

**GAS TURBINE SPRAY DYNAMICS AND  
COMBUSTION SIMULATION DESIGN**

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## INTRODUCTION

A gas turbine combustor is a complex combustion device within which there exists a wide range of coupled, interacting physical and chemical phenomena. The liquid fuel used as the energy source must be atomized into smaller droplets in order to increase the surface of fuel exposed to the hot gases and to facilitate rapid gasification and mixing with the oxygen rich ambience. The combustion performance and emissions are mainly influenced by the atomization of the liquid fuel, the motion and evaporation of the fuel droplets and mixing of fuel and air. Spray dynamics and combustion studies are extremely important to determine flame stability behavior at widely varying loads, to ensure safety and efficient utilization of energy, as well as to better understand the mechanisms of pollutants formation and destruction.

The spray combustion process can be divided into five elements: atomization, transport, vaporization, unmixedness, and combustion. In general, liquid fuel is injected through a nozzle system into the combustor chamber and is atomized to form a spray of droplets. Figure 1 shows a simple spray plume structure. In the atomization region, the liquid fuel disintegrates into ligaments and droplets. The dense spray region has significant liquid volume fraction and includes secondary break-up of drops and ligaments as well as drop-drop interactions, such as collisions and coalescence. In the dilute spray region, droplets are well formed and have strong interaction with turbulent airflow. In general, a spray structure depends on the injection pressure difference, injector size, fuel viscosity, and fuel density. With the initial injection velocity, fuel droplets penetrate into the high temperature air. The fuel spray advances with time until droplets are vaporized by the hot air and combustion gas.

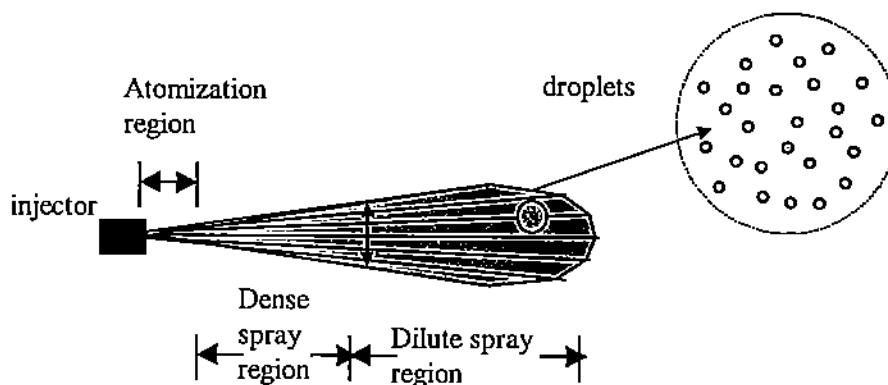


Figure 1. A Simple Spray Plume Structure

In a spray plume, fuel droplets heated by the surrounding hot air and combustion gas start to vaporize when the droplet temperature reaches the boiling point. The rate of vaporization depends mainly on the droplet size, boiling point and latent heat of fuel liquid, and gas

temperature. The fuel vapor mixes with the entrained air in the spray plume. The mixture starts to burn when the gas temperature reaches the ignition point and fuel/air mixture ratio is within the flammability limits. The burning produces heat and combustion products. The combustion products include mainly  $\text{CO}_2$ ,  $\text{H}_2\text{O}$ , and a small amount of pollutants such as  $\text{NO}_x$ .

The exchanges of mass, momentum, and energy between the gas and liquid phase in a spray combustor are critical features of the combustion process. Since the spray consists of droplets, it is reasonable to expect that the collective properties of the droplets would influence the bulk spray vaporization characteristics, which in turn determine the combustor performance. The rate of combustion in part of the combustor will be controlled by the rate of vaporization. Droplet trajectories affect the local vaporization rates, and droplet drag affects drop trajectories.

Spray combustion processes have long been a major engineering concern, and efforts have been made to achieve more economical use of fuels, better control of pollutants in combustion products, and longer lifetime of engineering devices. However, due to the complex nature of the spray atomization and combustion processes, many practical devices were designed based upon the trial-and-error approach (Kuo 1996), which is very expensive.

Recently, it has become apparent that an understanding of the mechanisms related to spray combustion is the key to the development of non-polluting and high performance devices. An important approach is to use advanced computer models for such fundamental studies and for developing practical devices. The development of advanced computers with large memories and high speed processors enables theoreticians to formulate and numerically solve comprehensive models with more detailed consideration of physical and chemical processes involved in spray combustion.

