Numerical Investigation of the Turbulent Combustion in a Direct-Injection Stratified Charge Engine with Emphasis on Pollutant Formation

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Abstract

Three-dimensional, time-dependent calculations have been performed to simulate a turbulent air swirl with spray, mixing, and combustion in the UPS-292 General Motors direct-injection stratified charge (DISC) engine. The present study focusses on the prediction of pollutant formation: detailed chemical reactions as well as the coupling of turbulence and chemistry are included. The engine burns most of the fuel in diffusion flames, and the combustion occurs in the flamelet regime of turbulent combustion. The present model extends the standard diffusion flamelet model to incorporate the time-dependent processes of internal engine combustion. The computations are performed using the KIVA-II code for three different engine load conditions at a speed of 2000 rpm. For comparison with the present results, there are calcualations with simplified chemistry as well as measurements of both the pressure history and the chemical composition of the exhaust gas. It appears that the present model greatly improves the predictions of pollutant emission for all conditions investigated.

Introduction

The simulation of turbulent combustion including detailed chemistry in internal combustion engines is a quite complex problem, and mathematical models need to be used which simplify physical and chemical processes. Typically, the chemical reactions are approximated using simplified reaction models such as global kinetic steps or assumption of chemical equilibrium. Moreover, the effect of turbulent fluctuations of the turbulent flow on the concentrations of chemical reactive species most often are neglected in numerical simulations of internal combustion engines. The present study employs an extended flamelet model to improve these simplified models.

The laminar flamelet concept considers the turbulent flame consisting of a set of laminar flamelets. These are well understood, and they are precalculated using a detailed reaction mechanism. In the present engine, about 95 % of the injected fuel is consumed in diffusion flames. Therefore, the diffusion flamelet model seems appropriate here. The structure of the laminar diffusion flame is characterized by a mixture fraction and its scalar dissipation rate. A statistical description of these variables accounts for interactions between non-equilibrium chemistry and turbulence. The model has been extended in order to describe the time-dependent fuel injection and the burn-out of the flame.

The reference fuel used in the computations is n-octane, and a detailed chemical kinetic mechanism is incorporated to predict pollutant formation, e.g. of nitrogen oxide and of carbon monoxide. The structure of laminar strained counterflow diffusion flames at various pressures, strain rates, and feed temperatures are stored in a flamelet library. These results enter the three-dimensional, time-dependent calculations performed with the KIVA-II code. A turbulent air swirl with fuel spray, mixing, and combustion under spark-ignition engine conditions in the UPS-292 direct-injection stratified charge engine is simulated. The engine operates at a speed of 2000 rpm, and three different engine load conditions are investigated. The results are compared to both experiments and to simulations using a simplified model.

Engine and Operating Conditions

The geometry of the combustion chamber and the schematic depiction of events occuring during injection and combustion are shown in Fig. 1. The engine combustion system is known as the TCCS (Texaco Controlled Combustion System). The UPS-292 stratified charge engine investigated operates at a speed of 2000 rpm, the initial rotating gas velocity is assumed to be 40 m/s. The bore is 9.843 cm, stroke and connecting rod are 10.46 cm and 17.186 cm, respectively. The compression ratio is 13:1. Bowl volume and diameter are 54.8 cm^3 and 5.05 cm, respectively.

In the experiments, the fuel Amoco 91 gasoline is used at a temperature of 358 K. The H/C ratio of this fuel is 1.85, and its lower heating value is 43.67 MJ/kg. Experimental results for three different engine load cases – the full-load and two different underload conditions – are available [1]. The overall equivalence ratios for the three load cases are 0.67 (case 1), 0.41 (case 2), and 0.24 (case 3), respectively. These values demonstrate the typical lean DISC engine concept. The measured

