

# Unsteady simulation of spray in moderately high pressure environment

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*Abstract:* - The present study is mainly motivated to develop an unsteady computational code which is simulating a transient behaviour of the spray injected into moderately high pressure environment (For a phenomenological study of the pressure effect on the spray, Aggarwal [3] divided pressure range into two regimes: moderately high pressure regime and critical/supercritical regime). In order to represent the spray development, the DDM (Discrete Droplet Model), which is often identified as the PSIC (Particle-Source-In-Cell) model, is employed among the SF (Separate Flow) models. Here, the Eulerian-Lagrangian formulation is used to analyze the two-phase interactions. For an accurate prediction of droplet evaporation rate in high pressure, a proper high pressure evaporation model is applied. Also, the effects of high pressure as well as high temperature are considered in the calculation of liquid and gas properties. Throughout the numerical simulation, transient thermo-fluid mechanical behaviour of spray in high pressure as well as normal pressure is traced and visualized.

*Keywords:* - Numerical simulation, droplet combustion, spray combustion, moderately high pressure, evaporation model, two-phase interaction

## 1 Introduction

In most spray systems, evaporation and combustion of liquid fuels take place in high pressure. However, due to its inherent complexities, study on the behaviour of spray in high pressure has been generally conducted through a more fundamental point of view. Since an investigation of spray is based on the evaporation and combustion processes of a droplet, many researchers have carried out numerical and experimental studies on a single droplet in high pressure environment. Extensive reviews of this subject were given by Bellan [1] and Givler and Abraham [2]. In the field of theoretical investigation on spray, previous studies have been mostly accomplished in normal pressure. Because some assumptions may be introduced, numerical simulation becomes easier than in high pressure case. Aggarwal [3] and Faeth [4-5] comprehensively reviewed the studies

on the behaviour of spray.

In this study, moderately high pressure regime is introduced. In order to phenomenologically discuss the pressure effect on the spray behaviour, Aggarwal [3] divided pressure range into two regimes: moderately high pressure regime (say, for pressure less than 75 % of the critical pressure of fuel) and critical/supercritical regime. In the first regime, the quasi-steady model for evaporation rate can still be used since gas density is small compared to liquid density and thermo-transport properties are relatively independent of pressure. Also, droplet dynamics are only weakly affected by pressure. Therefore, within this regime, high pressure effect on the spray behaviour can be favorably investigated even through the use of some simplifications.

The present investigation is a combined work of two previous studies [6-7]. Throughout the current study, it is aimed to simulate a transient behaviour of the spray as

well as to investigate pressure effect on its evaporation and combustion. An exact numerical simulation of spray in high pressure still remains a challenging task which requires overcoming several difficulties. Afterwards, if a more accurate as well as realistic representation for the spray in high pressure is further to be considered, it would be possible successive to the present study.

## 2 Formulation

### 2.1 Spray model

As schematized in Fig. 1, a liquid fuel spray is injected into a two-dimensional, axisymmetric, and cylindrical combustor which is initially filled with a quiescent hot air. Despite the complexities by the additional equations generated from the consideration for discrete droplets, the SF model has an advantage that it is able to simulate a spray realistically [8]. The present study employed the DDM (or the PSIC model [9]). Here, the gas field is formulated using the Eulerian approach while the droplets are described using the Lagrangian approach. The interactions between two different phases are considered by the source terms appearing in gas field governing equations.

### 2.2 High pressure evaporation model

An evaporation of fuel is caused by the fuel concentration gradient between gas field and liquid droplet. In normal pressure, it can be easily determined

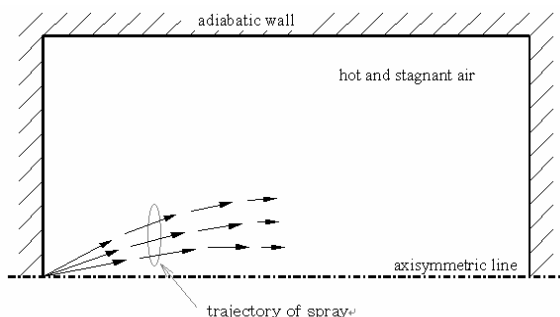


Fig.1 Schematic of the liquid spray in combustor

using the ideal gas equation of state. However, in high pressure, the real gas effect must be considered. In the present study, the fuel concentration at droplet surface is determined using thermodynamic and phase equilibrium, and the real gas effect is considered by the Redlich-Kwong equation of state. In addition, liquid-phase gas solubility effect is taken into account by considering the variations of droplet heat of vaporization. The high pressure evaporation model applied to this study, which can be referred from the works by various researchers [10-13], is as follows.

