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A pressure coupled Representative Interactive Linear Eddy Model (RILEM) for heavy-duty truck engine combustion simulations

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THESIS FOR THE DEGREE OF LICENTIATE OF ENGINEERING IN THERMO
AND FLUID DYNAMICS

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ABSTRACT

Internal combustion engines (ICE) are frequently debated due to their environmental consequences. Although the switch to electromobility is currently happening for light and medium-duty vessels, the transition for ships and heavy-duty trucks is more complex. The primary problem in the shift is the incapability of matching the range of ICE. Maintaining the ICE for large vessels is inevitable, requiring intensive research to improve the combustion engine technology to reduce their impact on the environment.

Operating engines in nonstandard conditions, such as low-temperature ranges or utilizing partially premixed mixtures, reduces emissions such as NO_x or soot. Simulating these scenarios requires special modeling techniques that can advance finite rate chemistry and simulate mixed combustion modes. The Linear Eddy Model (LEM) is a potential candidate to simulate these methods. LEM is a regime and mode-independent mixing model initially developed for nonreactive flows [1] and later extended to include reactive flows [2]. LEM advances finite rate chemistry, solves turbulence on a one-dimensional line, and advances molecular diffusion and heat convection. It offers the possibility of capturing the turbulence-chemistry interaction directly, which is essential for predicting pollutants formation. In this thesis, the coupling of LEM to a CFD code that simulates the spray chamber geometry is referred to as the Representative Interactive LEM (RILEM). RILEM describes the combustion chamber key parameters and interacts with the CFD in real-time as a combustion model to update its chemical state. RILEM shares similarities with the Representative Interactive Flamelet model (RIF) [3]. RIF is essentially the coupling of a CFD domain to laminar flamelets embedded in a turbulent flow; the coupling is based on the scalar dissipation rate χ for non-premixed [4], and on combustion progress variable c or level set approach for premixed cases [5]. RILEM features distinct differences compared to RIF, mainly the possibility of simulating partially premixed combustion modes and the ability to represent combustion on a physical one-dimensional line. A previous version of RILEM was implemented where the CFD and LEM were coupled based on a volume constraint. The volume-coupled RILEM was successfully validated against experiments [6]. A recent version of RILEM using pressure coupling is the objective of the presented thesis. It has been tested using a stand-alone code operating with driving parameters extracted from a reactive case [7]. The fundamental advantage of a pressure-coupled RILEM is the intrinsic inclusion of latent heat of evaporation effects and wall heat losses in the pressure trace communicated from the CFD. These effects need separate modeling on the LEM side in the case of volume coupling.

The recently developed RILEM utilizes a spherical formulation of the LEM that allows the line to maintain the characteristic length and the volume effects constant between the CFD and the LEM. An additional model was developed in this project's scope titled multiple Representative Interactive Linear Eddy Model (mRILEMs). mRILEMs advance multiple LEM lines in parallel, where different turbulent statistics are enforced in each line to illustrate the stochastic behavior of the eddies. Both RILEM and mRILEMs utilize scalars conditioned on mixture fraction Z and combustion progress variable space c to update the CFD chemical state. The local temperatures on the CFD are iterated by

utilizing the species mass fractions and the solution of the energy equation in its total enthalpy form.

RILEM and mRILEMs were tested on a single cylinder case of a heavy-duty truck engine. The pressure trace was compared against the experimental data and reached a reasonable agreement. The two models allowed the quantification of intermediate species such as CO and OH. RILEM provided accurate results by manipulating the probability density functions of the turbulent scalars combined with different initialization techniques, where utilizing mRILEMs ensured that the LEM side exclusively controls the combustion process.

Keywords: Representative interactive linear eddy model, multiple LEM lines, pressure coupling, turbulent chemistry interaction, pollutants formation.

LIST OF PUBLICATIONS

This thesis is based on the work contained in the following publications:

Publication I Doubiani. N., Menon. A., Kerstein. A., Oevermann. M. "Pressure Coupling Of the Spherical Linear Eddy Model to RANS-CFD for Internal-Combustion Engine Simulation" in *MHMT'21: World Congress on Momentum, Heat and Mass Transfer, Lisbon, PT*

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1 Introduction

1.1 Background

The internal combustion engine faces complex challenges due to the increased production and sales of electric drivetrains in automotive vehicles. Although light and medium-duty vehicles are going through a fast electrification process, the transition for airplanes, ships, and heavy-duty trucks is more challenging. Operating light- and medium-duty automobiles with electricity generated from sustainable resources contributes to transportation's zero-emissions objective. However, driving extended distances with heavy-duty vehicles or ships transporting a significant amount of merchandise requires enormous battery capacities. However, electricity production is not always realized with sustainable resources; in the case of electricity shortage, producers often pivot to less sustainable techniques such as coal combustion. This solution leads to emitting more significant quantities of CO₂ rather than using the internal combustion engine efficiently. Consequently, research in optimizing the emissions of internal combustion engines is continuously evolving. It suggests using diverse techniques, such as renewable fuels, and operating the engine under different configurations and combustion modes. Research on internal combustion engines is accomplished using experimental hardware or numerical models. Emissions from ICE depend heavily on the combustion quality, which is determined by the mixing process taking place in the combustion chamber. This mixing can happen either in a large-scale motion, namely the swirl or tumble motions, or by the small eddies that originate from the injection process. It is safe to say that the turbulence level in the combustion chamber is an essential parameter for the engine's performance.

Turbulent combustion modeling is a complex field of research; this complexity is due to the interaction of multiple physical disciplines such as turbulence, chemistry, and thermodynamics. Combustion can exist in various forms in an internal combustion engine: it can be non-premixed, premixed, or partially premixed in different turbulent regimes. Turbulent combustion modeling requires advancing convection, diffusion, and chemistry, all happening under different time scales; for non-premixed combustion, the slowest time scale is diffusion, which is also the controlling time scale. Chemistry, however, has a more minor time step making it substantially faster than diffusion. Specific models, such as Bray–Moss–Libby Model for non-premixed cases and the Equilibrium Model for premixed ones, are based on the assumption of infinitely fast chemistry. The chemical time scales, however, have significant differences. This premise results in assuming that the heat generation and NO_x formation occur simultaneously, which is not necessarily the case. Furthermore, this hypothesis can also neglect non-equilibrium effects such as flame extinction and lift-off, which are essential to capture in turbulent combustion modeling. It is, therefore, crucial to utilize models capable of advancing finite rate chemistry to investigate such phenomena.

Combustion models such as the Representative Interactive Flamelet (RIF) model are extensively used in industrial and academic studies. RIF simulates finite rate combustion

in a parametric way; non-premixed flames are modeled using the concept of mixture fraction and scalar dissipation rate [3, 4, 8–10]. On the other hand, premixed combustion is simulated using either the combustion progress variable or the mean turbulent flame front, also known as the G equation [5, 11]. This separation in the techniques utilized in simulating the two modes makes it challenging for RIF to simulate mixed modes combustion scenarios. Additionally, the representation of turbulence via the scalar dissipation rate deprives RIF of directly capturing turbulence chemistry interaction (TCI) effects. The transported PDF (TPDF) is a combustion model that advances a transport equation of the probability density function (PDF) [12, 13]. Its formulation makes it suitable to simulate both premixed, non-premixed modes and partially-premixed combustion with advancing finite rate chemistry. These features make it an appealing model to simulate non-standard combustion scenarios in low-temperature environments. It is, however, limited by its need for an additional mixing model. The effects of the TCI in the TPDF model, such as extinction and re-ignition, directly depend on the level of mixing that the additional mixing model presents. The Well Stirred Reactor (WSR) is another combustion model utilized for both premixed and non-premixed modes. WSR assumes that each CFD cell is a thermally insulated volume with a nearly uniform distribution of the scalars because of the intense turbulence mixing. The controlling time scale in WSR is the chemical process since the mixing is assumed to be infinitely fast. Although implementing the WSR is relatively simple, it has shown encouraging results compared with other combustion models [14, 15] and experiments in [16]. However, this agreement is reached by tuning the parameters of the WSR. In addition, WSR lacks appropriate sensitivity to turbulence chemistry interaction due to its infinitely fast mixing time scales assumption.

