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# Modification of Droplet Models for Numerical Simulation in Spray Combustion Investigation

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**Abstract:** A comparative assessment of the new droplet model including the multi-state behavior (MDCM4) is conducted using the droplet models which are currently available and have been applied in modern spray calculation. This investigation compares the trajectory, state transition, flame transformation and burn-out of a droplet which was injected into the combustion chamber with a known combustion flow structure. In order to represent droplet state quantitatively, an index of group combustion IGC is introduced. The state of evolution of a tested droplet is described by IGC along its trajectory. The results predicted by different droplet models show different characteristics which will ultimately influence the accuracy of the analysis of a spray combustion system. By analyzing the effects of different injection velocities and angles on the trajectory of the tested droplet, the validity of the new droplet model including the multi-state behavior (MDCM4) are examined by qualitatively comparing the results with experimental observation.

**Key words:** Droplet model, multi-state behavior, group combustion

## INTRODUCTION

Droplets play different roles in the transport of fuel vapor, oxidizer vapor and energy in different droplet states (Chiu, 2000). Therefore the selection of an accurate, versatile droplet model constitutes the primary consideration in spray calculation and the analysis of spray structure.

It is recognized that droplets may undergo various sub-processes such as heat-up, vaporization, ignition, burning and extinction based on their atomization conditions and local environmental conditions in the complex flow-field (Leu, 2008) and actual combustion phenomena (Leu and Ho, 1997). However, most computational models for spray combustion (El Banhawy and Whitelaw, 1980; Bayson *et al*., 1982; Faeth, 1987; Weber *et al*., 1987; Asheim and Peters, 1989) simply assumed that droplets could only evaporate [Droplet Evaporation Model (DEM)] and neglected all effects caused by possible droplet burning. Since droplet burning did occur in spray combustion, a Droplet Combustion Model (DCM) was proposed by Jiang and Chiu (1992) to employ local reactivity as the criterion for droplet burning based on group combustion theory (Suzuki and Chiu, 1971; Chiu *et al*., 1982; Gung and Gomez, 1997; Chiu and Lin, 1996). In this model, all droplets in the oxidizer-rich mixture are assumed in the state of burning once the droplets are heated up to their boiling point. Since only the local equivalent ratio is considered in this simple model, local gas temperature, oxidizer mass fraction and droplet size become irrelevant to the determination of droplet burning. So Jiang and Chiu further proposed that, in addition to local reactivity, droplet ignitability [Modified Droplet Combustion Model (MDCM1)] should also be considered to meet with the results of ignition study for a stationary droplet (Law and Chung, 1980). Jiang and Hsu (1993) applied the above three models, including DEM, DCM and MDCM1, to evaluate for spray combustion through a qualitative comparison of their predictions with experimental observations (Yule and Bolado, 1984). Among the three models, it may be concluded that MDCM1 is the most accurate model. They suggested the droplet ignition criterion in MDCM1 should include the effects of surrounding convective flow to have more realistic prediction of spray combustion. The ignition-extinction and flame structures of a combusting droplet in a convective flow field, however, are quite different from

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those of a stationary droplet because of the appearance of two types of flame configurations: an envelope flame at a low relative speed and a wake flame at a high relative speed. Many experimental studies have already addressed the subject of the transformation of an envelope flame into a wake flame under a high convective flow field (Spalding, 1953; Sami and Ogasawara, 1970; Udelson, 1962; Emmons, 1971; Gollahalli and Brzustowski, 1973; Leu and Liu, 2003). Chiu and coworkers (Chiu, 1993; Chiu and Huang, 1996; Jiang *et al*., 1995; Huang and Chiu, 1997, 2008) further perceive that a convection droplet exhibits much more complex multi-state behaviors including envelope flame combustion, wake flame combustion and vaporization mode. Huang and Chiu (1997) present an analysis of droplet states, including preheating, vaporization, combustion with an envelope flame or wake flame, which account for multi-state behavior in a general environment and to examine the criterion of droplet state transition. Finally, they presented a flow chart of the applications of this newly-presented droplet model in spray calculations.

In the present study, a comparative assessment of the new droplet model formulated by Huang and Chiu (1997) is conducted using DEM, DCM and MDCM1 which have been used in modern spray calculation. The investigation compares the trajectory, state transition, flame transformation and burn out of a droplet which was injected in the combustion chamber with a known combustion flow structure. In order to represent droplet state quantitatively, an index of group combustion IGC is introduced. The state of evolution of a tested droplet is described by IGC along its trajectory. The validity of the new droplet model including the multi-state behavior (MDCM4) is examined by qualitatively comparing the results with experimental observation in different injection velocities and angles.

