, Astec, and many others.

The workshop was also used to connect to the FP7 project (ITN) **T-MAPPP** (www.t-mappp.eu).

Additionally, there was a presentation in the frame of the "Multiphase Flows" session of the conference, and other contributions by NanoSim consortium members as shown in Table 2:

Multiphase Flows III	**WeA06** **Room: VS214** **Chair: Mojtaba Ghadiri**
CFD-DEM prediction of heat transfer in Packed Beds using commercial and open source codes ***A. Singhal*, S. Cloete, F. Municchi, S. Radl and S. Amini***	
IS-High Performance Computing for Particle Methods: New Trends, Algorithms and Applications II **Invited Session organized by Peter Wriggers, Eugenio Oñate, Bircan Avci and Pooyan Dadvand**	**TuM02** **Room: VS217** **Chair: Pooyan Dadvand**
Speeding up LIGGGHTS using a MPI/OpenMP hybrid parallelization and the road towards adaptive time stepping ***R. Berger*, C. Kloss and S. Pirker***	
IS-Multiscale Analysis of Multiphase Particulate Systems (T-MAPPP Symposium) II **Invited Session organized by Jin Ooi, Antonia Larese and Martin Crapper**	**TuE03** **Room: VS218** **Chair: Jin Ooi**
A contact detection method between two convex super-quadric particles based on an Interior Point algorithm in the Discrete Element Method ***A. Podlozhnyuk* and C. Kloss***	

Table 2: Other contributions of NanoSim consortium members at the Particles 2015 conference

Figure 1 shows the consortium members at the Particles 2015 conference.

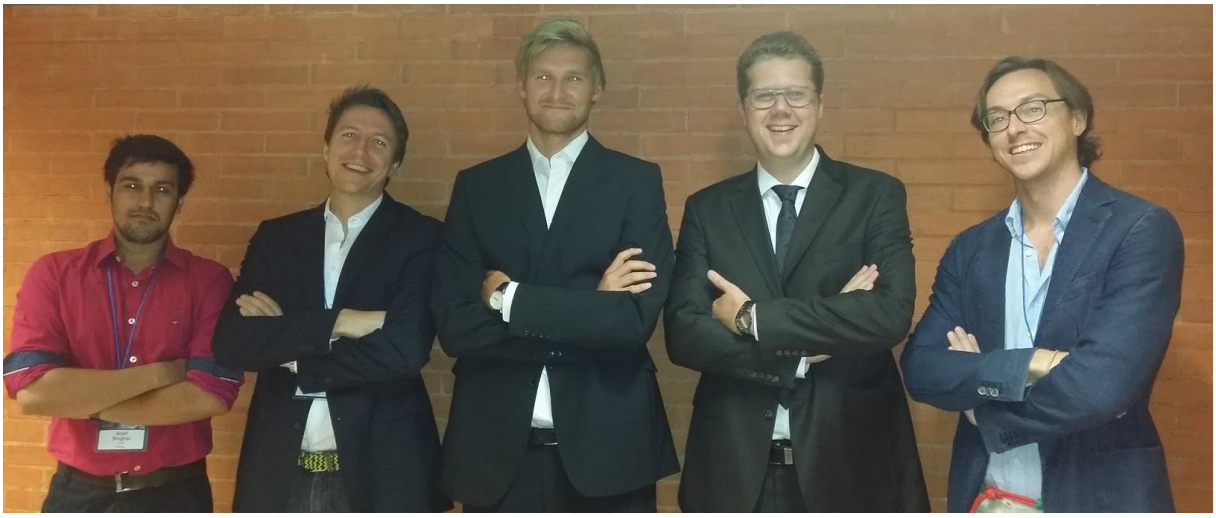

Figure 1: NanoSim consortium members at the Particles 2015 conference: from left to right: Arpit Singhal (SINTEF), Christoph Kloss (DCS Computing), Thomas Forgber (TU Graz), Stefan Radl (TU Graz), Christoph Goniva (DCS Computing)