ABSTRACT
Evolution of liquid spray in the combustion process behaves group combustion modal transition and characteristics and has been successfully confirmed by theoretically and experimentally since 1971. The group combustion modal transition plays a crucial role in the performance and emission issues in realistic spray system. Statistically distributed mesoscale structures have been observed experimentally in turbulent premixed sprays and combust with either a primarily external or an internal group combustion mode. The statistical theory describing group combustion transition of droplet clusters as spray evolves will be established in this study. The cluster statistical equation of spray is constructed to formulate the conservation of the probability of finding cluster of a specific group combustion number and cluster size at a given time, space and velocity and describe the group modal transition along spray evolution and the liquid phase contributions to gas-phase governing equations with establishments of the coupling integral correlation function. Further calculation for one simple spray combustion case will be performed to investigate the spray structural evolution and group combustion modal transition.

Keywords: spray combustion, group combustion, droplet cluster, statistical theory

INTRODUCTION
Spray combustion technology is widely applied in various applications wherein the liquid fuel or oxidizer is injected into the combustion chamber by the injection system to form the spray patterns and atomization characteristics that facilitate droplet penetration, vaporization and mixing with gas phase for combustion and power output. The research and development has been emerged in this topic for many decades. Modern structural theory of sprays has its base on the fundamental view that an isolated droplet is the building block of the sprays. Post-modern structural theory of sprays emphasizes the collective processes of many-droplet system as one of the fundamental contributing factor in building practical sprays. Chiu and co-workers [1-2] advocated the phenomena of group combustion of sprays, which comprises four principal group combustion modes according group combustion number and was confirmed by experimental studies by Chigier [3], Onuma [4], Mizutani [5] and others [6]. Recent experimental investigation of turbulent premixed sprays by Akamatsu [7] reveals that the spray structures constitute of a statistical collection of droplet clusters, which undergo group combustion modal transition, as shown in Fig.1. Chiu [8] proposed the theory of the mesoscale spray structures to interpret the Akamatsu’s results and elucidate the structures and combustion of practical sprays. Akamatsu’s results clearly indicate that turbulent premixed sprays consist of the connected chains of the clusters of variable density, size and complex geometrical configurations, depending on the dense spray formed along the direction of the injector. Relaxation of the clusters at given G value will enhance the interphase transport of energy, momentum and mass and subsequently facilitate the overall combustion. The physics of a statistical collection of droplet cluster in sprays constitute the new concept to elucidate the collective phenomena of all practical sprays. Representation of cluster based spray model provides alternative description of non-dilute, inhomogeneous sprays by the statistical distribution of group combustion modes including external group, internal group and isolated droplet combustion modes. In this study, the cluster statistical theory will be presented to describe the formation, structural
evolution, vaporization ignition and combustion of droplet clusters in typical hydrodynamic environment of sprays.

**MATHEMATICAL FORMULATION**

*Cluster Probability Distribution Function:*

Theoretical approach of many cluster system begins with the generalization from the equation of spray statistics introduced by Williams [9].

The generalization is carried out to allow the changes in the group combustion number of droplet cluster and droplet cluster size.

The distributions of internal and external group combustion modes of distributed clusters in a turbulent spray can be determined by the number density of the clusters and the probability of internal group combustion mode of each cluster [8] as follows:

$$\ln P_t = -1.89 + 0.278 \ln \Lambda - 0.278 \ln G_c$$  \hspace{1cm} (1)

where \( P_t \) is probability of the excitation of internal group combustion mode.

We define a cluster distribution function in a 8-dimensional space, including 3 spatial dimensions, \( \mathbf{x}, \mathbf{v} \), 3 velocity dimensions, \( \mathbf{v}, \mathbf{c} \), cluster radius, \( R_c \) and group combustion number, \( G_c \), to express the probable number of clusters in the cluster's radius range \( dR_c \) about \( G_c \), group combustion number \( dG_c \) range about \( G_c \) which are in the spatial range \( d\mathbf{x} \) about \( \mathbf{x} \) with velocity in the range \( d\mathbf{v} \) about \( \mathbf{v} \), as follows:

$$f(\mathbf{x},\mathbf{v},t,G_c,R_c) d\mathbf{x}d\mathbf{v}dR_c dG_c$$  \hspace{1cm} (2)

where \( \ell_c \) is the cluster radius. \( G_c = KLeN_T/\ell_c \), which \( K=2/3, \) \( N_T \) is total number of fuel droplets in a cluster and \( Le \) is Lewis number.

