SPIRE 8 – 2015 – Solids handling for intensified process technology

Title: Intensified by Design© for the intensification of processes involving solids handling

Acronym: IbD

Grant Agreement No: 680565

Deliverable 2.9	Public/publishable outputs from WP2
Associated WP	WP2 PI
Associated Tasks	Tasks 2.1-2.5
Due Date	31/08/2018
Date Delivered	14/09/2018
Prepared by (Lead Partner)	ULEEDS
Partners involved	ULEEDS, DRA, TUE, DSC, LEITAT,HSO
Authors	Andrew Bayly (ULEEDS) with support from partners
Dissemination Level	Public

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1 Introduction

WP2 of the IbD project focused on the development of design methodologies and computational tools for application to selection, development and design of intensified solids based process technologies.

The partners involved with WP3 are ULEEDS, DRA, TUE, DSC, LEITAT, HSO.

2 Objectives of WP2

(1) To develop the chemical process design methodologies for a) the design of PI innovative solutions based on the TRIZ methodology for new PI concept development, and b) PI implementation based on the Knowledge-based Engineering (KBE) methodology that will be programmed into the IbD® Platform.

(2) To develop the key computational tools that will be coded into the IbD® Platform. These include models for the design and application of PI technologies, focusing on ensuring the the capability required for the case studies in WP6 is available. The overall framework for linking models will also be addressed

3 Key achievements of WP2

- New Process design methodologies have been developed. (i) HSO identified that most of the inventions related with PI face secondary problems implying the presence of unsolved contradictions and developed the concepts for a TRIZ Methodology for Process Intensification to resolve these contradictions. (ii) DRA developed a knowledge-based engineering (KBE) approach to evaluating and rank existing PI solutions for implementation into chemical processes where solids are an intrinsic part of the process. This is based on a database of 154 technologies, each scored on 17 functionality criteria. For both methodologies backlogs have been developed, and implemented in the IbD Platform
- Phenomenological model for fluidized bed dryer was created. Latest correlations for hydrodynamics were used. Backlogs and codes were developed for implementation into the IBD platform.
- Detailed research on hydrodynamics of fluidized bed was initiated in order to further upgrade the correlations used in phenomenological model.
- Three significant novel methodologies were developed for application to fluid-particle processes that are seen in PI technologies involving solids:
    - Coupling of DEM (discrete element method) and dynamic meshing to enable large objects to modelled in particulate systems
    - A new SPH-DEM (SPH-smooth particle hydrodynamics) method to analyse particulate flows with free surfaces
    - A novel parallel implementation of CFD-DEM integrating a GPU based DEM method into a commercail software code

- A new programming language was developed to define process flows of PI equipment. A open source tool 'KinSolve' is written in MS Excel which interpretes the new language, as well as numerically solves the models. A new implementation of the Rosenbrock ODE solution method has been developed which robustly solves process models where other solvers typically produce unreliable results. These were implemented in the IBD platform.
- Development of immersed boundary and direct numerical simulation methods in order to develop correlations for deposition and resuspension of particles in turbulent flows
- A procedure to predict the working conditions of a PI technology has been developed and implemented for the selected case studies. For each case study, the control variables are identified, and some combinations of variables are simulated by means of Computational Fluid Dynamics (CFD) tools. The combinations of variables to be studied by CFD are obtained by means of Monte Carlo and Latin Hypercube sampling algorithms. The output data is fitted with a response surface (Radial Basis function), in order to predict the working conditions of the PI, without the need to perform a new CFD simulation every time new values of variables are requested. Lastly, the response surface has been integrated into the IBD platform. In that manner, the final user will have a real time response of the PI behaviour subjected to changes in the input variables. The whole procedure has been impleneted in the IRIS platform.
- Life Cycle Assessment and Life Cycle Cost of the case studies.

  Potential environmental impacts and benefits of the intensified processes has been quantified, allowing to compare the results between the conventional and the intensified process. For each case study the impacts related to the current process and the intensified one have been divided in 8 different categories in order to compare in detail the effects on the environment: Global warming potential, ozone depletion, human toxicity non-cancer effects, particulate matter, water depletion, mineral fossil & renewable resource depletion, cumulative energy demand and waste.

  This analysis include an economic assessment, comparing the costs of the production process for the conventional process and the intensified process, giving thus an overall vision of the benefits of the process intensification.

- Environmental impact tool

  The IbD Tool includes an LCA section in which users can perform an LCA with a database settled from the IbD project case studies, defining the requirements to build a standard Life Cycle Assessment tool.

  As an output of the LCA IbD tool the user is able to identify the environmental and cost impacts, comparing the results from conventional and intensified process.

4 Public outputs from WP2

4.1 Journal papers

4.1.1 Published papers

H. Wang, A. Mustaffar, A. Phan, V. Zivkovic, D. Reay, R. Law, K.V.K. Boodhoo, 2017, "A review of process intensification applied to solids handling", Chem Eng & Processing: Process Intensification, 118, pp. 78 – 107, https://doi.org/10.1016/j.cep.2017.04.007.

R. Law, C. Ramshaw and D.A. Reay, 2017. Process intensification – Overcoming impediments to heat and mass transfer enhancement when solids are present, via the IbD project. Thermal Science and Engineering Progress, 1, pp. 53-58, https://doi.org/10.1016/j.tsep.2017.02.004

Yi. He, Andrew E. Bayly, Ali Hassanpour, Coupling CFD-DEM with dynamic meshing: A new approach for fluid-structure interaction in particle-fluid flows, Powder Technology, 325, 2018, Pages 620-631, ISSN 0032-5910, https://doi.org/10.1016/j.powtec.2017.11.045.