1.2 CFD and LEM

The linear eddy model (LEM) by Kerstein [1] is a one-dimensional scalar mixing model for reactive flows. LEM directly advances turbulent advection using stochastic triplet maps allowing the eddies to interact directly with the flame structures. LEM advances molecular and heat diffusion by solving the reacting 1-D zero Mach number equations and advancing chemistry in each cell.

LEM was used as a stand-alone combustion model and then coupled to an LES simulation, titled LES-LEM [17–19]. In LES-LEM, LEM lines are implemented independently in each computational cell where turbulence, chemistry, and diffusion effects are solved for all temporal and physical scales. Although LES-LEM is a promising technique, the simulation cost is substantially high, making it an unrealistic approach for industrial investigations. The LES-LEM model has recently been modified to hold an LEM line in each cluster of neighboring LES cells instead of individual computation cells. This adjustment was shown to significantly reduce the simulation time without compromising the quality of the results. A more extreme version of this adjustment is the Representative Interactive Linear Eddy Model (RILEM)[20, 21]. RILEM is an attempt to reduce the simulation cost of LES-LEM by running a RANS simulation instead of an LES and utilizing a single LEM line to represent the statistical state of the CFD domain. RILEM shares many features with the Representative Interactive Flamelet (RIF) model, such as the

conditioning of the reactive scalars on mixture fraction and combustion progress variable spaces, the utilization of the presumed PDF for mixture fraction, and the real-time interaction between the CFD and the subgrid model. However, the two models have distinct differences, mainly in turbulence representation. RIF describes turbulence using the scalar dissipation rate, where turbulence in RILEM is represented directly, making it a suitable model for capturing turbulence chemistry effects that are essential for pollutant formation.

Coupling the LEM with a CFD domain in a represent way can be reached in two strategies. A previous version of RILEM was conceived for ICE simulations based on a volume coupling. The varying volume of the combustion chamber was enforced on the LEM line, which improved the representative aspect of the LEM to the CFD. Utilizing a volume constraint for the coupling process neglected the heat effects on the CFD side, such as the latent heat of evaporation and the wall heat losses; these effects were addressed by an additional enthalpy defect on the LEM side. The volume coupled RILEM utilized the spherical formulation of the LEM to reinforce a constant pressure on the line and was successfully validated against experiments for a heavy-duty compression ignition engine in [6, 16]. A recently developed RILEM version that uses a pressure coupling is presented in this thesis. The new coupling approach is motivated by the intrinsic inclusion of the latent heat of evaporation and wall heat loss effects in the pressure trace. The spherical geometry of the LEM was essential for the pressure-coupled RILEM to maintain the characteristic length and volume of the LEM constant between the two sides.

1.3 Objectives

The first objective was to create a stand-alone pressure coupled spherical LEM to run initial parameter investigations. The second goal was to assemble a pressure-coupled version of RILEM and compare it with experimental data. The thesis is organized in five chapters, starting with an introduction, presenting the rationale for utilizing LEM as a combustion model. The second chapter will present the mathematical models used to build the spherical stand-alone LEM and RILEM. In the third, the RILEM and mRILEM combustion closures will be described. The collected results will be presented and discussed in the fifth chapter. The thesis is finalized with a conclusion and a future work chapter.

2 Mathematical models

The work described in this thesis was performed using the open-source Computational Fluid Dynamics solver OpenFOAM v2.2.3. The following chapter will describe the governing equations used to characterize the fluid motion, the turbulence model utilized, and finally, a detailed description of the employed combustion model.

2.1 Flow simulation

2.1.1 Governing equations of fluid dynamics

Turbulent advection, molecular diffusion, and chemical reactions govern the development of the fuel and oxidizer inside the combustion chamber. Simulating reacting flows requires advancing the following equations, also known as the governing equations:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot [\rho \mathbf{u}] = \dot{\rho}_s, \quad (2.1)$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot [\rho \mathbf{u} \mathbf{u}] = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \mathbf{F} + \rho \mathbf{g} + \rho \dot{\mathbf{S}}, \quad (2.2)$$

$$\frac{\partial \rho Y_s}{\partial t} + \nabla \cdot [\rho \mathbf{u}_s Y_s] = \nabla \cdot [\rho D_s \nabla Y_s] + \dot{w}_s. \quad (2.3)$$

where ρ denotes density, u the velocity, $\dot{\rho}_s$ the source term due to evaporation. In addition, p symbolizes the pressure, $\boldsymbol{\tau}$ the stress tensor, $\mathbf{F}$ all the forces that can be applied externally on the fluid, $\mathbf{g}$ the vector of gravitational acceleration, $\dot{\mathbf{S}}$ the liquid phase source term. Y_s characterizes the species mass fractions, $\mathbf{u}_s$ the velocity, D_s the diffusion coefficient, and $\dot{w}_s$ the mass source term due to chemical reactions of each species s in the mixture.

An additional equation that accounts for the system's energy balance must be solved. The energy equation can exist in different formats: Internal energy, enthalpy, or temperature. Here, the energy equation in the total enthalpy form h is utilized:

$$\frac{\partial \rho h}{\partial t} + \nabla \cdot [\rho \mathbf{u} h] = \frac{dp}{dt} - \nabla \cdot \mathbf{j} + \dot{q}_{ev}, \quad (2.4)$$

where $\mathbf{j}$ represents the heat flux vector, $\dot{q}_{ev}$ the total enthalpy source term due to droplet evaporation provided by the spray model, viscous heating was neglected because of the low-Mach number assumption.

Solving a transport equation (2.3) for each species in the mixture with corresponding source terms is computationally expensive, especially for large chemical mechanisms with hundreds of species. Instead of advancing a transport equation for each species of the chemical mechanism, an alternative method, inspired from flamelet non-premixed reactive flow modeling [8] has been adopted. It solves a transport equation for mixture fraction

Z (2.5) to represent the amount of fuel in each CFD cell. The mixture fraction Z is a conserved scalar that does change solely due to diffusion and convection but not chemical reactions.

$$\frac{\partial \rho Z}{\partial t} + \nabla \cdot [\rho \mathbf{u} Z] = \nabla \cdot [\rho D \nabla Z] + \dot{\rho}_s, \quad (2.5)$$

The evolution of the fuel state from the unburnt to the burnt state is key in turbulent combustion modeling. For that, an additional generalized "time" coordinate in the form of a combustion progress variable c is introduced. Different definitions of the combustion progress variable exist in literature [22]. The definition based on oxygen mass fraction has been chosen for this thesis. The temperature definition was avoided because of its sensitivity to both chemistry and the compression of the combustion chamber. It is preferable to choose a quantity that is sensitive uniquely to the chemical advancement to capture the progress of the fuel.

$$\frac{\partial \rho c}{\partial t} + \nabla \cdot [\rho \mathbf{u} c] = \nabla \cdot [\rho D \nabla c] + \rho \dot{c}, \quad (2.6)$$

where c denotes the combustion progress variable that takes the value of 0 for the unburnt state and 1 for the completely burnt state as defined in [22]. c is defined based on the following formula:

$$c = \frac{Y_{O_2} - Y_{O_2,u}}{Y_{O_2,b} - Y_{O_2,u}}, \quad (2.7)$$

where Y_{O_2} denotes the oxygen mass fraction, $Y_{O_2,u}$ and $Y_{O_2,b}$ are the unburnt and the burnt oxygen mass fractions, respectively. In addition, $\dot{c}$ in equation (2.6) represents the source term of the combustion progress variable c , which will be discussed later in the thesis.

2.2 Turbulence modeling

The size of the turbulent eddies exists in a spectrum defined by two limits: The integral length scale, which is characterized by the geometry, which describes the large turbulent eddies, and the Kolmogorov scale that represents the smallest turbulent eddies that are determined by the fluid viscosity and the dissipation rate. Solving the governing equations requires a fine computational grid combined with small time steps to capture structures down to the Kolmogorov length and time scales. It is realized using direct numerical simulations (DNS) for simple geometries with moderate Reynolds numbers. However, for combustion chamber simulations, which imply complex moving geometries with significantly high Reynolds number flows, a substantial range of scales of eddies with different length and times scales exist between the integral and the Kolmogorov scales. A DNS solution for a combustion chamber simulation is unrealistic with the current computational hardware.