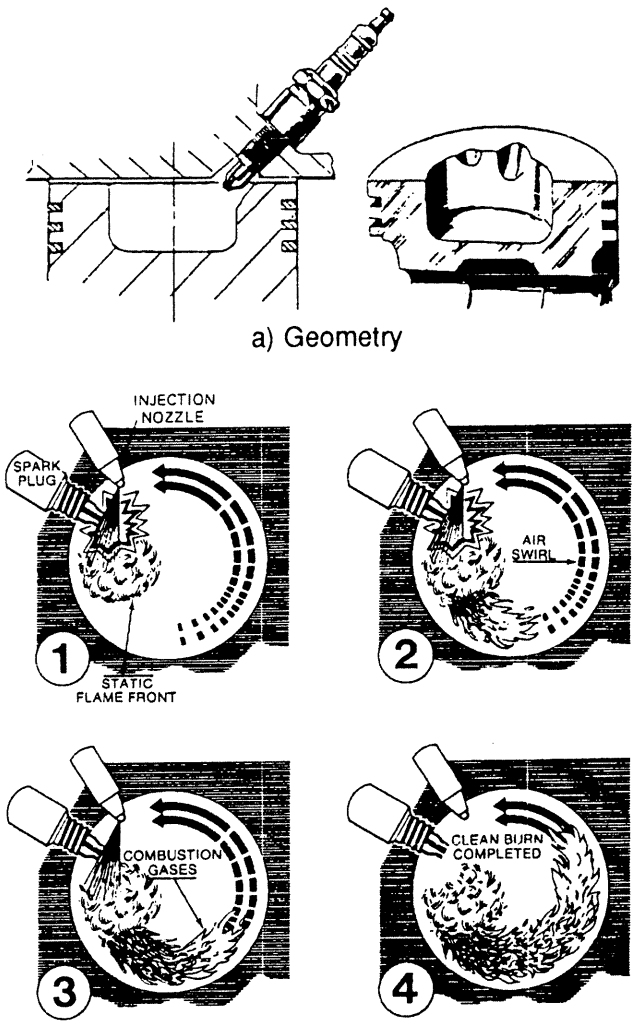

Figure 1: a) Geometry of the combustion chamber; b) schematic depiction of events occuring during injection and combustion in the UPS-292 GM DISC engine [1] .

quantities are the in-cylinder pressure history and the composition of the exhaust gas. The experiments were performed at the General Motors Research Laboratories [1]. Experimental results will be given later together with results of the numerical calculations.

Formulation

The model comprises the turbulent gas phase including chemical reactions as well as spray dynamics. Since the combustion is associated with steep density gradients, Favre averaged conservation equations for mass, momentum, energy, and mass fractions of chemical species are formulated.

The gas-phase equations are closed using a $k-\varepsilon$ turbulence model that accounts for volumetric expansion effects due to combustion [2]. Furthermore, the k and ε conservation equations involve source terms for the interaction with the spray [2]. For the present conditions, the turbulent Reynolds number is about 5000.

The directly injected fuel spray is described with the KIVA-II spray model [1, 2]. Spray dynamics like oscillations, collisions, distortions, coalescence and breakup of the droplets are considered. The liquid fuel spray is calculated using a stochastic particle technique which calculates the evolution of the probability distribution function of locations, velocities, sizes, and temperatures of the droplets. The present computation considers about 100,000 single droplets. The spray terms are coupled to the mass, momentum, energy, and species equations of the gas phase. Turbulence effects on the spray particles are modelled by adding a fluctuating velocity to the gas velocity.

The spark ignition in the DISC engine is modelled defining ignitor cells around the tip of the spark plug. Fuel and oxygen in these ignitor cells react infinitely fast to products and hence release ignition energy.

The present study focusses on both implementing effects of turbulence on chemistry and on improved models for chemical reactions. For this purpose the flamelet model is used.

If chemical reactions are faster than molecular diffusion (that is for large Damköhler numbers) the turbulent flame may be considered as an ensemble of asymptotically thin flamelets [3, 4]. For the present situation this assumption is shown to be appropriate [5]. Moreover, combustion in the DISC engine is known to take place almost entirely in diffusion flames [1, 6], so that the diffusion flamelet model is applied here [7]. Thus, the mixture fraction determines the flame location and the scalar dissipation rate characterizes the flame stretch – both variables determine the composition and temperature of a laminar diffusion flame.

The present mixture fraction ξ is based on the element C since fuel injection requires a modification of the standard flamelet model developed by Peters [3, 4] for steady flames (the element H leads to very small values of ξ_H at stoichiometricy and was not chosen here). If Z_c describes the element mass fraction, the mixture fraction is defined as

$$\xi_c \equiv \frac{Z_c - Z_{c,ox}}{Z_{c,fuel} - Z_{c,ox}}. \qquad (1)$$

In Eq.(1), *fuel* and *ox* denote conditions in the pure fuel and oxidizer stream, respectively.