For thermodynamic equilibrium, the following conditions between temperature, pressure, and fugacity of each species must be satisfied at droplet surface.

$$T^v = T^l \quad ; \quad p^v = p^l \quad ; \quad f_i^v = f_i^l \quad (1)$$

The mole fraction at droplet surface is determined using the following vapour-liquid phase equilibrium relation.

$$X_{fs}(p, T) = \frac{P_{vp,f}(T) \phi_f^{sat}(T)}{p \phi_f} \exp\left(\int_{P_{vp,f}}^p \frac{v_f^l(T, p)}{R_u T} dp\right) \quad (2)$$

The fugacity coefficient is obtained by the following thermodynamic relation.

$$R_u T \ln \phi_i = \int_v^\infty \left[ \left( \frac{\partial p}{\partial N_i} \right)_{T, v, N_j} - \frac{R_u T}{v} \right] dv - R_u T \ln Z \quad (3)$$

Also, the energy required for phase change is given by

$$\Delta h = \sum_i X_i^l \bar{H}_i(T, p, X_i^v) - \sum_i X_i^l H_i^l(T, p) \quad (4)$$

where the partial enthalpy for vaporizing component  $i$  and its ideal gas enthalpy at the same temperature are related through the following relation.

$$\left( \bar{H}_i - H_i^0 \right)_T = -R_u T^2 \left( \frac{\partial \ln \phi_i}{\partial T} \right)_{p, X^v} \quad (5)$$

### 2.3 Governing equations for gas field

A general form of gas field governing equation in axisymmetric coordinate is presented by

$$\frac{\partial(\rho\phi)}{\partial t} + \frac{\partial}{\partial x} \left( \rho u \phi - \Gamma_\phi \frac{\partial \phi}{\partial x} \right) + \frac{1}{y} \frac{\partial}{\partial y} \left( y \rho v \phi - y \Gamma_\phi \frac{\partial \phi}{\partial y} \right) = S_{\phi, s} + S_{\phi, l} \quad (6)$$

Table 1 Variables and source terms for gas field governing equation

Equation	$\phi$	$\Gamma_\phi$	$S_{\phi,g}$	$dV_\phi S_{\phi,l}$
Continuity	1	0	0	$\Sigma n\dot{m}$
Axial momentum	$u$	$\mu$	$-\frac{\partial p}{\partial x} + \frac{\partial}{\partial x}\left(\mu \frac{\partial u}{\partial x}\right) + \frac{1}{y} \frac{\partial}{\partial y}\left(y\mu \frac{\partial v}{\partial x}\right)$	$\Sigma\left(n\dot{m}u - \frac{4}{3}\pi\rho_d r_d^3 n F_\phi\right)$
Radial momentum	$v$	$\mu$	$-\frac{\partial p}{\partial y} - \frac{2\mu v}{y^2} + \frac{\rho v^2}{y} + \frac{\partial}{\partial x}\left(\mu \frac{\partial u}{\partial y}\right) + \frac{1}{y} \frac{\partial}{\partial y}\left(y\mu \frac{\partial v}{\partial y}\right)$	$\Sigma\left(n\dot{m}v - \frac{4}{3}\pi\rho_d r_d^3 n F_\phi\right)$
Energy	$h$	$\Gamma$	$\frac{\partial P}{\partial t} + \mu G + W_f Q R_f$	$\Sigma\left\{-n\dot{m}\left(C_p(T_g - T_d) + L\right)\right\}$
Mass fraction (fuel)	$Y_f$	$\Gamma$	$-W_f R_f$	$\Sigma n\dot{m}$
Mass fraction (other species)	$Y_i$	$\Gamma$	$\mp v_i W_i R_f$ (- for O <sub>2</sub> , + for product)	0

where,  $\Gamma = \frac{\mu}{\sigma_\phi}$ ,  $G = 2\left[\left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial v}{\partial y}\right)^2 + \left(\frac{v}{y}\right)^2\right] + \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)^2$ ,  $F_\phi = \frac{\partial \phi_d}{\partial t}$

Specific representations of the variables and source terms are tabulated in Table 1.