The simulation of complex geometries with high turbulent flows is achieved by modeling the small turbulent structures. This modeling is usually achieved by averaging the

governing equations where each variable is decomposed into a mean $\bar{\psi}$ and a fluctuating ψ' component:

$$\psi = \bar{\psi} + \psi'. \quad (2.8)$$

The Reynolds Averaged Navier Stocks (RANS) turbulence model implies a time averaging of the governing equations. For non-constant-density flows, a density-weighted averaging is applied, known as Favre averaging:

$$\psi = \tilde{\psi} + \psi''. \quad (2.9)$$

Applying time averaging on a quantity $\rho\psi$ results to:

$$\rho\psi = \overline{\rho\psi} + (\rho\psi)', \quad (2.10)$$

with

$$\tilde{\psi} = \frac{\overline{\rho\psi}}{\bar{\rho}} \quad \text{and} \quad \psi'' = \frac{(\rho\psi)'}{\bar{\rho}}. \quad (2.11)$$

The Favre averaging is applied for all quantities in the governing equations except for the pressure, diffusive fluxes, and density. The averaging implies that only the integral time and length scales will be solved, whereas the small scales need to be modeled even if the computational grid size is smaller than the integral length scale. Resolving structures with sizes between the integral and Kolmogorov scales is achieved using another turbulence model called large-eddy simulations (LES), where the filter width is smaller than the integral length scale; this approach, however, is more expensive than RANS. The work described in this thesis was done using a RANS turbulence model [23], although it is cheaper than LES, it lacks a great degree of detail because of the modeling of all the structures below the integral scale. RANS' low resolution was addressed with additional modeling employing the linear eddy model (LEM). Applying Reynolds averaging on the governing equation reduces the computational cost of the simulation but generates more unknown terms that need to be closed, as shown in the following equations :

$$\frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot [\bar{\rho} \tilde{\mathbf{u}}] = \tilde{\rho}_s, \quad (2.12)$$

$$\frac{\partial \bar{\rho} \tilde{\mathbf{u}}}{\partial t} + \nabla \cdot [\bar{\rho} \tilde{\mathbf{u}} \tilde{\mathbf{u}}] = -\nabla \bar{p} - \nabla \cdot [\widetilde{\bar{\rho} u_i'' u_j''}] + \nabla \cdot \tilde{\boldsymbol{\tau}} + \tilde{\mathbf{F}} + \bar{\rho} \mathbf{g} + \bar{\rho} \tilde{\mathbf{S}}, \quad (2.13)$$

$$\frac{\partial \bar{\rho} \tilde{h}}{\partial t} + \nabla \cdot [\bar{\rho} \tilde{\mathbf{u}} \tilde{h}] = \frac{d\bar{p}}{dt} - \nabla \cdot [\widetilde{\bar{\rho} u_i'' h''}] - \nabla \cdot \tilde{\mathbf{j}} + \tilde{q}_s, \quad (2.14)$$

$$\frac{\partial \bar{\rho} \tilde{Z}}{\partial t} + \nabla \cdot [\bar{\rho} \tilde{\mathbf{u}} \tilde{Z}] = \nabla \cdot \left[\frac{\mu_t}{Sc_t} \nabla \tilde{Z} \right] + \tilde{\rho}_s, \quad (2.15)$$

$$\frac{\partial \bar{\rho} \tilde{Z}''^2}{\partial t} + \nabla \cdot [\bar{\rho} \tilde{\mathbf{u}} \tilde{Z}''^2] = \nabla \cdot \left[\frac{\mu}{Sc_t} \nabla \tilde{Z}''^2 \right] + \frac{2\mu_t}{Sc_t} (\nabla \tilde{Z})^2 - \bar{\rho} \tilde{\chi}, \quad (2.16)$$

$$\frac{\partial \bar{\rho} \tilde{c}}{\partial t} + \nabla \cdot [\bar{\rho} \tilde{\mathbf{u}} \tilde{c}] = \nabla \cdot [\bar{\rho} D \nabla \tilde{c}] - \nabla \cdot [\widetilde{\bar{\rho} u_i'' c''}] + \bar{\rho} \tilde{c}, \quad (2.17)$$

where

$$\tilde{\chi} = C_\chi \frac{\epsilon}{k} \widetilde{Z''^2}, \quad (2.18)$$

and $C_\chi = 2.0$. These equations will be advanced using OpenFOAM at each time step. The solutions of equations (2.15), (2.16), (2.17) will be used in the mapping process of LEM.

It can be noticed that the application of the Reynolds averaging lead to the appearance of an unclosed term know as the Reynolds stress term in the moment equation :

$$\overline{\tau_{ij}} = -\widetilde{\bar{\rho} u_i'' u_j''}. \quad (2.19)$$

The Boussinesq assumption for turbulent eddy viscosity [24] is utilized to model the Reynolds stress term by linking it to the mean velocity gradient in the flow using the turbulent viscosity also knows as the eddy viscosity:

$$\widetilde{\bar{\rho} u_i'' u_j''} = \frac{2}{3} \bar{\rho} \tilde{k} - \mu_t [(\nabla \tilde{\mathbf{u}}) + (\nabla \tilde{\mathbf{u}})^T - \frac{2}{3} \nabla \tilde{\mathbf{u}}]. \quad (2.20)$$

The eddy viscosity is usually modeled as the following [25]:

$$\mu_t = \bar{\rho} C_\mu \frac{\tilde{k}^2}{\tilde{\epsilon}}, \quad C_\mu = 0.09. \quad (2.21)$$

The turbulent kinetic energy k and the turbulent dissipation rate ϵ are calculated using the classical $k - \epsilon$ model by Launder and Spalding [26] that advances the transport equations for these two terms in its compressible form.

$$\frac{\partial(\bar{\rho} \tilde{k})}{\partial t} + \nabla \cdot [\bar{\rho} \tilde{\mathbf{u}} \tilde{k}] = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \nabla \tilde{k} \right] + P_k - \bar{\rho} \tilde{\epsilon}, \quad (2.22)$$

$$\frac{\partial(\bar{\rho} \tilde{\epsilon})}{\partial t} + \nabla \cdot [\bar{\rho} \tilde{\mathbf{u}} \tilde{\epsilon}] = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_\epsilon} \right) \nabla \tilde{\epsilon} \right] + C_{\epsilon 1} \frac{\tilde{\epsilon}}{\tilde{k}} P_k - C_{\epsilon 2} \bar{\rho} \frac{\tilde{\epsilon}^2}{\tilde{k}}, \quad (2.23)$$

where the models constants are the following:

$$C_\mu = 0.09; \quad k = 1.0; \quad \sigma_\epsilon = 1.3; \quad C_{\epsilon 1} = 1.44; \quad C_{\epsilon 2} = 1.92 \quad (2.24)$$

and the source term P_k is provided as:

$$P_k = -\widetilde{\bar{\rho} u_i'' u_j''} \frac{\partial \tilde{u}_i}{\partial x_j} \quad (2.25)$$

The turbulent transport terms in the form of $\widetilde{\bar{\rho} u_i'' \phi''}$ in the Reynolds averaged equations can be approximated with the gradient flux assumption in equation (2.20) as the following:

$$\widetilde{\bar{\rho} u_i'' \phi''} = -\frac{\mu_t}{Sc_t} \nabla \tilde{\phi}. \quad (2.26)$$

Using this approximation in equations (2.13), (2.14), and (2.17), the system of Reynolds averaged equations can be closed.

2.2.1 Spray Modeling

A *spray* is characterized as a collection of liquid droplets in a gaseous phase. An injection process generates the fuel spray from the injecting nozzle in the combustion chamber. An injected spray can exist inside the combustion chamber for direct injection (DI) or in the inlet port for PPCI engines. The high injection pressure of the fuel causes the jet to break up; this process is known as the primary break-up, where different regimes can be identified. The most pertinent regime for high-pressure injections is the atomization regime that characterizes the interaction between the gas and the small perturbations generated by the turbulent motion in the nozzle. Additionally, a secondary process called the secondary break-up occurs due to the large drag forces generated from the high velocities. This process continues to decompose the liquid particles into smaller droplets. The direct injection for diesel engines occurs around the Top Dead Center (TDC), where the ambient temperature is relatively high, which causes the evaporation of the droplets generated by the secondary break-up. Spray simulation is critical for turbulent combustion simulation since the atomization process prescribes the amount of fuel evaporating to the gaseous phase in the secondary break-up. The contribution of the gaseous phase of the fuel determines the combustion level in the chamber, which will raise the temperature leading to evaporating more liquid fuel. Several models exist to simulate spray development under different conditions. A Lagrangian model was utilized in this study to characterize the spray in the diesel engine. The Huh Gosmann model [27] models the atomization process in this study, where the secondary break-up was simulated using Kelvin-Helmholtz model [28] where the KH instabilities are considered the leading cause of spray break-up.

