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Combustion Modeling with the G-Equation

M. Dekena[1*] and N. Peters[2]

1 Volkswagen AG
2 Institut für Technische Mechanik, RWTH D52056 Aachen - Germany

* now at AUDI AG, D85045 Ingolstadt

Résumé — Modélisation de la combustion avec l'équation de G — Une investigation numérique relative à la propagation des fronts de flammes turbulents dans les moteurs à essence à injection directe (GDI) a été menée en implantant un modèle de "flamelet" dans le code 3D Fire. L'avantage de ce modèle de combustion est de découpler la chimie de l'écoulement turbulent en divisant la chambre de combustion en deux zones : brûlée et imbrûlée, à l'aide d'une équation de transport d'un scalaire (équation de G). Une valeur de référence de ce scalaire définit la position moyenne de la flamme. Une chimie complète est calculée interactivement avec le calcul 3D à l'aide d'un code monodimensionnel RIF (*Representative Interactive Flamelet*). Le modèle de combustion a été validé sur la simulation d'un moteur 2 litres à 2 soupapes en combustion homogène pour vérifier la représentativité de l'approche "flamelet". Puis, le potentiel du modèle de combustion a été étudié en simulant un moteur modèle 2 litres 4 soupapes GDI.

Abstract — Combustion Modeling with the G-Equation — *Numerical investigations concerning the turbulent flame front propagation in Gasoline Direct Injection (GDI) engines were made by implementing a flamelet model in the CFD code Fire. The advantage of this combustion model is the decoupling of the chemistry from the turbulent flow. For this purpose the combustion chamber has to be divided into a burned and an unburned area, which is realized by transporting a scalar field (G-Equation). The reference value defines the present averaged flame position. The complete reaction kinetics is calculated interactively with the CFD code in a one dimensional Representative Interactive Flamelet (RIF) code. This combustion model was verified by simulating a 2.0 l-2 V gasoline engine with homogeneous combustion where a parameter study was conducted to check the flamelet model for plausibility. Finally, the potential of this combustion model was investigated by simulating a hypothetical 2.0 l-4 V GDI engine.*

INTRODUCTION

Because of increasing worldwide passenger car traffic especially in urban centers, the automotive industry is being forced to drastically reduce fuel consumptions and exhaust emissions.

It is for this reason that many automobile manufacturers are aiming to design cleaner and more efficient engines. What is desired is an engine with the advantages of gasoline engines (i.e. high specific power and good exhaust gas quality) at full load operation conditions and those of Diesel engines at part load. One possibility to reach this target is the use of engines with Gasoline Direct Injection (GDI). The optimization of those combustion processes is so complex, that advanced methods need to be used to develop a GDI engine in a suitable period.

In recent years, the computer programs have become so improved, that the realistic flow simulation of industrial applications by 3D Computational Fluid Dynamics (CFD) has become practicable. A special challenge for CFD is the simulation of GDI engine combustion with pollutant formation because every occuring phenomenon (turbulent flow, spray kinematics, evaporation of droplets and combustion) is very complex and needs to be modelled exactly.

In the present paper, a flamelet model for partial premixed combustion is implemented in the CFD code Fire in order to simulate GDI engine combustion. In order to test this model, two operating conditions of a 2.0 l-2 V gasoline engine with

homogeneous combustion have been simulated and compared with experimental results. The simulation of a hypothetical 2.0 l - 4 V GDI engine further demonstrates the benefit of the flamelet model.

1 METHOD OF NUMERICAL ANALYSIS

1.1 The Flamelet Model for Partial Premixed Combustion

Because of the assumption that the chemical time scales are much smaller than the turbulent time scales, a thin reaction layer exists in which the chemical reactions precedes. Peters [1] showed that this zone can be approximated by several counter diffusion flames, so-called flamelets. In the same paper a transformation of the cartesian coordinates into a newly defined *Z*-coordinate system leads the conservation equations for enthalpy respectively temperature and species into a one dimensional system which depends only on the mixture fraction *Z*. With this approach the chemistry can be regarded as decoupled from the turbulent flow.

