D4.2. Report on the modeling approach to model turbulent spray flames using large-eddy simulation

Version 0.2

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1. Introduction

In moving towards alternative fuels for sustainable powertrains, biofuel combustion and performance optimisation become increasingly important from perspectives of both fundamental study and practical application (Demirbas, 2008). To meet the challenges of understanding and optimising liquid biofuel combustion, a practical framework connecting the sub-process models to provide a full description from the macroscopic scales through to the very detailed microscopic kinetic and turbulent mixing scales is essential. In addressing these research challenges, each step needs to be considered with extreme care to satisfy key matrices of the technical foundation, which define the performance of the engine combustor. These include liquid fuel properties, optimisation of fuel injection and thermodynamic conditions, chemical kinetics, pollutant formation, as well as design optimisation (Robbins et al., 2012). To achieve these goals, truly predictive tools using HPC would be of significant value and therefore high-fidelity modelling and simulations using HPC are essential. Using advanced modelling and simulation, the activities conducted in ENERXICO aim to develop predictive methods to characterize reacting sprays at engine-like conditions. This framework will enable the investigation of cleaner and more sustainable propulsion systems based on biofuels while reducing risks associated with their usage.

The state-of-the-art in the development and assessment of biofuels in practical engines includes mainly experimental work. The use of numerical simulations in this context is rather low due to the large computational resources needed to describe accurately the physico-chemical evolution of the reacting multiphase flow at conditions of relevance for engine operation. In fact, spray modelling is very challenging in turbulent combustion systems being fed with liquid fuels (Oefelein et al., 2006). Primary atomization and secondary breakup, droplet collision, coalescence, vaporization, and turbulent interactions between phases are fundamental processes that take place in the formation of the spray (Lebas et al., 2009). These have to be solved at conditions of high Reynolds and Weber numbers, which may occur within a high speed and small nozzle diameter imposed by current injection technologies (~500 m/s and ~100 μm for Compression Ignition Engines, CIE). In order to avoid the resolution of primary breakup at engine-like conditions with accurate, but expensive approaches (García-Oliver et al, 2013) or (Lehmkuhl et al., 2018), since the internal nozzle needs to be solved with the smallest scales associated to the high velocity expansion at the nozzle, a Lagrangian Particle Tracking (LPT) method for droplet evolution and evaporation is proposed here to solve the multiphase flow (Kaario et al., 2019). This approach has been found to be appropriate to characterize reacting sprays in the Engine Combustion Network (ECN) in numerous cases and will also be employed here. The combustion process will

be described by the flamelet concept for partially premixed flames (Gövert et al, 2018), as it is a computationally efficient approach and compatible with detailed kinetics of fuel oxidation. Finally, as the originally developed steady flamelet approaches (Peters, 2000) were appropriate only for the description of mixing controlled flames in steady combustion systems, a more complete unsteady approach based on the tabulation of unsteady flamelets during autoignition including heat loss along with the stable branch will be used for steady and unsteady combustion processes.

2. Modelling approach for spray flames under engine-like conditions

This section describes the computational framework developed in the multiphysics code Alya to study and characterize alternative fuels for transportation using virtual testing. Details of the principal elements required by the numerical simulations are described below.

2.1 Dispersed phase

Alya utilizes a Lagrangian spray model with two way coupling for the representation of the evaporating droplet cloud. This approach is widely used for the modelling of dilute sprays. A fuel droplet is represented by a point mass, that does not occupy volume, thus the gas phase partial differential equations only need to account for the interaction between the two phases via source terms. Otherwise these already validated modules remain unchanged. This approximation is valid for dilute sprays, where the volume fraction of the liquid phase is below 0.001 (Jenny et al., 2012).

To describe the state of a parcel, we need to track its location, velocity, temperature, and size by solving ordinary differential equations for particular quantities. The first two variables are treated with the kinematic model, while the last two one with coupled heat and mass transfer models. The dominant force considered in the kinematic modelling of droplets this size is drag.

