Novel Approach for Efficient Modelling of Mixing and Reaction in Turbulent Flow Based on Discrete Distributions

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For many technical applications in combustion as well as process engineering, turbulent flow conditions are prevalent. This flow regime is characterized by large mixing rates, which make possible high reaction densities and therefore smaller combustors or chemical reactors. On the other hand, strong turbulent fluctuations in velocity, temperature, composition, etc., make the numerical simulation of the relevant physico-chemical processes a very difficult task.

For numerical simulation of such flows, **R**eynolds **A**veraged **N**avier **S**tokes (RANS) or **L**arge **E**ddy **S**imulation (LES) models are often employed. With RANS models, it has become feasible to carry out extensive studies during the design phase even for configurations of technical interest. For the LES approach, this is not yet possible with present computational means. Both modelling strategies do not resolve all length scales of the turbulent flow down to the Kolmogorov-scale (smallest turbulent eddies) or the Bachelor-scale, on which reactions take place. Hence turbulence models are required to take into account at least in an approximate manner the influence of unresolved fluctuations on, e.g., reaction rates.

Turbulent fluctuations can be charactierized by a probability density function (PDF). A new method for the approximation of multivariate scalar PDFs in turbulent reacting flow by means of a *joint presumed discrete distribution* (jPDD) is presented. The jPDDs can be generated with specified mean values and variances as well as covariances. Correlations between variables -- e.g. fluctuating mixture fractions and/or reaction progress -- can thereby be taken into account. In this way the important limitation of ordinary presumed PDF methods can be overcome, where statistical independence between the variables is usually assumed for lack of a better alternative. Different methods are presented to generate discrete distributions, based either on biased random number generators or on mixing models familiar from PDF transport models. Results of validation studies are presented, potential future applications of the approach are indicated.

In summary, the new jPDD model - which can be applied both in the RANS and the LES context - has the potential to be significantly more accurate than established presumed PDF methods, because correlations between fluctuating variables can be taken into account. At the same time, the new approach is nearly as efficient as standard presumed PDF formulations, since mean rates are computed in a pre-processing step and stored in lookup-tables as a function of the first and second moments of the relevant variables.

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