Stochastic Spray and Chemically Reacting Flow In LS-DYNA®

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1   Introduction

The injection of fuel sprays into an automotive engine and liquid jets into a high-speed flow stream is an important process in modern automotive gasoline and diesel engines, and propulsion in gas turbine and supersonic vehicles. In such applications, the combustion performance depends strongly on spray atomization, penetration, and the mixing process between the free stream air and the liquid fuel. As a result, the study of liquid spray in such areas has become an important research topic.

The spray can be represented by a stochastic equation giving the rate of change of the distribution function, $f = f(\mathbf{x}, \mathbf{v}, r, T, y, \dot{y}, t)$, which at a given time changes the positions, x, velocities, v, equilibrium radius, r, temperature, T, distortion from sphericity, y, and the time rate of change dy/dt[1,2]. This equation is then coupled with ensemble averaged gas phase equations of mass, momentum, and energy conservation. In addition, for many engineering sprays, drop breakup and collisions must be considered when the drop Webber number is larger than a critical value. Thus the essential dynamics of spray and its interaction with a gas is an extremely complicated physical phenomenon.

Much attention has recently been devoted to the chemically reactive simulation models in the fields of subsonic, supersonic, and hypersonic combustion. However, the modeling of chemically reacting flow is a challenging task because of the simultaneous contribution of a wide range of time scales to the system dynamics. For example, the spectrum for the time scales of the flow, transport, or turbulence is much narrower than that of the chemical time scales as shown in Fig.1[3]. Such a wide range of time scales, especially the extremely fast ones in chemistry, makes the set of governing equation stiff and expensive numerically. This is due to the fact that modeling of the detailed chemistry requires the use of an implicit ordinary differential equation (ODE) solver. For example, the computational expense is proportional to the square of the number of equations. For a system with n_s molecular species, the number of ODEs is approximately equal to n_s if n_s is large (where the atomic elements involved can be ignored). For typical reacting flows involving hydrocarbon combustion, n_s could be of order 50, so that the computational time is a factor of 50^2 greater than the time needed for the flow calculation without computing the combustion or an equivalent one-step reaction model[4].
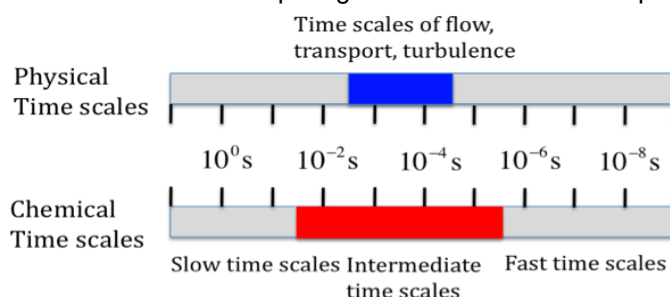

Fig.1. Schematic illustration of the time scales governing a chemically reacting flow.

In the LS-DYNA stochastic particle solver, we have diverse initial injection modes such as mono-dispersed, Rosin-Rammler, chi-squared distributions, and user-specified distribution of the stochastic particles as an initial condition over the computational domain. Industrial applications include dust, aerosol, and cosmetics problems. Currently, the LS-DYNA spray solver has two breakup modes, Taylor analogy breakup (TAB), and modified Kelvin-Helmholtz/Rayleigh-Taylor (K-H/R-T)[5].

The user can select the non-evaporating or the evaporating spray, which is now connected with chemistry solvers to provide information about the evaporating molecular species. In addition, the property libraries of a total of 10 liquid fuels are available for spray combustion, so that the user can select the corresponding fuel in an input keyword file.

The ultimate choice for the chemistry model that can generate accurate simulation results as compared with experimental data is the use of detailed reaction mechanisms. These mechanisms are described by a list of elementary reactions among the species involved with an Arrhenius-type rate expression for each reaction.