By assuming $Le = 1$, the flamelet equations are defined as follows:

– Species:

$$\rho\frac{\partial Y_i}{\partial t} - \rho\frac{\chi}{2}\frac{\partial^2 Y_i}{\partial Z^2} - \dot{m}_i = 0 \tag{1}$$

– Temperature:

$$\rho\frac{\partial T}{\partial t} - \rho\frac{\chi}{2}\frac{\partial^2 T}{\partial Z^2} + \sum_i^N \frac{h_i}{c_p}\dot{m}_i - \frac{1}{c_p}\left(\frac{\partial p}{\partial t} + q_R\right) = 0 \tag{2}$$

where the scalar dissipation rate χ is defined by:

$$\chi = 2D\left(\frac{\partial Z}{\partial \chi_\alpha}\right)^2 \tag{3}$$

and q_R stands for the radiation loss and Y_i symbolizes the mass fraction of the species *i*. The production rate due to the chemical reaction $\dot{m}_i$ is calculated by:

$$\dot{m}_i = W_i\sum_k \nu_{ik} w_k \tag{4}$$

where W_i is the molar weight of the species *i*, ν_{ik} is the matrix of stochiometric coefficients and w_k the reaction rate of the reaction *k*.

The flamelet model solves the species composition in dependence of the mixture fraction interactively with the CFD code. The boundary conditions are the temperature at the oxygen side, the temperature at the fuel side, the pressure and the stochiometric scalar dissipation and are obtained from the flow field.

In addition to the implemented transport equations in the FIRE code, two further equations are required:

– Mixture fraction:

$$\frac{\partial\left(\bar{\rho}\tilde{Z}\right)}{\partial t} + \frac{\partial\left(\bar{\rho}\tilde{\upsilon}_\alpha\tilde{Z}\right)}{\partial x_\alpha} = \frac{\partial}{\partial x_\alpha}\left(\frac{\mu_T}{Sc}\frac{\partial\tilde{Z}}{\partial x_\alpha}\right) + S_{Sp} \tag{5}$$

– Variance of mixture fraction:

$$\frac{\partial\left(\bar{\rho}\widetilde{Z''^2}\right)}{\partial t} + \frac{\partial\left(\bar{\rho}\tilde{\upsilon}_\alpha\widetilde{Z''^2}\right)}{\partial x_\alpha} = \frac{\partial}{\partial x_\alpha}\left(\frac{\mu_T}{Sc}\frac{\partial\widetilde{Z''^2}}{\partial x_\alpha}\right) + 2\frac{\mu_T}{Sc}\left(\frac{\partial\tilde{Z}}{\partial x_\alpha}\right) - \bar{\rho}\tilde{\chi} \tag{6}$$

S_{Sp} in Equation 5 stands for the fuel source which results from the spray.

1.2 The G-Equation for Turbulent, Partial Premixed Combustion

By definition, *G* values in the burned area are smaller than zero and in the unburned greater than zero.The flame front is determined at the reference *G* value G_0. Because of a kinematic balance at the flame front, the laminar G-Equation is defined as:

$$\frac{\partial G}{\partial t} + \upsilon_{\alpha,u}\frac{\partial G}{\partial x_\alpha} = S_L(Z)|\nabla G| \tag{7}$$

The G-Equation for turbulent combustion is derived by dividing the scalar *G* and the flow velocity υ into mean and fluctuating components.

$$\begin{aligned} G(x,t) &= \overline{G}(x,t) + G'(x,t) \\ \upsilon(x,t) &= \overline{\upsilon}(x,t) + \upsilon'(x,t) \end{aligned} \tag{8}$$

After inserting Equation (8) in Equation (7) and following ensemble-averaging as shown in [2] the turbulent G-Equation is defined by:

$$\frac{\partial\overline{G}}{\partial t} + \overline{\upsilon_{\alpha,u}}\frac{\partial}{\partial x_\alpha}\left(\overline{\upsilon'_{\alpha,u}G'}\right) = \overline{S_L^0\sigma} - \overline{D_L\kappa|\nabla G|} + \overline{Ln_\alpha\frac{\partial\upsilon_\alpha}{\partial x_\beta}n_\beta|\nabla G|} \tag{9}$$

where σ stands for the absolute value of the scalar gradient, κ for the flame curvature, *L* for the markstein length and D_L for the markstein diffusivity.

