Modeling Diesel Engine Combustion and Pollutant Formation Using a Stochastic Reactor Model Approach

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Abstract

A stochastic reactor model is used in order to study combustion and pollutant formation in a diesel engine. For modeling the in-cylinder gases a probability density function (PDF) approach is used combined with detailed chemistry. The soot particle size distribution transport equations are solved using the method of moments. Parameter studies are carried out in order to assess the influence of the turbulence intensity on autoignition. The results obtained with the stochastic model concerning ignition conditions and soot formation are compared to CFD calculations. The capability of the tool to reproduce the pressure trace, the ignition onset, and to indicate some trends related to particulate formation is demonstrated.

INTRODUCTION

In the past, the stochastic reactor model approach has been used successfully to model the HCCI (homogeneous charge compression ignition) combustion process [1] and to study the effects of turbulent mixing and inhomogeneities on knock in SI engines [2, 3]. In the case of diesel engine, because of the strong non-homogeneous aspect of the cylinder charge and of the complexity of the physical phenomena involved, until now stochastic reactor models have only been used in simplified conditions and with no or minimal chemistry. This study is a step towards using detailed kinetic models, sustaining affordable CPU-times in diesel engine simulations; models capable to account to a certain degree for the inhomogeneous and turbulent combustion in such engines.

METHOD

The partially stirred plug flow reactor (PaSPFR) model [4] has been recently applied in order to model partial HCCI combustion [5]. A stochastic reactor model (SRM) for SI engine calculation [2,3] was used as basis for this development. In regular HCCI combustion, the fuel is port injected, as in SI engines, whereas in partial HCCI, the fuel is injected into the combustion chamber, as in diesel engines. The model developed in [5] is used in the present study.

In the SRM/PaSPFR methods applied to engines the cylinder charge is considered to be represented by gas particles having different properties (composition, temperature). Interaction of particles is allowed only through mixing. The resulting system of differential equations is solved using operator splitting. With this approach in each time step each event is solved separately, as: piston movement, inlet/vaporization of fuel, mixing, chemical reactions and convective heat losses. The set of differential equations [2] is modified in order to account for the fuel intake in direct injection engines. Local quantities such as mass fractions, $Y_i(t)$, i = 1,...,S, temperature, T(t), and the moments M_0 , M_1 , M_2 of the soot particle size distribution are treated as random variables. Let $f(t) = (f_{1},...f_{s},f_{s+1},f_{s+2},f_{s+3},f_{s+4},f_{1};t) = (Y_{1},...,Y_{s},M_{0},M_{1},M_{2},T;t)$ denote the vector containing the random variables and let $y_{1},...,y_{s+4}$ denote the realizations (sample space variables) of the corresponding random variables $f_{1},...,f_{s+4}$. The time evolution of their joint scalar mass density function (MDF), $F_{t}(y_{1},...,y_{s+4};t)$, assuming statistical homogeneity is given by