In the LS-DYNA chemistry solver, the detailed chemistry modeling is implemented with an adaptive moving mesh technology, so that if the user has a simple mixture to solve such as an H_2-O_2 system, this is the best choice for simulating the problem. When the detailed model is too expensive due to involving a large number of species, there is another option, and that is the option of using reduced reaction models.

Although several methods for reducing reaction mechanism have been recently proposed, two reduced modeling methods have been implemented in the LS-DYNA chemistry solver; The G-scheme and the computational singular peturbation(CSP) method. The common idea in both reduced methods is to decouple the slow and fast time scales in given a stiff system of ODEs, so that only reduced equations are integrated by an explicit numerical scheme such as Runge-Kutta. However, unlike the CSP method which is used to identify the slow/fast components of the vector field at given state, the decomposition in the G-scheme is used to identify the slow/fast components of the perturbation of the state vector at given state. The original ideas and the detailed mathematical background on the CSP method can be found in the literature by Lam's work[6]. More details about the G-scheme can be also found in Valorani and Paolucci's work[7].

2   Theoretical Models

2.1   Stochastic Spray

A mathematical formulation that is capable of representing these complex physical processes is the spray equation.

$$\frac{\partial f}{\partial t} = -\frac{\partial}{\partial r}(Rf) - \nabla_x(\mathbf{v}f) - \nabla_v(\mathbf{F}f) - \frac{\partial}{\partial T}(\dot{T}f) - \frac{\partial}{\partial r}(\dot{y}f) - \frac{\partial}{\partial r}(\ddot{y}f) + Q \tag{1}$$

where $R = dr/dt$ is the particle growth rate, $\mathbf{F} = d\mathbf{v}/dt$ is the particle acceleration, the source term $Q\left(= \dot{f}_{breakup} + \dot{f}_{collision}\right)$ may account for the formation of new particles and rate of increase of the function f caused by collision between the particles.

In a Lagrangian reference frame, each computational particle, individually labeled by subscript k, represents a number of droplets with the same size, position, and velocity. This is required in the discrete particle method described in [8]. As a result, the required equation to trace the position for each individual droplet is given by

$$\frac{d\vec{x}_k}{dt} = \vec{u}_k \tag{2}$$

Next, the droplet velocity at an arbitrary time instant is determined by solving its momentum equation as

$$m_k \frac{d\vec{u}_k}{dt} = m_k\vec{g} + D_k(\vec{u}_k)(\vec{u} - \vec{u}_k). \tag{3}$$

Here, $m_k\left(= 4/3\,\pi\rho r_k^3$, where r is the particle radius$\right)$ is the droplet mass, $\vec{g}(\approx 9.8\ m/s^2)$ is the standard gravity for droplets, and we assume no turbulent effects on the droplet trajectory, i.e., no turbulent dispersion. In addition, $D_k(\vec{u})$ is the drag function

$$D_k(\vec{u}) = \frac{1}{2}\pi r_k^2 \rho_g C_D|\vec{u} - \vec{u}_k|. \tag{4}$$

In Eq. (4), the drag coefficient C_D is determined as

$$C_D = \frac{24}{Re_k}\left[1.0 + 0.15\,Re_k^{0.687}\right] \qquad Re_k < 10^3$$
$$= 0.44, \qquad\qquad\qquad\qquad Re_k > 10^3 \tag{5}$$

where Re_k is the particle Reynolds number, which is evaluated by using the relative velocity between the gas and the droplet, i.e.,

$$Re_k = \frac{2r_k|\vec{u} - \vec{u}_k|\rho_g}{\mu}. \tag{6}$$

Note that Eqs. (2) through (6) are the equation sets for the non-eqvporating spray flows.

2.2 Chemistry

The space-time conservation element solution element(CESE) method has been developed and applied as a compressible flow solver[9]. The compressible solver in LS-DYNA now has capable to solve any FSI problem with moving mesh technology. The governing system equations are either Euler or Navier-Stocks equation, which are strongly combined with the chemistry solver.

