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A Numerical Approach for the Prediction of Unburned Hydrocarbon Emissions in Gas Engines

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Abstract

Unburnt hydrocarbon (UHC) emission can be a significant green house gas contribution for gas engines. Aim of this work is the development of a calculation procedure to quantify the local UHC sources in the burning chamber which is applicable also for complex three dimensional geometries and which regards the local flow and turbulence conditions. A direct integration of the reaction rate calculation into the computational fluid dynamic (CFD) flow calculation is not possible. Hence, a hybrid-model is proposed to integrate the detailed reaction kinetics via separate sub models coupled with CFD. For that a model for turbulent flame propagation is based on detailed laminar flame calculation, flame wall quenching is modelled and the post oxidation of UHC will be regarded with a separate reaction model.

1. INTRODUCTION

Gas engines have raised a growing interest during the last years because of economical and technical advantages. Natural gas, mainly methane, because of its low carbon level C/H=1/4, is one of the less polluting fuels in terms of CO_2. On the otherside gas engines emissions comprises of high concentrations of unburned hydrocarbons (UHC) with up to 5% of the exhaust. Methane has a GWP value (Global Warming Potential) of 21, i.e, it is 21 times more harmful than CO2 as a greenhouse gas [1]. Moreover the loss of fuel leads to decrease in the efficiency of the engine. Hence the reduction of the UHC emissions is a necessity.

Different posssible sources for the UHC emissions in the engine could be found in the literature [2, 3]. The quenching of the flame on the cylinder walls and the fuel trapped in the crevices are one of the major sources of the UHCs. Numerical predictions of the UHCs have been previously made using the zonal-methods, but it has been difficult to incorporate detailed chemistry since the reaction rates vary strongly with local temperatures and pressures. One possible solution is the 3D-CFD simulation, to resolve the whole transient flow field inside the engine. But the direct integration of detailed chemistry with the local flow and turbulence conditions is not possible. The transport equations solved in the CFD simulations using the RANS (Reynolds Averaged Navier Stokes) methods, fail to make correct predictions, when detailed chemistry is involved, this is to the strong non-linear variation of reaction rates with temperature [4]. Hence proper “reaction kinetic models” are necessary for the predictions of UHCs [4,5,6].

2. APPROACH

A hybrid-model is proposed to integrate the detailed reaction kinetics via separate sub models coupled with CFD as shown in the diagram below.

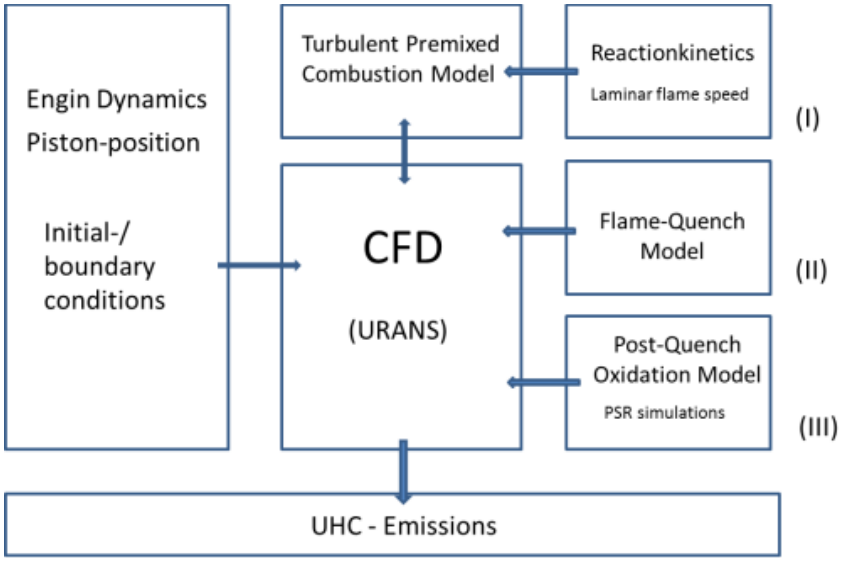

Figure 1: Schematic of the Hybrid-Model

Block (1) includes 1-D reaction kinetic simulations, the detailed reaction mechanism GRI-Mech 3.0 [7], which comprises 325 elementary reactions of 53 chemical species, is used. It is coupled with thermodynamical data and transfer coefficients from Burcat [8] and McBride [9] and solved by the simulation tool Cosilab [10]. A database for laminar flame speeds is created relevant to gas engine conditions, i.e, pressure: 0.1 MPa to 20 MPa, temperature: 300 K to 1500 K, equivalence ratios: 1.1 to 0.4 and the exhaust gas recirculation rates (EGR): 0 % to 30 %. This laminar flame speed data-base is used to compute the turbulent flame propagation. Different combustion models are tested, it is observed that the AFSW (Algebraic Flame surface wrinkling model) [11] provides better results compared to the other tested combustion models for the high pressure engine conditions. The AFSW model is implemented through a user defined function in ANSYS Fluent for the CFD simulations. Block (II) includes a computational model implemented to determine the distance at which the flame quenches on the cold walls during the numerical simulation. This model is developed by Ratzke et al. [12] and is based on the experimental work done by Boust et al. [13]. The distance for post-quench oxidation of the boundary fuel after the flame quench is calculated through the 0-D perfectly stirred reactors simulations in block (III), the GRI 3.0 Mechanism is used for the kinetic simulations. The diffusion will be taken into account solving the Fick's diffusion equation. The 0-D simulations are performed for ranges of temperature, pressures, equivalence ratios and EGR for the engine conditions. The validation experiments are currently performed in collaboration with the Institute of Internal Combustion Engines TU Munich.