Peters derived in [3] an approach for the term $\overline{S_L^0\sigma}$ by introducing an equation for the variance of the scalar *G*.

$$\frac{\partial \overline{G'^2}}{\partial t} + \overline{\upsilon_{\alpha,u}} \frac{\partial \overline{G'^2}}{\partial x_\alpha} = -\frac{\partial}{\partial x_\alpha}\left(\overline{\upsilon'_{\alpha,u} G'^2}\right) - 2\overline{\upsilon'_{\alpha,u} G'} - \overline{\omega} - \overline{\chi_L} - \overline{\Sigma_L} \quad (10)$$

where $\overline{\omega}$ is the scalar restauration, $\overline{\chi_L}$ the scalar dissipation and $\overline{\Sigma_L}$ the covariance of scalar fluctuation and of the stretch.

The variance of G is then used to determine the turbulent flame thickness which is defined as:

$$l_{F,t} = 2\frac{\sqrt{\overline{G'^2}}}{|\nabla \overline{G}|}\bigg|_{\overline{G}=G_0} \quad (11)$$

In order to close the system of equations an approch was used for the scalar restauration by an equation for the two point correlation of the scalar fluctuations [3] in the limit $\nu'/S_L^0 \to \infty$. After investigations by direct numerical simulation for finite ratios of ν'/S_L^0, [4] proposed the turbulent G-Equation be used in analogy to the laminar G-Equation:

$$\frac{\partial \overline{G}}{\partial t} + \overline{\upsilon_{\alpha,u}} \frac{\partial \overline{G}}{\partial x_\alpha} = S_T |\nabla \overline{G}| \quad (12)$$

where S_T is the turbulent burning velocity which is defined as:

$$S_T = \left(S_L^0 + b_1 \upsilon' + b_2 \sqrt{S_L^0 \upsilon'}\right)\left(1 - b_3 \frac{L}{l_t} \frac{\upsilon'}{S_L^0}\right) \quad (13)$$

Through direct numerical simulations [4, 5], the following constants were determined:

$$b_1 = 1.5 \; ; \; b_2 = 0.8 \; ; \; b_3 = 1.4 \quad (14)$$

The approximated turbulent flame thickness is simulated by:

$$l_{F,t} = 2\sqrt{\frac{2C_\mu}{c_\omega}} \frac{\tilde{k}^{3/2}}{\tilde{\varepsilon}} \quad (15)$$

The markstein length L is determined by the product of the markstein number and the laminar flame thickness:

$$L = M \cdot l_F \quad (16)$$

A semi-empirical approach for the laminar reference burning velocity S_L^0 is derived in [6]:

$$S_L^0 = F Y_{f,u}^m \exp\left(-G/T^0\right) \cdot \frac{T_u}{T^0}\left(\frac{T_b - T^0}{T_b - T_u}\right)^n \quad (17)$$

where T_u stands for the unburned temperature, T_b for the burned temperature and T^0 for the inner layer temperature. The constants F, G, m and n are fuel type dependent and defined in [2]. The unburned temperature is determined from the closest fully unburned cell to the flame front and the adiabatic flame temperature is obtained by the species composition and the total enthalpy in the fully burned cell closest to the flame front.

An approach for the laminar flame thickness is used in the following simulations and is shown in [6]:

$$l_F = \frac{\left(\lambda / C_p\right)\big|_{T^0}}{\rho_u S_L^0} \quad (18)$$

where the ratio λ/C_p is approximated by:

$$\frac{\lambda}{C_P} = 2.58 \text{ x } 10^{-5} \frac{\text{kg}}{\text{ms}}\left(\frac{T}{298 \text{ K}}\right)^{0.7} \quad (19)$$

The variable T^0 describes the inner layer temperature and is approximated according to [6] by:

$$p = B \exp(-E/T^0) \Rightarrow \text{T°} = \frac{E}{\ln(B/p)} \quad (20)$$

The constants B and E are fuel type dependent and are given in [2].

