MULTISCALE SOLID LIQUID MODELING

WHY WE NEED TO CONSIDER THE (STILL) UNUSUAL SCALE

Personal Point of View

- When I identified long term temporal forecasting model, it is unable to detect short term characteristics. When identified rich short term model, it didn't work to foresee with long time steps.
- The works with students of mine have more and more AFM, MicroBal Quartz-D, TEM, SEM, etc measurements but this is only very local data without glue with holistic properties.
- The current SBA15 (nanosilica support for catalyst) work has SAXS, XPS, XRD, TEM but our discussion about this measurements are very poor related with local catalyst sites impact for selectivity and conversion.

nanoscale is not enough

- In the traditional paradigm, the *analysis* means fractionation, scale reduction to small cell or unities and this basic elements representation improves our physical knowledge.
- NO more. But the reality and the physical modeling is more complicated and complex. We need a multiscale concept between atomistic, nano, micro, meso and macro scale.

- The Material Science (computational) models consider electronic/atomistic scale, atomistic/microscopic scale, and meso/macroscopic scale modeling. It is more difficult to define the objectives of the modeling and what small scale is enough to represent the material.
- The Chemical Engineering objective is more simple: how to use the results of the different scales models.

some CFD multiscale definition is misleading

- Local volume averaging method

$$\langle \nabla \psi_f \rangle = \nabla \langle \psi_f \rangle + \frac{1}{V} \int_{S_{fs}} \psi_f \mathbf{n}_{fs} dS$$

- EMMS (energy minimization multiscale) time average. Define some stable condition, that is, some energy variable to minimize

chemical engineering (CFD) scales examples

discrete bubble:
Lagrangean(gas); Eulerian(solid) ; bubble drag closures; scale=10 m

two fluids:
Eulerian(gas); Eulerian(solid) ; gas-solid drag closures; scale=1 m

discrete particle model:
Eulerian(gas); Lagrangean(solid) ; bubble drag closures; scale=0.01 m

molecular dynamics:
Lagrangean (gas); Lagrangean(solid) ; collision at particle surfaces;
scale=<0.001 m

multiscale relevance for chemical engineering (CFD)

- The computational challenge for a multiscale modeling is the coupling of the drastically different spatial and time scales information between molecular/local mechanics and macroscopic transport (phenomenological) models.

p.ex. the modeling of inorganic ceramic membrane reactor

basically two approaches

- Multiscale modeling from macroscopic through mesoscopic to microscopic. Ex: coupling of fluid FVM or FEM with particles DEM, it is a sort of particle based lagrangean method
- The traditional CFD hope to verify experimentally and to predict quantitative results, but limited to continuum system.

- (remember the instruments measurements delas with 10 nm – 100 micrometer). So the second approach is to model directly by discrete particle dissipative paradigms simulating heterogeneous fluid which are difficult to work in continuum model. Ex: Lattice-Boltzmann (LBG) atomistic-continuum hybrid algorithm from Material Science.
- Why not the third approach? The “pure” molecular dynamics?

another question, not exactly multiscale.
consider the fluid motion

- $$\rho\left(\frac{\partial \mathbf{u}}{\partial t}+\mathbf{u}\cdot\nabla\mathbf{u}\right)=\nabla p+\mathbf{F}+\mu\nabla^2\mathbf{u}$$ where $\mathbf{F}=\rho\mathbf{g}$

$$\nabla\cdot\mathbf{u}=0$$

- Normal and tangential stress in the interface of two fluids

$$\mathbf{n}\cdot\mathbf{T}\cdot\mathbf{n}=\sigma\left(\nabla\cdot\mathbf{n}\right) \qquad \mathbf{n}\cdot\mathbf{T}\cdot\mathbf{t}=\nabla\sigma\cdot\mathbf{t}$$

$$\mathbf{T}=-\mathbf{I}p+\mu\left[\nabla\mathbf{u}+\left(\nabla\mathbf{u}\right)^T\right]=-\mathbf{I}p+2\mu\mathbf{E}$$

$$\mathbf{E}=\frac{1}{2}\left[\nabla\mathbf{u}+\left(\nabla\mathbf{u}\right)^T\right]$$

consider the surface bertween two fluids

- balance of the forces gives

$$\int_V \rho\left(\frac{D\mathbf{u}}{Dt}\right)dV = \int_V \mathbf{f}\,dV + \int_S \left[\mathbf{n}\cdot\mathbf{T} - \mathbf{n}\cdot\hat{\mathbf{T}}\right]\underline{d}S + \int_C \sigma\mathbf{s}\,d\ell$$

Inertial force | Body force | Hydrodynamic forces | Surface tension force

when $V \to 0$

$$\int_S \left[\mathbf{n}\cdot\mathbf{T} - \mathbf{n}\cdot\hat{\mathbf{T}}\right]\underline{d}S + \int_C \sigma\mathbf{s}\,d\ell = 0$$

Stokes theorem

$$\int_S \left[\mathbf{n}\cdot\mathbf{T} - \mathbf{n}\cdot\hat{\mathbf{T}}\right]\underline{d}S = \int_S \left[\sigma\mathbf{n}(\nabla\cdot\mathbf{n}) - \nabla\sigma\right]\underline{d}S$$

$$\mathbf{n}\cdot\mathbf{T} - \mathbf{n}\cdot\hat{\mathbf{T}} = \sigma\mathbf{n}(\nabla\cdot\mathbf{n}) - \nabla\sigma$$

Stress = force/area | Normal force/area | TANGENTIAL stress

$$\mathbf{T} = -\mathbf{I}p + \mu\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right) = -\mathbf{I}p + 2\mu\mathbf{E}$$

- Normal stress balance

$$\mathbf{n}\cdot\mathbf{T}\cdot\mathbf{n}-\mathbf{n}\cdot\hat{\mathbf{T}}\cdot\mathbf{n}=\sigma(\nabla\cdot\mathbf{n})$$

$$\neq 0$$

so present curvature
tangential stress balance

- Tangential stress balance

$$\mathbf{n}\cdot\mathbf{T}\cdot\mathbf{s}-\mathbf{n}\cdot\hat{\mathbf{T}}\cdot\mathbf{s}=(\nabla\sigma\cdot\mathbf{s})$$

Jump in tangential component, has only velocity

$$if \quad \neq 0$$

implies motion drive

- so turbulence model RANS, RNG don't resolve
- (neither LES)

- Why not DNS (direct numerical simulation)?