

A Numerical Study of the Effect of EGR on Flame Lift-off in n-Heptane Sprays Using a Novel PaSR Model Implemented in OpenFOAM

Anne Kusters and Valeri Golovitchev
Chalmers Univ of Technology

Anders Karlsson
Volvo Technology Corp

ABSTRACT

The effect of exhaust gas recirculation (EGR) on flame lift-off in non-stationary n-heptane sprays was studied under Diesel engine-like conditions using numerical simulation involving complex chemistry and a novel partially stirred reactor (PaSR) model of subgrid turbulence-chemistry interaction.

The flame-stabilization mechanism is a result of complex physical and chemical interactions and cannot be described by a simplified theory. To leading order it is determined by the chemical reaction time at the leading edge, the turbulent diffusivity, and the flow velocity; so that there exists a balance between the local convection velocity and the triple-flame propagation speed. In this study of ignition and flame formation and stabilization processes, the VSB2 stochastic blob-and-bubble spray model was used in combination with the volume reactor fraction model (VRFM) implemented in OpenFOAM. The reacting volume fraction in the VRFM was determined by solving for mixture fraction, progress variable, and their variances in order to estimate the non-uniformities of the fluid cell; rather than simply taking the ratio of the mixing and chemistry time-scales. The chemistry is described by a reduced n-heptane mechanism with 36 species involved in 81 reactions.

The simulated lift-off trends are compared to available experimental data from the Engine Combustion Network, Sandia National Laboratories [1].

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INTRODUCTION

Flame lift-off and stabilization are of particular interest in the case of the turbulent combustion process occurring in a Diesel engine. Highly lifted flames are typical and the lift-off length influences the emissions. The lift-off length determines how much the fuel is mixed with air before the mixture reaches the flame. A broad discussion about the lift-off length of Diesel sprays and the parameters influencing it can be found in [2]. An increase in the ambient temperature and/or density decreases the lift-off length. An increase in temperature results in an increase in the laminar flame speed and thermal diffusivity, thereby decreasing lift-off length. In contrast, an increase in injection pressure, and hence an increase in injection velocity, results in an increase in lift-off length. In summary, the level of air entrainment is strongly

influenced by the lift-off length, which mostly depends on the ambient temperature and the injection pressure. Also, a smaller orifice diameter increases the level of air entrainment. Soot formation depends on how well the fuel is premixed with air upstream of the lift-off position. The better is fuel mixed with air, the lower is the soot formation during combustion.

In the initial phase of combustion, the premixed fraction of vapor fuel and air is consumed very fast; the combustion then continues under non-premixed conditions [3]. Modeling of turbulent combustion is very challenging since the turbulent mixing of vapor fuel with air and the interaction of the turbulence with the chemistry have to be described in a sufficient way.

The Eddy Dissipation Combustion Model (EDCM), introduced by Magnussen and Hjertager in 1976 [4], is an

empirical model that assumes the chemistry to be very fast and defines the rate of combustion to be controlled by the mixing process of oxygen and fuel (under the assumption that “mixed is burnt”). In diffusion flames, fuel and oxygen occur in separate eddies, hence the rate of combustion is defined by the rate of dissipation of the eddies [4]. Spalding already defined in 1970 an Eddy Break-Up (EBU) model [5] in which the velocity of the mixing process of unburned and burned gas is defined in terms of the decrease in the turbulent energy. The EDCM is related to the EBU model, but does not solve the equations for the concentration fluctuations, which are difficult to determine. Instead, the dissipation of turbulence is related to the mean concentration of the intermittent quantities [4]. With the EDCM, it was possible for the first time to describe turbulent diffusion combustion in a successful way. Since the model is very simple and robust it is widely used to describe turbulent combustion. One problem with this model is the lack of complex chemistry, which makes it impossible to take into account, for example, NO or soot formation or locally collapsing flames.

In 1981, Magnussen presented the Eddy Dissipation Concept (EDC) [6], a general concept for treating the turbulence-chemistry interaction in a turbulent flame. The concept defines the small structures of the flow, where the turbulence dissipates into heat, to be the structures where the reactants will be mixed at the molecular scale. These fine structures, where we have a molecularly well-mixed mixture, then account for a fraction of the volume of fluid. This fraction is defined to be the reactor volume in which chemical reactions are allowed to happen. The concept also considers the mass transfer between the reactor volume and the rest of the cell. With this model it was possible to include complex chemistry and consider the turbulence-chemistry interaction.

In the work presented here, the volume reactor fraction model (VRFM) was chosen and was implemented in OpenFOAM. The model was developed by Karlsson [7], and a study with an enhanced version of this model concerning flame lift-off length in Diesel sprays has been presented by Chomiak and Karlsson [8]. The model is based on the EDC, but considers the non-uniformities of the fluid cell. The results obtained from the VRFM are compared here to experimental data from the Engine Combustion Network, Sandia National Laboratories.

