REPORT DOCUMENTATION PAGE

Form Approved OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*	2. REPORT TYPE	3. DATES COVERED *(From - To)*
05-03-1998	Paper	

4. TITLE AND SUBTITLE

A Maximum Entropy Moment Closure Approach to Describing Spray Flows

5a. CONTRACT NUMBER

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)

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5d. PROJECT NUMBER
3058

5e. TASK NUMBER
RF9A

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) AND ADDRESS(ES)
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8. PERFORMING ORGANIZATION REPORT

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)

Air Force Research Laboratory (AFMC)
AFRL/PRS
5 Pollux Drive
Edwards AFB CA 93524-7048

10. SPONSOR/MONITOR'S ACRONYM(S)

11. SPONSOR/MONITOR'S NUMBER(S)
AFRL-PR-ED-TP-1998-062

12. DISTRIBUTION / AVAILABILITY STATEMENT
Approved for public release; distribution unlimited.

13. SUPPLEMENTARY NOTES

14. ABSTRACT

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			Doug Talley
Unclassified	Unclassified	Unclassified	A		19b. TELEPHONE NUMBER *(include area code)* (661) 275-6174

ILASS Americas, 11th Annual Conference on Liquid Atomization and Spray Systems, Sacramento, CA, May, 1998

A Maximum Entropy Moment Closure Approach to Describing Spray Flows

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This paper describes a method to obtain a complete description of a spray flow by computing the evolution of its probability density function simultaneously with the gas flow in which it is embedded. Transport equations describing the evolution of certain moments of the probability density function are closed using a Maximum Entropy Formalism. Work is currently underway to test whether this method will yield significant advantages over conventional approaches to predicting spray flows.

INTRODUCTION

Understanding and modeling multiphase flows have become of primary interest in a wide variety of applications. Of particular importance are spray flows such as those associated with liquid fuel injectors, industrial coating processes, and agricultural sprays. A spray flow can be defined as that regime downstream of an injector where a liquid column or sheet has broken up and atomized, but the resultant drops continue to have some mean velocity relative to the gas phase. Both the liquid phase and the gas phase continue to dynamically interact, exchanging not only momentum, but possibly mass and energy as well. This evolution can have a significant impact, for example, on the combustion processes inside a liquid rocket engine or on the coating produced by a spray application system. For this reason, it is necessary to have a full understanding of the physics of spray flows and to be able to accurately predict not only the distribution of the drops and their behavior, but also the dynamics of the gas phase, that is, the characteristics of the combined two-phase flow.

One common approach used in studying spray flows has been to use a Lagrangian-Eulerian, or particle tracking, method [1, 2]. The gas phase is predicted by solving the time-dependent, Reynolds-Averaged Navier-Stokes (RANS) equations with a suitable turbulence model and appropriate exchange terms. The drop trajectories are computed by integrating a Lagrangian equation of motion. While this approach has provided useful information in many applications, it also has some significant drawbacks.

For instance, as a drop's trajectory is not likely to coincide with the vertices of the numerical grid used to solve the gas equations, the issue of how to compute the exchange rates between phases must be resolved. As a drop travels, it deposits mass, momentum, and energy in a thin wake behind it. These quantities then diffuse or advect into the rest of the flow at a rate which depends on the gas properties and flow field. However, unless specifically accounted for by a subgrid model [3], the exchanged mass, momentum, and energy are immediately spread across the grid cell into which they were deposited. As they diffuse into neighboring cells, they are again instantly averaged over the cell. This has the effect of artificially increasing the transport rates of the exchanged quantities.

This error is compounded when we consider that a typical spray flow may have 10^6 or more drops per cubic centimeter. Current computer resources are inadequate to handle such a large number of particles. To compensate, computational drops are tracked, each computational drop often representing as many as 10^4 real drops. Thus, as one of these computational drops deposits mass, momentum, and energy into a grid cell, it must do so for 10^4 drops. Obviously this is not physical, as the actual drops would have different trajectories and their depositions would be more spread out through the gas phase.