The time-dependent conservation equations of Z_c and its variance account for time-dependent fuel injection ($\dot{Z}_c^s$ denotes the mass injection ratio based on element C):

$$\frac{\partial(\overline{\varrho}\widetilde{Z_c})}{\partial t} + \mathrm{div}(\overline{\varrho}\widetilde{\mathbf{u}}\widetilde{Z_c}) - \mathrm{div}(\Gamma_{eff}\mathrm{grad}\widetilde{Z_c}) = \overline{\varrho}\widetilde{\dot{Z}_c^s} \qquad (2)$$

$$\frac{\partial(\overline{\varrho}\widetilde{Z_c''^2})}{\partial t} + \mathrm{div}(\overline{\varrho}\widetilde{\mathbf{u}}\widetilde{Z_c''^2}) - \mathrm{div}(\Gamma_{eff}\mathrm{grad}\widetilde{Z_c''^2}) =$$

$$c_1\mu_{eff}(\mathrm{grad}\widetilde{Z_c})^2 - c_2\overline{\varrho}\frac{\widetilde{\varepsilon}}{\widetilde{k}}\widetilde{Z_c''^2} + 2\overline{\varrho}\widetilde{Z_c''^2}\frac{\widetilde{\dot{Z}_c^s}}{\widetilde{Z_c}}, \qquad (3)$$