MODELING ASPECTS

Spray combustion is a very complex process. All the different processes that happen in an evaporating spray need to be described. Typically, an Eulerian-Lagrangian approach is chosen to model the two-phase process. The liquid droplets are treated with a moving coordinate system, while the gas phase is described as a continuum with a fixed coordinate system. The coupling of the gas and liquid phases is done through a source term. In the work presented here, the VSB2 spray model was chosen. The model was implemented in OpenFOAM and a more detailed description can be found in

[9]. The main difference to a standard spray model is the replacement of the traditional parcel with a stochastic blob. That is, a droplet-size distribution is used instead of an assumption of equally sized droplets. Furthermore, the blob is assumed to interact with the gas phase in a bubble of locally varying size instead of with the gas phase of the whole cell. Robustness of the model is achieved by calculating the equilibrium values of the thermodynamics and the momentum. A tuned, standard k-ε model was chosen to treat the turbulence and was tuned as described in [9].

VRFM REACTOR FRACTION MODEL

Turbulent combustion is a complex process and the main difficulty is in describing the turbulence-chemistry interaction. The main combustion occurs under non-premixed conditions and the reaction rate is influenced by the turbulence time-scale. A combustible mixture is produced if fuel and oxygen are mixed on the molecular level. The turbulent mixing time is typically longer than the chemical-reaction time, hence the reaction rate of non-premixed combustion is influenced by turbulence. As described above, there exist different approaches to model these phenomena. The VRFM is a further developed version of the model that was developed by Karlsson [7], as discussed above. The main further development of the model is the definition of the reactor volume. Let us assume we have a computational cell and part of the cell is occupied by the reactor volume $V_{reactor} \leq V_{cell}$. The size of the reactor volume is defined by κ , see equation (1).

$$\kappa = \left(1 - \frac{\tilde{Z}^2}{\tilde{Z}(1-\tilde{Z})}\right) \cdot \left(1 - \frac{\tilde{c}^2}{\tilde{c}(1-\tilde{c})}\right) = \frac{V_{reactor}}{V_{cell}} \quad (1)$$

where $\tilde{Z}$ is the mixture fraction, $\tilde{Z}^2$ is the variance of the mixture fraction, $\tilde{c}$ is the chemical progress variable, and $\tilde{c}^2$ is its variance. In a two-feed system, as we have in an internal combustion engine with fuel and air, the mixture fraction can be understood as the local ratio of the injected fuel mass to the total local mass. It describes how well the fuel is mixed with the air. While the mixture fraction does not give any information about the chemistry, the progress variable is an indicator for the chemical state [10]. By using both variables in the definition of κ , the mixing process and the chemistry are considered. The equation for κ simply defines it as the product of the complements of the unmixedness in mixture space, $\frac{\tilde{Z}^2}{\tilde{Z}(1-\tilde{Z})}$, and in progress space, $\frac{\tilde{c}^2}{\tilde{c}(1-\tilde{c})}$. With this definition the problem of finding representative timescales of mixing and chemical reactions is removed. Furthermore, it correctly accounts for the unmixed situation created by evaporation, a feature that the traditional time-scale expression for κ could never describe. The variables are Favre averaged and the mixture fraction, $\tilde{Z}$, and its variance,

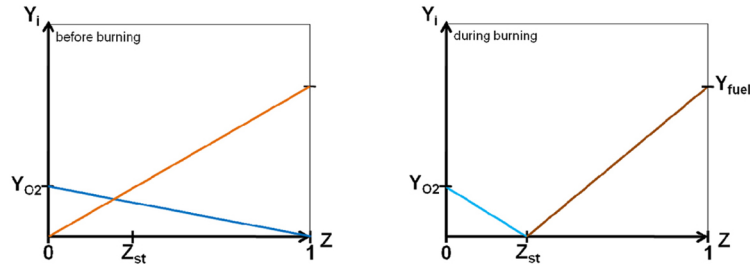


Figure 1. Correlation between oxygen and fuel mass fraction before and during combustion (adapted from [12])

$\tilde{Z}^2$, are defined according to Peters [11] by equations (2) and (3).

$$\frac{\partial(\tilde{\rho}\tilde{Z})}{\partial t} + \nabla \cdot (\tilde{\rho}\tilde{\mathbf{u}}\tilde{Z}) = \nabla \cdot \left[\frac{\mu_t}{Sc} \nabla \tilde{Z} \right] + \dot{S}_{evap} \quad (2)$$

$$\frac{\partial(\tilde{\rho}\tilde{Z}^2)}{\partial t} + \nabla \cdot (\tilde{\rho}\tilde{\mathbf{u}}\tilde{Z}^2) = \nabla \cdot \left[\frac{\mu_t}{Sc} \nabla \tilde{Z}^2 \right] + 2 \frac{\mu_t}{Sc} (\nabla \tilde{Z})^2 - \tilde{\rho}\tilde{\chi} + 2 \tilde{Z} \tilde{S}_{evap} \quad (3)$$

