Contribution ID: **106** Type: **Talk**

A multi-physics framework for modelling coupled heterogeneous transport and reaction kinetics

Wednesday, 2 December 2020 11:30 (30 minutes)

Conjugate coupled physics problems involving multiple materials and domains exist across industry, with various combinations of heat, mass, and momentum transport. Examples include automotive brake cooling, thermal cooling of electronics, and processing of chemical reactive species within packed bed reactors in the oil and gas industry [1]. With the ever-growing demand to produce more efficient, environmentally friendly, durable, and cost effective products, engineers seek to exploit ever more complex simulation capabilities to construct realistic virtual prototypes. Efficient parallel computing plays a crucial role in realising design decision making in a realistic time frame, and is complicated in this instance by the complexity of the multi-region system.

We describe a new framework to model conjugate heat, mass, and momentum transport within a chemically reacting system [2]. This forms part of the HELYX CFD package built on OpenFOAM technology. The multi-region, multi-physics framework is used to simulate the behaviour of a gas-phase packed-bed reactor composed of randomly packed particles within a tube region. Information about interstitial flow phenomena, global and local pressure profiles, and solid species transport phenomena is captured.

We discuss several challenges to performing a CFD analysis of these types of systems, including the creation of randomly packed domains; meshing of these complex structures; capturing the intricate transport phenomena between regions; and scaling of coupled multi-region systems with hundreds of separate domains to high core counts.

References

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Session Classification: HPC Applications

Track Classification: Computational Mechanics