1. INTRODUCTION

Since the early 1960's, it has been known that realistic combustion models for liquid fuel rocket engines should contain at least a rudimentary treatment of atomization and spray physics. This is of particular importance in transient operations. It has long been recognized that spray characteristics and droplet vaporization physics play a fundamental role in determining the stability behavior of liquid fuel rocket motors.

This paper gives an overview of work in progress on design of a numerical algorithm for practical studies of combustion instabilities in liquid rocket motors. For flexibility, the algorithm is composed of semi-independent solution modules, accounting for different physical processes. Current findings are reported and future work is indicated. The main emphasis of this research is the development of an efficient treatment to interactions between acoustic fields and liquid fuel/oxidizer sprays.

2. TECHNICAL DISCUSSION

2.1 General Approach

The presence of droplets and chemical reactions in the flow field is manifested as additional source terms in the gas-phase equation.

\[
\frac{dU}{dt} + \nabla F_c + \nabla F_d = S_{\text{drop}} + S_{\text{chem}}
\]  

(1)

where \( U \), \( F_c \) and \( F_d \) represent the conserved variables and convective and diffusive fluxes, respectively, and \( S \) denotes the source terms. Modularity of the algorithm is insured by accounting for each effect separately using the method of fractional steps:

\[
\frac{dU}{dt} + \nabla F_c = 0; \quad \frac{dU}{dt} + \nabla F_d = 0; \quad \frac{dU}{dt} = S_{\text{drop}}(U^*); \quad \frac{dU}{dt} = S_{\text{chem}}(U^{**})
\]  

(2)

The asterisks in the source terms represent evaluation using the results of the preceding calculation.

Second order accuracy is insured by using a Strang\(^3\)-type operator splitting. Thus, if \( L_c, L_d, L_{\text{drop}}, \) and \( L_{\text{react}} \) denote individual operators which advance the solution through a time increment \( \Delta t \), the solution at a new time lead can be expressed as:

\[
U^{n+2} = (L_c^{\Delta t} L_d^{\Delta t} L_{\text{drop}}^{2\Delta t} L_{\text{chem}}^{\Delta t} L_{\text{drop}}^{\Delta t} L_d^{\Delta t} L_c^{\Delta t})U^n
\]  

(3)

Although the overall solution is explicit, each solution operator may be implicit as desired.
2.2 Gas Dynamics

Convective and diffusion equations are solved on a BFC grid using finite volume methodology. Convective fluxes are evaluated explicitly using high order characteristic based methods. Diffusive fluxes are evaluated in a central difference algorithm using the Heun and Crank-Nicholson schemes for time integration.

2.3 Source Terms

2.3.1 Chemistry: Early studies of liquid rockets have indicated that at least at steady state the chemical time scales are several orders of magnitude smaller than time scales associated with the other combustion processes. For transient behavior the situation is not clear. Since chemistry calculations can be very expensive owing to the stiffness of the rate equations, a number of approaches for evaluation of chemical source terms are being tested. These include: direct solution of multi-step kinetics using solvers for stiff ODE's; lookup table based on source equation solutions; instantaneous kinetics based on ignition temperature.

2.3.2 Spray Production: Spray characteristics and droplet behavior are known to play a key role in determining stability behavior. Droplets are produced by disintegration of a liquid core injected into the combustor. Liquid core behavior is therefore expected to control the droplet and spray distribution. Role of injection mechanisms is illustrated in Figure 1 for two methods of introducing droplets into the computational domain. It is seen that considerations of liquid core behavior leads to a substantially different spray geometry.