## 2.4 Governing equations for liquid droplet

The following Ranz and Marshall experimental relation [19] is used for the mass conservation of droplet.

$$\frac{dm_d}{dt} = \dot{m}_s \left(1 + 0.3 \text{Re}^{1/2} \text{Pr}^{1/3}\right) \quad (7)$$

The stagnant evaporation rate can be determined by [3]

$$\dot{m}_s = 2\pi d \rho D \ln(1+B) \quad (8)$$

The Spalding's transfer number is expressed as follows

$$B = \frac{Y_{fs} - Y_f}{1 - Y_{fs}} \quad (9)$$

Neglecting the effects of gravity and Basset force, the momentum conservation for droplet becomes

$$m_d \left(\frac{d\vec{V}_d}{dt}\right) = \frac{1}{2} \rho C_D (\vec{V} - \vec{V}_d) |\vec{V} - \vec{V}_d| A_d - \left(\frac{m_g}{\rho} \frac{\partial p}{\partial x}\right) \quad (10)$$

The drag coefficient is determined using the following relation proposed by Putnam [5].

$$C_D = 24(1 + \text{Re}^{2/3}/6)/\text{Re}, \quad \text{Re} < 1000 \quad (11)$$

The energy conservation for droplet is given by

$$m_d \frac{dT_d}{dt} = \frac{\text{Nu} \pi k d}{c_{pd}} (T - T_d) - \frac{L}{c_{pd}} \dot{m}_d \quad (12)$$

The Nusselt number is calculated from the experimental relation produced by Ranz and Marshall [19].

$$\text{Nu} = 2 + 0.6 \text{Re}^{1/2} \text{Pr}^{1/3} \quad (13)$$

## 2.5 Chemical reaction and properties

Since, in the current type of ignition, the droplet heat-up as well as the mass diffusion plays an important role, the physical time delay seems to be much longer than the chemical time delay. Therefore, even the single-step chemical reaction model is adequate for representing the reaction of spray. In this study, the Arrhenius form of reaction rate is used as follows

$$\dot{\omega} = A \left(\frac{\rho_g Y_f}{W_f}\right)^a \left(\frac{\rho_g Y_o}{W_o}\right)^b \exp\left(-\frac{E_a}{R_u T}\right) \quad (14)$$

where the model constants are taken from the data given by Westbrook and Dryer [14].

The present study considers the high pressure effect as well as the high temperature effect in the calculation of liquid and gas phase properties. In addition, the mixture properties are evaluated using the appropriate mixing rules based on the properties of each constituent species [15-18].

Table 2 Operating conditions for spray simulation

Fuel	n-heptane (C <sub>7</sub> H <sub>16</sub> )
Oxidizer	Air
Initial temperature of gas field	1000 K
Initial temperature of each droplet	300 K
Initial diameter of each droplet	100 μm
Spray injection velocity	15 m/s
Fuel inflow rate	0.001 kg/s
Injection time duration	1 ms

### 2.6 Numerical method

In order to get the finite difference forms of the gas field governing equations, the TEACH code [20], which had been used to modelling the spray combustion by Choi and Baek [21], is modified. Also, the SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) algorithm [22] is applied to solve these equations.

### 3 Results and Discussion

For the spray simulation in high pressure, the ambient pressure is set to 20 atm which corresponds to the upper bound for the moderately high pressure regime of n-heptane. Operating conditions are tabulated in Table 2.