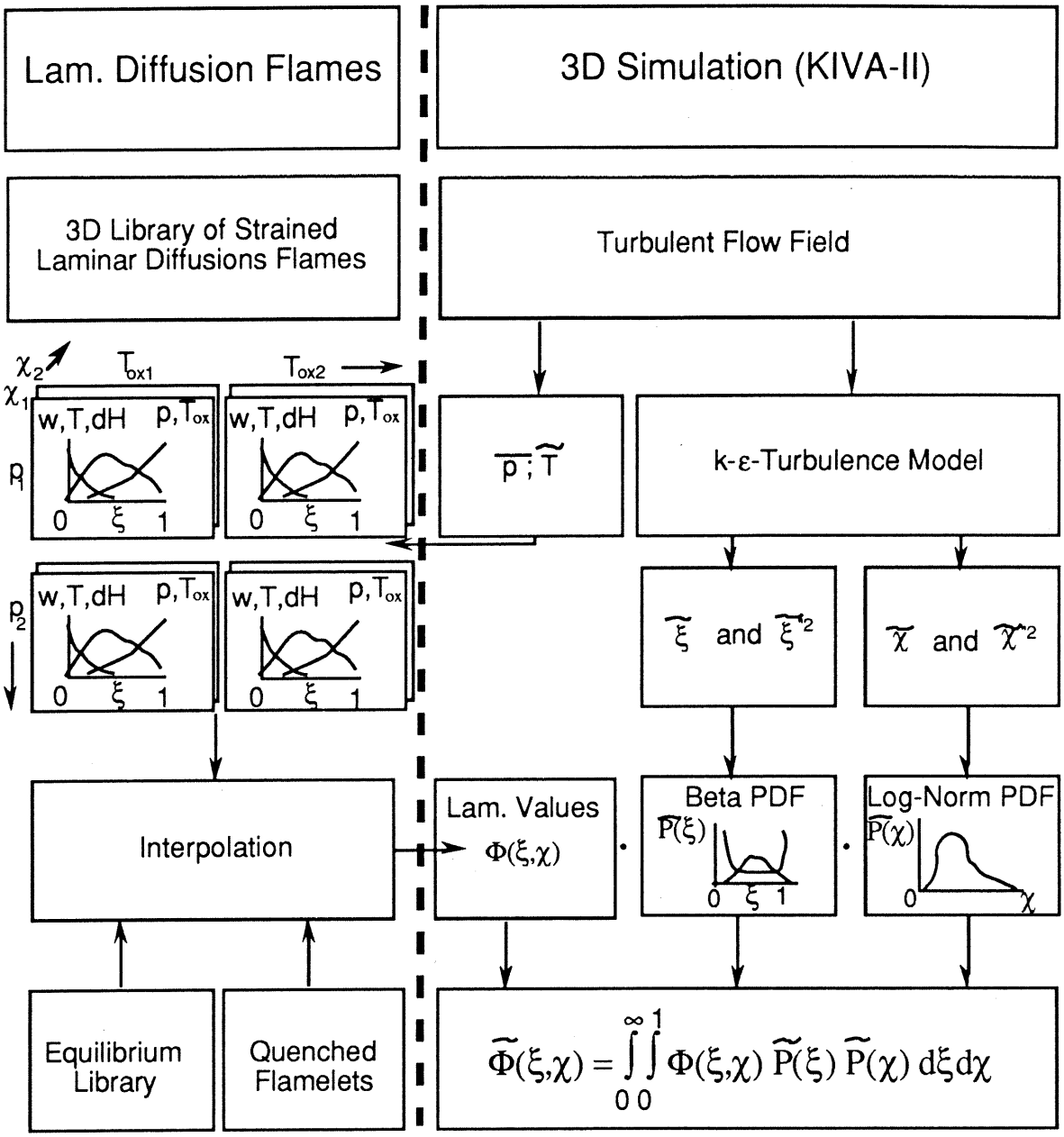

Figure 2: Schematic of the coupling of the flamelet library and the 3D internal engine simulation.

where the last term was modelled, for details see [7]. $\Gamma_{eff} = \mu_{eff}/\sigma$ is the effective exchange-coefficient and σ the turbulent Prandtl-Schmidt number, which is 0.9. The constants are $c_1 = 2/\sigma$ and $c_2 = 2$.

The second term of the rhs in Eq. (3) is associated with the scalar dissipation rate $\tilde{\chi}$ which is modelled using the turbulence kinetic energy k and its dissipation rate ϵ [3, 7]:

$$\tilde{\chi} \equiv 2\, D\, \overline{\mathrm{grad}^2 \xi_c''} = c_2 \frac{\tilde{\epsilon}}{\tilde{k}} \widetilde{\xi_c''^2} \quad \text{, where} \tag{4}$$

$$\widetilde{\xi_c''^2} = \frac{\widetilde{Z_c''^2}}{(Z_{c,fuel} - Z_{c,ox})^2} \,. \tag{5}$$

The coupling of non-equilibrium chemistry and turbulence is achieved using a statistical description of ξ and χ, where statistical independence of the two variables is assumed [3], c.f. Fig. 2. The probability density function (PDF) used for the mixture fraction is a beta-function the shape of which is determined by values of the local mean and the variance of the mixture fraction (c.f. Eqs. (2) and (3)). The scalar dissipation rate is assumed to be lognormal distributed with a constant variance that equals 2 [3]. For details see [3, 7].

The structures of laminar counterflow diffusion flames are precalculated [8] at strain rates of 15, 20, 60, 120, 250, 500, 750, 1000, 2000, and 3000 1/s at various pressures (20, 30, 40, and 50 bar). The feed temperature of the air stream is 900, 1050 and 1200 K, fuel enters at its pressure-dependent boiling temperature. The detailed reaction mechanism for n-octane comprises 67 species and 732 elementary reactions where some of the reaction rates are pressure-dependent.

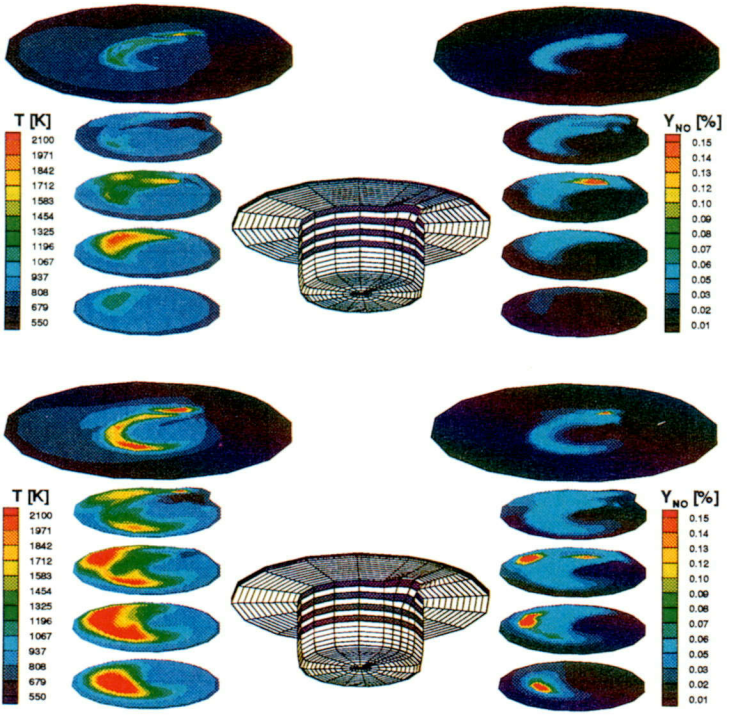

Figure 3: Contour plots of gas temperature T (left part) and of NO-mass fraction (right part) for case 2 at 5° CA BTDC (upper part) and at 0° CA BTDC (lower part) at five different locations (dark positions marked in the plot of the numerical grid) in the combustion chamber.