1.3 Interaction of the Flamelet Model with the Fire Code

Figure 1 shows the interaction of the flamelet model with the CFD code. A new timestep begins with the calculation of the flame propagation by the G-Equation. Then the CFD code

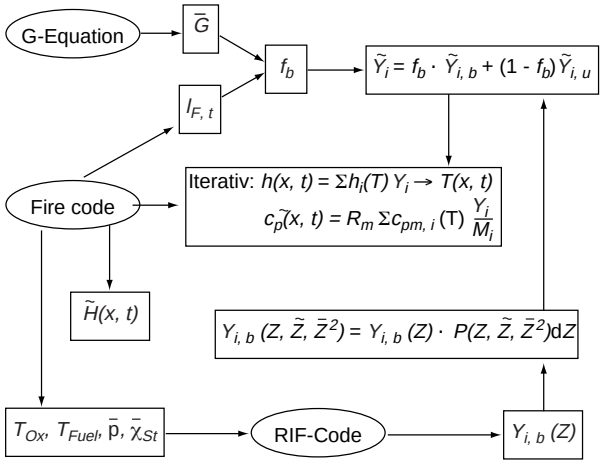


Figure 1

Interaction between the Fire code, G-Equation and the RIF code.

solves every transport equation for the new timestep and after this the RIF calculates the new species composition in dependence from the mixture fraction with the changed boundary conditions.

Because of the knowledge of the turbulent energy and dissipation from the CFD code, the turbulent flame thickness is determined by Equation (15). The burned fraction in each cell is calculated by the new *G*-field and the turbulent flame thickness. To obtain the species composition for the burned part in every cell, the solution of the RIF is weighted by a beta PDF.

The unburned flamelet contains only species of fuel, oxygen and nitrogen. The total species composition of a cell is calculated by an interpolation between the burned and the unburned averaged solutions with the burned fraction used as an interpolation factor. By transporting the total enthalpy in the CFD code iteratively, the new cell temperature is derived by a polynomial approach (NASA) for the enthalpy. The specific heat capacity is updated with the new cell temperature.

2 VALIDATION OF A 2.0 L-2 V GASOLINE ENGINE

A 2.0 l-2 V series engine was chosen to validate the flamelet model. The mesh of this simulated engine contained 42 000 cells. Initial conditions for turbulent kinetic energy and dissipation were obtained from previous theoretical investigations. The initial cylinder pressure and temperature resulted from indicated engine measurements. The ignition time was set to 24° CA BTDC.

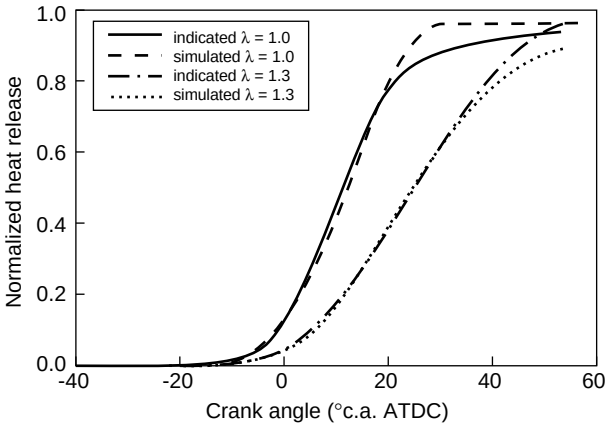
In Figure 2 the combustion chamber is shown with the isosurface of the reference value $\overline{G} = \overline{G}_0 = 0$ which describes the present averaged turbulent flame front.

A comparison of the indicated cylinder pressure and normalized heat release with the simulation in Figure 3 shows good agreement.

It is well-known that the $k - \varepsilon$ turbulence model calculates inaccurate values for the turbulent kinetic energy and dissipation at walls. This leads to inexact integral length scales at wall locations which has an effect on the calculation of the turbulent burning velocity. The local turbulent burning velocity in these regions are calculated too high. This occurs especially when large parts of the flame surface are near the wall and the simulated heat release rate is too high. It is for this reason that the normalized heat release and the cylinder pressure in the simulation shown in Figure 3 is overpredicted towards the end of the combustion period.

