SPRAY COMBUSTION STABILITY PROJECT

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ABSTRACT

This report summarizes research activity on the Spray Combustion Stability Project, characterizes accomplishments and current status, and discusses projected future work. The purpose is to provide a concise conceptual overview of the research effort so the reader can quickly assimilate the gist of the research results and place them within the context of their potential impact on liquid rocket engine design technology. Therefore, this report does not elaborate on many of the detailed technical aspects of the research program. Technical issues are addressed in substantial detail in recent AIAA papers which were presented at the 26^{th} Joint Propulsion Conference in July 1990 and are referenced herein.

I. Project Synopsis

The Spray Combustion Stability project is a research program which is cost shared by CASP and Rocketdyne Div., Rockwell Int. Corp. The principal goal of the project is to advance liquid rocket engine design technology, specifically analysis of resonant combustion instability. Project work began in fiscal year 1989 and is scheduled to continue through fiscal year 1991.

The specific objectives of the research effort as elaborated on in the Statement of Work (SOW) is to evaluate spray combustion physical submodels for application in CFD instability analyses. Submodels found deficient were to be refined or replaced by newly developed ones. In either case, the resulting submodels were to be validated with experimental data insofar as possible.

In the original SOW, Rocketdyne's ARICC spray combustion code was to serve as the testbed for submodel evaluation with improvements incorporated as second-generation code developments. During the initial part of the first year's effort, it became apparent that evaluation using the ARICC code was a tedious and lengthy procedure. Since a large amount of computer time and some degree of expertise with the code was required to obtain a converged solution, productivity was low. A decision was therefore made to evaluate and develop submodels independent of and external to ARICC. This method proved not only more efficient but more practical since physical processes could be studied independently. Final implementation of submodel improvements is being left to the discretion of code developers and users at Rocketdyne.

Based on a thorough review of the scientific literature and some contemplative reasoning, we have thus far concentrated our attention on two spray combustion physical processes which are inherently important in the proper assessment of resonant combustion instability and which are either inadequately or inefficiently simulated by current mathematical submodels. The physical processes considered are (a) high-pressure droplet gasification and (b) dispersion of the spray droplets and the associated spatial distribution of mass and energy release. These processes have been the focus for submodel development during this project. The technical progress achieved thus far is summarized in the following sections.

II. Technical Discussion

The guiding rationale in selecting spray combustion physical submodels for evaluation was the known or potential role of a particular physical process as a combustion instability mechanism or the pressing requirement to simulate a particular physical process with greater accuracy and efficiency during unstable combustion than is normally required during stable combustion. The basis of selection led to consideration of the two physical processes of high-pressure gasification and droplet dispersion. Other physical processes are certainly fundamental to combustion instability, but these seemed to have the greatest potential for significant improvement within the scope and limits of this project.

Because liquid rocket engines typically operate at high chamber pressures, generally above the critical pressure of the propellants, the process of high-pressure droplet gasification plays a fundamental role in combustor dynamics. This role can become even

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more central when considering acoustic pressure fluctuations associated with resonant instability. In instability analyses, it has become a common assumption to consider propellant vaporization as a rate-controlling feedback mechanism for Rayleigh-type driving of the acoustic waves. Thus, because the vaporization process is demonstrably sensitive to pressure, proper assessment of droplet gasification can be essential to the validity of the instability analysis. In many cases, this submodeling issue has been averted by the application of low-pressure models under high-pressure conditions with the hope that the low-pressure model sufficiently approximates the high-pressure process. Evaluation of high-pressure gasification submodeling was therefore seen to be and became a major concern of this research program.

Accurate description of droplet dispersion and the associated spatial distribution of mass and energy release was also found to be an important physical spray process that needed submodeling upgrades in obtaining an efficient technique suitable for instability analyses. The currently accepted modeling philosophy is to represent many physical droplets by a computational parcel which interacts with the flow as a single effective droplet. That is as a point source for interphase transport. To simulate dispersion due to turbulent fluctuations, a stochastic sampling procedure is conventionally utilized. However, the difficulty with this approach, particularly for instability analysis, is essentially one of computational efficiency. To obtain reasonable dispersion results using the current stochastic procedure, a statistically significant number of parcels (typically several thousand) must be evaluated. Similarly, to prevent the generation of large fluctuating interphase transport sources in space and time (computational shot noise), a large number of parcels must be evaluated to more uniformly distribute the source effects throughout the computational cells. The level of accuracy desired for instability analyses therefore imposes severe computational penalties by requiring an excessive number of parcels using current stochastic sampling techniques. Improved modeling of the dispersion process was needed and this problem has been addressed in our research effort.

