Please join us for a Chemical Engineering Seminar

Wednesday, June 1, 2011
325 Shillman Hall
11:45 a.m. – 1:00 p.m.

“Multiscale, Multiphysics Modeling of a Complex Chemical Engineering System”

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ABSTRACT

Formation of deposits inside the narrow nozzles in diesel engines disturbs fuel flow and adversely affects engine efficiency and emissions. Fuels and additives used to mitigate this problem are currently evaluated using very expensive tests in running engines. Modeling insights into this problem can therefore greatly reduce the cost of fuel and engine development.

The deposit formation process comprises different phenomena spanning multiple timescales. Free-radical chemical reactions, which are responsible for the deposit precursors, occur on a microsecond timescale. High-speed fuel injections, which cause washing and replenishment of the fuel film, occur on a millisecond timescale. The deposit itself accumulates over thousands of injection events, which occur over tens or hundreds of hours.

In this talk, I will describe how we are modeling these chemical and physical phenomena in a way that is computationally efficient and gives meaningful results. To model a system of this complexity requires estimation of many properties, such as temperature and injection velocity. Identifying which properties are most important, through computational experiments, has helped guide both model development and laboratory experiments. In addition to providing insight into the deposit formation process, this computational approach is suitable for other multi-scale models of chemical engineering systems.

Refreshments will be served.