The ordinary differential equation (ODE) system of location and velocity is solved by a combined Newmark/Newton-Raphson scheme (Houzeaux et al., 2016). The drag is determined based on Stokes flow around a sphere, considering the higher order Reynolds number effects with the Shiller-Neumann correction. The two ODEs are written below:

$$\frac{\mathrm{d}\mathbf{X}_p}{\mathrm{d}t} = \mathbf{U}_p$$
$$\frac{\mathrm{d}\mathbf{U}_p}{\mathrm{d}t} = \frac{\mathbf{U}_{seen} - \mathbf{U}_p}{\tau_p}$$

where $\boldsymbol{X_p}$ is the location of the particle, $\boldsymbol{U_p}$ is the velocity of the particle, Useen is the velocity of the surrounding gas, and $\boldsymbol{\tau_p}$ is the characteristic time scale

associated with drag given by the Schiller-Neumann correction of the Stokes drag as:

$$\tau_p = \frac{\tau_p^{St}}{C_D}$$

where the Stokes drag is given by:

$$\tau_p^{St} = \frac{\rho_p D_p^2}{18\mu_m}$$

and the correction factor by:

$$C_D = \begin{cases} 1 + 0.15 Re_p^{0.687}, & Re_p \leq 1000 \\ 0.44 \dfrac{Re_p}{24}, & Re_p > 1000 \end{cases}$$

D_p is the particle diameter, ρ_p is the liquid density, μ_m is the mean dynamic viscosity of the surrounding gas, Re_p is the particle Reynolds number.

The infinite conductivity model is implemented for the energy conservation. This implies a homogeneous but temporally changing droplet temperature (Ma and Roekaerts, 2017). The system of energy and mass ODEs is strongly coupled, since the droplet is significantly cooled by evaporation, and the fuel partial pressure on the droplet surface is predominantly influenced by the droplet surface temperature. We use the Ranz-Marshall correlation to determine the Nusselt and Sherwood numbers governing the heat and mass transfer:

$$Nu_m = 2 + 0.6 Re_p^{1/2} Pr_m^{1/3}$$
$$Sh_m = 2 + 0.6 Re_p^{1/2} Sc_m^{1/3}$$

where Pr_m and Sc_m are the Prandtl and Schmidt numbers of the surrounding gas. The ODEs for mass and temperature are written as:

$$\dot{m}_p = \frac{\mathrm{d}m_p}{\mathrm{d}t} = \pi D_p \mathcal{D}_m Sh_m \rho_m \ln\left(1 + \frac{Y_{f,surf} - Y_{f,seen}}{1 - Y_{f,surf}}\right)$$
$$\frac{\mathrm{d}T_p}{\mathrm{d}t} = \frac{\pi D_p \lambda_m Nu_m}{m_p c_{p,p}} (T_{seen} - T_p) + \frac{1}{m_p c_{p,p}} L_v \dot{m}_p$$

where $\mathcal{D}_m$, λ_m, and ρ_m are the fuel diffusivity, thermal conductivity, and density in the surrounding gas, Sh_m and Nu_m, are the Sherwood and Nusselt numbers of the surrounding gas, Y_f is the fuel mass fraction, $c_{p,p}$ is the specific heat of the particle, and L_v is the heat of vaporization. The heat transfer reducing effect of the evaporation is considered using the Abramzon and Sirignano model (Abramzon and WA Sirignano, 1989).

2.2 Gas-phase

The equations describing the gas phase corresponds to the low-Mach number approximation of the Navier-Stokes equations equations with the energy equation represented by the total enthalpy. A Favre-filtered description of the governing equations is followed to avoid modelling of terms including density fluctuations. The governing equations corresponding to the continuity, momentum and enthalpy are given by:

$$\frac{\partial \overline{\rho}}{\partial t} + \nabla \cdot (\overline{\rho}\widetilde{\mathrm{u}}) = 0$$

$$\frac{\partial \left(\overline{\rho}\widetilde{\mathbf{u}}\right)}{\partial t} + \nabla \cdot (\overline{\rho}\widetilde{\mathbf{u}}\widetilde{\mathbf{u}}) = -\nabla \overline{p} + \nabla \cdot \tau + \nabla \cdot \tau^{*}$$

$$\frac{\partial \left(\overline{\rho}\widetilde{h}\right)}{\partial t} + \nabla \cdot \left(\overline{\rho}\widetilde{\mathbf{u}}\widetilde{h}\right) = \nabla \cdot \left[\left(\overline{D} + \frac{\mu_t}{Sc_t}\right)\nabla \widetilde{h}\right]$$

where standard notation is used for all the quantites with ρ, u, D, μ_t, and Sc_t are the density, velocity, diffusivity, turbulent viscosity and turbulent Schimdt number respectively. The superscript * stands for the unclosed terms and has its origin in the filtering operation. Heating due to viscous forces is neglected in the enthalpy equation and the unresolved heat flux is modelled using a gradient diffusion approach (Mira et al., 2014). The formulation is closed by an appropriate expression for the subgrid-scale viscosity. In this paper the eddy-viscosity model proposed by Vreman (Vreman, 2004) is used. This model does not need complex averaging techniques to provide acceptable results for inhomogeneous flows using a single value of the model constant (in our case 0.1), and it is believed to be a good LES model for complex flows.