2.3 The Linear Eddy Model

The linear eddy model was introduced by Kerstein as a scalar mixing model for nonreactive flows in [1, 29, 30], and was later extended to include reactive flows [2, 31–33]. Developing LEM aims to have a regime and mode-independent model that provides an affordable full resolution of all spatial and temporal scales, including the minor scale effects in combustion. Compared to standard modeling approaches, e.g., gradient diffusion assumption, the LEM modeling is based on reducing the domain to one spatial dimension while still resolving all scales in space and time as in a DNS. This dimensional reduction requires a special approach to represent certain physical phenomena, particularly turbulent eddies. The flow in LEM is advanced by solving reactive 1-D zero Mach number equations on a one-dimensional line representing the simulated domain’s statistical state, which substantially reduces the simulation cost. The advancement of LEM is composed of diffusion of reactive scalars, chemical reactions, and turbulent advection. LEM is designed based on the one-dimensional turbulence (ODT) C++ code of Lignell [34] in its spherical format, which includes a mesh adaptor.

2.3.1 Diffusion and Chemistry in LEM

LEM advances the 1-D zero Mach equations of species mass fractions Y_s in (2.27) and the specific enthalpy of the mixture h in (2.28)

$$\rho \frac{DY_s}{Dt} = -\frac{dj_s}{dx} + M_s \dot{w}_s, \quad (2.27)$$

$$\rho \frac{Dh}{Dt} = -\frac{dp}{dt} - \frac{dq}{dx} - \sum_s j_s \frac{dh_s}{dx} - \sum_s h_s M_s \dot{w}_s, \quad (2.28)$$

where ρ denotes density, j_s the species diffusive flux, M_s the species molar mass, $\dot{w}_s$ the chemical source term for the species s . Additionally, p indicates the pressure, q the heat flux, and h_s the total enthalpy of species s . The equation of state of the mixture of ideal gases is expressed as the following in LEM:

$$p = \rho T \sum_s R_s Y_s, \quad (2.29)$$

where R_s conveys the individual gas constant of species s . The equations (2.27) and (2.28) are solved using a second-order accurate scheme using a central discretization of the diffusion terms. The temperature in the LEM cells is calculated using the calorific equation of state (3.20). The transport and thermodynamic parameters and the chemistry source chemistry are assessed using the CANTERA package [35], where the stiff chemical source term is integrated using SUNDIALS' implicit BDF method. [36]

2.3.2 Turbulent Advection in LEM

Turbulence is simulated on the LEM by executing independent eddy events. The simulation of the turbulent vortices on the line is performed by the triplet mapping process, which models the impact of the turbulent 3D vortices on the scalar profiles implemented on the one-dimensional line as described in figure 2.1. It is a technique that ensures continuity and conservation of mass. The triplet mapping process compresses the interval where the eddy has landed and creates three identical copies with inverting the middle one. It is a process that requires adaptation depending on the LEM chosen shape. In this case, the spherical shape of the LEM has been chosen; this choice will be explained in chapter 3.

A high pressurized fuel is injected into the combustion chamber or the inlet port in an ICE. This process creates a considerable number of eddies with a size distribution between the integral and the Kolmogorov length scales. These eddies are referred to as *small eddies*. The CFD provides the turbulence parameters $\bar{k}$ and $\bar{\epsilon}$ that determines the LEM parameters, namely, the turbulence diffusivity D_t , the integral length scale l_t , the Kolmogorov length scale η and the average time between the eddies. Initially, solely the small eddies were simulated on the LEM. However, the circumstances are different in a combustion chamber due to the large-scale motions such as tumble or swirl. These large movements significantly enhance the mixture in a real engine; ignoring them in a LEM simulation will lead to notable discrepancies between the LEM and CFD.

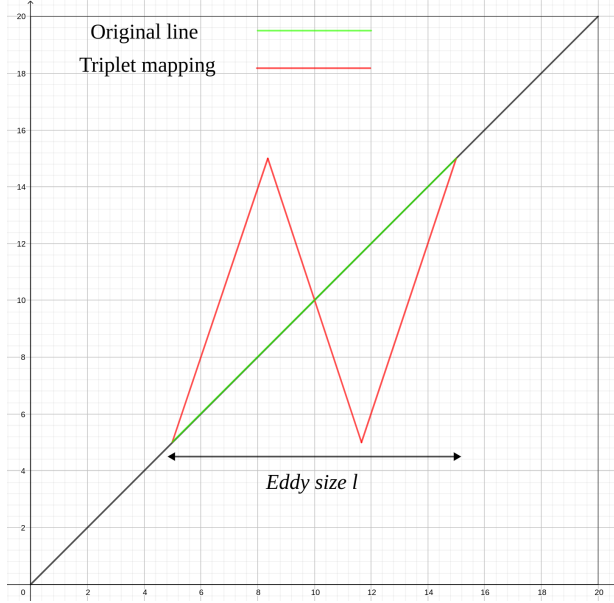


Figure 2.1: *Representation of a triplet map in a planar LEM*

Small eddies

The distribution defined in equation (2.30) and described in length in [1], determines the size distribution of eddies that exist between the integral and the Kolmogorov length scale.

$$f(l) = \frac{5}{3} \frac{l^{-8/3}}{\eta^{-5/3} - l_t^{-5/3}}, \quad (2.30)$$

where l indicates the size of the eddies, l_t is the integral length scale and η is the Kolmogorov length scale. The integral length scale l_t is defined as:

$$l_t = \frac{D_t}{u'}, \quad (2.31)$$

with D_t denotes the turbulent diffusivity:

$$D_t = \frac{C_\mu}{Sc_t} \frac{\tilde{k}^2}{\tilde{\epsilon}}, \quad (2.32)$$

and u' is the velocity fluctuations defined as:

$$u' = \sqrt{\frac{2\tilde{k}}{3}}. \quad (2.33)$$

η is calculated based on the inertial scaling law described in [1] with

$$\eta = N_\eta l_t Re_t^{-3/4}, \quad (2.34)$$

where Re_t is the turbulent Reynolds number:

$$Re_t = \frac{u' l_t}{\nu}. \quad (2.35)$$

The values assigned to the model constants $C_\lambda = 15$, $C_\mu = 0.09$ and $N_\eta = 10.76$ are based on literature values [37]

The eddy event frequency per unit length is determined using the above defined quantities, and is described as the following:

$$\lambda = \frac{54}{5} \frac{\nu Re_t}{C_\lambda l_t^3} \frac{(l_t/\eta)^{5/3} - 1}{1 - (\eta/l_t)^{4/3}}. \quad (2.36)$$

The eddy event time on the LEM domain is determined based on a sampling under a Poisson process assumption with mean eddy occurrence time:

$$\Delta\tau_{eddy} = (\lambda L)^{-1}, \quad (2.37)$$

where L characterizes the length of the LEM domain. Finally, the eddy location is specified based on the left edge of the eddy, and it is sampled uniformly on the LEM domain.

