Theses of the doctoral (PhD) dissertation

Application and development of two-phase models and simulators

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Introduction and the aim of the work

Fluid-solid two-phase flow occurs in many chemical engineering processes, such as in fluidization, pneumatic conveying, drying or catalytic cracking. Modelling and simulation are an effective way to understanding these processes and the detailed simulation studies can provide economic and environmental benefits. The quick development in information technology allows us to get a numerical solution of the detailed phase level models in a reasonable time because of the efficient methods and high performance of computers are available for the numerical solution of the models.

The aim of my dissertation is the model-based study of chemical engineering systems, in which I used the methods of computational fluid dynamics (CFD) at the model developing and simulation studies. In some cases I used a commercial program package, in which the flow model and the numerical method can be chosen for the solution of the given problem. In other cases the numerical solution of the model equations were performed by self-developed programs.

Additionally, I used, the residence time distribution analysis method, particle tracking and compartment modelling. The most frequently used modelling method was the immersed boundary method, which is a popular method that is used in the direct numerical simulations. This method allows detailed, particle level description of the systems. The results are shown in five case studies. They are: 1. the hydrodynamic study of a biomass gasification reactor by analysis of the residence time distribution, 2. evaluation of the mixing performance of a multijet mixer using data from the particle tracing study, 3. particle level modeling and simulation of a fluidized particle, 4. modelling and simulation of the saturation of adsorbent particle, and 5. settling a solid particle in Newtonian fluid.

New scientific results (theses)

1. I developed a new method based on residence time distribution analysis using computational fluid dynamics and a compartmental model to study the hydrodynamic behavior of the equipment with complex geometry. The residence time distribution curve obtained by using the heuristic compartmental model is in good agreement with the curve obtained by the detailed CFD model.

a) A three-dimensional CFD simulator of a biomass gasification device is developed, which is suitable for studying residence time distribution of systems with multiple inlets.

b) Using a compartmental model which is based on ideal flow units I showed that the hydrodynamic behavior of the detailed CFD model can be reproduced. With the application of the compartmental model we got a tool for the calculation of the residence time analysis with significantly less computational cost.

Related publications: 6., 10., 18.

2. **To evaluate the performance of continuous mixers, I defined a multi-aspect mixing measure and used it to develop an evaluation method. The advantage of the developed method is that in contrary to the traditional simulations based on the solution of the component balance equation, only the stationary velocity field has to be used for the calculations.**

   a) I developed metrics of mixing to define the mixedness. These metrics are applicable to qualify static and jet mixers.

   b) I defined the concept of local coverage, which can be used to qualify the mixer by interpreting the local coverage to the whole outlet boundary.

   c) I developed a calculation method that is suitable for determining the mixing performance of mixers based on the position data of the marked phase elements using the stationary velocity field obtained by the flow simulation.

   Related publications: 1., 13.

3. **Models using the immersed boundary method based on the direct numerical simulation modeling approach are developed for particle level modelling of two-phase flow including the**

phase interactions for different processes such as fluidization, adsorption and sedimentation.

a) A simulator of a two-phase system, including a fluidized particle is developed in which the gas-solid interaction is calculated by the immersed boundary method. The algorithm of the calculation is usable to calculate the moving of a solid particle considering the properties of the surrounding flow field.

b) I developed a particle level model to simulate the adsorption process on the surface of an adsorbent particle. I constructed a flow model of a two-phase system containing the adsorbent particle based on the immersed boundary method. The flow model is completed with a component balance for the component to be adsorbed and first-order kinetics describing the adsorption process. The developed method makes it possible to determine the degree of saturation of the adsorbed components on different surface elements of the particle.

c) I also developed a particle level model based on the immersed boundary method that can calculate the sedimentation of a solid particle in Newtonian fluid. The simulator is suitable to calculate the moving of the solid particle in still fluid based on the properties of the surrounding flow field.

Related publications: 3., 7., 8., 9., 11., 12., 14., 15., 16., 17., 19., 20.

Utilization of the work

The developed methods and simulators introduced in the dissertation are suitable for model-based study of one-phase or fluid-solid two phase systems. They are usable to study the processes in detail. Development of experimental devices to measure physical processes has a great importance in model validation, since it is essential part of the model development.

The developed models and the introduced methods in the case study of biomass gasification reactor are applicable for examining the hydrodynamics of other systems with multiple inlets.

The metrics developed to characterize mixing in the case of a multijet mixer can be used to qualify the mixing performance of other continuous mixers.

The advantage of particle level models of fluid-solid two-phase flow is that we can get detailed information about the motion and other relevant properties of the particles in the solid phase. Knowledge about the particle level properties is important to understanding the behavior of the whole particle population, which forms the basis of the entire modeling of the whole system. The particle level properties can contribute to the understanding of multiphase systems, and thus to their more economic operation.