Results and Discussion

The present study concerns both the incorporation of improved chemistry and the effects of turbulence on chemistry using the flamelet model. The applicability of the model and the occurrence of diffusion flames is discussed in more detail in Ref. [7]. The present calculations can be compared to both previous numerical results from O'Rourke and Amsden [1] using simplified chemistry and with experimental data [1]. The simplified model neglects turbulence-chemistry interactions. It comprises one kinetic step for the fuel consumption. Furthermore, an extended Zeldovich mechanism for thermal NO as well as 6 equilibrium reactions for the dissoziation of the species O_2, N_2, H_2, H_2O and CO_2 are implemented [2]. Hence, the simplified model comprises 12 species and 10 reactions.

At first, a general overview about the total combustion process is shown in Fig. 3. Here gas temperature (left part) and NO mass fraction (right part) are plotted at two different times during combustion, at 5° CA before top dead center (BTDC) (upper part) and at 0° CA BTDC (lower part). The figure shows five cuts through the combustion chamber at different locations which are marked through dark fields in the numerical grid (middle part). The location of the scallop of the spark plug can be seen in the second cut at the right-hand side of the combustion chamber. The position of ignition is seen in the third cut where gas temperature rises, c.f. Fig. 3. The results of the calculations have been obtained using the flamelet model. The figure shows the correlation of NO formation and high-temperature regions. The flame propagates in circumferential direction with the turbulent flow field through the combustion chamber. A comparison of the upper and lower NO contour plots shows that NO is formed in regions where the combus-