2.3 Combustion model

In the LES context, reacting sprays have been previously studied with different combustion models, going from the chemistry coordinated mapping (CCM) by Gong et al. (2014), the conditional moment closure (CMC) by Blomberg et al. (2016) or the dynamic thickened flame model with a Bayesian inference calibrated with a 2-step mechanism by Hakim et al. (2016). In contrast to these computationally demanding methods, another modeling approach is given by flamelet-based methods, where lookup-tables are computed to represent the chemical space. These methods applied to Spray A were addressed with the FGM model by Wehrfritz et al. (2014) or with the unsteady flamelet progress variable (UFPV) model by Ameen and Abraham (2014) or Perez-Sánchez et al. (2020). These studies show how the tabulation method can capture the ignition and flame characteristics of the complex non-premixed spray combustion process. In addition to the choice of the combustion model, the underlying chemical mechanism can vastly influence the results as discussed by Payri et al. (2019) using RANS. Results evidence the extreme importance of the low temperature chemistry including the period for which the cool flame extends. The different prediction of this stage between mechanisms leads to noticeable differences in

flame structures, which in turn produce substantially distinct turbulent flames, especially in the vicinity of the lift-off length (LOL). In order to account for the autoignition process and the stable burning of the flame, the flamelet manifold is constructed from the tabulation of strained autoigniting flamelets at different enthalpy levels. This approach allows to include the effect of heat loss and droplet evaporation on the ignition delay characteristics of the flame. This approach is similar to Wehrfritz et al. (2014), but with an additional dimension in the flamelet database.

The combustion process is described by the definition of three controlling variables, the progress variable Yc, the mixture fraction Z, and the normalized enthalpy *i*, which is computed from the transport of total enthalpy *h* described on the gas phase model.

$$i = \frac{h - h_{min}}{h_{max} - h_{min}}$$

The transport equations for Yc and Z are given by:

$$\frac{\partial\left(\overline{\rho}\widetilde{Y_c}\right)}{\partial t} + \nabla\cdot\left(\overline{\rho}\widetilde{\mathbf{u}}\widetilde{Y_c}\right) = \nabla\cdot\left[\overline{\rho}\left(\overline{D} + \frac{\nu_t}{Sc_t}\right)\nabla\widetilde{Y_c}\right] + \overline{\dot{\omega}}_{Y_c}$$

$$\frac{\partial\left(\overline{\rho}\widetilde{Z}\right)}{\partial t} + \nabla\cdot\left(\overline{\rho}\widetilde{\mathbf{u}}\widetilde{Z}\right) = \nabla\cdot\left[\overline{\rho}\left(\overline{D} + \frac{\nu_t}{Sc_t}\right)\nabla\widetilde{Z}\right]$$

The influence of the fluctuations in mixture fraction are included by a Probability Density Function (PDF) given by a beta-PDF (Gövert et al., 2018) using a variance of the mixture fraction transport equation Zv. The governing equations describing this process in LES are given by:

$$\frac{\partial\left(\overline{\rho}\widetilde{Z_v}\right)}{\partial t} + \nabla\cdot\left(\overline{\rho}\widetilde{\mathbf{u}}\widetilde{Z_v}\right) = \nabla\cdot\left[\left(\overline{D} + \frac{\mu_t}{Sc_t}\right)\nabla\widetilde{Z_v}\right] + 2\frac{\mu_t}{Sc_t}\left|\nabla\tilde{Z}\right|^2 - 2\frac{\mu_t}{\Delta^2 Sc_t}\widetilde{Z_v}$$

2.4 Chemical kinetics

The reaction mechanisms used to describe the combustion process of the different fuels under investigation correspond to well-established chemical kinetic mechanisms from the literature. As the mechanisms are rather large even for tabulation purposes, a systematically reduced mechanism optimized for autoignition using Path Flux Analysis (PFA) (Surapaneni, 2019) is employed to reduce the chemistry. This methodology facilitates the computations and reduce the stiffness without losing the accuracy. The base mechanism for each fuel are listed below