## MATHEMATICAL FORMULATION

**Droplet combustion models:** Six different droplet combustion models, presently available, were compared in the present study. All of the six models were used to identify the droplet state after the droplet temperature reached the boiling point. These six droplet models are depicted in the following section.

**Droplet evaporation model (DEM):** This model assumes that droplets evaporate and no droplet combustion occurs. This model is applied in most computational models for spray combustion (El Banhawy and Whitelaw, 1980; Bayson *et al*., 1982; Faeth, 1987; Weber *et al*., 1987; Asheim and Peters, 1989).

**Droplet combustion model (DCM):** Based on the group combustion theory, Suzuki and Chiu (1971), Chiu *et al*. (1982), Gung and Gomez (1997) and Jiang and Chiu (1992) proposed the local reactivity serves as the criterion to determine the droplet state. In this model, the equivalence ratio $\varphi$ is used to represent the local reactivity to determine whether or not the environment is suitable for droplet combustion. When $\varphi$ is less than unity, the environment is oxidizer-rich and the droplet combustion is able to take place. When $\varphi$ is greater than unity, the environment is classified as oxidizer-lean and the fuel droplet will simply evaporate. The flame type of a burning droplet is assumed to be an envelope flame which envelops the whole droplet.

**Modified droplet combustion model with ignition criterion (MDCM1):** The ability to ignite the droplet is not considered in DCM, the local temperature and droplet size becomes irrelevant to the determination of droplet state so that some modifications on DCM must be done. Jiang and Chiu (1987) modified the DCM by taking the droplet ignition criterion for a stationary droplet proposed by Law and Chung (1980) into the local reactivity criterion for the determination of droplet state. Thus the droplet combustion is assumed only when both criteria, i.e., the droplet ignitability and the local reactivity, are satisfied. The ignition criterion proposed by Law and Chung (1980) is established on the basis of the relative magnitude of the local Damköhler number, defined by:

$$\Delta = \frac{\rho}{\alpha}\left(\frac{a_f f'}{W_0}\right)\left(\frac{C_P}{Q}\right)^2 \frac{T^4 Y_O r_\infty^2}{T_s^2\left[\ln(\beta/H)\right]^2} \times \left(\frac{r_\infty}{r_s}-1\right)^2 \exp\left(\frac{-T_a}{T}\right) \quad (1)$$

and the ignition Damköhler number is given by

$$\Delta_i = \frac{3.6(\beta/Q)^{f(\gamma)}}{(\gamma+8)^{1.27}} \quad (2)$$

Where:

$$f(\gamma) = \frac{16}{(\gamma+32)^{0.8}} + 2$$

The ignitability of the droplet is assured if the local Damköhler number is greater than the ignition Damköhler number.

In this model, the flame type of a burning droplet is also assumed as the envelope flame.

**Modified droplet combustion model with convective motion and ignition (MDCM2):** The convective effect on the ignitability is not considered in MDCM1. From the

study of Huang and Chiu (1997), the droplet state in a convective flow depends on the initial state of the droplet and four critical Damköhler numbers.

The Damköhler number is defined (Mawid and Aggarwal, 1989) by

$$Da = \frac{Y_O^{a_O} \exp(-T_a/T) r_s^2 \ln^2(1+B)}{(C_P T/Q)^{a_O+a_F}(C_P T^2/T_a Q)^{3-a_F}} \times \frac{f' W_F^{1-a_F}}{\rho D W_O^{a_O}} \left(\frac{PC_P}{RQ}\right)^{a_O+a_F}$$

and four critical Damköhler numbers are given (Huang and Chiu, 1997) by

$$Da_I = 1.1(1+Re_l)^{1.5}(1+B)^{0.26} \quad (3)$$

$$Da_R = 0.84(1+Re_l)^{2.2}(1+B)^{0.12} \quad (4)$$

$$Da_B = 0.36(1+Re_l)^{1.5}(1+B)^{0.93} \quad (5)$$

$$Da_E = 0.76(1+Re_l)^{1.2}(1+B)^{0.29} \quad (6)$$

The ignition Damköhler number in Eq. 3 is formulated under the conditions that the droplet state transformed from vaporization to combustion with a wake flame or an envelope flame in a convective flow. In the presented model, the determination process of the droplet state is the same as MDCM1 except that the ignitability of the droplet is checked by the condition to include the convective effect. The flame type of a burning droplet is assumed as the envelope flame.

