

Invitation to lecture series „Simulation Sciences“

Wednesday, March 4th 2015, Multimedia auditorium Tannenhöhe (D5), TU
Clausthal, 4:30 pm

Prof. Dr. Ulrich Tallarek
Department of Chemistry, Philipps University Marburg

will talk about

Quantitative Morphology-Transport Relationships for Disordered Porous Media by Morphological Reconstruction and High-Performance Computing of Flow and Transport

Content of the lecture:

The discovery of the morphology-transport relationships for disordered porous media used in chemical engineering and separation science (packings, monoliths) is a major challenge, because it requires the 3D physical reconstruction and/or computer-generation of the materials followed by 3D mass transport simulations to collect meaningful data for a detailed analysis of morphological and transport properties. This approach is the only direct as well as the most realistic way to understand and optimize materials with applications in chromatography or catalysis. Our latest progress regarding the following issues will be reported: (1) Systematic study of how individual parameters, such as the packing density and packing protocol, affect the morphology of computer-generated packings. (2) Physical reconstruction of packed and monolithic beds to collect information on how experimental parameters of the packing and preparation process influence morphology. (3) 3D mass transport simulations performed on a high-performance computing platform to analyze in detail the hydrodynamics and resulting dispersion. (4) Analysis of computer-generated and physically reconstructed packed and monolithic beds with statistical methods to derive structural descriptors for mass transport (diffusion, dispersion), which have potential for refining the existing theoretical framework.

Guests are welcome.

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The SWZ is a common interdisciplinary research facility in simulation science of



TU Clausthal



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The lecture will be held in this building:

Multimedia auditorium
Department of Informatics, Auditorium building (D5)
Albrecht-von-Groddeck-Straße 7
38678 Clausthal-Zellerfeld



Navigation:

tu-c.de/d5