Large scale mixing

Large-scale 3D motion such as tumble and swirl needs dedicated modeling on a one-dimensional domain. Not considering the large-scale motions, small eddies, and diffusion effects alone will have difficulty creating sufficient stoichiometric regions for ignition, especially if the fuel is continuously injected, leading to a continuous increase of the mixture fraction solely in one region of the chamber, which can hinder the ignition of the fuel. Taking the large-scale motions into consideration contributes to creating several pockets with lower mixture fraction values. The distribution of the fuel regions increases the effect of the small eddies and diffusion to create ignitable regions. It is then essential to include the large-scale motions in the LEM simulation. The large-scale motions are described by the three introduced quantities (eddy size, length, and occurrence time) similar to the small eddies. The modeling of these three quantities is, however, different for the large-scale motions since they are generated by different physics, essentially the movement of the piston and the incoming flow from the inlet port. The length of the large-scale motions has been chosen to be equal to half of the combustion chamber's bore; this length ensures the fuel distribution to different parts of the chamber, which corresponds to the two sides of the LEM line. The time scale of these motions is determined based on the following scaling:

$$\tau_{bigeddy} = \theta \frac{v_N}{l_c}, \quad (2.38)$$

where θ refers to a mixing time constant that describes the effects of the combustion chamber geometry on the large-motion events times, which was fixed to unity in this study. v_N refers to the spray's velocity that influences the large-scale motion, and l_c is

the engine cylinder length scale. The number of large-scale motions occurring on one engine cycle is fixed at the start of the simulation by:

$$N_{bigeddy} = \frac{\tau_{engineCycle}}{\tau_{bigeddy}}, \quad (2.39)$$

where $\tau_{engineCycle}$ characterises the time required for one engine cycle. The occurrence times are independently sampled based on a uniform distribution of occurrence time during one engine cycle. Finally, the position of the large eddies is sampled uniformly across the LEM line.

2.3.3 LEM time advancement

The LEM framework incorporates three concurrent processes; Turbulent advection, molecular diffusion, and chemistry resolution. Diffusion and chemistry are implemented using a Strang operator splitting as presented in figure 2.2.

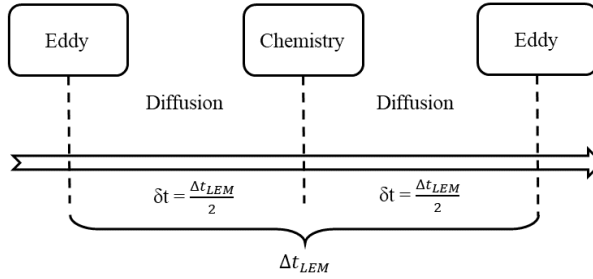


Figure 2.2: *Representation of the diffusion-chemistry process in LEM*

The time step Δt is defined as the duration between two consecutive eddy events in the original ODT code. The Strang Split Operator divides Δt into two halves δt on which the diffusion is advanced implicitly. The stiff chemical source term is integrated over the entire Δt time step in between the diffusion steps. Eddies events on the other hand are implemented instantaneously.

In the original ODT code used here, the LEM process is implemented in a way that the LEM time step Δt_{LEM} is decomposed into several Δt based on the sampled eddy occurrence times, which is decided based on the number of eddy events sampled in the corresponding time-step, this process is described in figure 2.3. Although this approach is considered the most consistent for turbulent chemistry interactions, the successive interruption and re-start of the CVODE chemistry solver substantially slows down the simulation. A substantial reduction of the overall simulation time was developed by employing two different strategies. The initial approach was to decompose the LEM line into several parts where chemistry is solved in parallel. This method utilizes OpenMP multithreading, where several chemistry solvers are initialized simultaneously, and each

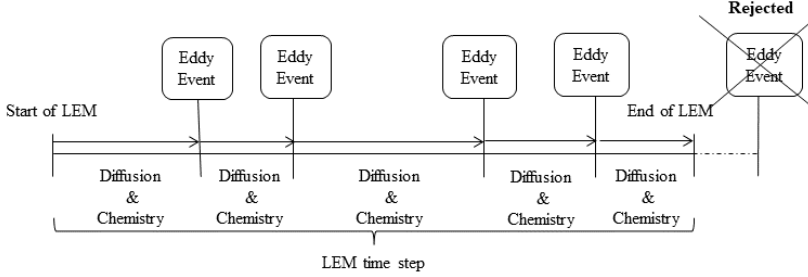


Figure 2.3: *Traditional LEM advancement framework*

solver integrates the chemical source terms for a dedicated section of the line. The second strategy was to cluster the eddies intended to be sampled on the corresponding LEM time step and implement them by sampling order at the start of the time step, as depicted in figure 2.4. The Strang Operator Strategy is correspondingly applied in this approach with $\delta t = \frac{\Delta t_{LEM}}{2}$, where the diffusion is advanced on δt and chemistry is integrated over Δt_{LEM} . The eddy clustering approach was created for a specific strategy where multiple LEMs were utilized. Advancing multiple LEMs in parallel using multi-threading to reduce

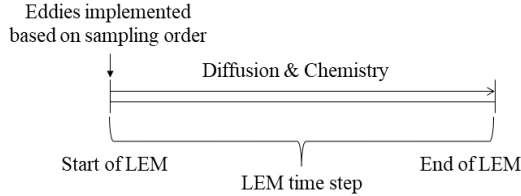


Figure 2.4: *Eddy clustering framework*

chemistry integration needed a forking operation which was avoided for the current version of the model. The first approach is the most convenient if enough computational resources are available. However, it will be shown later in the thesis that multiple LEM lines are required to acquire a reasonable simulation output. It is essential to state that the second approach is greatly sensitive to the selected time step. For large time steps, the LEM will implement numerous eddies and solve diffusion and chemistry over the extended time step. Choosing a large time step corresponds to clustering many eddies before running diffusion and chemistry, which neglects the turbulent chemistry interaction effects. Therefore, choosing a reasonable time step is crucial for the eddy clustering approach.

3 Combustion closure in RILEM

One of this project’s primary goals is to use the LEM as a combustion model for ICE. CFD and LEM require a coupling that ensures that the combustion information comes from LEM. The following section describes the adopted strategy.

The coupling between the CFD solver and the LEM combustion model should be pressure-based to include the heat effects, such as latent heat of evaporation and wall heat losses, in the LEM, which are modeled on the CFD solver. A volume coupling, for instance, demands separate modeling of these effects on the LEM side. These considerations motivated the development of a stand-alone LEM driven by input parameters extracted from a reactive CFD simulation, e.g., with the PaSR combustion model. Once the stand-alone code produces satisfactory results, the second step is to couple the CFD to the LEM using the same driving parameters as the stand-alone LEM. However, in this case, the chemical state of the CFD will be updated uniquely from LEM.

3.1 Spherical LEM

3.1.1 Spherical Triplet Maps

One of the objectives RILEM is to utilize a combustion model that represents the corresponding CFD domain. The original LEM code by Lignell [34] contains three different LEM geometries: planar, cylindrical, and spherical. To ensure the representative aspect between the LEM and the combustion chamber, the spherical LEM formulation was chosen with a characteristic length equal to the combustion chamber bore. This LEM formulation was useful in the CFD-LEM coupling method, described later in the thesis. The triplet maps for both small eddies and large-scale motions need to be updated for the spherical LEM. Both molecular and heat diffusion will be happening across a spherical boundary, which requires a spherical adaptation to the fluxes. Implementing a triplet map on a spherical LEM can occur in three possible scenarios, depending on where the eddy boundaries are landing. We name A the left boundary and $B = A + L$ the right boundary of the eddy, respectively, and L is the eddy size.

1. Both A and B land on the left cone of the line
2. A land on the left cone and B lands on the right cone.
3. Both A and B land on the right cone of the line

The LEM implementation suggests a different rearrangement for each scenario. The mathematical derivation has been discussed at length in [38]. The following figure represents the different implementation for each scenario.

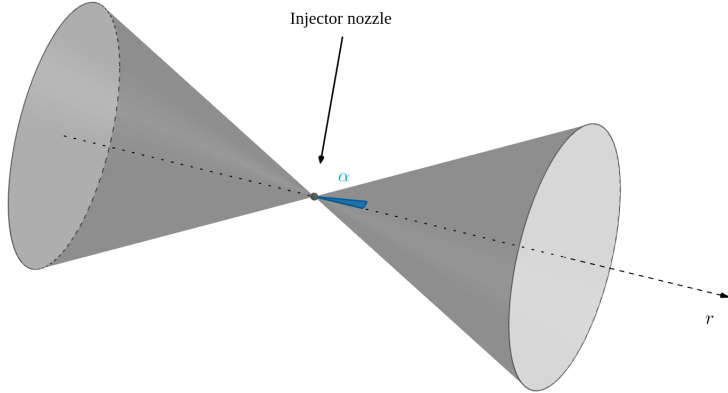


Figure 3.1: *Representation of the spherical LEM*

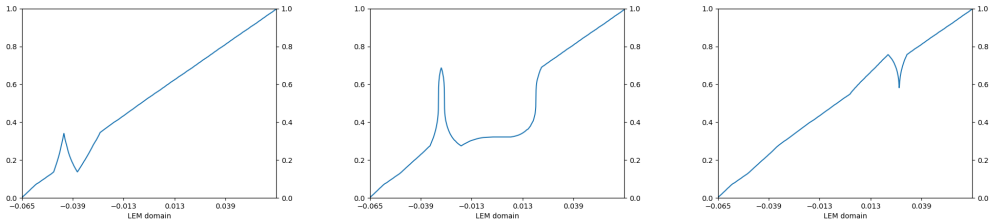


Figure 3.2: *Representation of spherical triplet maps per scenario: 1: To the left. 2: The middle. 3: To the right*

3.1.2 Pressure Coupling

The LEM line comprises several cells modeled as homogeneous reactors with constant volume or pressure for chemistry integration. The LEM line advances under a constant pressure condition, where the LEM pressure is equal to the CFD prescribed pressure. However, fuel injection and combustion are local processes in individual cells that lead to a change in the local pressure of the cells, which violates the constant pressure condition. Additionally, the length of the LEM line is required to be equal to the characteristic length of the CFD domain. These two constraints were possible to achieve using the spherical formulation of the LEM and the split operator strategy explained in the next paragraph.

