Overview of chemical processes with OpenFOAM

Assumption: The attendee has already completed basic/advanced OpenFOAM training
Focus is on "reactingFoam" type cases, with a brief survey of other solvers/methods

1. Introduction (0.25 hr)
    a. Motivation/chemical applications
    b. Flames, Sprays, Multiphase applications
2. Brief review (recap) of OpenFOAM (0.5 hr)
    a. OpenFOAM v11 … (focusing on chemistry)
        i. What's new in v11 (comparison to v10)
        ii. Comparison to chemistry in v2306
    b. Review of the OpenFOAM directory structure
    c. Running a case
        i. Parallel processing
        ii. Residual monitoring
    d. ParaView / paraFoam post processing
3. Dictionaries & case structure I (1.75 hrs)
    a. Key equations for single phase species transport and reaction
        i. Species transport equation overview (YEqn)
        ii. Energy equation overview (EEqn)
        iii. Changes to fvSchemes, fvSolution
    b. Files/dictionaries used for species transport & reaction
        i. Setting up species (0 directory, physicalProperties)
        ii. physicalProperties
            1. Thermo model selection (rho vs. psi thermos)
            2. Mixture options
        iii. Thermo file format
            1. NASA polynomials
            2. Sutherland properties
        iv. Reactions file format
            1. Structure
            2. Units
                a. Kmols
                b. Ta = EA/R
            3. Reaction types (Arrhenius, etc.)
            4. CHEMKIN mechanism conversion
        v. chemistryProperties
            1. Solver selection (Euler implicit, ODE)
            2. Chemical acceleration (more details later)
                a. ISAT
                b. DRM
        vi. combustionModel

                1. Overview of combustion model choices (more details later)
4. Example case #1 (part 1) – laminar flow species transport and homogeneous reaction (0.5 hr)
    a. Laminar flow case setup (Le = 1)
    b. Reactions off
    c. Reactions on
    d. Post process

End of Day #1

Day #2

1. Dictionaries & case structure II (0.5 hr)
    a. Basic case setup for species transport & reaction, continued
        i. Radiation modeling (brief overview -> more in Joel's heat transfer class)
            1. P1
            2. fvDOM
            3. view factors
        ii. Species transport (laminar)
            1. Le = 1
            2. Fickian diffusion
            3. Maxwell Stefan
            4. Using Cantera to get diffusion coefficients
        iii. Local time stepping
2. Example case #2 species transport & laminar reaction example (0.5 hr)
    a. Repeat Example case #1 but with different transport assumptions, LTS
3. Turbulent homogeneous chemistry (1 hr)
    a. Brief review of RANS
    b. Brief review of LES
    c. Turbulent combustion models
        i. EDC (multiple variants)
        ii. PaSR
    d. Species transport (turbulent)
4. Example case #3 turbulent flame (validation case) (0.5 hr)
    a. Convert CHEMKIN to OpenFOAM
    b. Transient vs. LTS
    c. Chemical acceleration (ISAT, DRM)
    d. Species transport model
    e. Radiation modeling
    f. Compare to data
5. Additional techniques (0.5 hr)
    a. Conjugate heat transfer (brief overview -> more in Joel's heat transfer class)
    b. Buoyancy
    c. Constant transport properties & liquid phase reactions

End Day #2

Start Day #3

1. Additional techniques (0.75 hr)
    a. chemFoam
    b. saving mole fractions
    c. Porous media
    d. Zone Combustion
    e. Membranes
    f. Real gas (Peng Robinson Equation of State)
    g. Adaptive mesh refinement
    h. Load balancing
2. Tips and tricks (0.25 hr)
    a. Start with chemistry off
    b. solverFreq for radiative heat transfer
    c. Time step size
    d. fvSchemes selection (upwind vs. Gauss limitedLinear01, etc.)
    e. fvModels selection (PBiCGStab, pressure solver, relaxation, etc.)
    f. RANS vs. LES chemistry
    g. Ideas for solving crashes…
3. Overview of other chemical tools in OpenFOAM (0.75 hr)
    a. XiFluid
    b. Lagrangian
        i. Sprays
        ii. Shrinking core/coal particle
    c. Films
    d. Multiphase
        i. Reactions
        ii. Mass transfer
        iii. Phase change
4. Summary (0.25 hr)
5. Q&A (1 hr)