1. nDodecane: as this is the reference fuel, several reaction mechanisms are tested. Those include:
    a. ERC Wisconsin (https://www.erc.wisc.edu/chemicalreaction.php)
    b. ECN recommended Yao et al. (2017)
    c. CRECK Modeling Group (Ranzi et al. 2014)
    d. Reduced mechanism with PFA from CRECK.
2. Conventional diesel : https://combustion.llnl.gov/mechanisms/surrogates/diesel-surrogate-detailed-and-reduced
3. HVO and OMEx: https://combustion.llnl.gov/mechanisms/alkanes/2-methyl-alkanes-and-n-alkanes, https://www.sciencedirect.com/science/article/pii/S0016236120308942
4. OME1: https://doi.org/10.1016/j.combustflame.2018.12.026

2.5 Computational approach

The code Alya will be used to conduct the numerical simulations of the project in the HPC context. Alya is a CFD code of the PRACE Benchmark Suite for HPC applications and has been highly optimized and tested independently in most European supercomputer platforms. The Alya code is developed at Case Department of the Barcelona Supercomputing Centre. Alya is a parallel multiphysics software developed using the Finite Element (FE) method to run applications on HPC facilities. The code has also been tested on 100,000 cores for multiphysics applications (Vázquez et al., 2016) indicating the parallel performance of the code for large-scale applications on complex problems.

The discretization strategy followed in the ENERXICO project is based on a recent publication (Both et al., 2020) where the conservative finite element convective scheme proposed by Charnyi et al. (Journal of Computational Physics 337, 2017, 289 - 308) originally formulated for incompressible flows to the low

Mach regime is extended. Similar to Lehmkuhl et al. (Journal of Computational Physics 390, 2019, 51 - 65) stabilization is only introduced for the continuity equation by means of a non-incremental fractional-step method, modified in order to account for variable density flows. The final scheme preserves momentum and angular momentum for variable density flows. The error of kinetic energy conservation is of order O(dt h^(k+1)), thus dissipation is limited. Standard stabilized finite elements are used for the scalars, while the time integration is carried out by means of an explicit third order Runge-Kutta scheme for momentum and scalars. The chosen low dissipation FE scheme presents good accuracy compared to other low dissipation Finite Volume and Finite Difference methods with the advantage of being able to increase the order of accuracy at will without breaking the fundamental symmetry properties of the discrete operators.

3. Validation and preliminary results

The ENERXICO project is dedicated to the study of alternative fuels for transportation using advanced numerical simulations based on LES employing different liquid biofuels (HVO, OME1 and OMEx) and compare them with reference fuels (n-dodecane and conventional diesel) at conditions of the spray A from the ECN. The ECN is an international initiative coordinated by Sandia National Laboratories that includes a forum for experimental and numerical collaboration to provide knowledge and further understanding on reacting sprays in internal combustion engines. It also includes an open-access data repository with well-established and documented experimental data for model validation. Baseline target conditions with guidelines for the diagnostic/post-processing techniques have been defined by the ECN for different spray cases. In particular, the application case in Enerxico is focused on the conditions of Spray A that features an ambient gas temperature of 900 K and ambient pressure of 6 MPa with 15% oxygen concentration.

The first stage for the modelling of the spray flames is the definition of the particle injection, which was addressed comparing different statistical distributions of particle sizes using Rosin-Rammler distributions and constant droplet size. Different refinement levels were also tested to evaluate the influence of mesh resolution on the predicted quantities. Results with finest grid are still in progress, though results of the other cases are now compiled.

The code has been tested for the prediction of liquid and vapor penetration lengths, and good agreement is found for both inert and reacting conditions using the chemical kinetic mechanism from Yao et al. (2017), see Figure 1. Comparison of the flow fields for velocity and mixture fraction are in progress. The inert condition has overpredicted the liquid length by less than 10%, while the vapor penetration is in good agreement with the experiments. The same observations can be made for the reacting case. Analysis of autoignition delay, and lift-off length are in progress, and so are the analysis of the flow fields for the reacting case. A visualization of the flow fields for the inert and reacting conditions of spray A are shown in Figures 2 and 3 respectively.