Split Operator Strategy

Combustion on the LEM is implemented as a constant volume process in each cell, where the pressure is allowed to change locally, and the volume stays constant. Similarly, the fuel injection process is also implemented as a constant volume process, where the new

local densities are calculated based on the injected mass in the cells. These two processes lead to a violation of the constant pressure constraint of the LEM. Additionally, the pressure on the LEM should be equal to the CFD pressure. The split operator strategy was the remedy to this issue. It goes through two processes; the first is an isentropic process that allows the cell's volumes to expand/compress to reach a target pressure:

$$V_2 = V_1 \left(\frac{p_1}{p_{CFD}} \right)^{1/\gamma}, \quad (3.1)$$

where p_{CFD} denote the target CFD pressure, $\gamma = c_p/c_v$, c_p and c_v the specific heat capacities under constant pressure and constant volume respectively. In addition, ρ_2 is estimated based on equation (3.9) and $Y_{2,s}$, and T_2 are deducted from equations (3.8). All LEM cells volume will change to match the CFD pressure in this operation.

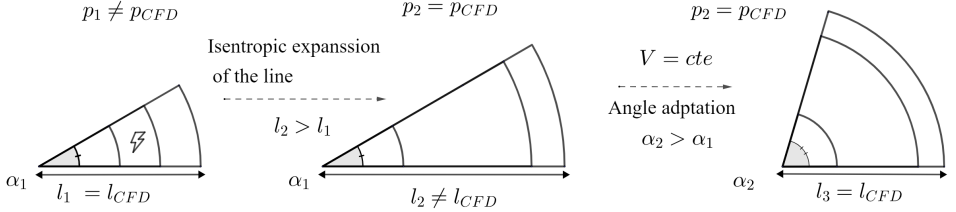


Figure 3.3: *Split Operator Strategy*

The first procedure guarantees the resolution of the constant pressure limitation; however, after applying the isentropic process on the line, the length of the line is different from the CFD characteristic length, which violates the representation aspect of the model. This problem is resolved by utilizing the spherical formulation of the LEM, which is the second step in the split operator strategy. A new cone angle α of the line is calculated based on the condition that the LEM length matches the characteristic CFD length, as the following formula shows:

$$\alpha = \arccos \left(1 - \frac{12V_{LEM}}{\pi D^3} \right), \quad (3.2)$$

where D represents the combustion chamber's bore, and V_{LEM} the total volume of the LEM line. This step ensures the conservation of the LEM's volume while matching the characteristic length. Finally, the LEM cell boundaries are recalculated based on the new cone angle.

3.1.3 Fuel Mapping Strategy

The fuel injection is simulated as a 3D process on the CFD side using a Lagrangian spray model. The LEM only accepts fuel in its vapor phase, so a specific strategy is required to correctly map the fuel on the LEM line. The first possible solution is to develop an independent spray model on the LEM side. Although this solution is realistic,

it was not adopted for complexity reasons. Instead, the following values provided from the spray model on the CFD determine the fuel mapping on the LEM: Evaporated fuel mass, vapor deposition length, and the volume of the cells that witness evaporation. The choice of the second alternative is motivated by its simple implementation and the sustained consistency between LEM and CFD compared to the first approach. The total volumes of LEM and CFD will not necessarily match. However, it is essential to reinforce it when extensive properties are communicated between the two sides; for this purpose, the volume ratio Q is introduced:

$$Q = \frac{V_{LEM}}{V_{CFD}}. \quad (3.3)$$

The fuel mapping strategy is based on two main quantities:

- **The vapor penetration length:** It determines the number of LEM cells on which the fuel will be mapped.
- **The evaporated fuel mass:** It specifies the amount of fuel vapor on the CFD that will be injected in the LEM.

The injector is defined as the meeting point of the two LEM cones. Due to the line's orientation along the spray axis, the two cones will receive equal amounts of fuel symmetrically. The LEM vapor penetration length is calculated by matching the volume of the cells with evaporation on the CFD.

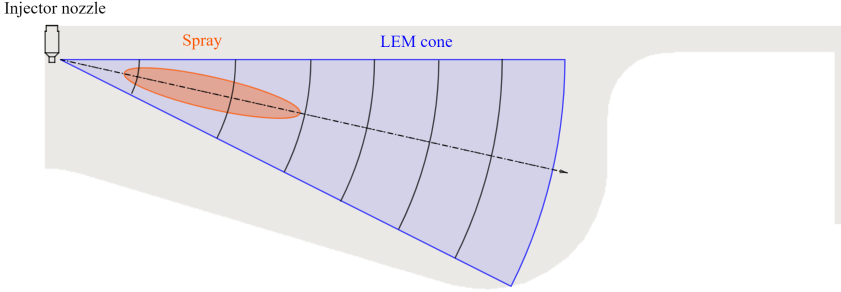


Figure 3.4: Representation of the LEM cone oriented towards the spray

We calculate the ratio of injected vapor fuel on the CFD side as:

$$\beta = \frac{\sum V_{ev,i}}{V_{CFD}}. \quad (3.4)$$

The volume with fuel evaporation can be calculated using β on the LEM side as:

$$V_{fuel} = \frac{\beta V_{LEM}}{Q} = \beta V_{CFD}. \quad (3.5)$$

Based on the spherical geometry of the LEM domain, the corresponding radius of fuel, which is the LEM fuel evaporation length, can be calculated as:

$$r_{fuel} = 3 \left(\frac{V_{fuel}}{2\pi(1 - \cos \alpha)} \right)^{1/3}. \quad (3.6)$$

Fuel vapor is added to all cells on the LEM domain with radius lower or equal that r_{fuel} . The second step is to determine the fuel mass that each LEM cell receives. The LEM cell's volume is the defining factor in determining the mass of each cell:

$$m_{ev,i}^{LEM} = m_{ev}^{CFD} Q \frac{V_{ev,i}^{LEM}}{\sum V_{ev,i}^{LEM}}. \quad (3.7)$$

The described method does not guarantee that the fuel vapor mass remains under the saturation level in each cell. However, this limit did not cause any issues in the simulations. Once the allocated mass in each LEM cell is determined, merging the existing quantities with the introduced ones in each cell receiving fuel occurs. The merging will apply to temperature, mass fractions, and densities, taking place using a constant volume process. For $\phi_i = \{Y_{i,s}, T_i\}$ we have equation (3.8) where ϕ^{old} denotes the scalars before adding the fuel vapor and ϕ^{add} the added ones:

$$\phi_i^{new} = \frac{\phi_i^{old} m_i^{old} + \phi_i^{add} m_i^{add}}{m_i^{old} + m_i^{add}}, \quad (3.8)$$

and for the density ρ :

$$\rho_i^{new} = \rho_i^{old} + \rho_i^{add} \frac{V_i^{add}}{V_i^{old}}. \quad (3.9)$$

The addition of vapor fuel to the LEM cells under a constant volume assumption leads to undesirable changes in the local pressure of the cells where the injection occurred. The Split Operator Strategy is used a second time to realize a homogeneous pressure on the LEM which matches the CFD target pressure.