High-Pressure Droplet Gasification

The high-pressure droplet gasification modeling effort has been ongoing since inception of this project. Early submodel development has been summarized in a 1989 interim report[1] with later developments included in a recent AIAA conference paper.[2] The reader is referred to these supplementary publications for mathematical details and graphical presentation of computational results. The intent of this section is to present a brief conceptual description of the formulated submodel and a summary of performance evaluation including current capabilitites and limits. Tasks accomplished in the high-pressure droplet gasification submodeling effort are summarized in Table 1.

TABLE 1
Gasification Modeling Accomplishments

(1) Formulation of transport model for subcritical vaporization including surface regression, bulk thermal expansion, and internal circulation effects.
(2) Implementation of a high-pressure thermodynamic vapor-liquid equilibria model to account for real-gas effects and ambient-gas absorption.
(3) Evaluation of submodel with experimental data for n-heptane droplets vaporizing in hot, high-pressure nitrogen gas.
(4) Calibration of thermodynamic model for O_2/H_2 phase equilibria.
(5) Analysis of LOX droplets vaporizing in high-pressure, hydrogen-rich gas.

The aim of the theoretical development was to obtain a realistic physical submodel with reasonable computational efficiency. A detailed comprehensive analysis is not our purpose. In particular, the desire was to bring high-pressure effects on thermodynamic and transport processes into consideration while maintaining mathematical simplicity. This required reformulation of the basic transport model and inclusion of a high-pressure multicomponent thermodynamic vapor-liquid equilibria model. In addition, supercritical gasification had to be considered since sufficiently high-pressures can drive the droplet surface to the thermodynamic critical state.

The reformulated subcritical transport equations for the gas-phase are based on the quasi-steady assumption with inclusion of surface regression and bulk thermal expansion effects which are neglected in low-pressure models. Transport is modeled as a spherically-symmetric, diffusion-controlled process with empirical corrections for convective effects. Liquid-phase energy transport is currently handeled using 3 alternative models: (1) infinite conductivity model, (2) pure conduction model, and (3) effective conductivity model. The effective conductivity model is the most sophisticated approach and attempts to account for internal circulation effects.

Because real-gas effects and ambient-gas absorption becomes important at higher pressures, a high-pressure thermodynamic model has been implemented to provide the species concentration boundary condition at the drop surface and to obtain a corrected enthalpy of vaporization which can devi-

ate substantially for the pure component latent heat of vaporization. The model is currently applicable to weakly polar molecules and mixtures containing quantum gases (eg. hydrogen). There are some extensions of the model that can handle aqueous mixtures which try to account for the large dipole moment of the H_2O molecule, but they are highly approximate.

Once the droplet surface reaches the critical state, a supercritical gasification model is needed. Unfortunately, there is as yet no definitive experimental description of the critical transition and supercritical gasification processes. It is therefore necessary to resort to ad hoc schemes based on plausible presuppositions. The simplest approach is to assume flash supercritical transition of the entire droplet, but this seems unrealistic since the droplet should actually have internal temperature and concentration gradients. To account for a presumed finite-rate process, two alternative schemes are utilized. In one scheme, the basic idea is to transform to a constant temperature boundary condition corresponding to the critical mixing point and apply the subcritical diffusion-controlled transport relationships. This is considered as a representative lower limit for the gasification rate. An alternative scheme is to model the process using an empirical stripping mode breakup expression. This is considered as a representative upper limit for the gasification rate.

A FORTRAN computer code was developed to evaluate the proposed submodel. Initially, validation calculations were made for comparison with experimental data on n-heptane droplets vaporizing in high-pressure nitrogen gas. Agreement was good verifying the basic validity of the code and the subcritical transport model. Because of unavailable experimental data, there was no way to evaluate the supercritical gasification schemes.

The code was further modified to consider LOX droplets vaporizing in high-pressure, hydrogen-rich gas since this propellant combination is of great interest for high-performance liquid rocket engines. The thermodynamic model was calibrated using high-pressure solid oxygen/hydrogen equilibria data. High-pressure effects on thermodynamic and thermophysical properties were also considered. Representative computations were then made to demonstrate the transition process from steady-state vaporization to fully transient heat-up to the critical state with subsequent supercritical vaporization. Presentation and discussion of the results are in an accompanying AIAA paper.[2]

Additional validation with experimental data would be desirable. It should also be stated that formulations for including an envelope flame have been constructed but not included in the code because of the additional complications which would result from the required extension of the thermodynamic model at this time. Extension of the thermodynamic model for a wider range of substances including polar molecules (eg., H_2O) will be necessary before practical implementation in a comprehensive combustor code. Nevertheless, the model is currently useful for examining the general effect of pressure on the vaporization process and the resulting influence on combustion instability.

Turbulent Droplet Dispersion

The turbulent droplet dispersion submodeling effort began in the latter part of 1989. Based on the difficulties encountered with current dispersion models as previously discussed, the conceptual basis for a novel modeling technique aimed at avoiding these deficiencies was conceived. Development of the model has proceeded at a quick pace, and technical progress has been summarized in a recent AIAA conference paper.[3] The reader is referred to this publication for mathematical details and presentation of computational results. This section will be devoted to providing a conceptual description of the model and a report of model evaluation efforts to date. Tasks accomplished in the droplet dispersion submodeling effort are summarized in Table 2.

The fundamental concept of this new model was to combine a statistical spatial distribution representation for each parcel with a statistical turbulent dispersion width transport scheme. Specifically, each parcel represents a group of physical droplets through a normal probability density function (PDF) in space. The instantaneous mean position of each parcel PDF is determined from Lagrangian tracking using either a deterministic or stochastic sampling procedure. In addition the variance of each parcel PDF is determined from a statistical, turbulence-induced mean-squared dispersion which depends upon previous parcel interactions with the characteristic turbulence

TABLE 2
Dispersion Modeling Accomplishments

(1) Conceptualization and mathematical formulation of a novel model for turbulent droplet dispersion with PDF representation for droplet parcels.
(2) Proof-of-concept computations for new model in comparison with conventional point source model for nonevaporating particles injected into nearly homogeneous turbulent flow.
(3) Proof-of-concept computations for new model in comparison with conventional point source model for nonevaporating particles injected into a round turbulent jet.

properties of the flow. This approach allows for a smooth distribution of source terms over the grid cells with reduced sampling requirements for obtaining the dispersion width. A concept schematic of the model with stochastic sampling for the mean parcel position is depicted in Figure 1.

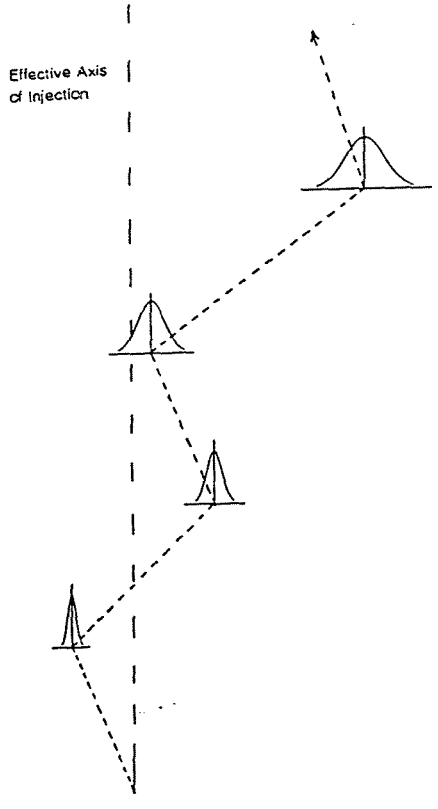

Figure 1. Concept schematic of proposed dispersion width transport model with stochastic sampling for mean parcel position.

The dispersion width transport scheme is the key to increased efficiency since it makes use of statistical generalizations allowing reduction in sampling. The idea is to retain the concept of parcels interacting with a sequence of turbulent eddies as in the stochastic point source method but to generalize it by formulating the mathematics in such a way to allow statistical treatment. This is accomplished by repeated application of the linearized particle equations of motion for each eddy interaction with successive substitution such that a single expression is obtained describing dispersion in terms of the turbulent velocity fluctuations in each eddy, parcel/eddy interaction times, and the inertial time lag for each interaction. By introduction of a characteristic turbulent velocity fluctuation, it then becomes possible to express the mean-squared dispersion as the variance of the PDF after the n^{th} eddy in terms of preceeding parcel/eddy interaction properties. With the mean and variance of each parcel PDF, it is possible to combine the PDF distributions to obtain the physical particle distribution profile.

After following through with the described mathematical formulation procedure, model evaluation was considered. Two simple test cases chosen were for nonevaporating particles injected into nearly-homogeneous grid-generated turbulence and into a round, turbulent air jet. In both cases particle loading was small and interphase momentum coupling was neglected. The new model was to be compared with the stochastic point source model which has been previously validated in the scientific literature. FORTRAN computer codes were developed for these purposes and computations carried out. Presentation and lengthy discussion of the results are in the accompanying AIAA paper.[3]

In summarizing these results, the new dispersion width transport model was found to have significantly improved computational efficiency over the stochastic point source method while producing good approximations for the physical particle spatial distribution profiles. Two schemes were considered for evaluating the mean parcel position: (a) Deterministic Dispersion Width Transport Model (DDWT) and (b) Stochastic Dispersion Width Transport Model (SDWT). For nearly-homogeneous turbulence, deterministic tracking with a single parcel (DDWT model) was found to sufficiently sample the turbulence properties and produce accurate dispersion results as shown in Figure 2. For the jet flow with nonhomogeneous turbulence, however, deterministic tracking was inadequate. More thorough sampling of the turbulence was required through stochastic tracking of the mean parcel position (SDWT model). Computational efficiency was still impressive, though, as dispersion results using no more than 200 parcels were found to produce a good approximation to dispersion results using 20,000 particles in the stochastic point source methodology. An example of such results is shown in Figure 3.

The potential impact of this new dispersion model on the accuracy and efficiency of spray combustion CFD codes, particularly with regard to instability analyses, is significant. Extension of the model to include evaporating droplets with interphase coupling of mass, momentum, and energy is obvious follow-up work for the future. It appears that additional adaptation for considering acoustic perturbations and improvements in efficiency are also possible, and model development is continuing.

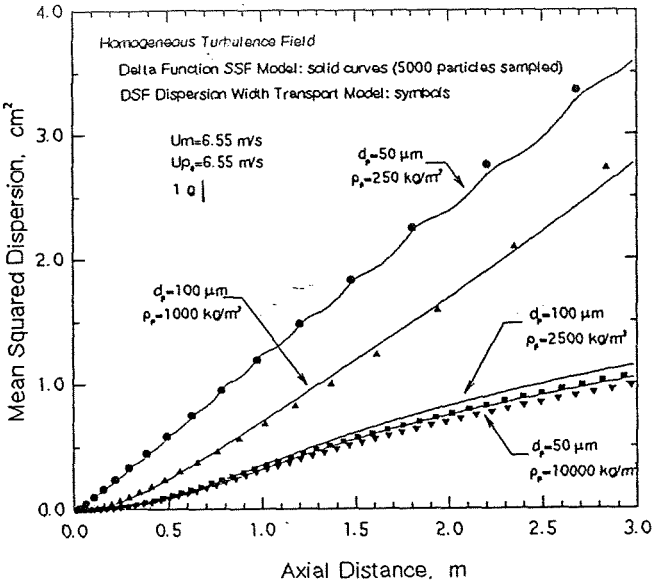

Figure 2. Proof-of-concept computations for the deterministic dispersion width transport model.