![Figure 1. Spray Shape Due to Two Modes of Injection](image)

(a) droplets injected individually from the left; (b) droplets injected from liquid core behavior calculations

Liquid Core: In the context of liquid rocket motors, atomization is typically achieved through breakup of liquid sheets and/or jets. This is true for impinging jets and shear-coaxial or swirl coaxial injectors. The common feature of such mechanisms is that before the breakup, the initial liquid stream has one dimension much smaller than the others: sheet thickness or the jet diameter. This disparity in dimensions is exploited by allowing the reduction in the problem dimensionality, essentially be constraining the fluid motion in the thin direction. This constraining is usually performed by integration of quantities such as velocity across the thickness conservation equations for mass, three momentum components and energy are:
\[ \varphi + \varphi (u_x + u_y) = 0 \quad ; \quad \rho \varphi u = -p_x + (\beta - q)\beta x - \rho \varphi \alpha_x \quad ; \quad \rho \varphi v = -p_y + (\beta - q)\beta y - \rho \varphi \alpha_y \quad ; \quad \rho \varphi \alpha = -\rho \varphi \beta + q + p \quad ; \quad \frac{1}{12} \rho \varphi \phi = \frac{p}{\varphi} - \frac{1}{2}(\beta - q + p) \]  

In the above equations the dot represents the material derivative. The surface tension \( q \) is a function of local liquid surface curvature. Position of top and bottom surfaces and the local thicknesses of the sheet are denoted by \( \beta, \alpha \) and \( \varphi \), respectively. The \( x, y, z \) velocity components are represented by \( u, v, \) and \( \lambda \), respectively.

A simplified treatment of this system assuming small curvatures and axial pressure gradients has been tested for the case of a developing sheet in an axial acoustic field. The results are shown in Figure 2.

![Figure 2. Liquid Sheet in an Acoustic Field](image)

The figure shows that the simple model is capable of responding to interactions with highly transient gas-phase field.

In rocket engine combustion, transverse pressure oscillations are expected to be of particular importance. Experiments carried out at MSFC indicate that acoustic fields can significantly alter a sheet’s geometry. Figure 3 shows some representative behavior of thin liquid sheets in a transverse acoustic field.

![Figure 3. Shape of a Liquid Sheet Under Transverse Acoustic Oscillations](image)
The figure shows that proper frequency matching can result in severe sheet distortions. It is interesting to note that in this configuration, sheet deformation does not necessarily lead to increased droplet production. Computations are currently being conducted to simulate this behavior numerically using equation (4).

Sheet models obtained from 3-D considerations are inexact by definition, and their corresponding equations are not necessarily invariant under superimposed rigid body motions (SRM). This is in contrast to the original 3D models which preserve such invariance. This is true from the constitutive as well as field equation point of view. This is of practical importance since invariance requirements may result in a different set of differential equations.

A different approach for the treatment of liquid sheets and jets involves an a-priori two and one-dimensional formulation using the theory of directed continua. Here the effects in the thin dimension are accounted for by specification of additional kinematic (vector) fields, each of which is described by its own differential equation. Constitutive relations are also two and one-dimensional and differ from the full three-dimensional formulations in that they may depend on the medium as well as the local geometry. This approach for solution of liquid core behavior is currently being investigated.

Liquid core calculations are performed using the Jet Embedding technique. This involves a separate calculation of the liquid phase, using the gas-phase velocity temperature and pressure data. Gas-phase data is interpolated unto a separate liquid-core computational mesh.

**Droplet Motion:** Liquid core calculations are followed by droplet injection. In a current implementation, droplet dynamics include: viscous and quasi-steady heatup of motion are solved for each droplet. This model is capable of displaying interactions with acoustic waves, as shown in Figures 4, 5, and 6. The figures show distortion of a spray by an axial acoustic wave (Figure 4); distortion of a droplet stream by a transverse acoustic wave (Figure 5); and droplet induced triggering of a shock in axial acoustic wave propagation.

![Figure 4. Spray Deformation in a Resonant Tube with Axial Acoustic Waves for: (a) unreacting flow and (b) flow with heat release](image_url)
3. CONCLUSIONS

The numerical model being developed during the course of this work, has shown strong coupling between acoustic waves and spray motion. The model is currently undergoing systematic parametric and verification studies for two and three-dimensional non-reacting and reacting flows. Liquid sheet (and jet) formulations, such as ones described by Equation s(4) are being developed for shear coaxial and impinging element injectors. Parametric studies will be conducted to quantify the dependence of combustion instabilities on: vaporization rate, droplet stripping rate model, droplet size spectrum, chemical kinetics, and liquid core formulations. Tests are also planned for comparisons with experimental data in single and multi-element injection configurations.

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5. REFERENCES