3.2 Spherical Stand Alone Linear Eddy Model (SSALEM)

A Spherical Stand-Alone LEM (SSALEM) was developed for debugging purposes and extensive parameter investigations. SSALEM was also used as a testing platform before proceeding to the CFD-LEM coupling. In a pre-processing step, a reacting CFD simulation was run using the Well Stirred Reactor model (WSR) to extract driving parameters for the SSALEM. A standard 1D slider-crank model has been used to calculate the combustion chamber volume as a function of the engine speed. In SSALEM, the coupling is meaningful only in one direction, from the CFD to the LEM, which means no feedback from the LEM to the CFD to update the chemical state. Ignition on the LEM was triggered by the enforced pressure trace extracted from the WSR simulation. Some snapshots of the SSALEM simulation are presented in the result chapter. In order to benefit from LEM's combustion closure, it is required to have a coupling to the CFD solver that goes in both

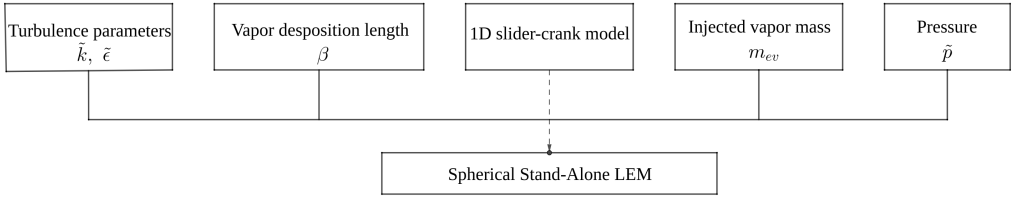


Figure 3.5: *SSALEM framework*

ways, creating a feedback loop that will influence the CFD parameters, such as the rate of evaporation of the fuel and the turbulence level due to the increase of temperature. RILEM always refers to the RANS-CFD coupling.

3.3 RILEM

The implementation of the CFD and LEM sides in different dimensions (3D for CFD 1D for LEM) makes the coupling between the two sides a complex exercise. The utilization of LEM as a combustion model for engine simulations follows a similar approach as in RIF models. The coupling is implemented by mapping of the LEM solution in physical space to a solution in a mixture fraction and progress variable space and calculation of the mean values via a presumed Probability Density Function (PDF) approach. If transport equations of species mass fractions are advanced on the CFD side, a source term for each individual species must be sent from the LEM to the CFD. This approach can be costly for substantially large chemical mechanisms as a transport equation for each species needs to be solved on the CFD side. Instead, equations for the mean and the variance of the mixture fraction Z are advanced. In addition, a transport equation for the combustion progress variable c is advanced. Figure 3.6 represents the framework of RILEM at one CFD time step. The left side of the figure shows the driving parameters extracted from the CFD and the different processes that occur in the LEM. The right side describes the conditioning operation of the selected reactive scalars, their mapping on the CFD from LEM, and the temperature calculation.

3.3.1 Reactive Scalars Integration

The LEM provides a distribution of the reactive scalars in 1D physical space, which needs to be communicated with the 3D CFD domain in a meaningful way. For that, RILEM adopts a similar coupling concept to the RIF approach, where the LEM reactive scalars are conditioned on a reference composed of either Z and c ; the chosen resolution was 200 bins in the Z direction and 100 bins in c , where a *bin* refers to a specific interval in a space. This operation results in matrices for the reactive scalars referred to as *solution tables*.

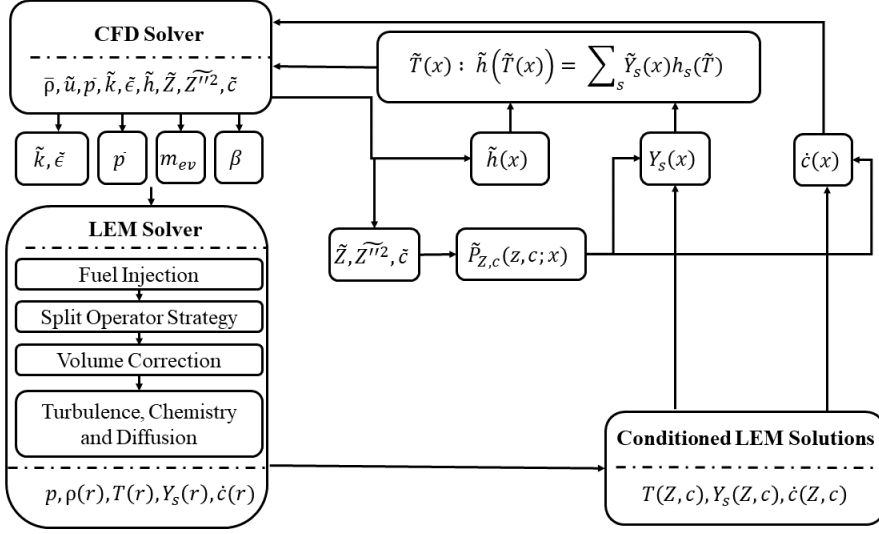


Figure 3.6: *RILEM* configuration

The communication between the CFD and LEM is conducted by the Joint PDFs of the mixture fraction Z and combustion progress variable c . The joint PDF is utilized to determine the mean value of the scalars in a specific CFD cell:

$$\widetilde{\phi}_k = \int_0^1 \int_0^1 \tilde{P}_{Z,c}(Z_k, c_k) \phi^{LEM}(Z, c) dZ dc. \quad (3.10)$$

Statistical independence is considered between Z and c , simplifying the problem by decomposing the joint PDFs to two independent PDFs:

$$P_{Z,c}(Z, c) = P_Z(Z; \tilde{Z}, \widetilde{Z'^2}) P_c(c; \tilde{c}). \quad (3.11)$$

The solution of the mean and the variance of mixture fractions transport equations provides a value of the two variables in each CFD cell, enabling us to utilize a presumed β -PDF for Z :

$$P_Z(Z; \tilde{Z}, \widetilde{Z'^2}) = \frac{\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(\beta)} Z^{\alpha-1} (1-Z)^{\beta-1}, \quad (3.12)$$

where Γ is the usual gamma function defined as:

$$\Gamma(t) = \int_0^\infty t^{x-1} e^{-t} dt, \quad (3.13)$$

and α , β and γ are three coefficients defined as:

$$\gamma = \frac{\tilde{Z}(1-\tilde{Z})}{\widetilde{Z'^2}}, \quad \alpha = \gamma\tilde{Z}, \quad \beta = \gamma(1-\tilde{Z}). \quad (3.14)$$

A β -PDF can likewise be used for the combustion progress variable if a transport equation of the combustion progress variable variance $\widetilde{c''^2}$ is solved. However, the complexity of formulating a transport equation of $\widetilde{c''^2}$ encourages exploring other functions that can describe the c distribution. More easily, one way to define it is as a step function based on the mean value of the progress variable as shown in the following:

$$P_c(c; \tilde{c}) = \begin{cases} \frac{1-\tilde{c}}{\tilde{c}} & 0 \leq c \leq \tilde{c} \\ \frac{\tilde{c}}{1-\tilde{c}} & \tilde{c} \leq c \leq 1 \end{cases} \quad (3.15)$$

Using $P_Z(Z)$ and $P_c(c)$, the integrated values of temperature and species mass fractions can be formulated as:

$$\widetilde{T}_k = \int_0^1 \int_0^1 \tilde{P}_Z(Z; \widetilde{Z}_k, \widetilde{Z}_k''^2) \tilde{P}_c(c; \tilde{c}_k) T^{LEM}(Z, c) dZ dc, \quad (3.16)$$

$$\widetilde{Y}_{k,s} = \int_0^1 \int_0^1 \tilde{P}_Z(Z; \widetilde{Z}_k, \widetilde{Z}_k''^2) \tilde{P}_c(c; \tilde{c}_k) Y_s^{LEM}(Z, c) dZ dc. \quad (3.17)$$

$$\tilde{\dot{c}}_k = \int_0^1 \int_0^1 \tilde{P}_Z(Z; \widetilde{Z}_k, \widetilde{Z}_k''^2) \tilde{P}_c(c; \tilde{c}_k) \dot{c}^{LEM}(Z, c) dZ dc, \quad (3.18)$$

where $\dot{c}$ denotes the source term of the combustion progress variable transport equation, which will be defined in the next section.