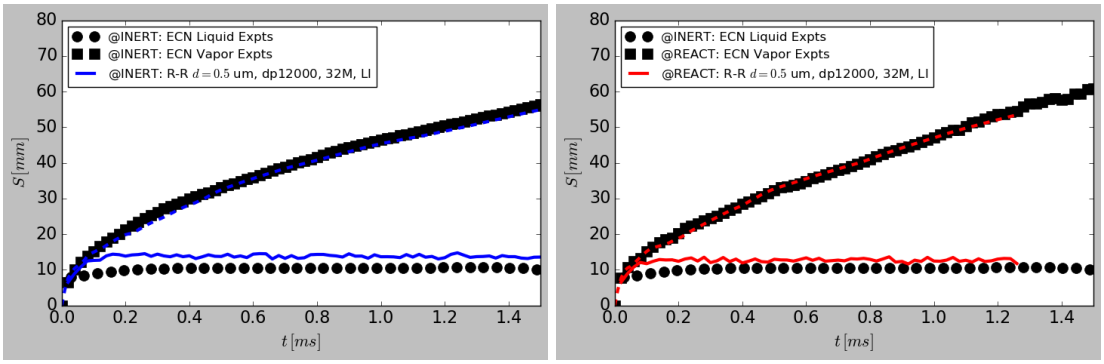

Figure 1. Liquid and vapor penetration for the inert (left) and reacting flow (right).

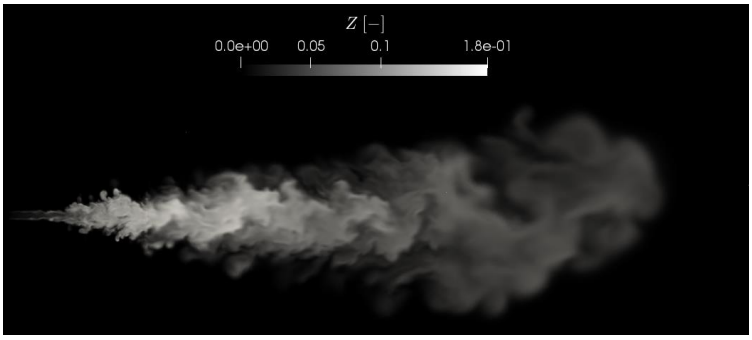

Figure 2. Mixture fraction field at t = 1.5 ms for the inert case.

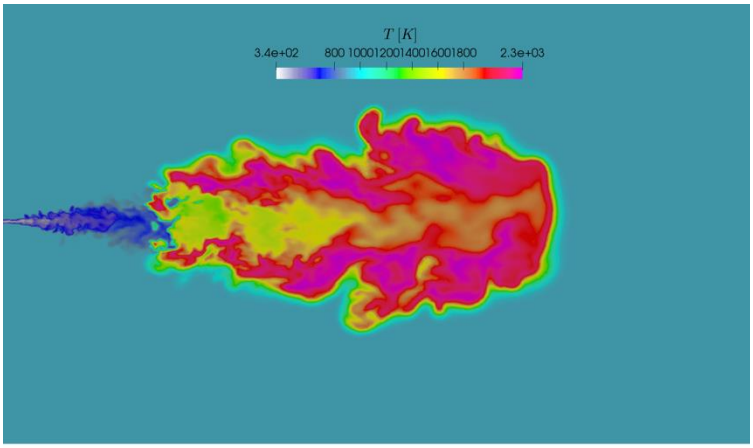

Figure 3. Temperature field at t = 1.5 ms for the reacting case.

4. Conclusions

The numerical framework for the investigation of liquid biofuels fuels for transportation at engine-like conditions for large-eddy simulation has been introduced. The modelling approach is based on a Lagrangian Particle Tracking method to describe the dispersed phase, while the gas-phase reacting flow is described the low Mach number approximation of the Navier-Stokes equations. The combustion model is based on the tabulation of igniting flamelets using different enthalpy levels and the definition of controlling variables to access the flamelet database. The resulting manifold is based on the progress variable, mixture fraction and normalized enthalpy, and the effect of turbulent fluctuations on the reacting layer is accounted for by a presumed-shape PDF using a beta function. The computational approach has been demonstrated for the Spray A conditions of the ECN and preliminary results are introduced. The current work is now focused on the study and characterization of the liquid biofuels and the comparison with the experimental data.

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