Use of the combustion and stochastic water spray modules in the LS-DYNA® Compressible Flow Solver

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Abstract

Recent development of the chemistry and stochastic water spray modules in the CESE LS-DYNA® compressible flow solver will be reported in this presentation. For the chemistry, detailed descriptions about CHEMKIN input files including the thermodynamics and transport data files will be presented. How to construct of the keyword files is also demonstrated for the various chemically reactive flows. Limitations of the current chemistry module and future development with reduced chemistry will be discussed. For the stochastic water spray, the concept of the stochastic particle, breakup models such as the TAB and KH&RT hybrid models, and collision models are described and corresponding keyword setups are explained with water spray flows. Limitation and current developments including fuel vaporization models will be also presented.

Chemistry Input File

The chemistry input file, which normally has extension .inp includes information on elements, species, thermodynamics data, and elementary chemical reaction mechanisms. The example a chemistry input file for LS-DYNA compressible flow is shown in Fig.1 for H2-O2 system, which is basically a CHEMKIN-compatible input file[1], *the chemical kinetics package of gas-phase chemical kinetics*. To solve a combustion problem, the user must construct this LS-DYNA chemistry input file prior to any combustion simulation.

Chemistry Solvers

After a chemistry keyword input file is correctly constructed, one of the chemistry solvers should be selected to simulate a chemically reactive flow. Currently, LS-DYNA has four different combustion modules including isobaric, isochoric, 1-step reaction, and multiple-species reaction mechanism. Except for the one-step reaction combustion, each solver requires the chemical composition, along with corresponding initial and boundary conditions. In the case of detonation problems, we designed a one-dimensional initiation model to be followed by two- or three- dimensional detonating flow simulations. The one-dimensional solution is automatically saved to a file which the user designates so that later on, one can use this file for several individual simulations. For general chemical reacting flow problems, we designed both inviscid and viscous flow, which typically solve the Euler or Navier-Stokes reactive flow equations, respectively. Details about the chemistry solvers will presented with selected example problems.

Stochastic Particles

The stochastic processes deal with systems which develop in time or space in accordance with probability theories. Such processes have now been added to LS-DYNA to simulate a water spray, aerosol, and any liquid particle flows using random variables and probability density functions. For the water spray, the existing basic breakup model and most advanced hybrid breakup model, TAB, and KH&RT, respectively are implemented with particle collision models. With these modules, one of the successful examples for the supersonic cross flow was reported [2] as shown in Fig.3. Moreover, the stochastic particle method could potentially apply to any particle-related flows. Details about keyword input will be presented. In addition, currently we are developing combined multi-physics modules such as simulations of spray (or liquid injection), evaporation, and combustion simultaneously.

```
                                SAMPLE 1
ELEMENTS
N  O
END
SPECIES
O2 N2 O N NO
END
THERMO
END
REACTIONS    CAL/MOLE
O2+M=2O+M                          3.6E+18  -1.00  -118240.
  N/1.0/ NO/1.0/
  REV /3.00E+15  -0.50        0./
N2+M=2N+M                          1.90E+17 -0.50  -224557.
  O/1.0/ NO/1.0/ O2/1.0/
  REV /1.10E+16  -0.50        0./
NO+M=N+O+M                         3.90E+20 -1.50  -150035.
  N2/1.0/   O2/1.0/
  REV /1.00E+20  -1.50        0./
O+NO=N+O2                          3.20E+09  1.00   -39148.
  REV /1.30E+10   1.00    -7114./
O+N2=N+NO                          7.00E+13  0.00   -75514.
  REV /1.56E+13   0.00        0./
N+N2=N+N+N                         4.085E+22 -1.50  -224557.
  REV /2.27E+21  -1.50        0./
O2+O=2O+O                          9.00E+19 -1.00  -118240.
  REV /7.50E+16  -0.50        0./
O2+O2=2O+O2                        3.24E+19 -1.00  -118240.
  REV /2.70E+16  -0.50        0./
O2+N2=2O+N2                        7.20E+18 -1.00  -118240.
  REV /6.00E+15  -0.50        0./
N2+N2=2N+N2                        4.70E+17 -0.50  -224557.
  REV /2.72E+16  -0.50        0./
NO+M=N+O+M                        7.80E+20 -1.50  -150035.
   O/1.0/  N/1.0/ NO/1.0/
  REV /2.00E+20  -1.50        0./
END
```

Fig. 1 Example of the LS-DYNA chemistry input file for an H2-O2 reaction mechanism.