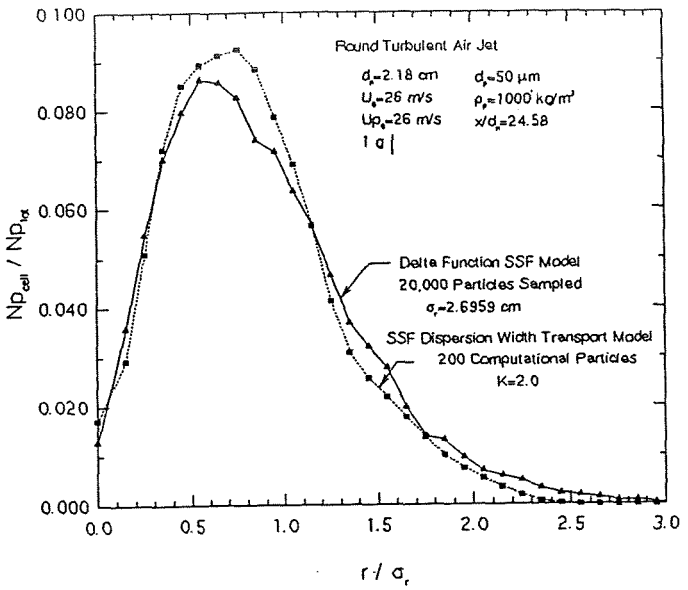

Figure 3. Proof-of-concept computations for the stochastic dispersion width transport model.

III. Project Direction

Research emphasis during the final phases of this project will be on development of the droplet dispersion model. The potential impact of this method on spray combustion modeling is sufficiently great to justify concentrated effort. Further development of the high-pressure droplet gasification model will require new experimental data which probably won't be available during the project lifetime. However, limited effort will be devoted to assessing the general influence of pressure on vaporization-controlled combustion instability using the current model.

Tentative plans for systematic development of the droplet dispersion model have been made. Work has already began on extension of the model to include evaporation effects.. Based on experimental work in the literature, evaluation of vaporizing monodispersed methanol droplets in a methane-fuelled jet diffusion flame is in progress. Eventually, interphase transport coupling will be addressed in an effective manner. Other plans include improving the efficiency of the procedure by limiting the number of interactions allowed to influence dispersion in a given eddy. Extension to recirculating flows and adaptation for acoustic perturbations are also under consideration at this time.

A simplified assessment of the high-pressure vaporization process on combustion instability is being undertaken concurrent with the droplet dispersion model development. The basic concept of this approach is to apply a simple analysis of the instability response factor using low-pressure and high-pressure vaporization models to quantify the effect of pressure on the feedback mechanism. Such an approach has practical application as a combustion response module for combustion instability design codes. The droplet vaporization code has been modified to simulate a simplified 1-D combustor with n-heptane droplets vaporizing in the stoichiometric products of combustion with oxygen. Sinusoidal oscillations characteristic of acoustic mode instability in a cylindrical chamber are superimposed on the combustor flow. The high-pressure thermodynamic model takes account of real-gas effects including H_2O molecules using an approximate engineering model. Absorption of ambient-gas into the droplet is neglected, however. The analysis is limited to subcritical vaporization since supercritical gasification models are dubious. A total of 36 droplets are injected per cycle of oscillation with the resulting vaporization histories combined to obtain the instability response factors based on the Rayleigh criteria. The response factors are to be evaluated for a given mean chamber pressure as a function of frequency. Comparison

of results for low-pressure and high-pressure vaporization models will yield a measure of importance of high-pressure vaporization effects on resonant combustion instability. The greater the response factor the greater the tendency to drive instability. Preliminary computations at moderate pressures indicate that consideration of high-pressure effects implies a substantial increase in the response factor. This increase is expected to be even larger at higher pressures.

IV. Concluding Remarks

This report has attempted to describe the accomplishments and current status of the Spray Combustion Stability Project as well as indicate the planned direction of future research. While research effort in this project has been primarily restricted to physical submodel development, it is desirable that these submodeling concepts be pursued to actual implementation into comprehensive CFD spray combustion codes. This will hopefully make full scale instability analyses more practicable and useful and improve spray combustor design technology.

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