Particle tracking also suffers from the fact that the tracking calculations are, by nature, simulations whereas the RANS equations constitute a model for the mean flow field. Some researchers [4, 5] have attempted to resolve this by using Large Eddy Simulation (LES) techniques. By simulating the gas flow (though subgrid processes must still be modeled), the approaches to predicting the two phases seem to be

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more compatible with each other than simply using the RANS equations, but the LES method still suffers from the same droplet tracking issues discussed above. Further, given that we are generally interested in average flow quantities rather than instantaneous values, all the data arising from any simulation must be post-processed. This may not pose a problem if we are only interested in overall statistics. For example, if we want to know the mean number density of drops in a particular cell, we can perform a simple time average. However, what if we are interested in the mean number density of drops in a particular size class? The averaging procedure might be similar, but the required computational time is significantly increased because a sufficient number of drops in the specific size class must pass through the cell to provide a data set large enough for a meaningful average. Now what if we want the mean number density of drops in a particular size and velocity class? The computational time will again increase as we wait for enough data on drops in these classes to be generated. As the quantity of interest becomes more specific, the necessary computation time becomes more prohibitive.

An alternative approach which does not involve simulation is to compute the evolution of the average quantities of the spray flow directly. Not only will this remove the need to post-average, but it will also resolve many of the other problems associated with particle tracking. The purpose of this work is to obtain a complete description of a spray flow by computing the evolution of its probability density function (pdf) along with the gas flow in which it is embedded.

GOVERNING EQUATIONS

Following Williams [6] and O'Rourke [7], let $F(\bar{x}, \bar{v}, \phi; t)d\bar{x}\,d\bar{v}\,d\phi$ denote the probability of finding a drop in $d\bar{x}$ about $\bar{x}$ with velocity in $d\bar{v}$ about $\bar{v}$ and diameter in $d\phi$ about ϕ at time t. Neglecting source terms and vaporization, the spray equation, which describes the evolution of the drop pdf, can be written

$$\frac{\partial F}{\partial t} + \nabla_x \cdot (F\bar{v}) + \nabla_v \cdot (F\bar{a}) = 0 \qquad (1)$$

The two gradient symbols denote a spatial and velocity gradient, respectively, and the quantity $\bar{a}$ is the expected time rate of change of velocity with the expectation being over the gas phase characteristics. Note that $\bar{v}$ is a coordinate of the space the pdf spans rather than the expected rate of change of position. The incompressible, ensemble-averaged Navier-Stokes equations are solved for the gas flow properties. The two sets of equations are coupled by a point force term in the gas equations and the droplet acceleration $\bar{a}$ in the spray equation. The Reynolds-stress terms are closed used using a standard $k-\varepsilon$ model that has been slightly modified to account for the generation and/or dissipation of turbulence due to the drops. The modification also adds another level of coupling between the two phases.

A straightforward solution of the spray equation is not possible given the number of dimensions that F spans. A finite volume mesh over the seven dimensions we are currently considering would require at least 50^7 grid cells—fifty in each coordinate direction. However, every pdf is expressible as an infinite set of moments. If we assume that a select number of low-order moments carry a predominant amount of the information about the spray, then an approximate solution of the spray equation may be found using moment methods.

Consider the following decomposition of F

$$F(\bar{x}, \bar{v}, \phi; t) = \lambda_c(\bar{x}; t) f_c(\phi, \bar{v}; \bar{x}, t) \qquad (2)$$

where $\lambda_c(\bar{x}; t)$ is the one-particle probability density function in physical space, $f_c(\phi, \bar{v}; \bar{x}, t)d\phi\,d\bar{v}$ is the probability that a drop found in $d\bar{x}$ at time t has size and velocity coordinates in $d\phi$ about ϕ and $d\bar{v}$ about $\bar{v}$, and the subscript c is used to denote concentration-based statistics. The quantity $\lambda_c(\bar{x}; t)$ may also be interpreted as the expected number density of drops at $(\bar{x}, t)$ [8]. Using (2), the spray equation may be split into two separate equations

$$\frac{\partial \lambda_c}{\partial t} + \nabla_x \cdot (\lambda_c \langle \bar{v} \rangle) = 0 \qquad (3)$$

$$\frac{\partial f_c}{\partial t} + \nabla_x \cdot (f_c \bar{v}) + \nabla_v \cdot (f_c \bar{a}) = f_c \left[\nabla_x \cdot \langle \bar{v} \rangle + (\langle \bar{v} \rangle - \bar{v}) \cdot \nabla_x \ln \lambda_c \right] \qquad (4)$$

The angled brackets denote the ensemble average over drop diameter and velocity space. Equation (3) describes the evolution of the expected number density of the spray. The terms on the left hand side of equation (4) are similar to those in the spray equation, however two new terms have been introduced on the right-hand side. The first represents a renormalization of the size/velocity pdf due to the gain or loss of drops in a grid cell in the presence of a gradient in the mean drop velocity. The second term is a redistribution of probability due to a number density gradient.