Publications of the author

Articles:

1. Gyurik, L., Ulbert, Zs., Molnár, B., Varga, T., Chován, T., Egedy, A., 2020, CFD Based Nozzle Design for a Multijet Mixer, **Chemical Engineering and Processing - Process Intensification** Vol. 157 /DOI: 10.1016/j.cep.2020.108121/ **Q1, IF: 3.731**
2. Egedy, A., Gyurik, L., Ulbert, Zs., Rado A., 2020, CFD modeling and environmental assessment of a VOC removal silo, **International Journal of Environmental Science and Technology** /DOI: 10.1007/s13762-020-02833-7 **Q2, IF: 2.540**
3. Gyurik, L., Egedy, A., Ulbert, Zs., Cronin, K., Ring, D., 2019, Modelling the Motion of a Single Solid Bead in a Newtonian Fluid by Two-Phase CFD Methods, **Chemical Engineering Transactions**, Vol. 76., pp. 175-180. /DOI: 10.3303/CET1976030/ **Q3, IF: -**
4. Egedy, A., Gyurik, L., Ulbert, Zs., Rado, A., 2019, CFD Modelling and Simulation of a VOC Removal Silo, **Chemical Engineering Transactions**, Vol. 76., pp. 163-168. /DOI: 10.3303/CET1976028/ **Q3, IF: -**
5. Egedy, A., Gyurik, L., Varga T., Zou, J., Miskolczi, N., Yang, H., 2018, Kinetic-compartmental modelling of potassium-containing cellulose feedstock gasification, **Frontiers of Chemical Science and Engineering**, Vol. 12., pp. 708-717. /DOI: 10.1007/s11705-018-1767-y/ **Q1, IF: 3.552**
6. Gyurik, L., Egedy, A., Zou, J., Miskolczi, N., Ulbert, Zs., Yang, H., 2018, Hydrodynamic modelling of a two-stage biomass gasification reactor, **Journal of the Energy Institute** Vol. 92., pp. 403-412. /DOI: 10.1016/j.joei.2018.05.007/ **Q1, IF: 4.748**

7. Gyurik, L., Egedy, A., Ulbert, Zs., 2018, Simulation of Gas-Solid Flow in Quasi-Two-Dimensional Fluidized Bed by Immersed Boundary Method, **Chemical Engineering Transactions**, Vol. 70., pp. 805-810. /DOI: 10.3303/CET1870135/ **Q3, IF: -**

Publications in conference proceedings:

8. Gyurik, L., Egedy, A., Varga, T., Ulbert, Zs., 2020, Two-phase Flow Modelling and Simulation of Gas Purification Column, **Proceedings of the 30th European Symposium on Computer Aided Process Engineering (ESCAPE30)** Part A, pp. 199-204. /ISBN: 978-0-12-823511-9/
9. Gyurik, L., Egedy, A., Ulbert, Zs., 2018, Modeling Solid-Liquid Settling System as a Two-Phase Flow Problem, **COMSOL Conference 2018 Lausanne** 6 p
10. Gyurik, L., Egedy, A., Zou, J., Miskolczi, N., Ulbert, Zs., Yang, H., 2017, Hydrodynamic Modelling of a Gasification Reactor, **Műszaki Kémiai Napok 2017**, pp. 11-16. /ISBN: 978-963-396-094-3/

Oral presentations, posters:

11. Gyurik, L., Egedy, A., Varga, T., Ulbert, Zs., 2020, Two-phase Flow Modelling and Simulation of Gas Purification Column, **30th European Symposium on Computer Aided Process Engineering – ESCAPE30 Virtual Symposium**, 2020. 08. 30. – 09. 02.
12. Gyurik, L., Egedy, A., Ulbert, Zs., Cronin, K., Ring, D., 2019, Modelling the Motion of a Single Solid Bead in a Newtonian Fluid by Two-Phase CFD Methods, **22nd Conference on Process Integration for Energy Saving and Pollution Reduction - PRES'19**, Agios Nikolaos, Greece, 2019. 10. 20-23.

13. Gyurik, L., Egedy, A., Ulbert, Zs., Diszperzer többcélú optimalizálása numerikus áramlástani szimulációk segítségével, **Műszaki Kémiai Napok 2019**, Veszprém, 2019. 04. 16-18.
14. Gyurik, L., Egedy, A., Ulbert, Zs., 2018, Modeling Solid-Liquid Settling System as a Two-Phase Flow Problem, **COMSOL Conference 2018**, Lausanne, Switzerland, 2018. 10. 22-24.
15. Gyurik, L., Egedy, A., Ulbert, Zs., 2018, Simulation of Gas-Solid Flow in Quasi-Two-Dimensional Fluidized Bed by Immersed Boundary Method, **21st Conference on Process Integration for Energy Saving and Pollution Reduction - PRES'18**, Prague, Czechia, 2018. 08. 25-29.
16. Gyurik, L., Egedy, A., Ulbert, Zs., 2018, Immersed Boundary módszer alkalmazása gáz-szilárd kétfázisú rendszerek modellezésére és szimulációjára, **Műszaki Kémiai Napok 2018** Veszprém, 2018. 04. 24-26.
17. Gyurik, L., Egedy, A., Ulbert, Zs., 2018, Immersed Boundary Method for Modelling of Multiphase Flow, **Tavaszi Szél Nemzetközi Multidiszciplináris Konferencia 2018**, Győr, 2018. 05. 04-06.
18. Gyurik, L., Egedy, A., Zou, J., Miskolczi, N., Ulbert, Zs., Yang, H., 2017, Hydrodynamic Modelling of a Gasification Reactor, **Műszaki Kémiai Napok 2017**, Veszprém, 2017. 04. 25-27.
19. Gyurik, L., Egedy, A., Ulbert, Zs., 2017, Modelling and Computer-aided Simulation of Gas-solid Two-phase Flows, **Tavaszi Szél Nemzetközi Multidiszciplináris Konferencia 2017**, Miskolc, 2017. 03. 31. – 04. 02.
20. Gyurik, L., Egedy, A., Ulbert, Zs., 2016, Gáz-szilárd kétfázisú áramlások modellezése és számítógépes szimulációja, **XXII. Nemzetközi Vegyészkonferencia**, Timisoara, Romania, 2016. 11. 03-06.