For a set of n_q elementary reactions involving n_s species, the rate equation can be written in the general form as,

$$\sum_{k=1}^{n_s} v'_{kl} X_k \Leftrightarrow \sum_{k=1}^{n_s} v''_{kl} X_k, \qquad l = 1,2,3,K,n_q \tag{7}$$

where v'_{kl} and v''_{kl} are the forward and backward stoichiometric coefficients for species k, X_k is the chemical symbol for the species k. Then, the net molar production rate of species k is given by,

$$\dot{\omega}_k = \sum_{l=1}^{n_s} v_{kl} \left(k_{fl} \prod_{k=1}^{n_s} [X_k]^{v'_{kl}} - k_{bl} \prod_{k=1}^{n_s} [X_k]^{v''_{kl}} \right) \tag{8}$$

where $v_{kl} = v''_{kl} - v'_{kl}$, k_{fl} and k_{bl} are the forward and backward rate coefficient of reaction l, and $[X_k]$ is the molar concentration of species k. The forward rate coefficient are typically expressed as,

$$k_{fl} = A_l T^{\beta_l} \exp\left(-\frac{E_{al}}{RT}\right) \tag{9}$$

whre A_l is the pre-exponential factor, β_l is the temperature exponent, E_{al} is the activation energy per unit mole, T is temperature, and R is the universal gas constant. The backward rate constants k_{bl} can be evaluated in terms of k_{fl} by chemical equilibrium consideration. The equation of state for a system of ideal gas is given,

$$P = \rho R_g(y_k) T(e, y_k) \tag{10}$$

R_g is the mixture gas constant given by,

$$R_g(y_k) = \frac{R}{W(y_k)} = R \sum_{k=1}^{n_s} \frac{y_k}{W_k} \tag{11}$$

where W is the mean molar of the mixture, y_k is the mass fraction of species k and W_k is the molar mass of species k.

