

Autoignition of sprays in a Cylindrical Combustor

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Introduction

Application of spray combustion can be found in many practical systems such as diesel engine, gas turbine combustor, industrial furnace and so on. Spray combustion includes a number of complicated physical processes such as vaporization, mixing, ignition, combustion and radiative heat transfer. Among them, the ignition phenomenon is a crucial process, since it is an incipient process required for major heat release as well as one of deterministic factors for the system efficiency. For example, in diesel engine system, the autoignition under high temperature and high pressure conditions influences the whole performance of engine system. Therefore, an understanding of the detailed physical and chemical processes, which govern an autoignition in spray combustion, is highly preferred from a practical point of view. However, there are many difficulties in analyzing the problem of autoignition and spray combustion due to their inherently complicated thermo-fluid mechanical characteristics. Hence, most of researchers used to choose physically simple as well as reliable models [1, 2]. In order to successfully model the autoignition, following unsteady behaviors must be taken into account: chemical reaction at related temperature range, fluid dynamics, heat transfer, phase changes and interactions between two phases.

In liquid fueled spray combustion, the fuel is injected into an environment of hot air as discrete droplet groups. Thus, the analysis must be extended to include two-phase coupling in the mass, momentum and energy equations. In this study, separated flow (SF) model [3] is used for detailed consideration of the finite rates of transports between phases. Ignition delay time, which is governed by various physical and chemical factors [4], is usually introduced to represent basic characteristics of autoignition, i.e., the rapid transition from non-reactive state to reactive state by a global heating of the mixture. Therefore, the parametric study of ignition delay is very important to fully understanding the autoignition process. Regarding this, a great deal of efforts has been exercised to explain the autoignition phenomena. Theoretical investigations have been done by adopting phenomenological models [5], transient one-dimensional models [6, 7, 8] and steady state multidimensional models [9] with single step or reduced multi-step chemical mechanisms. However, the unsteady multidimensional simulation has yet to be investigated in further detail.

Major objectives in this work are to examine the effects of various parameters on ignition phenomena by simulating developments of spray combustion in a confined cylindrical combustor. While the TEACH code is modified and used to solve the unsteady gas field, the PSI-Cell model is employed for finite transport rates between two phases and the infinite conduction model for the vaporization of droplets.

Formulations

The schematic for this study is represented in Fig. 1. Fuel droplets injected experience the heating up to boiling temperature by surrounding stagnant hot air, vaporization, mixing with air and combustion. In order to study the autoignition phenomena in a 2D axisymmetric combustor, the following assumptions are used: (1) unsteady and axisymmetric system, (2) negligible turbulence effect, (3) spherical droplets, (4) no interaction between droplets, (5) single reaction step with a second order, and (6) ideal gas. These physical processes can be represented by the following gas and droplet equations.

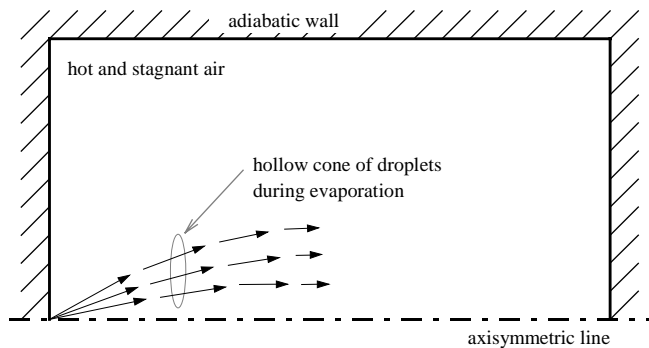


Fig. 1 Schematic of the axisymmetric combustor

The governing equation for the gas field in axisymmetric coordinates is presented in Eq. (1), which is based on the Eulerian approach. In this equation, ϕ , ρ and Γ are the general dependent variable (mass, momentum, energy, chemical species and etc.), gas density and diffusion coefficient. S_ϕ includes the source term of dependent variable and other terms, which are transposed from the left hand side of the equation. Specific representations of each dependent variable are tabulated in Table 1. $S_{\phi,g}$ and $S_{\phi,l}$ represent the source terms for the gas and liquid phase, respectively.

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

Since the existence of liquid droplets introduces phenomenon of droplet evaporation and mixing with air, the modeling appropriately describing interactions between gas and liquid phases is required. In order to deal with this problem, the PSI-Cell method [10] is adopted here in numerical analysis. With this model, droplet equations are case in Lagrangian formulation, coupled with the gas phase field through the source terms ($S_{\phi,l}$). In the PSI-Cell model all droplets injected are divided into a finite number of groups, each of which comprises a specified number of droplets. Droplet trajectory, velocity, temperature and droplet diameter could be obtained by solving the following governing equations for droplets.