MOMENT EQUATIONS

The decomposition expressed in equation (2) is a necessary and important step in our development because F is not a normalized pdf. The probability represented by F is directly dependent upon the amount of spray present across the ensemble at a given location

in physical space. By decomposing F, we are able to remove this dependency and obtain the normalized pdf, f_c, which is only defined across realizations of the ensemble in which a droplet is located at the point of interest. Unlike F, we are able to compute moments of f_c, and by making use of equation (4), we can derive transport equations for those moments. For example, by multiplying (4) by ϕ and integrating over all diameter and velocity space, we obtain an equation for the evolution of the expected drop diameter $\langle\phi\rangle$

$$\frac{\partial\langle\phi\rangle}{\partial t}+\nabla_x\cdot\langle\phi\,\bar{\mathrm{v}}\rangle = \langle\phi\rangle\nabla_x\cdot\langle\bar{\mathrm{v}}\rangle+\left(\langle\phi\rangle\langle\bar{\mathrm{v}}\rangle-\langle\phi\,\bar{\mathrm{v}}\rangle\right)\cdot\nabla_x\ln\lambda_c \tag{5}$$

Other moments that might be selected for a one-dimensional computation are the mean drop velocity, $\langle \mathrm{v}_x\rangle$, mean-squared velocity, $\langle \mathrm{v}_x^2\rangle$, and the diameter/velocity cross moment, $\langle\phi\,\mathrm{v}_x\rangle$. The transport equations for the these moments are, respectively,

$$\frac{\partial\langle \mathrm{v}_x\rangle}{\partial t}+\frac{\partial\langle \mathrm{v}_x^2\rangle}{\partial x}=\langle \mathrm{v}_x\rangle\frac{\partial\langle \mathrm{v}_x\rangle}{\partial x} +\left(\langle \mathrm{v}_x\rangle^2-\langle \mathrm{v}_x^2\rangle\right)\frac{\partial(\ln\lambda_c)}{\partial x}+\langle a_x\rangle \tag{6}$$

$$\frac{\partial(\lambda_c\sigma_{\mathrm{v}}^2)}{\partial t}+\frac{\partial}{\partial x}\left[\lambda_c\left(\langle \mathrm{v}_x^3\rangle-2\langle \mathrm{v}_x\rangle\langle \mathrm{v}_x^2\rangle+\langle \mathrm{v}_x\rangle^3\right)\right] +2\lambda_c\sigma_{\mathrm{v}}^2\frac{\partial\langle \mathrm{v}_x\rangle}{\partial x}=2\lambda_c\left(\langle a_x\mathrm{v}_x\rangle-\langle a_x\rangle\langle \mathrm{v}_x\rangle\right) \tag{7}$$

$$\frac{\partial\langle\phi\,\mathrm{v}_x\rangle}{\partial t}+\frac{\partial\langle\phi\,\mathrm{v}_x^2\rangle}{\partial x}=\langle\phi\,\mathrm{v}_x\rangle\frac{\partial\langle \mathrm{v}_x\rangle}{\partial x} +\left(\langle\phi\,\mathrm{v}_x\rangle\langle \mathrm{v}_x\rangle-\langle\phi\,\mathrm{v}_x^2\rangle\right)\frac{\partial(\ln\lambda_c)}{\partial x}+\langle\phi\,a_x\rangle \tag{8}$$

where equation (7) has been written in terms of a central moment, $\sigma_{\mathrm{v}}^2=\langle \mathrm{v}_x^2\rangle-\langle \mathrm{v}_x\rangle^2$, rather than a moment about the origin. When the method is extended to two-dimensional flow, additional moments will be required, such as $\langle \mathrm{v}_y\rangle$, $\langle \mathrm{v}_y^2\rangle$, $\langle\phi\,\mathrm{v}_y\rangle$, and $\langle \mathrm{v}_x\mathrm{v}_y\rangle$, along with their corresponding transport equations.