The simulation of flow field in a spray combustor is exceedingly complex and challenging. The spray combustion occurs in a three-dimensional, time-dependent system with two-phase turbulent flow, and incompletely understood chemical reactions. The combustion characteristics are greatly affected by the spray characteristics. The formation of  $\text{NO}_x$  and other pollutants are closely related to the spray combustion process itself. Other contributing factors include turbulence, radiation heat transfer, and fuel-air mixing. These factors are generally interrelated to one another. Computational fluid dynamics (CFD) models have become increasingly important in gaining insights of these processes for the improved combustion performance and reduced emissions while not compromising fuel economy.

Numerical spray combustion models have been proposed over the past two decades. The comprehensive reviews of spray and combustion models can be found in the literature (Chigger 1976, Law 1982, Faeth 1983, Crowe 1991, Sirignano 1993, Oefelein and Young 1996). In general, these models can be classified into three types: 1) two-fluid models which treat the particles as a continuum, (2) separated flow Lagrangian trajectory models which track individual particles in the gas field, and (3) direct numerical simulations.

Although much progress has been made in CFD model development for spray combustion in recent years, considerable work is still needed for the development of accurate and efficient

physical submodels. The submodels required in spray combustion include turbulence, spray injection, atomization, breakup, coalescence, turbulent dispersion, vaporization, ignition, combustion, wall heat transfer, and emissions ( $\text{NO}_x$ , etc.). Spray combustion modeling requires a knowledge of interactive transport processes which occur during gasification and combustion. Since the dimensions of a typical combustor are on the order of ten to one hundred centimeters while the drops are on the order of a few micros, and resolution on the order of the drop size is very difficult due to computational limitations, a cluster of droplets containing hundreds to thousands of representative drops is considered in spray modeling depending on the location of interest in the combustor.

### **DROPLET GROUP EFFECTS**

Sprays normally involve a large number of droplets. The simplest analysis is to estimate the combustion rate as a sum of combustion rate of isolated drops. However, interactions between the droplets alter the drag coefficient, change the flow field, increase or decrease the ignition delay depending on the denseness of the spray, compete for the heat and oxygen, and alter the fuel vapor distribution around drops.

The interactions of droplets with the environment and the droplets among themselves are generally termed as collective interactions or group effects. Collective phenomena can occur in a spatial extension ranging from few droplets to a large aggregate of droplets constituting a fraction or majority part of spray systems. The group phenomena, including group evaporation, group ignition, and group combustion, is the global collective behavior associated with the phase change, heat transfer, combustion and aerodynamics of many droplet systems under the effects of long range collective interaction. These phenomena are structurally different from that of the sum of each isolated droplet in the same hydrodynamic environment.

The collective phenomena of droplets have been observed by a number of experimental researchers. Experimental observations by Chigier and McCreath (1976) for the combustion of droplets in sprays showed that droplets in dense sprays vaporize as a group, with the group surrounded by an external flame zone during vaporization. The theoretical work of Chiu et al.(1982) attempted to categorize the experimental results with the application of group combustion theory. By simultaneous analysis of an inner heterogeneous region and an outer homogeneous gas phase region for a spherical droplet cloud, it was demonstrated that as the spray density increases or the droplet spacing decreases, the model of combustion first exists as single droplet combustion, then as internal group combustion, external group combustion, and finally external sheath combustion, as shown in Figure 2. A group combustion number ("G" number) was proposed to define the mode of combustion. Both internal and external group combustion occur, since the collective behavior of droplets in liquid sprays prevents air penetration and forms a nonflammable fuel-rich mixture in the core region of the spherical cloud, resulting no burning droplets therein, as shown in Figure 3.