$$\frac{dm_d}{dt} = -\dot{m}_{sphere} \left(1 + 0.3 \text{Re}^{0.5} \text{Pr}^{0.33} \right) \quad (2)$$

$$\dot{m}_{sphere} = 2\pi d \rho D \ln(1 + B) \quad (3)$$

$$m_d \left(\frac{du_d}{dt} \right) = \frac{1}{2} \rho_g C_d (u - u_d) |u - u_d| A_d - \left(\frac{m_g}{\rho_g} \frac{\partial p}{\partial x} \right) \quad (4)$$

$$m_d \frac{dT_d}{dt} = \frac{Nu \pi k d}{C_{pd}} (T - T_d) - \frac{L}{C_{pd}} \dot{m}_d \quad (5)$$

$$- \frac{d}{dt} \left(\frac{\rho_d \pi d^3}{6} \right) = \dot{m}_d \quad (6)$$

While equation (2) is the mass conservation for the droplet as proposed by Faeth [3], the droplet evaporation rate in quasi steady state, \dot{m}_{sphere} is empirically determined by Eq. (3) under the assumption of spherical shape. D and B are the diffusion coefficient and Spalding's transport coefficient, respectively. Equation (4) represents the momentum conservation equation for droplet, considering the effects of drag force and pressure gradient. While droplet velocity can be calculated by integrating du_d/dt , its trajectory is followed by integrating the droplet velocity. Energy conservation equation is represented by Eq. (5), in which Nu is the Nusselt number set to

Table 1. Variables and source terms appearing in Eq. (1)

Equation	ϕ	Γ_ϕ	$S_{\phi,g}$	$dV_\phi S_{\phi,l}$
Continuity	1	0	0	$\sum n \dot{m}$
Axial Momentum	u	μ	$-\frac{\partial p}{\partial x} + \frac{\partial}{\partial x} \left(\mu \frac{\partial u}{\partial x} \right) + \frac{1}{y} \frac{\partial}{\partial y} \left(y \mu \frac{\partial v}{\partial x} \right)$	$\sum \left(n \dot{m} u - \frac{4}{3} \pi \rho_d r_d^3 n F_\phi \right)$
Radial Momentum	v	μ	$-\frac{\partial p}{\partial y} - \frac{2\mu v}{y^2} + \frac{\partial}{\partial x} \left(\mu \frac{\partial u}{\partial y} \right) + \frac{1}{y} \frac{\partial}{\partial y} \left(y \mu \frac{\partial v}{\partial y} \right)$	$\sum \left(n \dot{m} v - \frac{4}{3} \pi \rho_d r_d^3 n F_\phi \right)$
Energy	h	Γ	$\frac{\partial p}{\partial t} + \mu G + W_f Q R_f$	$\sum \{ -n \dot{m} (C_p (T_g - T_d) + L) \}$
Mass Fraction (fuel)	Y_f	Γ	$-W_f R_f$	$\sum n \dot{m}$
Mass Fraction (other species)	Y_i	Γ	$\mp \nu_i W_i R_f$ (- for O_2 , + for products)	0
$\Gamma = \frac{\mu}{\sigma_\phi}, \quad G = 2 \left[\left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial v}{\partial y} \right)^2 + \left(\frac{v}{y} \right)^2 \right] + \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)^2, \quad F_\phi = \frac{\partial \phi_d}{\partial t}$				

$Nu = 2 + 0.6 Re^{0.5} Pr^{0.33}$ [11]. Latent heat of vaporization, specific heat of the droplet and thermal conductivity of the gas are denoted by L , C_{pd} and k . Finally, variation of droplet diameter can be traced using Eq. (6) with the mass flow rate determined by Eq. (2). The chemical reaction is assumed to be governed by a one step, second order reaction with Arrhenius form.

In order to check the effects of the time step in the calculation, a number of values had been tried [12]. Appropriate values of time steps for the gas field (Δt_g), the droplet trajectory (Δt_d) and the droplet injection (Δt_{inj}) were determined within given convergence criteria after many preliminary calculations.

Results and Discussion

The numerical simulation has been performed for nonpremixed two phase spray combustion in a confined cylindrical combustor. Unless otherwise mentioned, the reference conditions are as follows; (1) combustor is 0.05m radius and 0.1m long, (2) the air in combustor is initially hot and stagnant (1000K, 1atm), (3) the fuel is n-decane, (4) the total injection time is 1ms with fuel mass flow rate of 0.001kg/s, (5) the droplet diameter is 100 μ m and monodispersed, (6) initial velocities of all droplets are 15m/s, (7) droplets are injected in twelve different directions (three different radial positions of $y = 0.10, 0.25$, and 0.40 mm with four different angles of $\theta = 10^\circ, 12^\circ, 14^\circ$ and 16° at each position).