Following Williams [9], the cluster probability density equation of many cluster system is formulated as follows:

$$\frac{\partial f}{\partial t} + \nabla_\mathbf{x} \cdot (\mathbf{v} f) + \nabla_\mathbf{c} \cdot (\mathbf{c} f) + \frac{\partial}{\partial \ell_c} \left( \ell_c f \right) = \Gamma + J$$  \hspace{1cm} (3)

where \( \Gamma \) and \( J \) are rate of the formation and break up of clusters, \( F_t \) is the effective external force acting on a cluster. And, \( \ell_c \) and \( \dot{\ell}_c \) depend on \( (\ell_c, G_c, \mathbf{x}, \mathbf{v}, t) \) and local properties and are given by

$$\frac{d\ell_c}{dt} = \frac{-M_c}{4\pi\tau_c \ell_c}$$  \hspace{1cm} (4)

$$\dot{N}_c = \frac{1}{2\pi} \iint G_c^2 \ell_c d\Omega$$  \hspace{1cm} (5)

$$\frac{dG_c}{dt} = \left( \frac{\dot{N}_c - \dot{\ell}_c}{N_c - \ell_c} \right) G_c$$  \hspace{1cm} (6)

in which \( N_T \) is the total number of droplets in a cluster, \( \Omega \) is solid angle, \( M_c \) is the gasification rate of cluster, and \( F_c \) is the force acting on a cluster, given by,

$$F_c = \iiint nF_D \cdot dV = \sum_{i=1}^{N_T} F_{D_i}$$  \hspace{1cm} (7)

where \( F_{D_i} \) is the drag force acting on \( i \)-th droplet in a cluster.

Based on the statistical method, a mean cluster property \( \bar{Q}_c(\mathbf{x},\mathbf{u},t,G_c) \) can be determined, by

$$\bar{Q}_c(\mathbf{x},\mathbf{u},t,G_c) = \int_{\ell_c}^{\ell_c max} \frac{1}{\Delta \ell_c} \int_{\ell_c min} Q_c(\mathbf{x},\mathbf{u},t,G_c) d\ell_c$$  \hspace{1cm} (8)

*Two-Phase Coupling Terms:*

The structures of turbulent sprays are predicted by solving the conservation equation of turbulent two-phase flow with the source terms given by

$$S_{\text{ten}} = \iiint M_c f(x,v_c,t,\ell_c,G_c) d\ell_v d\ell_c dG_c$$  \hspace{1cm} (9)

$$S_{\text{hec}} = \iiint F_c f(x,v_c,t,\ell_c,G_c) d\ell_v d\ell_c dG_c$$  \hspace{1cm} (10)

$$S_{\text{hec}} = \iiint Q_c f(x,v_c,t,\ell_c,G_c) d\ell_v d\ell_c dG_c$$  \hspace{1cm} (11)

where \( \bar{Q}_c \) is the rate of the heat transfer from the environment to a cluster. Mathematical procedure involved in the determination of the flow field variables is the same as the sprays model with droplet as the building elements. The number density of the clusters, \( n_{IG} \), which are in the internal group combustion mode is calculated as follows,

$$n_{IG} = \iiint P_t f(x,v_c,t,\ell_c,G_c) d\ell_v d\ell_c dG_c$$  \hspace{1cm} (12)

**ANALYTICAL RESULTS**

In this part, we consider the case of steady state one-dimensional flow field in which the cluster velocity is the same as that of the fluid. And there is no cluster formation and breakups of clusters occur in the region of interest, i.e. \( \Gamma \) and \( J \) equal to zero. Under the same velocity order, the aerodynamic force is neglected due to that the velocity difference is zero. Since, the cluster statistical equation, Eq.(3), becomes as follows:

$$\frac{\partial}{\partial \ell_c} (\ell_c f) + \frac{\partial}{\partial G_c} \left( \ell_c f \right) = 0$$  \hspace{1cm} (13)

