Module: Modeling of Granular Materials

Courses:
- Multiscale simulation of granular materials (Lecture – 2 SWS) – M. Dosta
- Thermodynamic and kinetic modeling of the solid state (Lecture – 2 SWS) – P. Gurikov
- Multiscale simulation of granular materials (Recitation Section – 2 SWS) – M. Dosta

Language: English

ECTS-Credit Points Module: 6 LP

Examination: Written exam

Period: Winter semester

Admission Requirements: none

Recommended Previous Knowledge: Fundamentals in Mathematics, Physics and Mechanics; Module “Particle Technology for International Master Programs”

Workload in Hours: Independent Study Time: 110, Study Time in Lecture: 70

Professional Competence

Theoretical Knowledge
After successful completion of the module the students are able to:

- describe modern modeling approaches which can be applied for simulation of granular materials
- analyze and evaluate possibility to apply numerical simulations on different time and length scales: from description of single particle properties on micro scale up to process simulation on macro scale
- list modern simulation system and discuss possibility of their application
- explain fundamentals of main numerical methods which are used for modeling of particulate materials
- list experimental methods to characterize granular materials
- explain fundamental thermodynamic and kinetic relations for the processes with solids
- explain theoretical background and limitations of the discrete models for the processes with solids

Capabilities
After successful completion of the module the students are able to,

- perform flowsheet simulation of solids processes and analyze steady-state or dynamic process behavior
- simulate behavior of granular materials on the micro scale with Discrete Element Method (DEM)
• optimize processes of mechanical process engineering (mixing, separation, crushing, ...) with DEM
• apply multiscale simulations for modeling of particulate materials
• evaluate results of numerical simulations
• select and apply appropriate thermodynamic and kinetic models for processes with solids
• select and apply appropriate discrete models for the processes with solids.

Personal Competence

Social Competence

After completion of this module, participants will be able to debate technical questions in small teams to enhance the ability to take position to their own opinions and increase their capacity for teamwork.

Autonomy

After completion of this module, participants will be able to solve a technical problem independently including a presentation of the results. They are able to work out the knowledge that is necessary to solve the problem by themselves on the basis of the existing knowledge from the lecture.

Lecture: Multiscale simulation of granular materials

Language: English

Lecturer: Maksym Dosta

Period: Winter Semester

Content:

• Steady-state flowsheet simulation of solids processes
• Dynamic flowsheet simulation of solids processes
• Introduction to Discrete Element Method (DEM)
• Contact and breakage mechanics of granular materials
• Extension of DEM
• Modeling of Gas/Solid streams with coupled DEM and CFD methods
• Population balance modelling of solids processes
• Multiscale simulation of particulate materials

Literature:

M. Dosta: Lecture notes.
Recitation Section (small): Multiscale simulation of granular materials

Language: English

Lecturer: Maksym Dosta

Period: Winter Semester

Content:

- Introduction into simulation frameworks: Aspen Plus (Solids), Dyssol, MUSEN
- Steady-state flowsheet simulation of solids processes (Aspen Plus)
- Dynamic flowsheet simulation of solids processes (Dyssol)
- Implementation of new contact laws and calculation of particle interactions (Matlab)
- Simulation of granular materials with population balance models (Matlab)
- Simulation of granular materials with discrete element method (MUSEN)
- Optimization of several processes with discrete element method (MUSEN)

Literature:

M. Dosta: Lecture notes.


Other lecture materials to be distributed
Lecture: Thermodynamic and kinetic modeling of the solid state

Language: English

Lecturer: Pavel Gurikov

Period: Winter Semester

Content:

- Thermodynamics of pure solids: melting/crystallization; glassy and amorphous state.
- Thermodynamics of solid-gas equilibria: adsorption and sublimation.
- Thermodynamics of solid-liquid equilibria: solubility in aqueous and non-aqueous systems; solid solutions; supercritical fluids as solvents.
- Kinetics of dissolution/precipitation processes: chemical vapor deposition; drug release; hydrothermal processes.
- Characterization of solids: contact angle, adsorption techniques, IR spectroscopy, electron microscopy.
- Discrete models of dissolution/precipitation processes: diffusion limited aggregation; random-like and ballistic-like deposition models.
- Advanced discrete models: surface wettability; adsorption and precipitation of (bio)polymers.

Literature:

