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LIQUID-PROPELLANT DROPLET VAPORIZATION AND COMBUSTION IN HIGH PRESSURE ENVIRONMENTS

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I. Research Objectives and Potential Impact on Propulsion

Many practical liquid-propellant rocket propulsion systems involve droplet vaporization and spray combustion in high-pressure environments. Liquid propellants are usually delivered to combustion chambers as a spray of droplets, which then undergo a sequence of vaporization, ignition, and combustion processes at pressure levels well above the thermodynamic critical points of the liquids. Under these conditions, droplets initially injected at subcritical temperatures may heat up and experience a thermodynamic state transition into the supercritical regime during their lifetimes. Consequently, the sharp distinction between gas and liquid disappears, and the entire system exhibits many distinct characteristics which conventional droplet theories developed for low-pressure cases can not deal with.

Attempts to study droplet vaporization and combustion in the supercritical regime have been made for three decades. While these studies have provided significant information to understanding the physics and chemistry of droplet vaporization and combustion at high pressures, a number of fundamental problems remain unresolved. Much of the previous work employed certain assumptions and empirical correlations which were extrapolated from low-pressure cases and involved a considerable number of uncertainties. In order to correct the deficiencies of existing models for high-pressure droplet vaporization and combustion, a fundamental investigation into this matter is essential. The specific objectives of this research are:

1. to acquire basic understanding of physical and chemical mechanisms involved in the vaporization and combustion of isolated liquid-propellant droplets in both stagnant and forced-convective environments;
2. to establish droplet vaporization and combustion correlations for the study of liquid-propellant spray combustion and two-phase flowfields in rocket motors; and
3. to investigate the dynamic responses of multicomponent droplet vaporization and combustion to ambient flow oscillations.

II. Current Status and Results

During this report period, emphasis has been placed in three areas: (1) assessment of constitutive relations and property evaluation techniques for multicomponent mixtures at high pressures; (2) analysis of droplet vaporization at near and supercritical conditions; and (3) investigation of droplet combustion at near and supercritical conditions. The major status of our work is given below.

1. Assessment of Constitutive Relations and Property Evaluation Techniques for Multicomponent Mixtures at High Pressures

One of the fundamental difficulties in the study of supercritical droplet vaporization and combustion is the lack of reliable data on thermodynamic and transport properties of each constituent species as well as of the mixture at high pressures. The problem becomes even more severe at near-critical conditions (within a few percents of the critical temperature). The thermophysical properties usually exhibit anomalous behavior, and become very sensitive to both temperature and pressure due to a transition of molecular ordering or to small-scale circulation effects resulting from the migration of clusters of molecules . When generalized correlations are used, these property irregularities are smoothed out and may lead to inaccurate results. During the last year, efforts have been made continuously to assess (and occasionally establish) various property evaluation techniques and constitutive relations for multicomponent mixtures at high pressures. These relations include equations of state and mixing/combining rules with high-pressure corrections. In addition, a generalized methodology and an efficient numerical algorithm were developed to treat thermodynamic vapor-liquid phase equilibria for liquid propellants at high pressures. Specific outputs from the phase-equilibrium analysis include:

- latent heat of vaporization
- solubility of ambient gas in the liquid phase
- liquid and gas-phase species concentrations at the droplet surface

2. Analysis of Droplet Vaporization at Near and Supercritical Conditions

The specific objective of this work is to analyze, from first principles, the detailed physical processes involved in multicomponent liquid-propellant droplet vaporization at high pressures. The formulation is based on the full time-dependent conservation equations, and accommodates a thorough treatment of property variations and vapor-liquid phase equilibrium. Because of its completeness, the model enables a systematic examination of the droplet vaporization characteristics in a high-pressure environment. In particular, the effects of ambient gas solubility, property variation, transient diffusion, and multicomponent transport on the droplet behavior are investigated in depth.

3. Investigation of Droplet Combustion at Near and Supercritical Conditions

The analysis of droplet combustion extends the model for droplet vaporization and accommodates finite-rate chemical kinetics. Consequently, various combustion related problems (such as ignition, flame development, extinction, etc.) can be treated in detail. Specific results of this task include:

1. thermodynamic conditions for reaching supercritical combustion;

2. complete time history of the flowfield and interface transfer rates for evaporating or burning droplets at various ambient conditions; and
3. ignition criteria for a variety of liquid-propellant and ambient-gas situations.

The influences of volatility and miscibility of the liquid constituents on droplet vaporization and combustion characteristics are also addressed.

Calculations were first carried out to study the combustion process of a single droplet in a stagnant air environment, due to the availability of experimental data for model validation. At $t = 0$, a pure n-pentane droplet with a diameter of 100 µm is exposed suddenly to air. The initial droplet and air temperature are 300 and 1200 K, respectively. Figure 1 shows the distributions of the gas-phase temperature at various times. The air pressure is 50 atm. Initially, as a result of heat feedback to the droplet, the liquid fuel starts to evaporate. The resultant vapor then ignites with the ambient air, causing a small hump in the temperature profile at $t = 1$ msec. The rapid increase in the gas-phase temperature in the subsequent stage suggests the onset of flame development. Figure 2 presents the corresponding temperature distributions in the liquid phase. The penetration of thermal wave in the droplet is clearly observed.

Figure 3 presents the histories of the square of droplet diameter at various pressures. The droplet surface regression rate increases with pressure mainly as a result of reduced heat of vaporization at high pressures. In the initial period, the droplet diameter decreases slowly with only vaporization involved in the regression process. The regression rate then increases rapidly immediately after the onset of flame development in the gas phase, due to the enhanced heat transfer to the liquid phase.

The analysis was compared with the conventional low-pressure model in which Raoult's law is employed to determine the species concentrations at the droplet surface before the occurrence of the critical state. In addition, the ambient gas solubility is ignored and the latent heat of vaporization is taken to be that of the saturated pure liquid. Figure 4 presents the time variations of the square of the droplet diameter at $p = 50$ atm in accordance with both the high- and low-pressure models. Because of its inability to predict the correct droplet surface condition, the low-pressure model overpredicts the surface temperature, thereby leading to excessive volumetric dilatation. However, this effect is offset by the underpredicted latent heat of vaporization in the later stage of the droplet lifetime and consequently causes a faster regression rate. In regard to the mass evaporation rate, the discrepancy between these two models appears to be even greater due to the lower liquid density predicted by the low-pressure model.

VI. Proposed Work for Coming Year

Future work on high-pressure droplet vaporization and combustion will consist of the following tasks.

1. Vaporization and Combustion of Cryogenic Propellant Droplets

The specific objective of this task is to enhance our current understanding of cryogenic propellant droplet combustion at supercritical conditions. The work represents an outgrowth of the analysis developed in the last year and incorporates several unique characteristics of cryogenic propellants into the model. Special attention will be focused on the evaluation of thermophysical properties and establishment of constitutive relationships. Representative propellant combinations (such as LOX/RP-1 and LOX/LH_2) will be treated to simulate actual motor conditions.

2. Dynamic Responses of Droplet Vaporization and Combustion to Ambient Flow Oscillations

The purpose of this work is to identify some of the combustion instability driving mechanisms associated with supercritical droplet vaporization and combustion. The analysis will begin with essentially the same as that for a steady environment, but with appropriate modifications of the outer boundary conditions for the gas phase, various pressure-coupled combustion response functions can be obtained. Cases of both pulsed and periodic oscillations will be examined carefully. Results will be used to establish useful correlations for existing analyses of linear combustion instabilities in rocket motors.

3. Droplet Vaporization and Combustion in a Forced Convective Environment

The primary objective of this task is to investigate the effects of forced convection on droplet vaporization and combustion processes. The work will extend the analysis developed in the last year and solve the multi-dimensional flowfield surrounding the droplet. Results can be used to assess and/or establish useful correlations for heat, mass, and momentum transfer rates under forced convective situations. Special attention will be paid to the applications to the study of liquid-propellant spray combustion and two-phase flowfields in rocket motors.

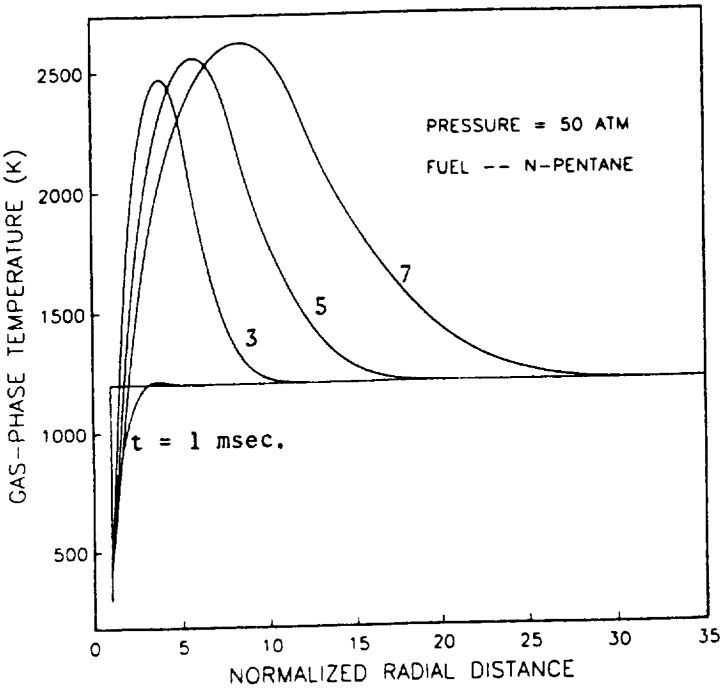

Fig. 1. Distributions of Gas-Phase Temperature at Various Times.

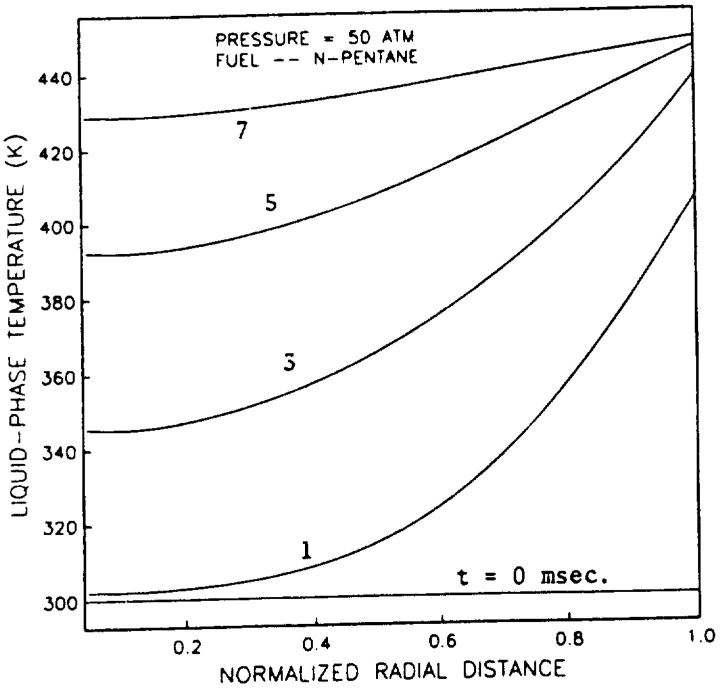

Fig.2. Distributions of Liquid-Phase Temperature at Various Times.

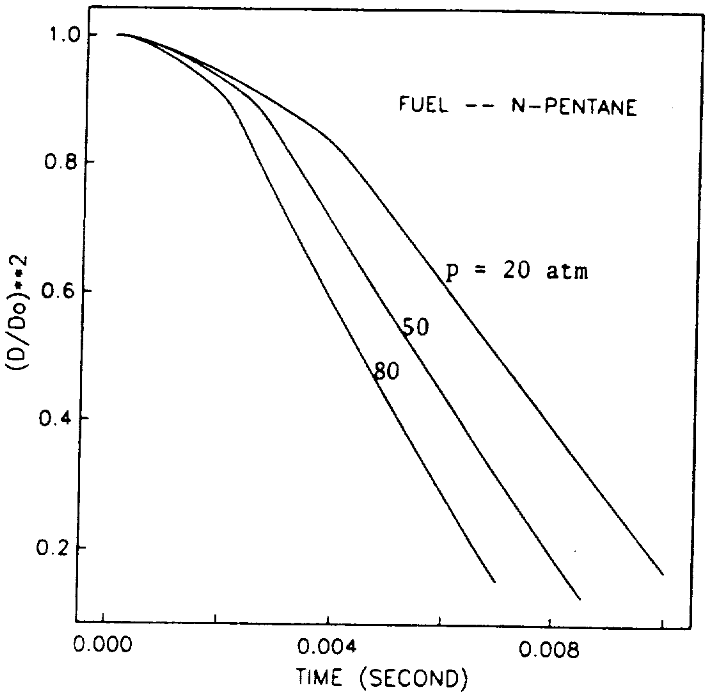

Fig. 3. Time Histories of the Square of Droplet Diameter at Various Pressures.

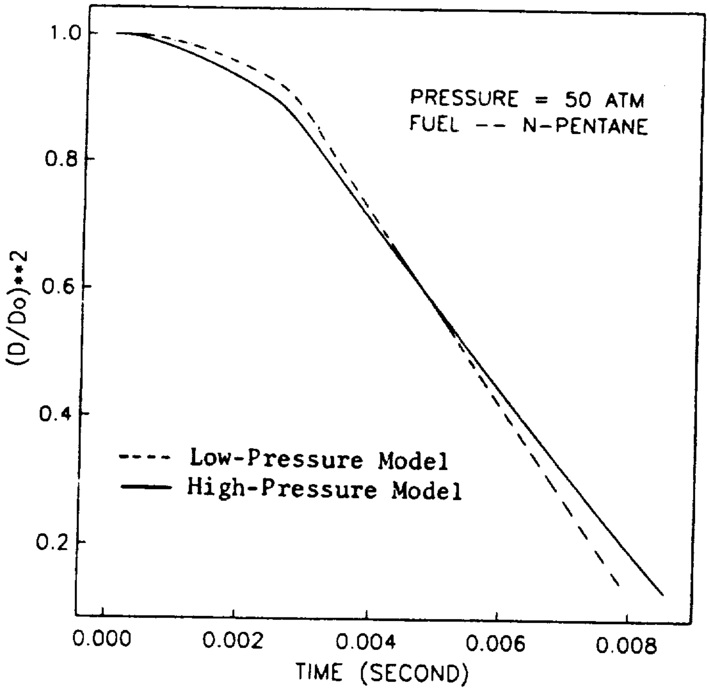

Fig. 4. Time Histories of the Square of Droplet Diameter at p = 50 atm.