The zeroth perturbation approximation can be obtained by assuming \( \ell_c = \ell_c^{(0)} + \ell_c^{(1)} \) and \( G_c^{(0)} = 0 \), which the first order term, \( \ell_c^{(1)} \), accounts for the cluster convective and interactive effects. For steady-state process, the cluster evaporation or burning rate is expressed as
\[ \dot{\eta}^{[0]} = -k_i / \ell_c \]  

(14)

After some manipulations of eqs (4)-(6), the rate of change of total number of droplets and group combustion number for a cluster are expresses respectively as follows:

\[
\dot{N}_c = -k_i / \ell_c \quad \text{and} \quad \dot{G}_c = k_i / \ell_c^* 
\]

(15)

where \( k_i, k_c, \) and \( k_3 \) are constants associated with spray properties.

By the perturbation method similar to the case by Williams [10], we substitute \( \dot{\ell}_c = \dot{\ell}_c^{[0]} + \dot{\ell}_c^{[1]} \), \( \dot{G}_c = \dot{G}_c^{[1]} \), and \( f^{[n]} = f^{[0]} + f^{[1]} + \ldots \) into Eq.(13). Then collecting the terms of the same order of magnitude, the equation for \( f^{[0]} \) is obtained as follows:

\[
\frac{\partial}{\partial x} \left( \frac{\eta f^{[0]}}{\ell_c} \right) - \frac{\partial}{\partial \ell_c} \left( \frac{k_i}{\ell_c} f^{[0]} \right) = \mathcal{J}_c 
\]

(16)

where \( \mathcal{J}_c \) is a known factor after \( f^{[n+1]} \) has been calculated.

Here, in order to obtain the analytical solution of Eq. (16), we make further assumption of \( \dot{\ell}_c^{[0]} = 0 \) and \( \dot{G}_c^{[1]} = 0 \) wherein the cluster convective and interactive effects are neglected and the clusters undergo the iso-Gc evolutational process respectively. Thus, the equation (16) can be reduced to the form without any source terms in the right hand side and we first define the new dependent variable as

\[
\Psi(x, \ell_c) = k_i f^{[0]} / \ell_c
\]

(17)

to transform Eq.(16) to the function of two new independent variables,

\[
\xi = \frac{\ell_c^2}{2} \int_0^x k_i dx
\]

(18)

\[
\eta = \frac{\ell_c^2}{2} + \frac{1}{v} \int_0^x k_i dx
\]

(19)

By the transformation of variables, the resulting equation can be found as

\[
\frac{\partial \Psi}{\partial \xi} = 0
\]

(20)

Clearly, it shows that \( \Psi \) is function of \( \eta \) only. The initial cluster distribution at \( x=0 \) is assumed as Rosin-Rammler distribution function, \( g_0(\ell_c) \), then \( \Psi(0, \ell_c) = k_i g_0(\ell_c)/\ell_c \). And \( g_0(\ell_c) \) can be expressed as follows:

\[
g_0(\ell_c) = \frac{\eta_0 s}{\langle \ell_c \rangle_0} \left[ \Gamma \left( \frac{\ell_c}{\langle \ell_c \rangle_0} \right) \right]^{-1} \left( \frac{\ell_c}{\langle \ell_c \rangle_0} \right)^{\eta_0} \cdot \exp \left\{ -\frac{\ell_c}{\langle \ell_c \rangle_0} \Gamma \left( \frac{\ell_c}{\langle \ell_c \rangle_0} \right) \right\} 
\]

(21)

where \( \Gamma(x) = \int_0^x y^{\ell_c-1} e^{-y} dy \) is gamma function, and \( s \) and \( t \) are the shape factors of the initial distribution function.