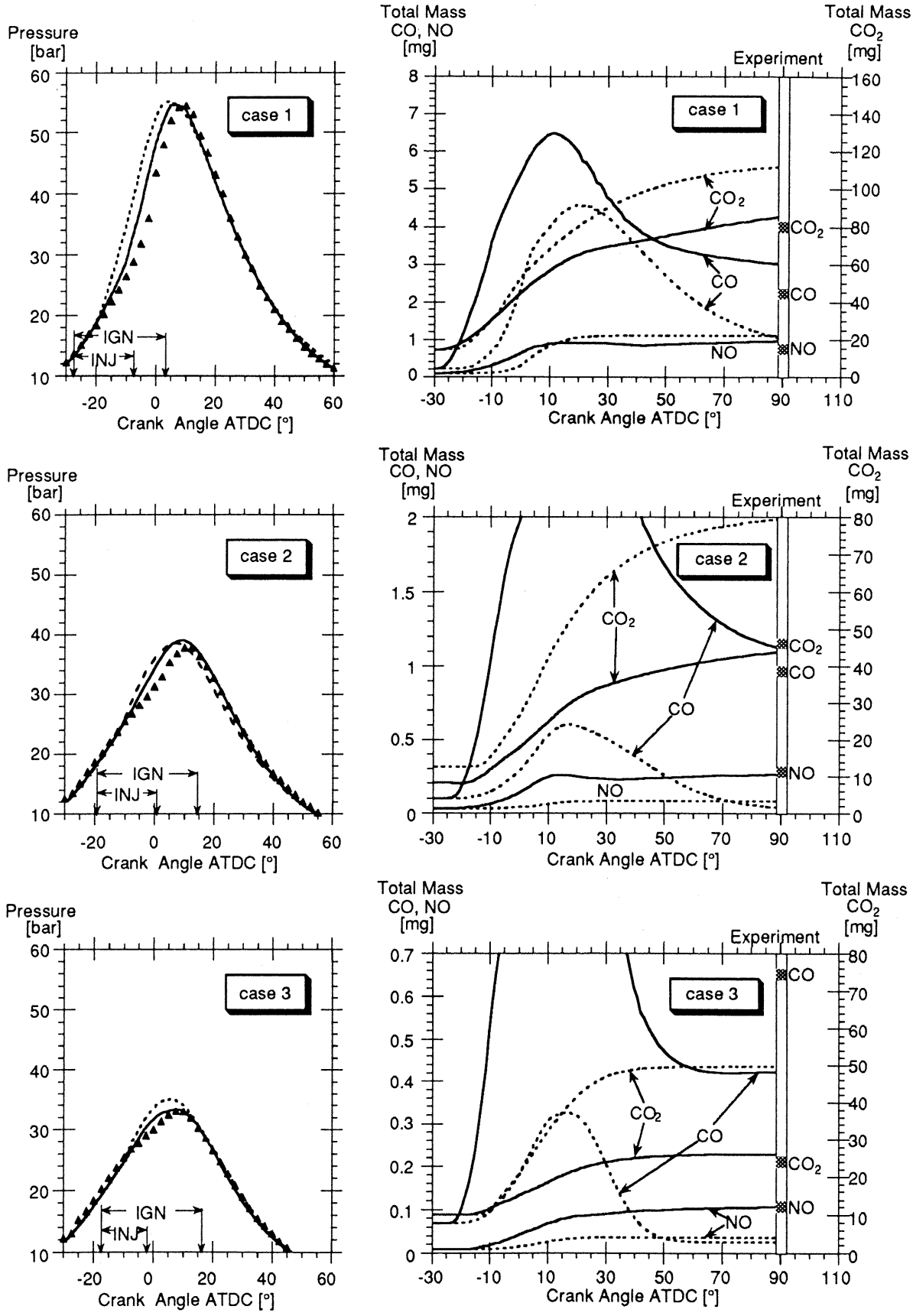

Figure 4: Left: In-cylinder pressure versus crank angle ATDC predicted by the flamelet model (solid line), the simplified model (dashed line), and experiment (symbols) for the full-load case 1 and two different underload cases 2 and 3. Right: Total mass of CO, NO, and CO_2 versus crank angle for the calculation with the flamelet model (solid line), the simplified chemistry model (dashed line), and experiments at 90° CA ATDC (symbols) for the three different load cases.

tion process proceeds and temperature rises.

Experimental data are available for the in-cylinder pressure and the total mass of CO, CO_2, and NO in the hot exhaust. In Fig. 4, both previous calculations and experimental results are compared to the present numerical results. The left part of Fig. 4 shows the measured and calculated in-cylinder pressure histories for cases 1, 2, and 3, respectively. It can be seen that the simplified chemistry releases heat faster in comparison with the flamelet model and the experiment, which leads to a higher pressure increase seen in the figure. This is due to endothermic decomposition of the fuel in rich flame regions which are neglected in the simplified model but are considered using detailed chemistry.

The right part of Fig. 4 gives a quantitative comparison of the measured and calculated species mass of CO_2, CO, and NO for the 3 different cases. The species mass of CO_2 in the exhaust gas characterizing the total chemical conversion differs between 3.7 % and 7.7 % if flamelet calculations and the experiment are compared whereas the simplified chemistry calculation differs between 40.9 % and 99.6 % from experiment.

The species mass CO, which strongly influences the chemical heat release, departs from 56.2 % to 96.2 % from experiment compared with the simplified model. The flamelet model predicts a value of CO mass which differs between 19.3 % and 36.2 % from experiment.

Comparing the NO mass at 90 degree crank angle after top dead center, the flamelet model predicts a value which departs between 4.6 % and 15.0 % from the experimental value. The simplified model predicts a NO mass which differs between from 31.9 % and 70.1 % from the measured NO mass. Apart from the differences in the reaction mechanism, this may be caused by the effect of turbulence on the chemical reactions which is included in the flamelet model but not in the simplified model.

Conclusions

The simulation of the combustion process in a stratified charge engine including spray dynamics, evaporation, mixing, and combustion has been performed using the code KIVA-II. The effects of turbulence on chemistry were included using a flamelet model for turbulent non-premixed combustion which enables consideration of detailed chemistry. The standard flamelet model was extended to account for time-dependent fuel injection. The modified model has been applied to three-dimensinal internal engine combustion. Flamelet calculations were compared with calculations using a simple combustion model which neglects turbulence-chemistry interactions. Moreover, the computational results were compared with experimental data for pressure and for some chemical species.

In general, it can be seen that the flamelet model is able to describe overall heat release and chemical species concentrations significantly better than the simplified combustion model. Hence, the influence of detailed chemistry and the interactions between turbulence and chemistry should be considered in internal engine combustion simulations. In order to improve the flamelet results, a more detailed flamelet library with partially premixed reactant streams may be used in future calculations.

Considering the real combustion process, models for soot formation and radiation would be helpful to render simulations of the combustion process more predictive.

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