**Modified droplet combustion model with convective motion, ignition and reattachment (MDCM3):** In this model, the flame type of a burning droplet is further divided into the wake flame type and the envelope flame type. Both the ignition Damköhler and the reattachment Damköhler number shown in Eq. 3 and 4 are used to identify the droplet state. The identification of droplet state in this model is checked in two steps. The first step is to check whether the droplet combustion is possible or not by the same process as MDCM2 i.e. convective motion and ignition criterion. The second step is to identify the type of flame i.e. the envelope flame for $Da>Da_R$, or a wake flame for $Da<Da_R$.

**Modified droplet combustion model with multi-state behavior (MDCM4):** In this model, the multi-state behavior of a convection droplet is adopted. If the local reactivity does not meet the combustion criterion, the droplet is assumed to be in the state of vaporization. However when the local reactivity satisfies the combustion criteria, the appropriate combustion state is determined by local Damköhler numbers and the initial state of the droplet. The detail procedures for the determination of the state follow the scheme shown in the study of Huang and Chiu (1997).

In the following sections, each of the six models mentioned will be compared and the results obtained by MDCM4 will be discussed in detail to assess versatility of the model.

**State evolution of a droplet in a simulated combustion chamber:** Six different droplet models depicted in above sections are used to examine the trajectory, state transition, flame transformation and burn out of a droplet which was injected into the combustion chamber (Fig. 1) with a known combustion flow structure. The inlet conditions of spray combustion processes are listed in Table 1. The overall fuel-air ratio is 0.0166 and the group combustion number $G = (4\pi\lambda^0 C^0_{f\,lm} n^0_{lm} r^0)/(\rho^0_g C^0_\rho \mu^0_g)$. The droplet size distribution obeys the Rosin-Rammler relation whereas gas velocity distribution for the outer annular inlet assumes 1/7 power laws. The numerically predicted distribution of gas phase temperature and the gas concentration are shown in Fig. 2 and 3, respectively (Jiang and Hsu, 1993).

The governing equations for the injected droplet are described below:

$$\frac{d\vec{x}}{dt} = \vec{V}_l \quad (7)$$

$$\frac{d}{dt}(m_l \vec{V}_l) = \vec{F}_l \quad (8)$$

$$\frac{d}{dt}(m_l C_{Pl} T_l) = \dot{q}_l \quad (9)$$

$$\frac{dr_l}{dt} = \frac{\dot{m}_l}{4\pi r_l^2 \rho_l} \quad (10)$$

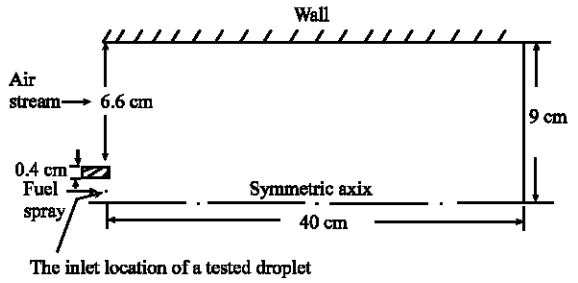


Fig. 1: Schematic diagram for the cylindrical non-premixed combustor

Table 1: The inlet condition of the simulated combustor

| | $M_{f,in}$ (kg sec$^{-1}$) | $M_{air,in}$ (kg sec$^{-1}$) | $u^0_g$ (m sec$^{-1}$) | $u^0_l$ (m sec$^{-1}$) | $T^0_g$ (K) | $T^0_l$ (K) | $P^0_g$ (atm) |
|---|---|---|---|---|---|---|---|
| Fuel spray | 0.00366 | 0.00 | 30 | 25 | 600 | 298 | 1.0 |
| Air stream | 0.00 | 0.22 | 20 | NA | 600 | NA | 1.0 |

