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Particle Methods in Turbulent Combustion: Numerical Simulation of Pollutant Formation

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Existing commercial CFD codes offer a number of different models for calculating pollutant (NOx, CO, soot, unreacted hydrocarbons, etc.) formation in burners and transportation engines. The models are of different complexity ranging from a kind of correlation-based approaches to a detailed chemical kinetics based models. The general drawback of the most of these models is that they calculate the local mean rates of pollutant formation without taking into account turbulence-induced differences in residence times of fluid elements in a given location as well as differences in their temperature and species concentrations. However, if one properly takes into account the spectrum of turbulent velocity fluctuations,

this can influence pollutant production considerably, in particular in hot recirculation zones.

The objective of the work briefly outlined in this paper was to develop a hierarchy of subgrid Particle methods for simulating pollutant formation in turbulent flames with different levels of approximation. The Particle method implies continuous monitoring (in a Lagrangian manner) of multiple local instantaneous states of combustion products in the turbulent flow field thus allowing for intrinsically correct treatment of turbulence – chemistry interaction [1]. The simplest Particle methods imply one-way coupling with a finite-volume CFD code, whereas the most sophisticated methods are based on the two-way coupling.

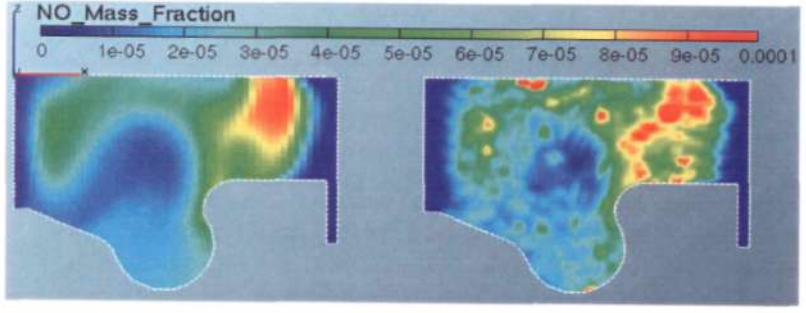

Fig.1 Spatial distributions of NOx mass fraction in Diesel engine at crank angle 760°. Left: standard model, right: Particle method

In the simplest Particle method, the reaction rates of pollutant formation are modified with due regard for statistical residence time distribution in computational cells. Each notional particle evolves in time and space according to the ordinary differential equations of motion with a stochastic source term. As an example, Fig. 1 compares the spatial distributions of NOx mass fraction in a Diesel engine obtained with standard model and Particle method. Due to accounting the local distributions of residence time, the Particle method resolves multiple locations of NOx production, whereas the standard model smears them out.

In the most sophisticated Particle method, each notional particle evolves in time and space according to the ordinary differential equations of mass, species, momentum, and energy conservation with due regard for chemical reactions, as well as mass, momentum and energy exchange between particles. The effect of turbulence is modeled by stochastic source terms in the momentum equation. The mean reaction rate of pollutant formation is taken as the local instantaneous ensemble-mean value. As an example of method implementation, Fig. 2 compares the predicted and measured values of NOx concentration at the end of constant-volume combustion of propane – air mixtures of different composition at normal initial pressure and temperature. The Particle method is seen to provide excellent qualitative and quantitative predictions for NOx emissions.

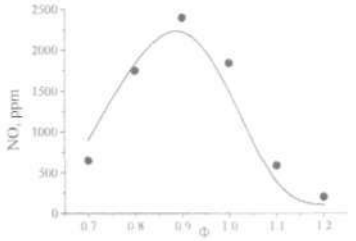

Fig. 2. Comparison of predicted and measured [1] values of NOx concentration at the end of constant-volume combustion of propane – air mixture of different equivalence ratios at normal initial pressure and temperature

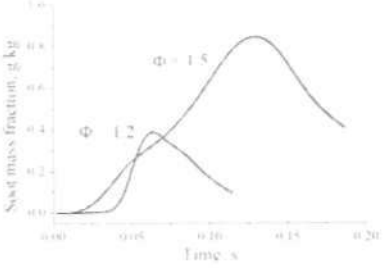

Fig. 3. Predicted time histories of mean soot mass fraction in the course of constant-volume combustion of fuel-rich n-heptane – air mixtures with equivalence ratios 1.2 and 1.5 at normal initial conditions

In addition to NOx, the Particle method is capable of predicting the formation of other pollutants. For example, Fig. 3 shows the results of 3D CFD calculations of soot production at combustion of fuel-rich n-heptane – air mixtures with equivalence ratios 1.2 and 1.5 in a cylindrical enclosure at normal initial conditions.

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2. Huzayyin A.S., Moneib H.A., Shehatta M.S., Attia A.M.A. Laminar burning velocity and explosion index of LPG – air and propane – air mixtures. Fuel, 2008, Vol.87, pp. 39 – 57.

PL-3

Application of the Multireference Configuration Interaction (MRD-CI) Method to Study Collisions of Alkali Atoms with Helium

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The multireference configuration interaction (MRD-CI) method allows one to compute total energies and wave functions of molecular systems at a high level of accuracy for all types of electronic states over a wide range of nuclear conformations. This method has been employed to describe the potential curves of the Na(3s,3p)He complex for use in a coupled channel treatment of the corresponding inelastic collision processes [C. Y. Lin et al., Phys. Rev. A **78**, 052706 (2008)]. A similar series of calculations has been carried out for the K (n,l) + He potentials in order to study the interactions of high-lying Rydberg states with neutral particles. Results for low-lying Rydberg states are obtained with high accuracy by employing quantum mechanical methods and these are in turn used to generate the corresponding data for their counterparts at higher energy with a much larger electronic cloud radius that are required for applications in astrophysics and plasma chemistry. Calculations for autoionizing states produced by electron collisions will also be presented.