Simulation of Turbulent Non-reactive and Reactive, Dilute Spray Flows

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ABSTRACT

Introduction

Turbulent spray flows are vital for many technical applications such as industrial furnaces, gas turbine combustors, internal engine combustion, and liquid rocket propulsion systems. Even though there has been a big effort in modeling and simulating of both non-reacting and reacting spray flows, there is still a big lack of knowledge in the fundamental understanding of these systems. The present paper gives a survey of the status of modeling and simulation of dilute spray systems where different aspects are taken into account. First, non-reactive sprays will be considered where a number of different modeling approaches are compared. They comprise the standard κ – ε model, which is widely used in industry, as well as the Reynolds stress model and pdf (probability density function) methods. Moreover, reactive sprays are addressed where the flamelet model for turbulent spray diffusion flames is an excellent tool to provide information on pollutant formation as well as production of intermediates that are relevant for soot formation.

Reynolds-Stress Model

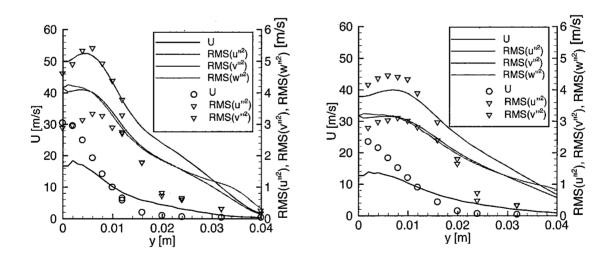


Figure 1: Comparison of experimental [1] (symbols) and computed [2] (lines) root mean square velocity components of a turbulent non-reactive methanol/air spray flow at two axial distances of x = 75 mm (left) and x = 100 mm (right).

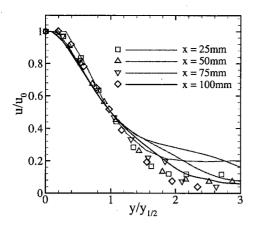


Figure 2: Similarity profiles of the axial velocity component at various downstream positions.

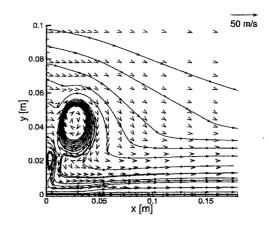


Figure 3: Gas velocity streamlines of a recirculating turbulent spray flow.

A Reynolds stress model has been developed for turbulent spray flows, and it is applied to an experimental configuration investigated by McDonell and Samuelsen [1] where experimental data of the second moments of the velocity components are available. Figure 1 shows the Favre mean values of the axial velocity, U, as well as the root mean square of the velocity components in axial and radial direction. It appears that the Reynolds stress model [2] is capable of predicting the principal profiles of the experimental values. However, it is poor near the axis of symmetry. The discrepancies here are attributable to the lack of information of radial velocities near the inlet whose influence is considerable due to the sensitivity of numerical results to the inlet conditions. Figure 2 shows that the prediction of similarity profiles is good.

The present experiment shows some very light recirculation, and therefore, the model cannot be tested to its full extend. The next step here will be the simulation of a strong swirling flow. The model, however, is suitable to simulate recirculation zones that are not predictable with the κ - ε model, c.f. Fig. 3.

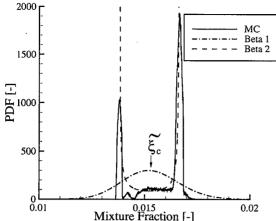
PDF Model

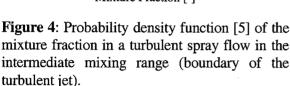
The probability density function (pdf) of both scalars (e.g. species mass fractions, enthalpy) and vectors (gas and/or droplet velocity) may be presumed (presumed pdf methods), modeled using trenaport equations for their moments (RANS models), or modeled using a transport equation for the probability density function (called pdf method in the remainder of the text).

It appears [3] that the presumed pdf for the turbulent mixing in gas flows [4] that typically is modeled using a β function is poor in turbulent spray flows. Therefore, a transport equation of the mixture fraction is derived and solved for use in turbulent spray flows [5]. From these results, a modified β function is suggested and tested for use in turbulent spray flows. It appears that the deviation of the mixture fraction in the initial air and fuel streams which typically are zero and unity, resp., in gas flows, cause the problems in spray flows where the gas-phase mixture fraction deviates from these values due to the vaporization process causing a source term in the gas-phase conservation equations.

Figures 4 and 5 show profiles of probability density functions of the mixture fraction obtained with the pdf method (MC), the presumed β function (Beta 1) and the modified β function (Beta 2). Figure 4 displays results in the jet boundary where the mixing level is high whereas Fig. 5 shows a pdf in the air regime of the flow, which can also be seen from the absolute values of the Favre averaged mixture fraction, $\tilde{\xi}_C$.

With this method, the profiles of the Favre-averaged fuel vapor fraction [5] may be computed and compared to experiment [1]. It appears that the pdf method greatly improves the simulation.





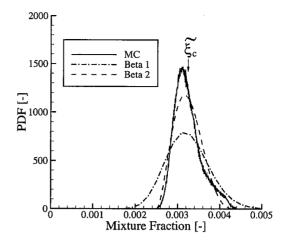


Figure 5: Probability density function [5] of the mixture fraction in a turbulent spray flow in the air-sided mixing range (outer regime of the turbulent jet).

Thus, the pdf method is a powerful method not only to predict improved computational results in turbulent spray flows, but it is also a suitable tool to derive simplified models for use in complex technical applications.

Flamelet Model for Turbulent Reactive Spray Flows

The presentation includes the simulation of turbulent spray flows with chemical reactions where the combustion intermediates may be predicted by use of the flamelet model for turbulent spray diffusion flames. Here, a new way of incorporating structures of laminar spray flamelets is presented that makes use of novel evidence on the structures of laminar spray flame computations.

Conclusions

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There is a need for the development of efficient models for the prediction of turbulent non-reactive and reactive spray flows for complex technical applications. These may be derived from more complex modeling approaches such as the pdf methods for turbulent processes. The pdf methods as well as LES and DNS approaches are not suitable for use in complex processes that occur in technical applications such as gas turbines, liquid rocket propulsion, internal engine combustion, and similar systems.

References

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