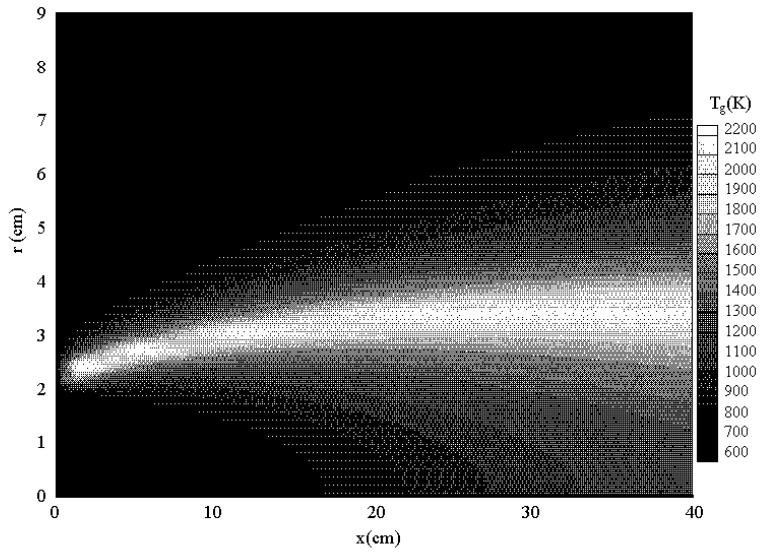


Fig. 2: The distribution of gas temperature in the simulated combustor

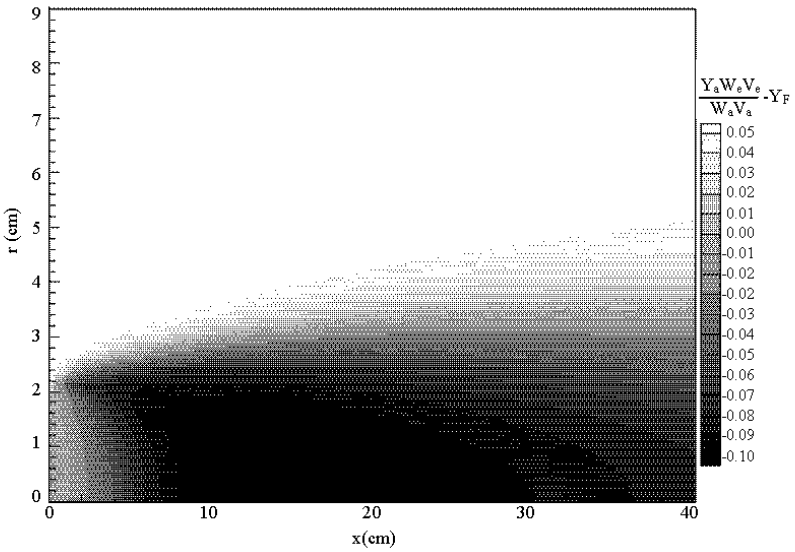


Fig. 3: The distribution of gas concentration in the simulated combustor

Where:

$$\dot{m}_l = C_f 4\pi\rho_g D_g r_l \ln(1+B) \quad (11)$$

$$\dot{q}_l = 2\pi r_l \lambda_g Nu(T_g - T_l)\delta(T_l) \quad (12)$$

$$\vec{F}_l = 0.5\pi\rho_g r_l^2 C_D \left|\vec{V}_g - \vec{V}_l\right|(\vec{V}_g - \vec{V}_l) \quad (13)$$

The values of $C_f$ and $C_D$ for each droplet state can be found in the study of Huang and Chiu[22]. Since no superheating is assumed, the value of $\delta(t_L)$ is 1 when $T_l<T_b$ or 0 when $T_l>T_b$.

In order to represent droplet state quantitatively, an index of group combustion IGC is introduced according to the following convention. For a droplet in the state of preheating, IGC is assigned the value of -1. Likewise, the IGC for the state of vaporization, combustion with a wake flame and combustion with an envelope flame are assigned with the value of 0, 1 and 2, respectively. A mean state of the droplet group is defined by an arithmetic mean of IGC (MIGC) as follows:

$$MIGC = \frac{\sum_{i=1}^{N} n_i (IGC)_i}{\sum n_i} \quad (14)$$

Where, $n_i$ is the number density of droplets in the ith size group. Thus, the global distribution of MIGC serves as a new index expressing group combustion behavior (state) and spray structure. A low-MIGC spray implies a spray with a small number of burning droplets and its structure is more original for its state is approaching preheating quantitatively. On the other hand, a high-MIGC spray represents a spray with a large number of burning droplets and, its structure is more destroyed for its state is approaching fully combusted quantitatively. According to the group combustion theory by Chiu *et al.* (1982), Gung and Gomez (1997) and Chiu and Lin (1996), the group combustion modes of a low-MIGC spray and a high-MIGC spray will be external group combustion mode and internal combustion mode, respectively. In the present study, the state of evolution of a tested droplet is described by IGC along its trajectory.

## RESULTS AND DISCUSSION

**Comparison of different droplet models:** Six different droplet models depicted in the above section are used to examine the trajectory of a droplet injected into the combustion chamber with an initial radius of 50 μm, injection velocity of 80 m $sec^{-1}$ and the injection angle of 15°. The predicted results by different droplet models have different characteristics on both the trajectory and the value of IGC shown in Fig. 4. The results show that the DCM predicts a shorter axial distance for droplet burn out because the DCM criterion leads to the occurrence of combustion without ignition delay and the envelope flame overestimates the combustion rate. The results predicted by MDCM1 yield a longer axial distance for droplet burnout because of the ignition delay adopted by MDCM1. Furthermore, the criterion prohibits the combustion of smaller sized droplets. The convective effect on the ignitability in MDCM2 is pronounced because convective motion causes further spatial delays in ignition. In MDCM3, the flame type of droplet combustion is further divided into the envelope flame and the wake flame so that the droplet burns more slowly than those predicted by MDCM2. Since the droplet is not burn in DEM, vaporization does not complete even at the terminus of the chamber.