MAXIMUM ENTROPY CLOSURE

This moment method suffers, however, from the same fundamental closure problem encountered in turbulence modeling. As each successive moment transport equation is derived, at least one new, higher-order moment is introduced that must be determined. These unclosed moments can be evaluated by making use of the Maximum Entropy principle. In his study of communications theory, Shannon [9] developed the concept of information entropy as a measure of probabilistic uncertainty. Later, Jaynes [10] showed that an infinite number of pdf's are consistent with a set of known constraints, but the one that should be chosen is the one with maximum entropy. If a pdf with less entropy (i.e., less uncertainty) were used, it would imply the existence of some additional knowledge. However, since all the available knowledge was applied in the form of constraints, no additional knowledge would exist, thus it would be inappropriate to choose any pdf other than the one with maximum entropy. This pdf is the most unbiased distribution possible within the given constraints. Figure 1 shows some examples of common distributions predicted by the Maximum Entropy Formalism (MEF). The uniform distribution shows that in the absence of any constraints other than the endpoints of its domain, every value in the domain is equally probable since there is no information to the contrary. The other three distributions show the results of different moment constraints. It is interesting to note that the parameters used to characterize these distributions, for example, the mean and variance of a Gaussian distribution, are the same quantities used as constraints in the Maximum Entropy Formalism. This lends a high degree of confidence to the validity of the Maximum Entropy approach.

Though various types of constraints have been used in different applications of the MEF, we will require that the low-order moments that we selected earlier have a specified value. The maximization is carried out by way of the method of Lagrange multipliers. This leads to a pdf of the form

$$f_c=\exp\left[-\lambda_0-\sum_{r=1}^{M}\lambda_r A_r\right] \tag{9}$$

where the λ's are the Lagrange multipliers, A_r is the quantity to be averaged, and M is the number of moment constraints. The coefficients must be determined from a non-linear system of coupled, differential equations which, in general, must be solved numerically. Figure 2 shows a typical distribution for a drop's diameter and one component of velocity constrained by the mean velocity and diameter, the mean-squared velocity and diameter, the mean-cubed diameter, and the diameter/velocity cross moment. Notice how the drop diameter and velocity are correlated due to the influence of the constrained cross moment and that there is some skewness in the diameter direction imparted by the mean-cubed diameter constraint.

Sellens, Tankin, and others [11, 12] have made use of the Maximum Entropy Formalism in their work on predicting droplet distributions resulting from the breakup of a liquid sheet or jet. In this work, the breakup process is considered independently from gas-phase constraints, and it was not their intention to solve for the evolution of the droplet distribution throughout space and time, but rather to obtain a distribution for all the drops in the spray. In contrast, our work is focused on describing the *evolution* of a droplet pdf at every point in the flow domain and how that evolution is influenced by and interacts with the gas phase. In our approach, we model the evolution of the complete, coupled spray flow using moment equations. The MEF is introduced as a method to close those equations. For this reason, we refer to this approach as MEMC, the Maximum Entropy Moment Closure approach to modeling spray flows.

CURRENT STATUS

At the time of this writing, the theoretical framework has been established, and though there still exist some numerical issues which need to be addressed, we have proceeded to compute some simple test cases. The moment transport equations have been solved without the gas phase (though an artificial drag was imposed). The results agree with our expectations that a distribution would propagate from the injector through the flow domain. Secondly, a gas-phase flow solver has been programmed and validated using a number of standard test cases. The two solution algorithms have been incorporated into a new code and we are presently working on smoothly integrating the computation of the two sets of equations.

Calculations are currently being carried out on a single-processor work station, however the simple tests performed thus far have shown that there could be significant advantages to transporting the code to a mutli-processor platform. Certain aspects of the solution procedure seem particularly well-suited to parallel computation. Once we have completed the one-dimensional tests, we will begin exploring this option in more detail.