Figure 2

Turbulent flame front at 5 degrees c.a. ATDC; n = 2000 tr/min; ignition time = 24° CA BTDC.



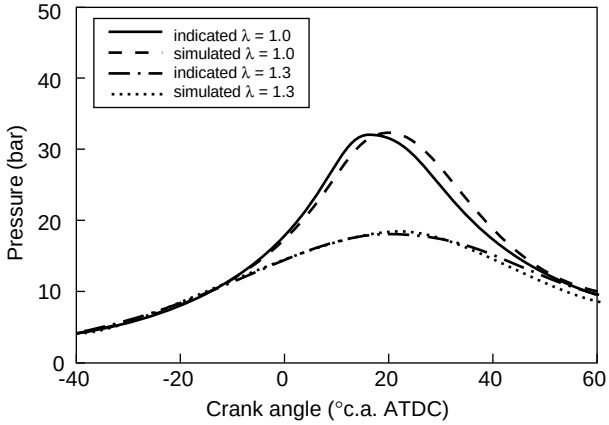


Figure 3

Comparison of measured and simulated heat release and pressure at n = 2000 tr/min.

3 SIMULATION OF A 2.0 L-4 V GDI ENGINE

In the following section the simulation of a simplified hypothetical 2.0 l-4 V GDI engine at full load operation conditions at 2000 tr/min will show the potential of the flamelet model for partial premixed combustion.

The piston bowl shape is cylindrical and placed in the center of the cylinder. For simplification purposes the inlet ports are omitted and replaced by appropriate boundary conditions which forces a swirl flow (Fig. 4).

The injection start time began at 30° CA BBDC, the injection duration equaled 60 degrees c.a. and the ignition time was set to 20° CA BTDC. The injected fuel mass at full load amounted to 35 mg.

The fuel was vertically injected by a 60° CA. hollow cone nozzle which was placed in the center of the cylinder. The spray kinematics and evaporation of the droplets was simulated by a discrete-droplet model which is implemented in the Fire code.

An example of the resulting droplet and fuel vapour distribution is shown in Figure 5 at 90° CA BTDC. Because of the hollow cone nozzle, the droplets move to the cylinder wall and form a rich mixture in the squish area at the time of ignition time the mixture at the spark plug is flammable so that a combustion can be initiated. While ignition period the burning velocity of the flame front starts with the laminar burning velocity till a fully turbulent flame front is developed. ignition. In contrast to the squish area at the same time, the mixture in the piston bowl is extremly lean. At

From then on the flame front propagates unattached into the unburned mixture.

In Figure 6, the position of the turbulent flame front and the exhaust gas concentrations for carbonmonoxide, nitrogenoxide and fuel is demonstrated at 25° CA ATDC. At this time, there is the flame front no longer propagates because in the squish area the mixture is too rich and in the piston bowl it is too lean for a further growth of the flame front surface.

Figure 7 shows the global quantities of the cylinder pressure, normalized heat release, carbonmonoxide and nitrogenoxide concentrations.

Global quantities of exhaust gas concentrations are obtained by density weightning of the total integration domain.

The normalized heat release clearly indicates that only 70% of the injected fuel has been burned. The exhaust gas contains 30% unburned fuel, 2% carbonmonoxid and 0.5% nitrogenoxide.

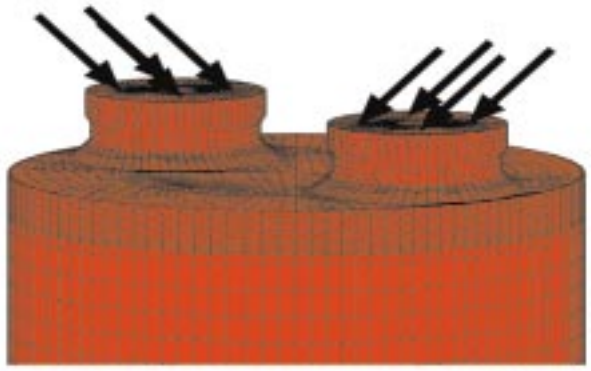


Figure 4

Direction of the mass flow boundary conditions for both inlet ports.