The results predicted by MDCM4 show that the droplet burns out at a smaller axial distance than that predicted by MDCM2. The results predicted by different

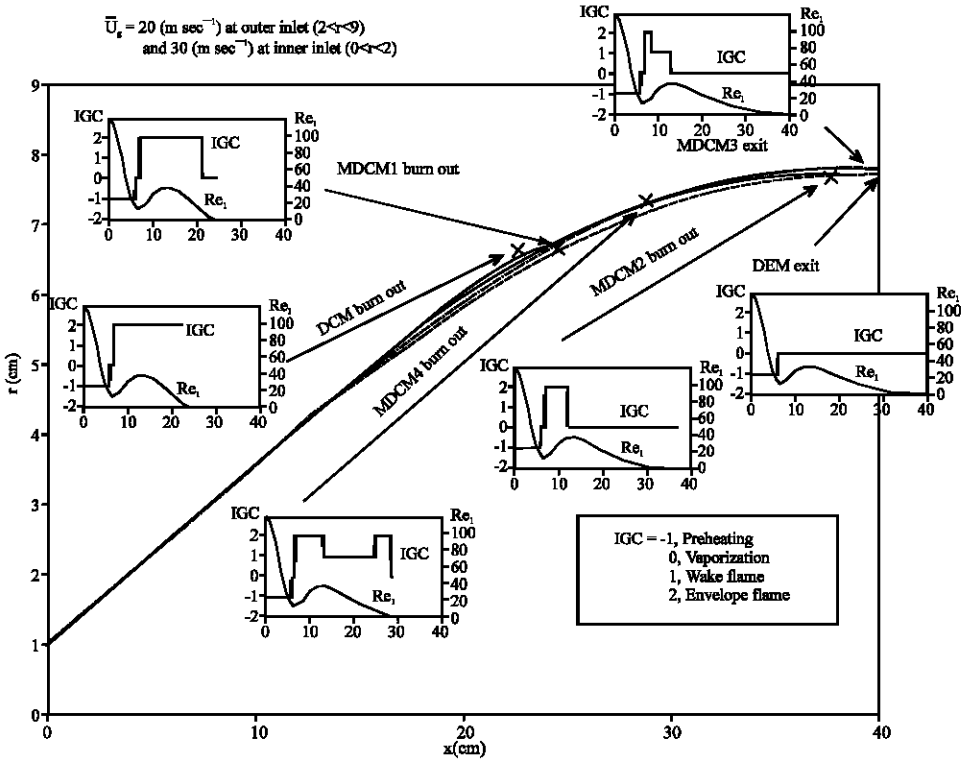


Fig. 4: The trajectory of a tested droplet with the injected angle θ = 15° and injection velocity $U_{10}$ = 80 (m $sec^{-1}$) by different droplet combustion models

droplet models show different characteristics, which will ultimately influence the accuracy of the analysis of a spray combustion system. The validity of each model must be carefully examined by comparing the results with experimental observation.

**Effects of velocities and angles of injection:** In this section, the effects of injection velocities and injection angles on the trajectory of the tested droplet are examined by using MDCM4. Test droplets with an initial radius of 50 μm are injected at four selected velocities; 10, 20, 40 and 80 m sec$^{-1}$ and at four injection angles; 50°, 15°, 25° and 35°. At a small injection angle, say, as shown in Fig. 5, all droplets at the four selected injection velocities start preheating and subsequently vaporize as shown in the IGC diagrams in the insets. Clearly the droplets that remain in the spray core form a vaporizing droplet cloud to support an external group flame. At injection angle, Fig. 6, the droplet at the lowest velocity evolves from the state of preheating to that of vaporization, whereas droplets at 20 and 40 m sec$^{-1}$ both experience preheating, vaporization and combustion with an envelope flame before burning out. The critical Damköhler number reaches at x = 8 cm downstream of injection and burnout at x = 15 cm for the injection velocity of 20 m sec$^{-1}$. At the injection velocity of 80 m sec$^{-1}$, the droplet goes through preheating, followed by a brief period of vaporization. After which it is ignited and burns with an envelope flame that subsequently transforms into a wake flame for a substantial period of time until the Reynolds number decreases below the critical value at which time an envelope flame is reestablished. It is interesting to note that there is an optimal velocity, 20 m sec$^{-1}$, among the four selected injection velocities, at which the droplet burnout occurs with the minimum axial location as shown in Fig. 6. At the injection angle, all the droplets go through the states of preheating, vaporization and combustion, Fig. 7. At a lower velocity, 10 m sec$^{-1}$, a droplet has a significantly longer vaporization time. This becomes shorter at higher velocities.