Yi He, Andrew E. Bayly, Ali Hassanpour, Frans Muller, Ke Wu, Dongmin Yang. A GPU-based coupled SPH-DEM method for particle-fluid flow with free surfaces, Powder Technology, 338 (2018) 548-562, https://doi.org/10.1016/j.powtec.2017.11.045

4.1.2 Papers under review or in preparation

Yi He, Andrew E. Bayly, Ali Hassanpour, Frans Muller, An Efficient Parallelism for Complex Particle-Fluid flows: Coupling ANSYS/Fluent with GPU-based DEM via Network Communication (to be submitted).

Yi He, Andrew E. Bayly, Ali Hassanpour, Michael Fairweather, Frans Muller. Large Eddy Simulations on the Flow in an Agitated Tubular Reactor Using Lattice Boltzmann Method (in preparation).

Yi He, Andrew E. Bayly, Ali Hassanpour, Michael Fairweather, Frans Muller. CFD simulation of Tubular Reactor Agitated by A Solid Bar (to be submitted).

M. Mihajlovic, I. Roghair, M. van Sint Annaland, Modified calculation of the van der Waals force for Geldart A and B type particles for the DEM simulations (in preparation).

M. Akhami, M. Fairweather, A.E. Bayly, F. Muller, Particle Re-Suspension in Turbulent Channel Flow using Direct Numerical Simulation and Immersed Boundary Method *(in preparation).*

M. Akhami, M. Fairweather, A.E. Bayly, F. Muller, Particle Deposition in Turbulent Flow using Direct Numerical Simulation and Immersed Boundary Method (in preparation).

4.2 Conference publications

4.2.1 Conference presentations

Y. He, A.E. Bayly, Recent advances in multiphase flow modelling, Granular Flow SIG Meeting, 21-22 June 2018, Edinburgh, UK.

Yi He, Andrew E. Bayly, Ali Hassanpour, Michael Fairweather, Frans Muller, CFD-DEM modelling on complex particle-fluid flow with fluid-structure interaction. Particle 2017, Germany

Livotov, P., Sekaran, A. P. C., Law, R., Mas'udah, Reay, D. A. (2017) Systematic innovation in process engineering: Linking TRIZ and process intensification. TRIZ Future Conference 2017, Lappeenranta, Finland, October 2017. [Oral presentation and full paper]

M. Mihajlovic, I. Roghair, M. van Sint Annaland, High temperature fluidization - Van der Waals influence, CFD 2017, Trondheim, Norway

M. Mihajlovic, F. Xu, I. Roghair, M. van Sint Annaland, Influence of particle collision properties on fluidization behavior at elevated temperatures, ISCRE 2018, Florence, Italy

M. Mihajlovic, I. Roghair, M. van Sint Annaland, Influence of inter-particle forces and particle collision properties on fluidization behavior at elevated temperatures, 8th World Congress on Particle Technology, Orlando, Florida

Reay, D. A., Law, R. (2016) PI – overcoming impediments to heat and mass transfer when solids are present, via the IbD project. International Heat Transfer Symposium, Nottingham, UK, June 2016 [Oral presentation]

4.2.2 Conference posters

CFD Modelling of Agitated Tubular Reactor Using Discrete Element Method and Dynamic Meshing Approach. 10th World Congress of Chemical Engineering, 1-5th October, 2017.

Law, R., Reay, D. (2018) Towards standardisation of process intensification in solids-handling processes – the IbD platform. AIChE Spring Meeting, Orlando, FL, USA, April 2018 [Poster presentation and demonstration]

4.3 Other technical presentations (e.g seminars, invited talks etc.)

D.A. Reay, 2016. Intensified by Design – The IbD Project. Process Intensification Group Meeting, School of Chemical Engineering, Newcastle University, 4 March.
H. Wang, 2016, Taylor-Couette reactor for solids processing applications, Process Intensification Group (PIG) Seminar, Newcastle, United Kingdom.

F.L. Muller and D.A. Reay, 2016. 'Intensified by Design' – Overview of the IbD project and the Case Studies. Leeds University and David Reay & Associates. Proc. 24^{th} Process Intensification Network Meeting, Newcastle University, June 2016.

Yi He, 2016, University of Leeds Post-Docs Conference, Dec.2016

A.E.Bayly, 2017, Overview of modelling of particulate system modelling Granular Flow SIG meetings, April 2017

A.E.Bayly, 2017, As part of presentation on current activity in CFD and DEM Granular Flow SIG meetings, Sept 2017

D.A. Reay, Ramshaw, C., Law, R., Mustaffar, A. 2017. The fear of fouling and solid streams – Overcoming this barrier to improve energy efficiency in intensified processes. 16th International Conference on Susdtainable Energy Technologies (SET2017), Bologna, July 2017

D.A. Reay, 2017. Process Intensification: Overcoming impediments to heat and mass transfer enhancement when solids are present. 24th SC-SCCST (Anglo-Chinese) Conference, Northumbria University, June 2017

5 Appendices

Relevant websites with links (where available) to abstracts/presentations highlighted above:

www.hexag.org

www.pinetwork.org

http://wcce10.org/index.php/program/st-program

https://www.aiche.org/conferences/aiche-spring-meeting-and-global-congress-on-process-safety/2018

Particles 2017: http://congress.cimne.com/particles2017/frontal/default.asp