Boulder Fluid and Thermal Sciences Seminar Series

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porousGasificationFoam and GRPY: open-source contributions to research computing.

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We present two open-source computational tools. The **porousGasificationFoam** solver and libraries were developed using the open-source C++ library OpenFOAM to simulate the thermochemical conversion in porous media. They integrate gas flow through a porous media with the models of heterogeneous (drying, gasification, pyrolysis, solid combustion, precipitation) and homogeneous (gas combustion) chemical reactions. Inside porous media transport equations are formulated applying the spatial averaging methodology. The mass and enthalpy transfer between solid and gas phases is suitable for systems out of the thermal equilibrium. We validate the model against two Thermogravimetric Analysis experiments and theoretical results for macroscopic char bed smoldering. We designed the library to improve studies of wildfires and the design of large-scale reactors. The **GRPY** was developed to calculate the hydrodynamic properties of particles having an arbitrary shape, e.g., proteins. It is one of the tools implementing the Generalized Rotne-Prager-Yamakawa model of hydrodynamic interactions.

Biography: Paweł Żuk obtained his Ph.D. in theoretical physics at the University of Warsaw. He developed the Generalized Rotne-Prager-Yamakawa model of hydrodynamic interactions, widely applied in colloidal suspensions and biomolecules studies. He did a post-doc at Princeton University with Prof. Howard Stone. He developed and used OpenFOAM codes to study ionic solutions in confinement. Currently, he holds a joint position at the Institute of Physical Chemistry Polish Academy of Sciences and Lancaster University, UK. In his current research, he focuses on nonequilibrium thermal processes.