In Fig. 2, the unsteady variations of the maximum temperature and the maximum reaction rate in gas field are plotted. However, it must be noted that their maximum values do not always occur at the same position as time passes by. The maximum reaction rate starts to increase rapidly at about 4.2 ms. The maximum temperature is seen to behave in a very similar manner. Before this time, the liquid fuel undergoes evaporation while its vapor being mixed with air forming the combustible mixture. After the onset of ignition, the maximum reaction rate reaches an approximately constant average value. Thus, the time at an incipience of the rapid increase in the maximum reaction rate is defined as an ignition delay time here. Fig. 3 shows an unsteady variation of droplet temperature and droplet diameter squared. Depending on the injection position and angle, droplets experience different thermal history. Except for an initial heating period and last burn-out period, all the variations of diameter squared (d^2) are seemingly linear. A discontinuous change in d^2 for each type of droplets after 6 ms is caused by a full development of gaseous flame. Among others, the droplets injected far from the symmetric axis, i.e., at larger y and θ undergoes faster heating and thereby, faster decrease in d^2 . This results from that fact those droplets are less influenced by a reduction in the gas temperature due to heat transfer to the droplets than inner droplets.

There are also other parameters influencing the ignition delay; injection velocity, initial gas pressure and temperature, fuel type, droplet size and distribution in the chamber. The effect of the initial gas temperature on the ignition delay time is represented in Fig. 4. As expected, the ignition delay time rapidly decreases at low temperature zone while it slowly decreases in high temperature zone as the initial gas temperature increases. In Fig. 5, the effect of the droplet diameter on the ignition delay time is presented when the total amount of fuel injected is fixed. When the droplet size becomes larger, the ignition delay steadily increases since the total evaporation rate must be reduced because of smaller total surface area.

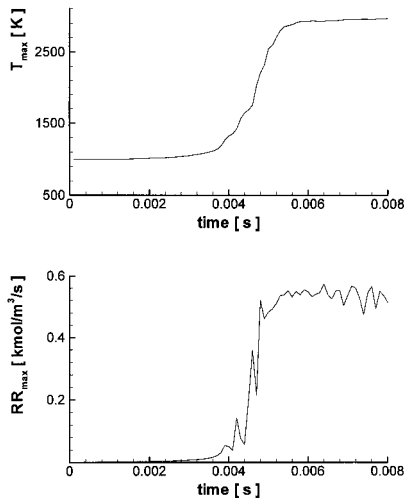


Fig. 2 Maximum temperature and reaction rate variation

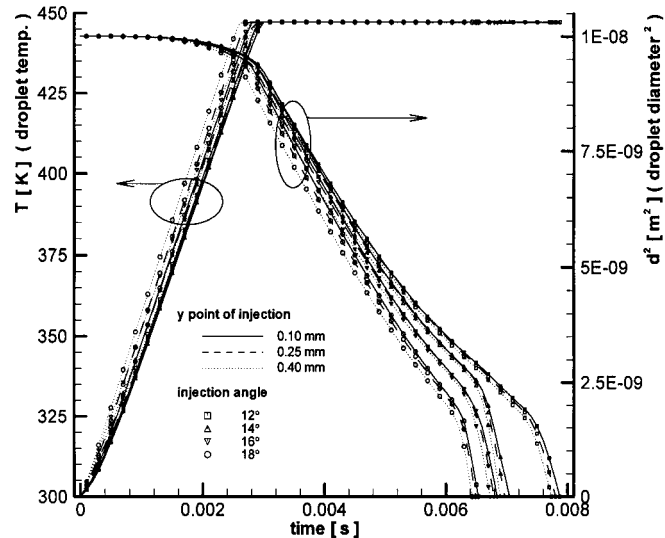


Fig. 3 Droplet history (injected at $t=0$) temperature and diameter² variation

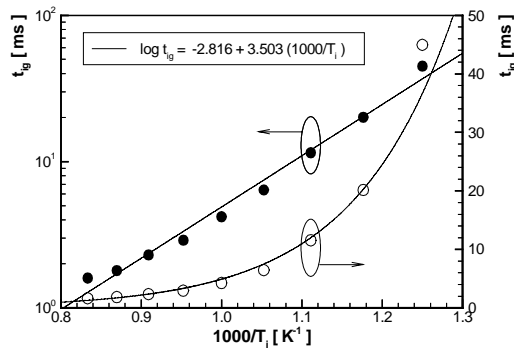


Fig. 4 Ignition delay vs. initial reciprocal temperature

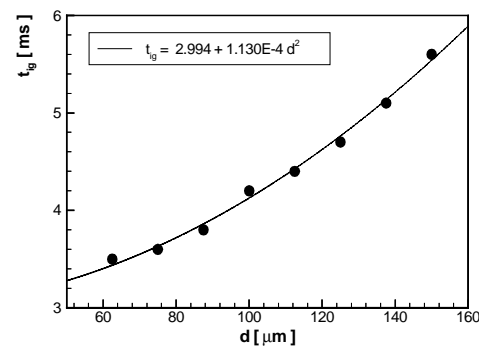


Fig. 5 Ignition delay vs. droplet diameter ($T_i = 1000\text{K}$)

Conclusion

An ignition of a spray injected into a cylindrical combustion chamber has been numerically investigated. Herein, their heating and ignition behaviors could be predicted and discussed by changing such various parameters as injection type, initial gas temperature and droplet size. The effects of other factors would also be sought in the work to be continued.

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