In order to quantitatively verify the present code, the calculated ignition delay is compared with both experimental and numerical results produced by Sato *et*

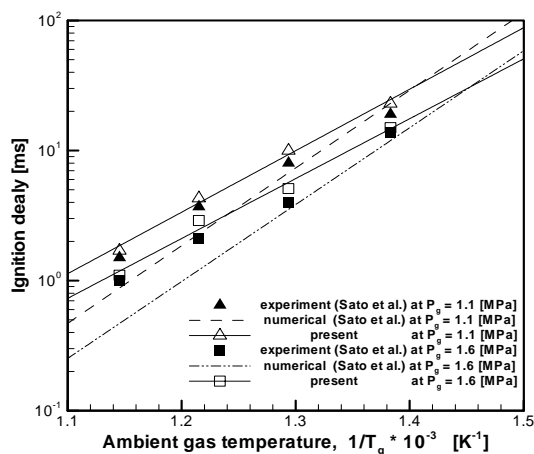


Fig.2 Comparisons of the spray ignition delay time

*al.* [23]. In their study, ignition delays of the n-decane spray injected into the air at high pressure are experimentally measured as well as numerically predicted through a simple modelling. The comparison is plotted in Fig. 2. The conditions for calculations are the same as those for their numerical predictions.

Figure 3 presents the evaporation histories of both spray and single droplet for normal and high pressure environment. The spray case corresponds to the histories of 12 representative droplets originally injected with 12 different trajectories. The single droplet case is when only one droplet is injected. As shown in Fig. 3, the life-time of single droplet is shorter than that of spray droplets in normal pressure, whereas it becomes vice-versa in high pressure. In normal pressure, a smaller concentration gradient of fuel is developed around the spray droplets so that the life-time of each droplet in spray is longer than that of single droplet. On the other hand, in high pressure, the life-time of each droplet in spray becomes shorter than that of single droplet. This is mainly due to the fact that each droplet in spray reaches the wet-bulb temperature earlier than the single droplet case. In high pressure, the high temperature flame zone

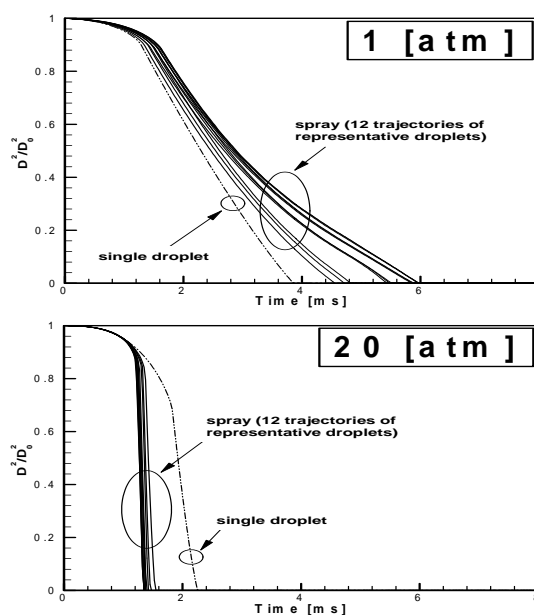


Fig.3 Evaporation histories in normal and high pressure environment (single droplet vs. spray)

is formed faster because of a larger reaction rate, which results in a more rapid increase in temperature of spray droplets than the single droplet case.

Figure 4 displays the results of spray penetration. The spray penetration depth in high pressure is shown to be shorter than that of normal pressure. Here, we can think of the following two factors affecting it. The one is a larger droplet evaporation rate in high pressure which leads to a small life-time of each droplet. The other is a drag force exerted on the droplet. At the early time of injection, the gas field density has the biggest influence on determining the drag because the other parameters are almost the same. Thus a larger drag induced in high pressure leads to shorter depth of spray penetration.