In practical combustor, it is of importance to obtain the combustion efficiency. In this study, we assume the clusters are in the mode of external group combustion and the reaction occurs as soon as the fuel of cluster evaporates emanated from the cluster boundary, then the heat release rate is proportional to the cluster evaporation rate. So the combustion efficiency is defined as the change of the mass due to the evaporation or burning process between 0 and \( x \) to the initial mass of the spray at \( x=0 \) and given by

\[
\eta_c = 1 - \frac{\int_0^x \frac{1}{2} \pi \ell_c^2 f(x, \ell_c) d\ell_c}{\int_0^\infty \frac{1}{2} \pi \ell_c^2 g_0(0, \ell_c) d\ell_c}
\]

(22)

Rearrange the above equation as

\[
\eta_c = 1 - \frac{\int_0^x \frac{1}{2} \pi \ell_c^2 f(x, \ell_c) d\ell_c}{\int_0^\infty \frac{1}{2} \pi \ell_c^2 g_0(0, \ell_c) d\ell_c}
\]

(23)

So, the above equation shows that the combustion efficiency is in terms of the initial cluster distribution for the iso-Gc spray combustion and \( \eta \) is the variable, i.e. Eq. (19).

This results by the mathematical operations has been performed by Williams [9] following Probert's calculation [11] and the result can be expressed as follows:

\[
\eta_c = 1 - \frac{e^{-s}}{\Gamma \left( \frac{\ell_c}{\langle \ell_c \rangle_0} \right)} \int_0^\infty \left[ \left( y + z \right)^{\eta_0} - 2 \right]^{\eta_0} dy
\]

(24)

where the variables \( y \) and \( z \) are defined as follows:

\[
y = \left[ \frac{\Gamma \left( \frac{\ell_c}{\langle \ell_c \rangle_0} \right)}{\Gamma \left( \frac{\ell_c}{\langle \ell_c \rangle_0} \right)} \right] \left[ \left( \frac{\ell_c}{\langle \ell_c \rangle_0} \right)^2 - \frac{2}{\langle \ell_c \rangle_0^2} \int_0^\infty k_i dx \right]^{1/2} \]

(25)

\[
z = \left[ \frac{\Gamma \left( \frac{\ell_c}{\langle \ell_c \rangle_0} \right)}{\Gamma \left( \frac{\ell_c}{\langle \ell_c \rangle_0} \right)} \right] \left[ \frac{2}{\langle \ell_c \rangle_0^2} \int_0^\infty k_i dx \right]^{1/2} \]

(26)

For most values of \( r \), \( y<<z \), we can expand the first two factors in the integral of Eq.(24) in powers of \( y \) and keeping the first term to obtain the approximation of \( \eta_c \) as follows:

\[
\eta_c \approx 1 - \left( \frac{2}{s} \right)^{1/2} \frac{\Gamma \left( \frac{\ell_c}{\langle \ell_c \rangle_0} \right)}{\Gamma \left( \frac{\ell_c}{\langle \ell_c \rangle_0} \right)} y \left( \frac{\ell_c}{\langle \ell_c \rangle_0} \right)^{1/2} e^{-z}
\]

(27)
Figure 2 shows the combustion efficiency obtained by the above asymptotic expression is plotted against the dimensionless chamber length \( z \) by selecting \( t=s-4 \). By increasing \( s \) value, the combustion efficiency increases simultaneously.

The result is the same as the one of the droplet-based spray statistics by Williams [9]. According to Eq.(27), the exponent term dominates the \( \eta_c \) values and concludes that for smaller cluster size, but larger \( k_i \), \( s \), and \( t \), the better combustion efficiency is obtained in this study.

CONCLUSIONS

The advantages of the cluster-based spray statistical model are: (1) characterization of collective phenomena in practical cluster based spray combustion, and (2) determination of the clusters interior structures and burning characteristics, i.e. the distribution of the group combustion mode and its transition mechanisms. These two advantages lend to significant saving in the computational time than the droplet based spray model.

The calculation of the ideal iso-Gc cluster in steady-state spray combustion has been performed to examine the feasibility of the cluster statistical theory. And, the combustion efficiency for the ideal iso-Gc cluster has been calculated against the dimensionless chamber length to investigate the effects by varying the initial shape factors. The result has been found to be the same as the ideal droplet-based spray statistics by Williams [9]. In practical combustor, the clusters relax along the injection direction and undergo the group combustion modal transition. Further studies of the submodel for group combustion modal transition theoretically and experimentally will aid to develop the more realistic and reasonable computation for the cluster-based statistical spray modeling.

REFERENCES


![Fig.1 Schematic diagram of group combustion modal transition of ideal cluster.](image)

![Fig. 2 Combustion efficiency against dimensionless chamber length, z by the asymptotic expression in the ideal iso-Gc many cluster system.](image)