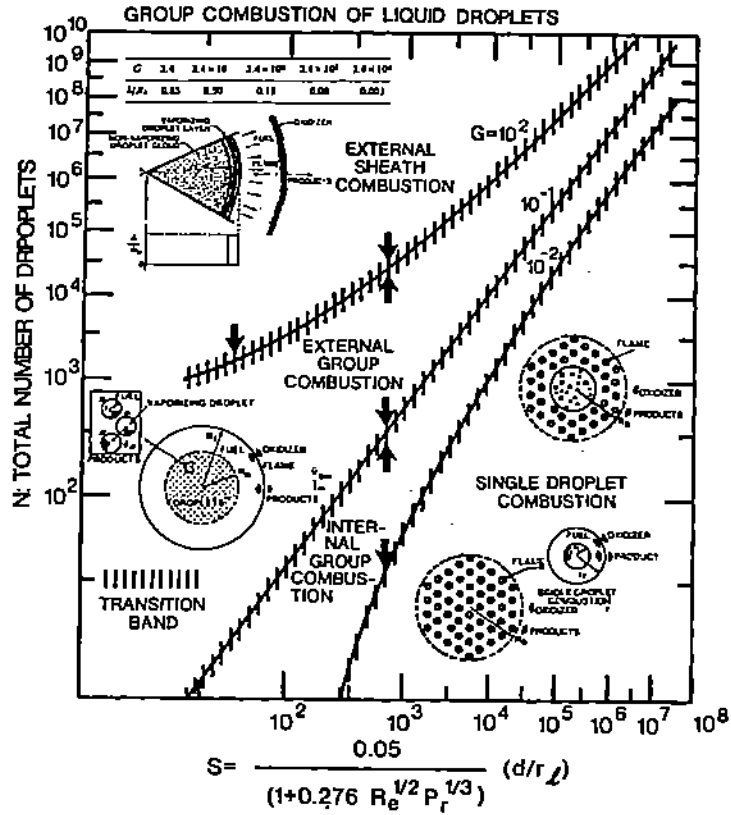


Figure 2 Four group combustion modes of a droplet cloud (Chiu et al. 1982)

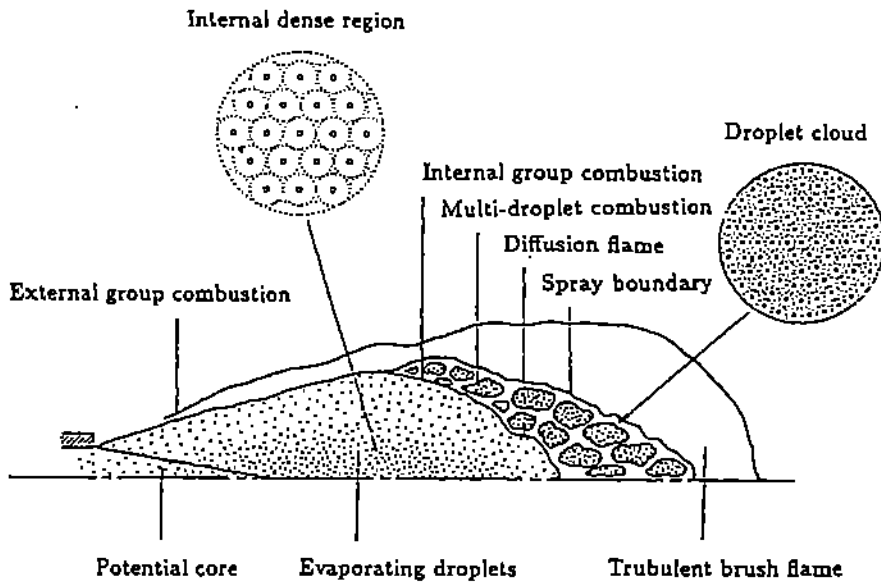


Figure 3 Schematic of liquid-spray group combustion (Chiu, 1999)

Group combustion phenomena in sprays, in general, have common features as those of the clouds, however, the collective effects tend to create axially elongated group flame in axial direction and lesser group effects in the direction perpendicular to the streaming flow. It is found that both the dense and dilute sprays exhibit the group combustion phenomena.

According to the group combustion model of Chiu et al. (1982), however, the droplets in a group are uniformly distributed and stationary droplets were assumed. The droplet vaporization rate is estimated by the classical single droplet vaporization theory (Williams 1985), with an empirical correlation for connective effects. Classical single droplet vaporization theory assumes an infinite surrounding of the droplet and neglects the interaction effects of adjacent droplets. However, with a reduction in the amount of gaseous oxidizer supplied to each fuel droplet from the surroundings, a reduced droplet vaporization rate is experimentally observed (Miyasaka and Law 1981) for interactive droplets. Bellan and Cuffel (1983) further demonstrated that an infinite droplet surrounding cannot provide adequate predictions for nondilute sprays.