3 Key Words

Example segments of a spray and a chemistry keyword file for LS-DYNA compressible flow are shown in Fig.2. The chemistry keyword file includes the chemistry input file, and thermodynamics and transport data files. The chemistry input file which has the chemistry information such as elementry reaction kinetics, reaction rates, and the involved species is a CHEMKIN-compatible input format, where CHEMKIN is a chemical kinetics package of gas-phase chemical kinetics [10]. To solve the spray and the combustion problem, the user must first construct the keyword files, and for more detail, we would refer the reader to Volume 2 of the LS-DYNA Keyword User's Manual.

```
                                              *CHEMISTRY_COMPOSITION
                                              $  comp_id
                                                     41
                                              $  MoleNo   Species
                                                    2.0       H2
                                                    1.0       O2
                                                    7.0       AR
                                              $*CHEMISTRY_CONTROL_FULL
$ Setup stochastic particles                  $      ID    errlim
*STOCHASTIC_SPRAY_PARTICLES                            5
$       1       2       3       4       5       6       7   det2.inp
$ injdist  ibrkup  icollde  ievap  ipulse  limpar  idfuel  therm.dat
        3       2       0       0       0  100000       1   tran.dat
$                                                           *CESE_INITIAL_CHEM
$    rhop   tip pmass[kg]  prtrte  strinj  durinj          $  ChemID    compID
     998.0   300.0  6.391e-3  1.0e6     0.0    10.0               5      41
$                                                           $INITIAL CONDITIONS
$ the next card is needed for initial position and particle velocity:  $     uic      vic      wic      ric      pic      tic      hic
$  XORIG   YORIG   ZORIG    SMR  Velinj  Drnoz  Dthnoz          -478.5     0.0      0.0   0.2231  36679.6   624.0      0.0
   0.0463  0.0253  1.0e-5  5.0e-5  32.625  2.5e-4             *CESE_INITIAL_CHEM_SET
$   0.139   0.076  1.0e-5  5.0e-5  32.625  2.5e-4             $ elesetID   chemID   compID
$ TILTXY  TILTXZ    CONE   DCONE    ANOZ    AMP0                 111       5       41
     0.0     0.0     2.5     2.5 1.963e-7    0.0             $INITIAL_SET CONDITIONS
                                                            $     uic      vic      wic      ric      pic      tic      hic
                                                                 -478.5     0.0      0.0   0.2231  36679.6   624.0      0.0
                 (a)                                                           (b)
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Fig.2 Part of key word files for the stochastic particle and the chemically reacting flow solvers in LS-DYNA.

4   Results and Discussion

4.1   Stochastic Spray