At higher injection velocities of 40 and 80 m sec$^{-1}$, the droplets are ignited in the state of preheating and form an envelope flame proceeded by a negligible period of vaporization. This is explained on the grounds that the ignition occurs when the droplet passes through the group envelope flame zone where the droplet is exposed to the high environmental temperature of nearly 2000 K. Note also that at the injection velocity of 80 m sec$^{-1}$, the droplet collides at the wall. At the injection angle of, all the droplets appear to penetrate group envelope flame, Fig. 8. Thus, all droplets under such conditions appear to have shorter preheating and vaporization times. Droplets at all the injection velocities, except at 80 m sec$^{-1}$, burn out in relatively short axial distances.

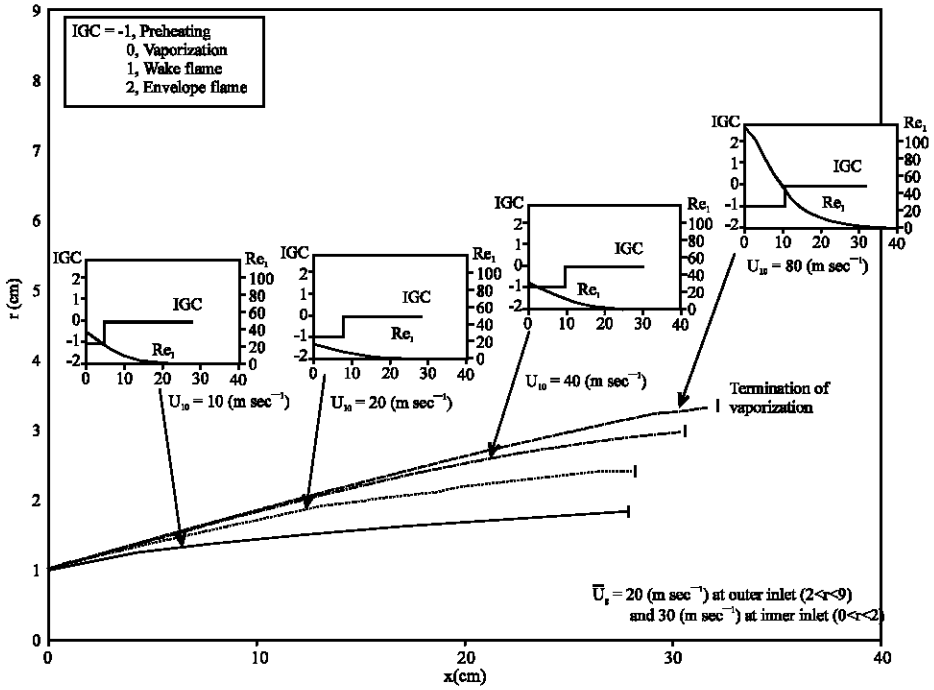


Fig. 5: The trajectory of a tested droplet with the injected angle θ = 5° by different droplet combustion models

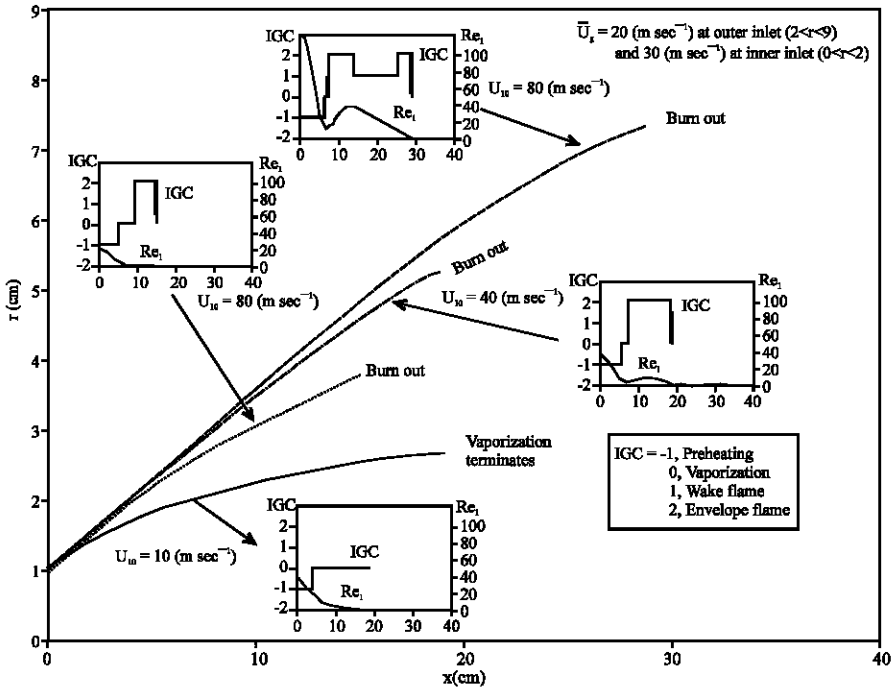


Fig. 6: The trajectory of a tested droplet with the injected angle θ = 15° by different droplet combustion models