Figure 5 displays the transient temperature variations within the gas field. At the early two scenes of normal pressure case, the low temperature zone appears along the trajectory of spray since the droplets are initially injected with lower temperature than the gas field. The result at 3.75 ms shows that an ignition occurs in the

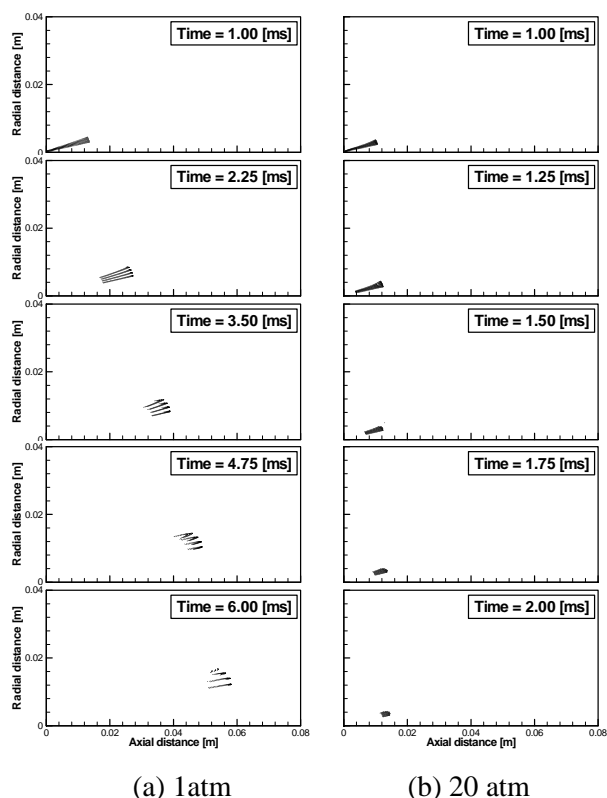


Fig.4 Spray trajectory at normal(a) and high(b) pressure

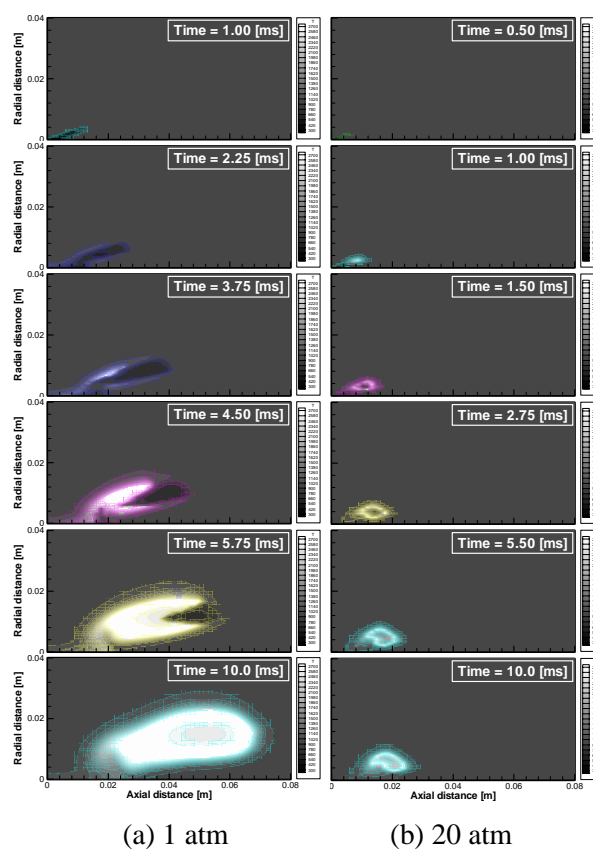


Fig.5 Temperature distribution in gas field at normal(a) and high(b) pressure

rear zone of spray. Afterwards, the flame is observed to propagate downstream of the pre-vaporized zone. In high pressure, the high temperature zone appears at 1.00 ms. Thus it can be inferred that the ignition has already taken place at this time. This is mainly due to a shorter life-time of spray as well as a larger reaction rate. Also, vigorous reaction in high pressure makes the flame zone more compact than the case of normal pressure.

## 4 Conclusion

Throughout this study, simulations of the liquid fuel spray injected into a confined combustor have been conducted. The summary of the results is as follows.

The evaporation and combustion in high pressure were observed to occur more rapidly and vigorously so that the reaction was completed in more compact zone

compared to the case of normal pressure.

In normal pressure, the life-time of spray was longer than that of single droplet because evaporation was suppressed by neighboring droplets. However, in high pressure, flame was formed earlier for the spray case so that the spray life-time became shorter.

