1/ Suggest to elaborate assumption: is prior knowledge of openFoam for compressible flow and heat transfer assumed? Compressible flow, radiative heat transfer and conjugate heat transfer can be treated with switching to reactive flow.

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 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

2/ How does this differ to basic training? Intended as recap? Something new?

3/ Does reactive flow impose new challenges for mesh generation?

4/ Switch order around? First assume transport of hot gas? Subsequently add chemistry?

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. Basic case setup for species transport & reaction
        i. Setting up species (0 directory, physicalProperties)
        ii. chemistryProperties
            1. Solver selection (Euler implicit, ODE)
            2. Chemical acceleration
                a. ISAT
                b. DRM
        iii. combustionModel
            1. Overview of combustion model choices
        iv. physicalProperties
            1. Thermo model selection (rho vs. psi thermos)
            2. Mixture options
        v. Thermo file format
            1. NASA polynomials
            2. Sutherland properties
        vi. Reactions file format
            1. Structure
            2. Units
                a. Kmols
                b. Ta = EA/R
            3. Reaction types (Arrhenius, etc.)

5/ Include LTS (here or later?) and adaptive mesh generation?

6/ Not sure to what extend chemistry can be accelerated in case that combustion is switched off.

7/ (again) Switch order around?

8/ Previous exposure to laminar combustion has been very limited. Not sure what to expect here.
Does “laminar” immediately imply “incompressible”. What Mach number is intended to be used here?

4. CHEMKIN mechanism conversion

4. Example case #1 (part 1) – laminar 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
            1. P1
            2. fvDOM
            3. view factors

11/ Also applies to heat transfer for non-reactive flow.
What is scope of the course?

        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 10/ Cool! Should be fun!
3. Turbulent homogeneous chemistry (1 hr)
    a. Brief review of RANS
    b. Brief review of LES
    c. Turbulent combustion models
        i. EDC (multiple variants) 11/ Some like neither and argue for theoretically sound models.
        ii. PaSR
    d. Species transport (turbulent)
4. Example case #3 turbulent flame (validation case) (0.5 hr)
    a. Convert CHEMKIN to OpenFOAM 12/ Valuable discussion on cfd-online forum.
    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 13/ Again, scope of prior knowledge would be good to have. Good video tutorials are now available.
    b. Buoyancy
    c. Constant transport properties & liquid phase reactions

End Day #2

Start Day #3

14/ Cool!

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. Time step size
    c. fvSchemes selection (upwind vs. Gauss limitedLinear01, etc.)
    d. fvModels selection (PBiCGStab..)
    e. RANS vs. LES chemistry
    f. Ideas for solving crashes…

15/ Freeze radiative heat transfer for number of steps using solverFreq (as in non-reactive heat transfer).

16/ Important? Focus instead on pressure solve and prospect of p-U coupled solver?

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)

17/ Would love to discuss details of both.