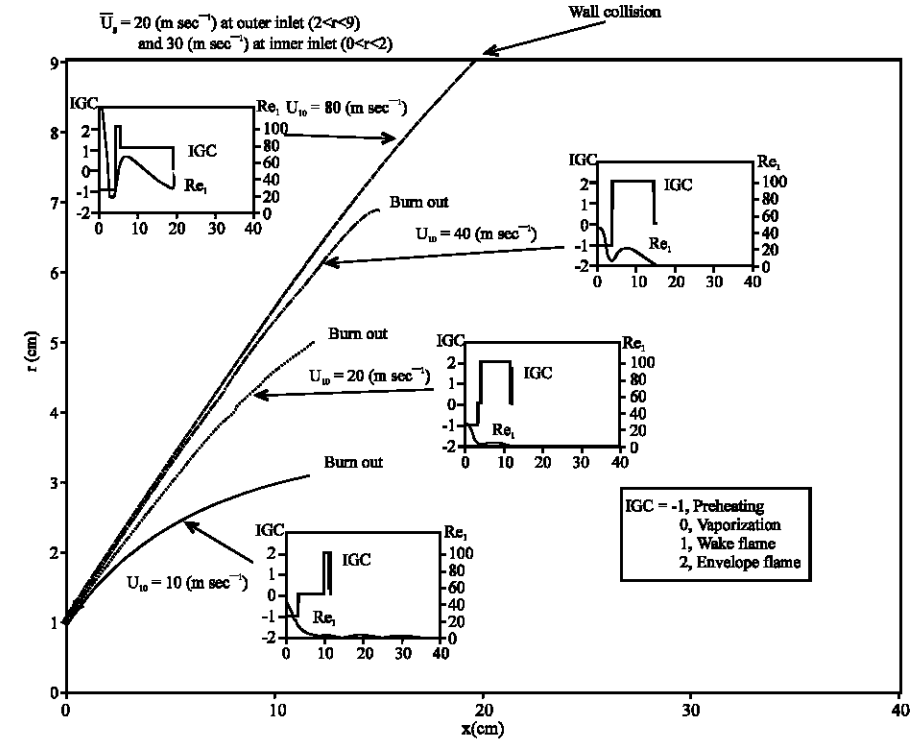


Fig.7: The trajectory of a tested droplet with the injected angle θ = 25° by different droplet combustion models