3. RESULTS AND DISCUSSIONS

Several laminar flame speed correlations are available in literature [14, 15, 16, 17], these correlations predict the laminar flame speeds accurately for near stoichiometric regions and for low pressure and low temperature conditions. However, they fail to provide proper predictions when applied for gas engine conditions. Hence detailed reaction kinetic simulations are performed for the proper predictions of laminar flame speeds for the gas engine. Though the engine relevant temperature and pressure exceed the validated region of the detailed reaction mechanism, the provided flame speeds are in good agreement to measurement data available in the literature, cf. Elia et al. [17] and Gu et al. [18]. However, the measured flame speeds from [17] at high pressure are of lower values as compared to those calculated by the chemical simulations by about 15 %.

Figure 2 shows the computed laminar flame speeds of methane-air-mixtures as a function of pressure for several equivalence ratios and EGR rates. With increasing pressure, the laminar flame speed drops. This influence is important for moderate pressure up to 5 MPa. At higher pressures, the flame speed approaches a steady value. Charge dilution by air (which affects the stoichiometry) and by exhaust gas reduces the flame speed; the influence of the same amount of exhaust gas is larger as compared to the diluting air.

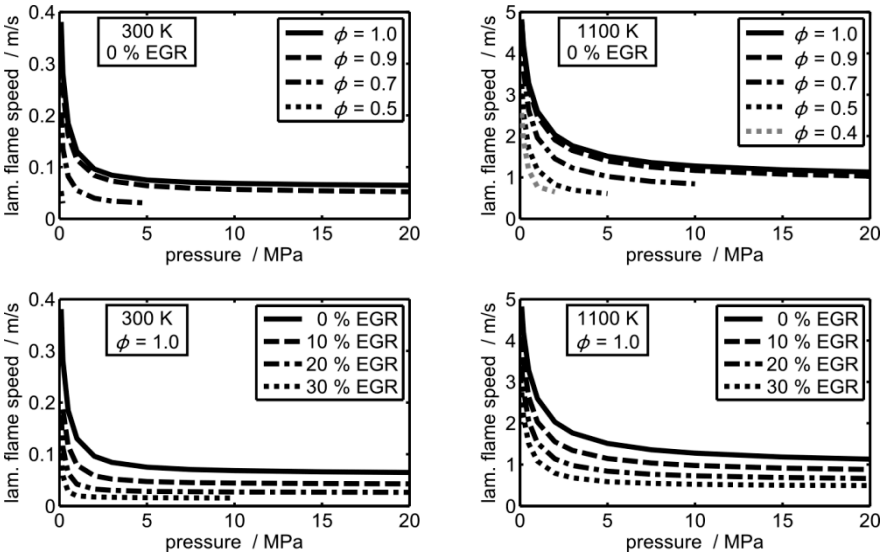

Figure 2: Laminar flame speed of methane-air-mixtures from reaction kinetic calculations within a pressure range of 0.1 to 20 MPa for unburned gas temperatures of 300 and 1100 K, shown for varying equivalence ratios (top) and EGR rates (bottom).

The turbulent flame propagation is simulated in the CFD calculations using the RANS method. The turbulent flame speed closure correlation suggested by Muppala-Dinkelacker [11] is incorporated (AFSW model)

$$s_T = s_L \cdot \left(1 + \frac{0.46}{Le} \cdot \mathrm{Re}_t^{0.25} \cdot \left(\frac{u'}{s_L} \right)^{0.3} \cdot \left(\frac{p}{p_0} \right)^{0.2} \right)$$

The flamequench model suggested by Ratzke et al. [12] is used to calculate the quench distance as a post-processing process. Further post-flame oxidation is incorporated as a function developed from the 0-D PSR simulations. These functions are incorporated in CFD by means of user defined functions.

4. CONCLUSIONS

A hybrid-model is suggested for the incestigation of the unburned hydrocarbon emmisions in gas engines. An extension to biogas is planned. The detailed chemistry is taken into account through 1-D and 0-D chemical kinetic simulations, the obtained chemistry results are coupled with CFD in the form of user defined functions. The validation studies will be performed in the near future.

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