Figure 3 shows a spray flow illustrating the detailed breakup process in a 3-dimensional domain with the air stream velocity of *Mach* number 1.94, and jet-to-air momentum of $Q_0 = 7$. The snapshot was taken when the spray flow reached a steady-state condition. Although the initial spray started with big droplets having the same size of the nozzle diameter, many small drops in the leeward side were clearly observed, indicating that the K-H breakup mode was performing well. On the other hand, large droplets deformed like ligaments still exist up to the highest vertical position of the spray, and thereafter, only small droplets generated by column breakup are clearly observed. More dispersion in normal direction and less dense sprays are obvious in the downstream region, suggesting that the spray undergoes a further breakup process downstream. The spray behaviors described in present study agrees well qualitatively with the experiment results in high speed cross flow[5].
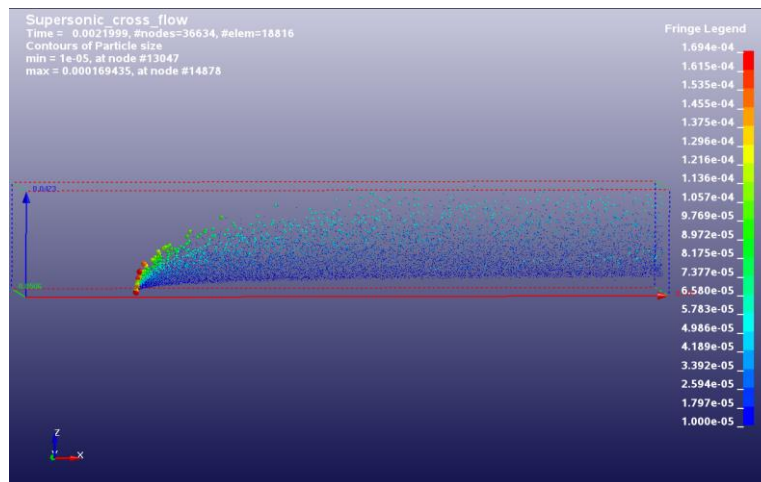

Fig. 3 Stochastic particle flows with supersonic cross velocity at Mach 1.94. The KH&RT hybrid breakup model with collision model.

4.2   Chemically Reacting Flows

Figure 4 shows comparisons among the developed models in LS-DYNA's chemistry solver: detailed full chemistry, CSP, and G-scheme. Fig.4(a) shows the constant volume results for the temperature[K], H2, and H mass fractions[%] and Fig.4(b) shows the constant pressure results. The detailed full chemistry model is considered as a reference, and the reduced models are compared with this reference result. Clearly, all results are well-matched with the full model except for a little overshoot for the H species mass fraction in the case of the CSP reduced model.
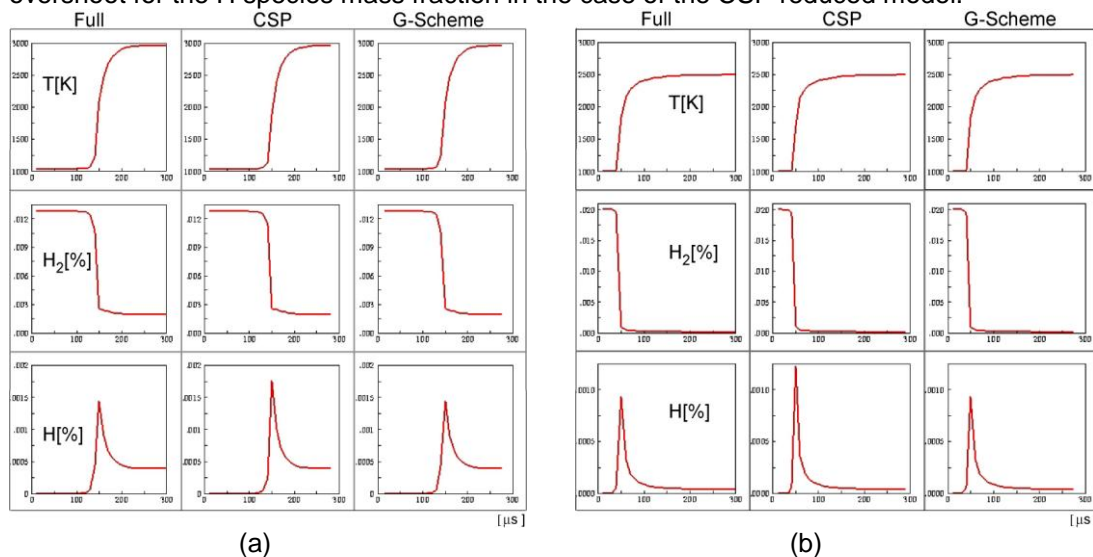

(a)   (b)

Fig. 4 Comparisons among the chemistry models: a) Constant volume combustions with stoichometric of H_2-O_2-Ar system, b) Constant pressure combustions with H_2-O_2-N_2 system.

Figure 5 show the 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 chemistry system. The results are excellent agree ment with those in reference [11].
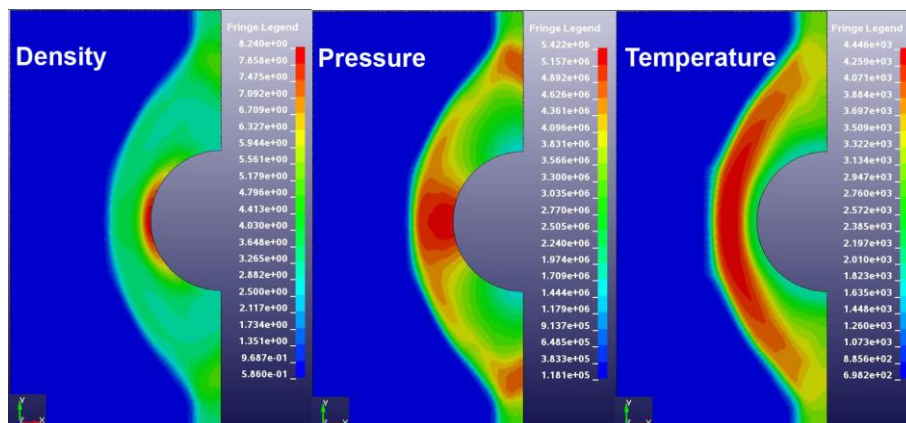

Fig. 5 Blunt body flow with hypersonic inflow at Mach 7. The simulation was conducted by Navier-Stokes chemically reactive flow modeling with 5 species(O2, N2, O, N, NO) and 11 elementary reaction steps for the dissociation and recombination of air.

5   Summary

Recent development of the chemistry solver and stochastic water spray modules in the CESE LS-DYNA$^{®}$ compressible flow solver is reported in this presentation. For the stochastic particle solver, the initial injection modes, breakup models, collision models, and vaporization models are developed and described. The stochastic particle solver in LS-DYNA will keep on expanding to cover various applications such as automotive spray painting, spray cooling, and the cosmetics industry. Planned improvements include developing a realistic breakup model, as well as practical simulation using a number of particles more closely matching the true number of particles in conjunction with MPP parallel computing technology.

For the chemistry, detailed and reduced models are develped based on theoretical models and the keyword input files including thermodynamics and transport data files are also demonstrated. The combustion solver in LS-DYNA will also continue to develop to address other application areas such as detonating flow with FSI, and heterogeneous combustion with MPP parallel computing technology.

6   References

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