

Spring 2015

Summary of general multiscale concepts (molecular, single eddy, single particle, reactor scale) to be covered and illustrated:

1. Stoichiometry, reaction progress, relationship to measures of composition, independent reactions.
2. Chemical and physical equilibria and equilibrium composition calculations.
3. Mechanisms and derivation of reaction rates.
4. Local transport effects on observed reaction rates.
5. Ideal reactor models (isothermal and non-isothermal systems)
6. Obtaining reaction rates in absence of transport limitations.
7. Accounting for non-idealities in macro- mixing and micro-mixing.
8. Modeling and scale-up of multiphase reactor types (stirred tanks, packed beds, trickle beds, slurry systems, etc.)
9. Applications to waste reduction and pollution abatement problems.
10. Applications to more efficient chemical process and/or material synthesis.