Two stochastic approximations of the chemical source term in the PDF transport equation

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Abstract

The need to include many species as variables for the probability density function (PDF) transport equation to describe emissions in turbulent reactive flow appropriately is the motivation and starting point for this paper. The numerical method for solving the PDF transport equation employs a Monte Carlo technique combined with an operator splitting approach. The Monte Carlo technique is based on a stochastic particle-mesh method. One problem

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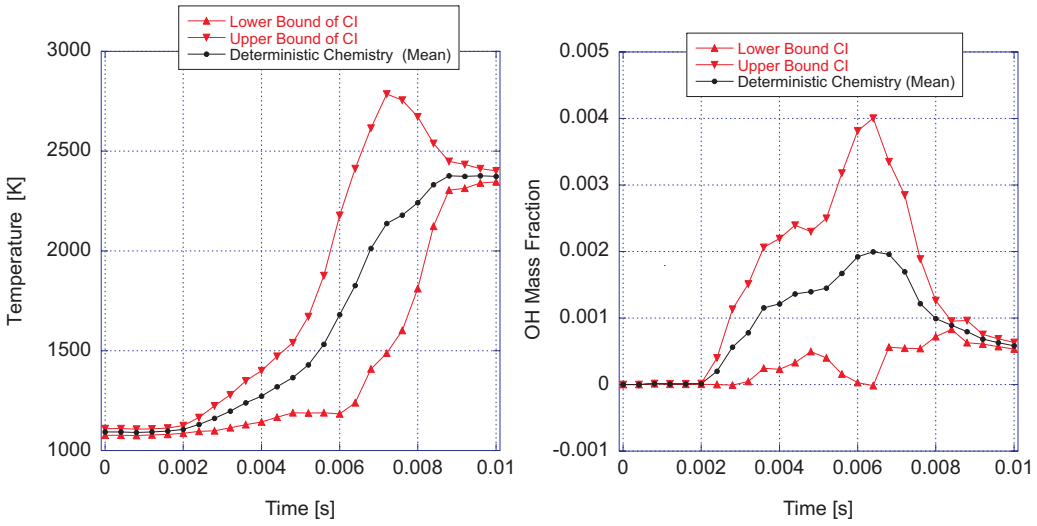
that arises when using this method is the need to cut down the computational cost for the chemistry step. In the chemistry step the chemical species and the temperature are advanced in time which means for each stochastic particle a system of ordinary differential equations (ODE) has to be solved numerically. This system of ODE is usually stiff and special solvers are required to obtain the numerical solution. For chemistry models describing practical combustion systems the number of chemical species is quite large and the computational time that is needed to solve the system of ODE for each particle is prohibitive.

Table 1: *Non-premixed combustion of n-heptane. Initial concentrations.*

	Fuel	Air
	$\dot{n}_1$	$\dot{n}_2$
	2 mol/min	52 mol/min
X(nC7H16)	1	0
X(N2)	0	0.7900
X(O2)	0	0.2100

From the computational procedure described above it is clear that the trajectory of each stochastic particle evolves deterministically according to the chemical source term. However, other processes like mixing make the trajectories intrinsically stochastic. This is a characteristic feature of all particle interaction models, e.g. the CURL model just to name one representative of this model class. Consequently, although we compute the trajectories of each particle deterministically when we evaluate the chemistry we do not make use of this detailed information. We are only interested in the PDF as a whole or functionals of the PDF such as the mean and variance. In this paper we present two stochastic approximations of the chemical source term in the PDF transport equation. Both approximate the deterministic trajectories of the particles by a jump process. The first method, described in [1], is based on a direct stochastic simulation of the chemical reactions. The second method presented makes use of the mathematical result that (almost) every system of ordinary differential equation can be approximated by a jump



(a) (b)

Figure 1: *Time evolution of the empirical mean of (a) temperature and (b) OH mass fraction with confidence bounds for four repetitions.*

Markov process. Both methods will be discussed and the corresponding simulation algorithms will be explained. Then, in the second part of the paper, the numerical performance of this new algorithm is investigated in the context of Monte Carlo methods for the PDF transport equation following the ideas in [2]. We consider a non-premixed combustion problem. A fuel stream consisting of n-heptane, which is injected into hot air is studied, similar to the configuration described in [4]. For the purpose of this numerical investigation it is assumed that the joint scalar PDF is homogeneous in space and the combustion can be modelled using the PaSPFR model. In **Table 1** flow rate and composition of the two streams are given. The PDF model is solved by a particle based Monte Carlo method and a standard splitting technique as described by Pope [3]. **Figure 1** shows the time evolution of the mean temperature and mean OH massfraction with their confidence bands as a measure of the statistical error. In this example the stiff ODE solver DASSL has been used to calculate the chemical source term in the PDF equation. Given the magnitude of the statistical error it is quite clear that we do not need to calculate the trajectories for each particle with a very high accuracy. In order to assess the computational speed up of the stochastic chemistry

approximations we implement both approaches in the Monte Carlo method for the PDF transport equation. It is found that the new stochastic methods clearly outperform the deterministic method for the cases studied.

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