$\dot{S}_{evap}$ is the source term due to evaporation and Sc is the turbulent Schmidt number with a constant value of 0.7. The scalar dissipation rate, $\tilde{\chi}$, is modeled with equation (4).

$$\tilde{\chi} = C \frac{1}{k/\varepsilon + \sqrt{\nu/\varepsilon}} \tilde{Z}^2 \quad (4)$$

The addition of the Kolmogorov time scale, $(\nu/\varepsilon)^{1/2}$, is to overcome shortcomings in the turbulence model by preventing the time scale from becoming infinitely small, near wall, say. This is also in agreement with the model assumptions, the reactor volume cannot be smaller than a volume based on the Kolmogorov scale.

The progress variable, $\tilde{c}$, is defined by equation (5).

$$\tilde{c} = \begin{cases} 1 - \frac{\tilde{Y}_{fuel}}{\tilde{Z}} & \text{if } \tilde{Z} \leq \tilde{Z}_{st} \\ 1 - \frac{\tilde{Y}_{O2}}{(\tilde{Y}_{O2})_{air}(1-\tilde{Z})} & \text{if } \tilde{Z} > \tilde{Z}_{st} \end{cases} \quad (5)$$

The definition of the progress variable can be explained with Figure 1. Before burning, we have a linear correlation between oxygen (air) and fuel in the Z -space. During burning, the stoichiometric mixture of fuel and oxygen continuously reacts. Both mixture fractions (Y_{O2} and Y_{fuel}) are zero at Z_{st} . For $Z \leq Z_{st}$, the mass fraction of O_2 is an indicator for the chemical progress, whereas for $Z > Z_{st}$, the fuel mass fraction is an indicator for the chemical progress.

This definition of the chemical progress is the most simple definition possible; a similar definition was used by, for example, Magnussen in [13]. Other definitions can be considered; for example, based on how “far” the current chemical state of the mixture is from chemical equilibrium. Although this is outside the scope of the present work, it will be investigated in future work.

The variance of the progress variable, $\tilde{c}^2$, (eq. (6)) is defined according to the variance of the mixture fraction variable (eq. (3)).

$$\frac{\partial(\tilde{\rho}\tilde{c}^2)}{\partial t} + \nabla \cdot (\tilde{\rho}\tilde{\mathbf{u}}\tilde{c}^2) = \nabla \cdot \left[\frac{\mu_t}{Sc} \nabla \tilde{c}^2 \right] + 2 \frac{\mu_t}{Sc} (\nabla \tilde{c})^2 + \tilde{\rho}\tilde{\chi} + 2 \tilde{c} \tilde{S}_{evap} \quad (6)$$

Thus the model takes into account both the chemical progress and how well the fuel is mixed with the oxidant.

Owing to turbulence, the reactor species will continuously mix with the mean species, hence the first step considered in the VRFM is the mixing of the reactor species with the mean species, with the mixing time defined by equation (7).

$$\tau_{mix} = \frac{\tilde{\kappa}}{\varepsilon} \quad (7)$$

The reactor properties are then updated by equation (8) and used as the input to the chemistry calculation.

$$\tilde{Y}_i^R = \tilde{Y}_i^R + \frac{\tilde{Y}_i - \tilde{Y}_i^R}{\tau_{mix}} \Delta t \quad (8)$$

The chemistry calculation gives the chemical source term for the reactor, $\dot{\omega}_i^R$, which is then included in the transport equation of the mean species concentration, $\tilde{Y}_i$, considering the reactor volume κ . The transport equation of the mean mass fraction, $\tilde{Y}_i$, is then given by equation (9).

$$\frac{\partial}{\partial t} \tilde{\rho}\tilde{Y}_i + \nabla \cdot (\tilde{\rho}\tilde{\mathbf{u}}\tilde{Y}_i) = -\Delta\mu_{eff}\tilde{Y}_i + \kappa\dot{\omega}_i^R + \dot{S}_{i,evap} \quad (9)$$

where $\dot{S}_{i,evap}$ is the source term due to evaporation. The definition of the molecularly mixed fraction of the cell volume available for chemical processes, κ , directly influences the rate of change of the mean species concentration. The transport equation for the reactor species is shown in equation (10).

$$\frac{\partial}{\partial t} \tilde{\rho}\tilde{Y}_i^R + \nabla \cdot (\tilde{\rho}\tilde{\mathbf{u}}\tilde{Y}_i^R) = -\Delta\mu_{eff}\tilde{Y}_i^R + \dot{\omega}_i^R + \tilde{\rho} \frac{\tilde{Y}_i - \tilde{Y}_i^R}{\tau_{mix}} \quad (10)$$