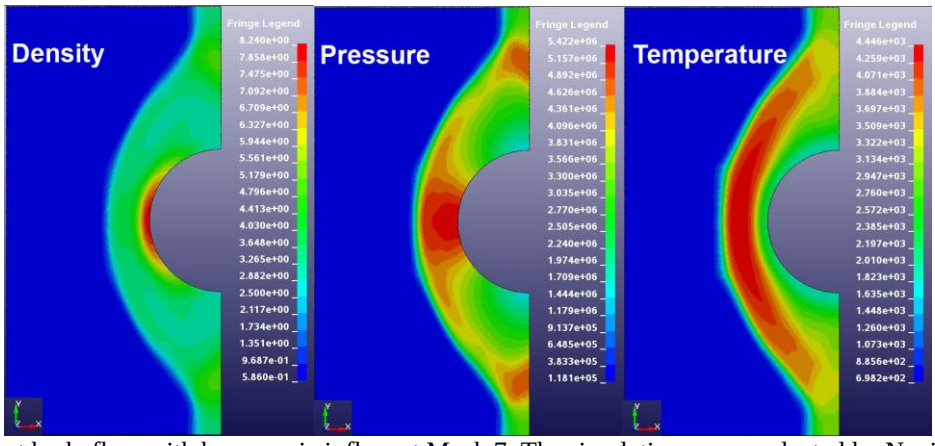

Fig. 2 Blunt body flow with hypersonic inflow at Mach 7. The simulation was conducted by Navier-Stokes chemically reactive flow modeling with 5 species(O2, N2, O, N, NO) and 11 elementary reaction steps for the dissociation and recombination of air.

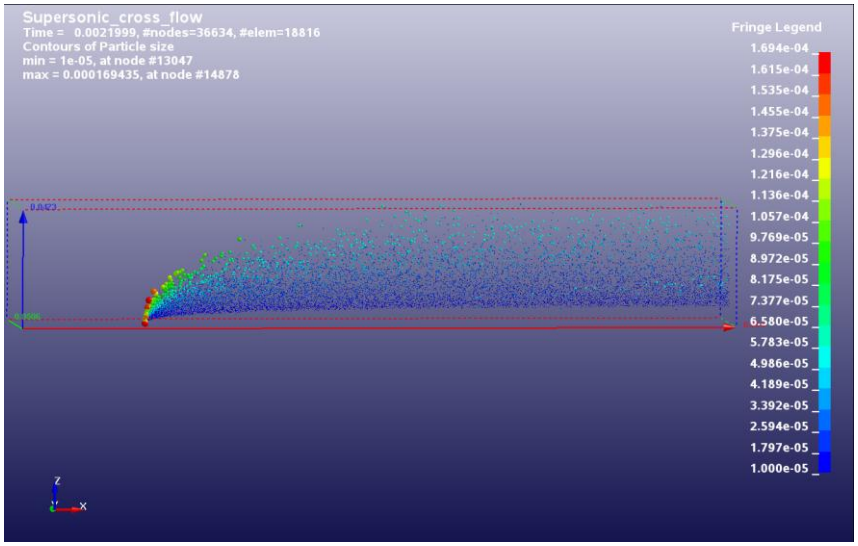

Fig. 3 Stochastic particle flows with supersonic cross velocity at Mach 1.7. The KH&RT hybrid breakup model with collision model was applied.

References

[1] R. J. Kee, F. M. Rupley, and J. A. Miller. *Chemkin-II: A Fortran chemical kinetics package for the analysis of gas-phase chemical kinetics.* SAND89-8009, Sandia National Laboratories, Livermore, California Sep. (1989)

[2] K.-S. Im, K.-C. Lin, M.-C. Lai, and M.-S. Chon,"Breakup modeling of liuqid jet in cross flow," International Journal of Automotive Technology, Vol. 12., No. 4 pp01-08 (2011).