The assumption of stationary droplet vaporization in the group combustion theory by Chiu is only justified for a large-droplet spray, since, due to a droplets' large inertia, the relative motion between droplets and their surrounding gas-phase flow is significantly small so that the convective effects on droplets vaporization cannot be neglected. However, the theory overestimates convective effects on the droplet vaporization rate of small droplet sprays in order to account for the effects of droplet movement on vaporization in sprays. Bellan and Harstad (1990) have developed a nondilute convective droplet vaporization model. This model considers both gas and droplet velocities at the cloud surface by solving the gas and droplet momentum equations, respectively, with an assumption of self-similar radial velocities for gas and droplet flows inside the cloud. The analytical results using this model exhibit very different characteristics from those in the group combustion of Chiu et al. (1982).

Jiang and Chiang (1994) studied vaporization of a dense spherical cloud of droplets at subcritical and supercritical conditions. They conducted a complete variable transient analysis of both the inner heterogeneous region and an outer homogeneous region comprised of a spherical cloud of monosized droplets distributed uniformly. The analysis included effects of ambient gas solubility, property variation, thermodynamic non-ideality, and transient diffusion. However, the analysis was conducted for only one single spherical cloud in a quiescent hot nitrogen.

Annamalai et al. (1995) tried to implement the group combustion theory to the CFD modeling of coal/char particle combustion. An effectiveness factor was introduced to account for the group combustion effects.

Recently, Kawahara et. al. (1999) attempted to investigate the applicability of group combustion theory to real spray combustion situations. Various cluster sizes, consisting of inhomogeneous droplets, are characterized by a turbulent coherent vortex and the flowability of individual droplets.

The experimental investigation indicated that the interaction between the turbulent coherent vortex structure and small droplets generates the clustering of the droplets and results in their

group combustion as shown in Figure 4. The Stokes effect causes the small droplets to be entrained into the turbulent vortices, to form droplet clusters. Each droplet cluster is formed by a homogeneous collection of droplets with the same momentum. Multiple clusters are formed from these homogeneous clusters, and can simultaneously include various cluster sizes. Moreover, these droplet clusters cause external or internal group combustion in actual spray flames. In contrast, large droplets travel individually along the spray cone, showing no group combustion behavior. The “compound-cluster combustion” is defined as the droplet combustion of multiple clusters formed by various sizes of smaller homogeneous droplet clusters formed by a coherent turbulent structure. This concept is especially useful for the dense spray combustion found in gas turbines.

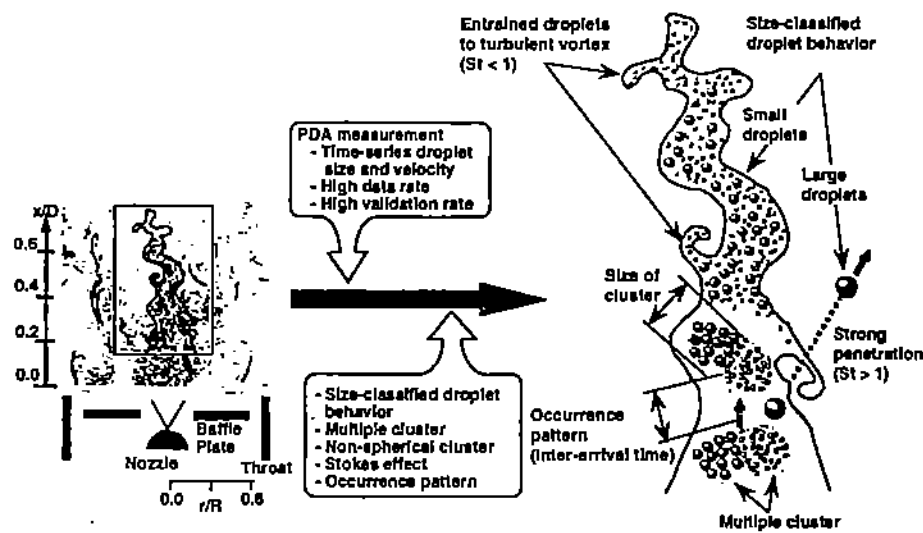


Figure 4 Concept of “compound-cluster combustion” (Kawahara et al. 1999)

## RESEARCH OBJECTIVE

The major objective of this research is to simulate the interactive transport processes in the dispersion, evaporation and combustion of droplets and droplet groups. Both dense and dilute spray regions will be included. The group theory will be implemented in the modeling of spray combustion in a gas turbine combustor. Simplified group numbers for the CFD simulation of spray dynamics and combustion will be defined. This will provide realistic and accurate spray model for the simulation of actual physical processes.