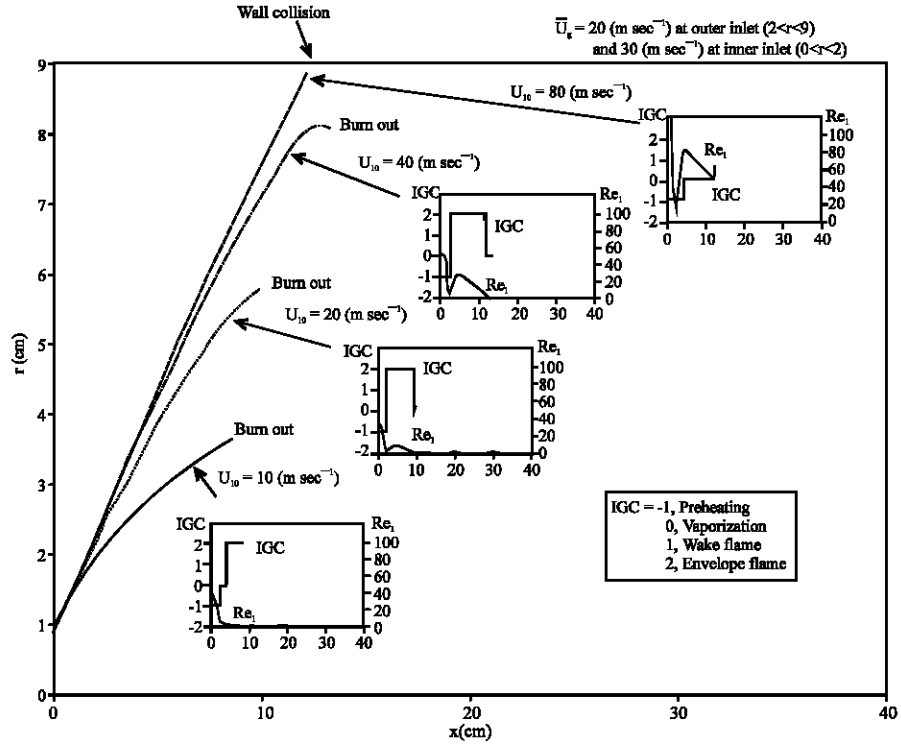


Fig. 8: The trajectory of a tested droplet with the injected angle $\theta$ = 35° by different droplet combustion models

From the results of the simulation of droplet state evolution, one arrives at the following specific conclusions for a spray operating at a moderately high group combustion number. The analysis confirms that the droplets injected in the spray core with relatively smaller injection angles, virtually remain practically in the states of vaporization and preheating without the combustion predicted in group combustion model (Suzuki and Chiu, 1971; Chiu *et al.*, 1982; Gung and Gomez, 1997). The group envelope flame which is stabilized at the radial distance comparable to the size of the spray core is supported by the fuel vapor produced by the vaporizing droplet cloud in the core region of the spray. The droplets injected at larger spray angles are all ignited as they pass through the hot group region and burn with envelope flames. Some of those larger droplets with higher velocities may transform into wake flame combustion mode when the environmental temperature is reduced so that reaches. When the relative velocity and droplet size become smaller, a wake flame may revert to an envelope flame prior to droplet burnout. The appearance of combusting droplets in the outer region of the group flame has been observed experimentally by McDonell *et al.* (1993).

## CONCLUSIONS

Six droplet combustion models, including DEM, DCM, MDCM1, MDCM2, MDCM3 and MDCM4, have been evaluated for a droplet which was injected into the combustion chamber with a known combustion flow structure through a qualitative comparison of their predictions about the trajectory, state transition, flame transformation and burn out. The results predicted by different droplet models show different characteristics, which will ultimately influence the accuracy of the analysis of a spray combustion system. The validity of each model must be carefully examined by comparing the results with experimental observation.

The major results of the analysis by MDCM4 are summarized as follows:

- The droplets injected in the spray core with relatively smaller injection angles, virtually remain practically in the states of vaporization and preheating.
- The droplets injected at larger spray angles are all ignited as they pass through the hot group region and burn with envelope flames.
- Some of those larger droplets with higher velocities may transform into wake flame combustion mode when local environmental temperature is reduced so that reaches.
- When the relative velocity and droplet size become smaller, a wake flame may revert to an envelope flame prior to droplet burnout.

By qualitatively comparing the above results with experimental observation (Suzuki and Chiu, 1971;

Chiu *et al*., 1982) and theoretical study (McDonell *et al*., 1993; Gung and Gomez, 1997), it may be concluded that MDCM4 is the most accurate and realistic model for spray combustion.

The investigation of the present study is conducted based on the behavior of a droplet which was injected in the combustion chamber with a known combustion flow structure. For more realistic assessment, the comparison of different droplet models in the two-phase flow computation should be conducted; work that is currently in progress.

## ACKNOWLEDGMENT

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## NOMENCLATURE

$\alpha$ = Stoichiometric coefficient of reactant
B = Transfer number
f = Frequency factor
$G_i$ = Drag coefficient
$G_f$ = Correction factor for the droplet gasification rate due to the convective effect
$C_p$ = Specific heat at constant pressure
D = Diffusivity coefficient
E = Activation energy
$\bar{F}$ = Aerodynamic drag force
G = Group Combustion number
H = Effective droplet heat of vaporization
$\dot{m}$ = Droplet vaporization/combustion rate
P = Pressure
Q = Heat of combustion
R = Universal gas constant
Re = Reynolds number
$r_l$ = Droplet radius
$r_\infty$ = Distance from droplet center to where ignition takes place
$r_0$ = Radius of fuel nozzle
T = Temperature
$T_a$ = E/R
$T_b$ = Boiling temperature
t = Time
u = Axial velocity
$\bar{V}$ = Velocity vector
W = Molecular weight
Y = Species concentration as mass fraction
$\alpha$ = Thermal diffusivity
$\beta$ = $C_p(T - T_b) + H$
$\gamma$ = $(T_a Y_f Q)/T^2 C_p$
$\lambda$ = Thermal conductivity
$\rho$ = Density
$\phi$ = Equivalence ratio

**Superscripts**
0 = Inlet condition

**Subscripts**
0 = Inlet condition

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