Spray penetration depth was found to be shorter in high pressure environment because the life-time of each droplet in spray was shorter and the drag force was larger at the early stage of injection.

#### References:

- [1] Bellan J., Supercritical (and subcritical) fluid behaviour and modeling: drops, streams, shear and mixing layers, jets and sprays, *Prog. E. C. Sci.*, **26**, 2000, 329-366.
- [2] Givler S. D. and Abraham J., Supercritical droplet evaporation and combustion studies, *Prog. E. C. Sci.*, **22**, 1996, 1-28.
- [3] Aggarwal S. K., A review of spray ignition phenomena: present status and future research, *Prog. E. C. Sci.*, **24**, 1998, 565-600.
- [4] Faeth G. M., Mixing, transport and combustion in sprays, *Prog. E. C. Sci.*, **13**, 1987, 293-345.
- [5] Faeth G. M., Evaporation and combustion of sprays, *Prog. E. C. Sci.*, **9**, 1983, 1-76.
- [6] Kang S. H. and Baek S. W., Natural convection effect on the droplet ignition in high pressure condition, *Combust. Sci. Tech.*, **164**, 2001, 279-305.
- [7] Kang S. H., Baek S. W. and Choi J. H., Autoignition of sprays in a cylindrical combustor, *Int. J. Heat Mass Transfer*, **44**, 2001, 2413-2422.
- [8] Kuo K. K., *Principles of Combustion*, John Wiley and Sons Incorporated, 1986.
- [9] Crowe C. T., Sharma M. P. and Stock D. E., The particle-source-in cell (PSI-Cell) model for gas-droplet flows, *J. Fluids Eng.*, 1977, 325-332.
- [10] Delplanque J.P. and Sirignano W. A., Numerical study of the transient evaporation of an oxygen droplet at sub- and super-critical conditions. *AIAA* 91-0075.
- [11] Jia H. and Gogos G., High pressure droplet evaporation; effects of liquid-phase gas solubility, *Int. J. Heat Mass Transfer*, **36**, 1993, 4419-4431.
- [12] Jia H. and Gogos G., Investigation of liquid droplet evaporation in subcritical and supercritical gaseous environments, *J. Th. H. T.*, **6**, 1992, 738-745.
- [13] Yang A. S., Hsieh W. H., Kuo K. K. and Brown J. J., Evaporation of LOX under supercritical and subcritical conditions, *AIAA* 93-2188.
- [14] Westbrook C. K. and Dryer F. L., Chemical kinetic modeling of hydrocarbon combustion, *Prog. E. C. Sci.*, **10**, 1984, 1-57.
- [15] Reid R. C., Prausnitz J. M. and Poling B. E., *The Properties of Gases and Liquids (Fourth edition)*, McGRAW-HILL, 1987.
- [16] Takahashi S., Preparation of a generalized chart for the diffusion coefficients of gases at high pressures, *J. Chem. E. Japan*, **7**, 1974, 417-420.
- [17] Daubert D. E. and Danner R. P., *Physical and Thermodynamic Properties of Pure Chemicals*, Hemisphere Publishing Corporation, 1989.
- [18] Incropera F. P. and DeWitt D. P., *Fundamentals of Heat and Mass Transfer (Fourth edition)*, John Wiley and Sons Incorporated, 1996.
- [19] Ranz W. E. and Marshall W. R., Evaporation from drops, *Chemical Eng. Prog.*, **48**(3), 1952, 141-146.
- [20] Gosman A. D. and Ideriah F. J. K., *TEACH-T: A General Computer Program for Two-Dimensional Recirculating Flow*, Imperial College, 1976.
- [21] Choi C. E. and Baek S. W., Numerical analysis of a spray combustion with nongray radiation using weighted sum of gray gasses model, *Combust. Sci. Tech.*, **115**, 1996, 297-315.
- [22] Patankar S. V., *Numerical Heat Transfer and Fluid Flow*, Hemisphere Publishing Corporation, 1980.
- [23] Sato J., Konishi K., Okada H. and Niioka T., Ignition process of fuel spray injected into high pressure high temperature atmosphere, *21th (Int.) Symp. on Combustion*, 1986, 695-702.