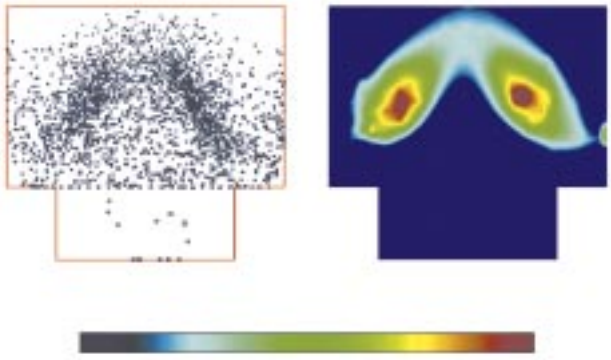


Figure 5

Droplet and vapour distribution at 90° CA BTDC.

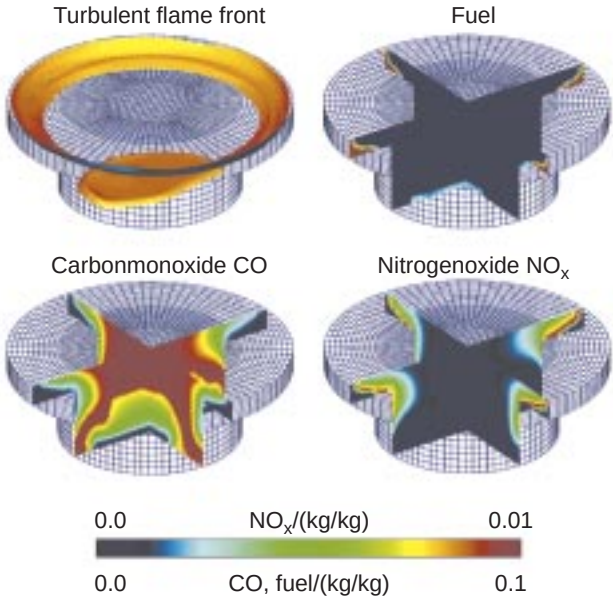


Figure 6

Turbulent flame front and exhaust gas concentration at 25° CA TDC.

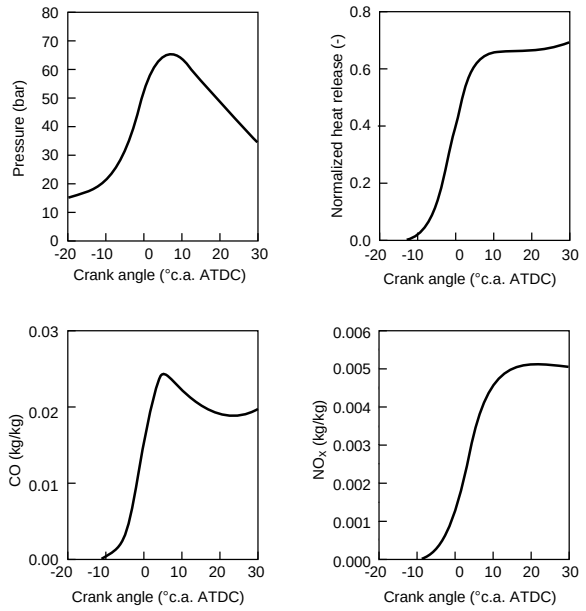


Figure 7

Global quantities of the simulated GDI engine.

CONCLUSION

A flamelet model for partial premixed combustion has been coded into a commercial CFD code. The model was tested and the numerical results compared to measurements. Good agreement with experimental results were obtained for the case of a homogeneous combustion engine. The flamelet model was further applied to a hypothetical GDI engine which allowed the calculation of numerous exhaust gas concentrations including carbonmonoxide and nitrogenoxide. Further investigations need to be conducted to a real GDI engine in order to check the quality of the flamelet model with regards to exhaust gas concentrations.

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