## TECHNICAL APPROACH

The technical approach is to develop a spray model to include the droplet group effects. These include droplet dispersion, evaporation, and combustion.

## Droplet Dispersion and Evaporation

The droplet dispersion and evaporation are two key processes in the spray combustion. They govern the fuel-air mixing process and consequently affect the performance of liquid-fired combustion systems such as flame stability and  $\text{NO}_x$  and other pollutant emissions. The precise prediction of the evaporation time and the movement of droplets is crucial for optimum design and performance of modern gas turbine combustion chambers

During the transport of droplets in a turbulent spray, droplets are dispersed by turbulence. In a realistic spray model, this phenomena should be considered not only in the movement of a cluster of droplets, but also within the cluster. A group modeling of droplet dispersions in nonevaporating sprays has been developed (Zhou and Yao 1988, 1992, 1994). It uses droplet groups to represent the spray. Each group contains many droplets, having the same size and properties. When a group of droplets leaves the exit of the nozzle, these droplets are all originally located at one point and then dispersed away due to turbulence. Therefore, a droplet group has dimensions and grows up due to the turbulent droplet dispersion during its traveling. The droplet distribution within a group is described by a Gaussian probability density function. The instantaneous location of center point of a group is determined from Lagrangian tracking.

The group model of droplet dispersion closely simulates a real flow, because in a real flow the droplets within a group are dispersed by turbulence instead of staying at one point. This is consistent with the conceptual situation that if the droplets in a small region of a spray are dyed with a red color, this dyed group of droplets will disperse in time within the spray. The group approach essentially traces this dyed group of droplets in the spray.

In a spray-fired reaction, it is the vapor that burns. As a result, the step from atomization to combustion requires vaporization. Vaporization has proven to be especially difficult to characterize within the spray. The study of the vapor concentration within the spray is progressing slowly but is critically needed to bridge the gap between the fuel injection process and the resulting combustion. To develop simplified but accurate evaporation models is one of the essential types of droplet dynamics studies required for successful spray combustor analysis. These models must be efficient to calculate the average characteristics of droplet group behavior in the combustor with reasonable approximations.

The accurate prediction of vaporization rate of droplets depends on 1) droplet surface temperature since the fuel vapor mass fraction at the surface generally has an exponential dependence on this temperature, 2) realistic representation of gas-phase convection, 3) property effects because the thermophysical properties on the gas film outside the droplet can vary significantly during the droplet lifetime at its traveling, and 4) droplet trajectory calculations that determine the instantaneous droplet locations and hence the local environment for calculating the vaporization rate.

Interactive evaporation studies are important from two perspectives: 1) many finer droplets and droplets in a spray core simply vaporize without combusting (e.g. dense clouds); 2) solutions

for vaporization can also be applied to diffusion controlled combustion with suitable transformations.

### Research Plan

The research for the group effects on the droplet dispersion and evaporation includes the following tasks:

- 1) Further validation of group modeling for droplet dispersion in non-evaporating sprays by comparing the computational results with the recent published experimental data.
- 2) Development of a new group modeling for droplet evaporation in turbulent sprays with the consideration of the multiple-droplet interaction effects on droplet vaporization within a droplet group.
- 3) Validation of the new group evaporation modeling by comparisons between computational results and published experimental data.
- 4) Study parametric effects on droplet dispersion and evaporation.

### **Group Combustion**

The group combustion phenomena has been observed by experimental research and characterized by the group combustion theory. Due to the complexity and idealized assumptions, the implementation of the group combustion in the spray combustion modeling has been limited. A realistic and accurate spray combustion modeling is essential to determine the effects of turbulent mixing, fuel and air parameters, etc. on the overall performance of the combustor.

### Research Plan

The research for the spray combustion modeling with group combustion includes the following tasks:

- 1) Thoroughly exam all the assumptions in the group combustion theory. .
- 2) Classify the modes of combustion in the gas turbine combustor.
- 3) Define simplified group numbers for the group effects on combustion
- 4) Implement the group combustion model in KIVA code.
- 5) Validate the group combustion modeling by comparisons between computational results and published experimental data.
- 6) Investigate parametric effects on group combustion.

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