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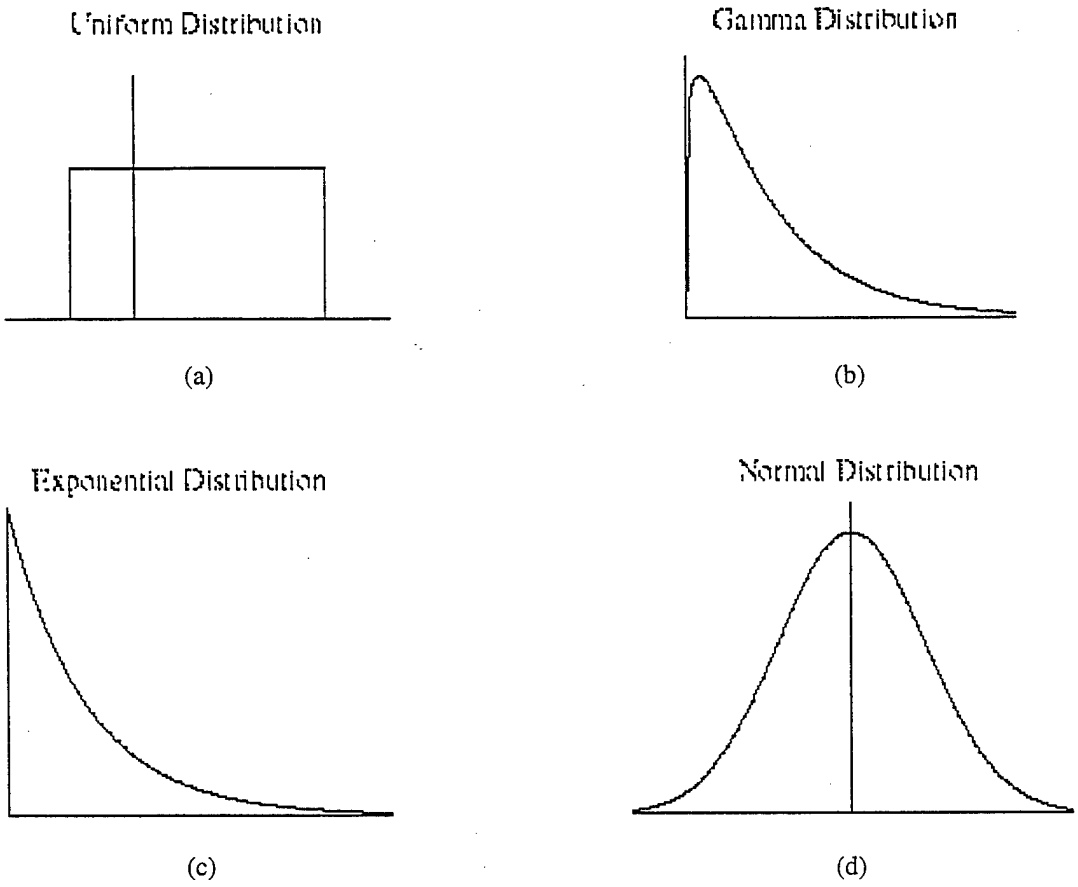

Fig. 1: Distributions produced by the Maximum Entropy Formalism using various constraints. (a) No constraints on a finite domain. (b) Arithmetic and geometric means constrained on a semi-infinite domain. (c) Mean constrained on a semi-infinite domain. (d) Mean and variance constrained on an infinite domain.

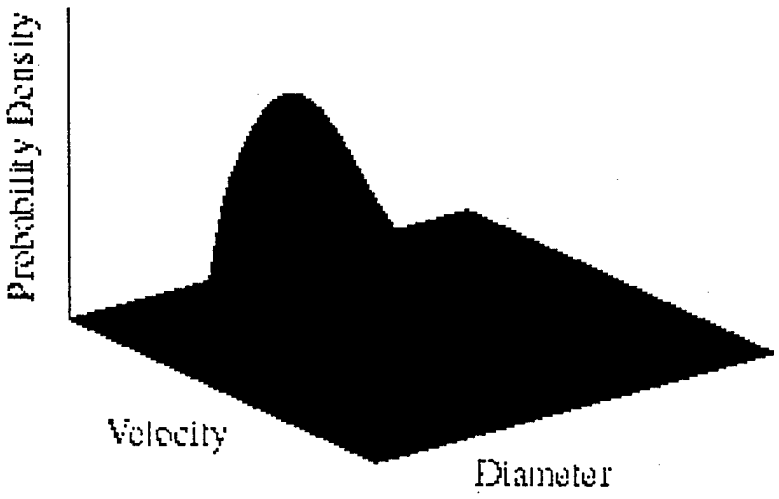

Fig. 2: Sample spray probability density function over diameter and x-velocity space.