3.3.2 Reactive Scalars Exploitation

3.3.2.1 Temperature and Species Mass Fractions

The mean temperature value in each CFD cell can be directly calculated from the temperature solution table extracted from the LEM, as described in the previous section. The temperature was, however, iterated based on the calculated species mass fractions and the solution of the total enthalpy transport equation based on calorific heat equation:

$$\tilde{h}_k(\tilde{T}) = \sum_{s=1}^N \tilde{Y}_{s,k}(t) h_s(\tilde{T}), \quad (3.19)$$

with

$$h_s(T) = \Delta h_s^0 + \int_{T^0}^T c_{p,s}(T) dT, \quad (3.20)$$

where h_s denotes the mass-specific enthalpy values of the species s , Δh_s^0 the standard heat of formation, and $c_{p,s}$ the mass specific heat capacity at constant pressure. Two values of temperatures can be calculated on the CFD side. $\tilde{T}_{pdf,k}$ which is the mean value of temperature from the temperature solution table from the LEM, and $\tilde{T}_k$, which is calculated based on the mean value of species mass fractions and the solution of the total enthalpy transport equation. The two temperature values should ideally closely match in case that the LEM is representative of the combustion process. The similitude is possible

due to the intrinsic inclusion of the communicated pressure to the heat effects that appear as a source term for the total enthalpy equation. However, $\tilde{T}_k$ and $\tilde{T}_{pdf,k}$ do not match in the volume coupling; The heat loss effects on the CFD are intrinsically communicated via the pressure trace on the pressure coupling. In the volume coupling, however, the LEM requires a heat loss term in the heat equation to account for the heat losses on the CFD.

3.3.2.2 Combustion progress variable

The source term of combustion progress variable $\dot{c}$ describes the evolution of the fuel state. Since LEM is responsible for the chemical closure, the $\dot{c}$ has to be provided by the LEM, and its choice is crucially important. Since the progress variable c is determined based on O_2 mass fractions, the $\dot{c}$ should respect the same choice, and it was defined as the following:

$$\dot{c} = \frac{dY_{O_2}/dt}{Y_{O_2,b} - Y_{O_2,u}}, \quad (3.21)$$

where $\frac{dY_{O_2}}{dt}$ is defined as the following:

$$\frac{dY_{O_2}}{dt} = \frac{R[O_2]W_{O_2}}{\rho}, \quad (3.22)$$

where $R[O_2]$ denotes the net production rate of O_2 and W_{O_2} represents the molecular weight of O_2 . As described in the previous section, $\dot{c}$ is conditioned on Z and c spaces on the LEM and $\tilde{c}$ is calculated based on both $P_z(Z)$ and $P_c(c)$ to advance the transport equation of the progress variable on the CFD.

3.4 mRILEMs

The current version of RILEM successfully considers the 3D effects by using the spherical geometry of the LEM. However, the stochastic nature of the eddies causes an issue in the construction of the solution table. The problem is formulated as follows: The LEM line implements a sequence of eddy events that generates a distribution of the turbulent scalars in the LEM space. This distribution will be reflected in the conditioning step, which leads to filling the table uniquely with the data that the line has discovered on the corresponding time step. Based on the chosen eddy sequence and the resolution in the Z and c spaces, only specific locations in the table are filled, leaving other parts undefined. Initially, data exists only for $Z_i = 0$ since injection did not happen yet. The concern occurs in the integration process according to (3.10), which uses $P_z(Z)$ and $P_c(c)$ and data over the whole Z and c spaces. If the LEM fails to encounter that required combination, the CFD cell will be calculating the mean values with not enough data for the two spaces. The solution to the presented problem is to advance multiple LEMs by changing the eddy sequences solely and maintaining the rest of the driving parameters identical between the lines. Each LEM line builds a solution table corresponding to the distribution generated by its corresponding eddy sequence. The data from each table are averaged to generate a general representative table that the CFD will utilize to calculate the mean values of the reactive scalars. This approach is referred to as mRILEMs and

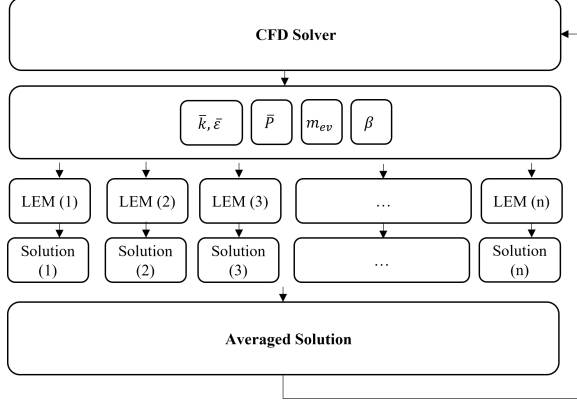


Figure 3.7: *mRILEMs* configuration

sketched in Figure 3.7. The averaging process between the tables created by each LEM line is done as simple arithmetic mean value:

$$\phi_{ij} = \frac{\sum_{k=1}^{n_{ij}} \phi_{ij}^k}{n_{ij}}, \quad (3.23)$$

where n_{ij} denotes the total number of hits for a position i, j in a table (Z_i, c_j) , where $i \in [1, n_Z]$ and $j \in [1, n_c]$, and n_Z and n_c the resolution (number of bins) of the Z space and c space respectively. This approach is valid only if all the tables have significant values for the corresponding Z and c combination, i.e., n_{ij} equal to the number of the LEM realizations.

A series of simulations have been done using the mRILEMs approach with 24 LEMs. The findings displayed in the results chapter demonstrate that utilization of 24 lines appears to be not enough to complete the solution table. This issue can be solved in principle by utilizing substantially more LEM lines. Here we suggest an alternative approach by following a method that suggests the following:

1. ϕ built from 24 LEM lines
2. Scaling the $P_Z(Z)$ and $P_c(c)$ of the turbulent scalars
3. Maintaining the LEM time history

The motivation behind this method is to avoid integrating empty data on Z and c bins, which boils down to having as much data as possible on the averaged solution table ϕ and scaling the integral of the PDFs to unity.

PDF scaling

The PDF scaling will be explained in this section. Calculating a mean value of a turbulent scalar conditioned on Z and c spaces is done by utilizing the following formula:

$$\tilde{\phi} = \int_0^1 \int_0^1 \tilde{P}_Z(Z; \tilde{Z}_k, \tilde{Z}_k^{''2}) \tilde{P}_c(c; \tilde{c}_k) \phi^{LEM}(Z, c) dZ dc \quad (3.24)$$

However, the holes in the solution tables of ϕ represent discontinuities in the distribution of the turbulent scalar in Z and c spaces, which means that utilizing an integral formulation as depicted in (3.24) to express the mean value calculation is incorrect; Equation (3.24) will instead be expressed as a discrete sum as described in the following:

$$\tilde{\phi} = \sum_{i \in N(z)} \sum_{j \in N(c)} \tilde{P}_Z(Z_i; \tilde{Z}_k, \tilde{Z}_k^{''2}) \tilde{P}_c(c_j; \tilde{c}_k) \phi^{LEM}(Z_i, c_j) \Delta Z \Delta c, \quad (3.25)$$

where $N(z)$ and $N(c)$ correspond to the set of solutions found in the corresponding solution space. $\tilde{Z}_k$, $\tilde{Z}_k^{''2}$, and $\tilde{c}_k$ represent respectively the mean of the mixture fraction, the variance of the mixture fraction and the mean of the progress variable in a CFD cell k .

Scaling the PDFs is essentially utilizing the following formula:

$$\tilde{\phi} = \sum_{i \in N(z)} \sum_{j \in N(c)} \tilde{P}_Z^*(Z_i; \tilde{Z}_k, \tilde{Z}_k^{''2}) \tilde{P}_c^*(c_j; \tilde{c}_k) \phi^{LEM}(Z_i, c_j) \Delta Z \Delta c, \quad (3.26)$$

where P_z^* and P_c^* are the scales PDFs expressed as the following:

$$P_z^*(z_i) = \frac{P_z(z_i)}{\sum_{i \in N(z)} P_z(z_i)}, \quad P_c^*(c_j) = \frac{P_c(c_j)}{\sum_{j \in N(c)} P_c(c_j)} \quad (3.27)$$

Persistence of the LEM results

The persistence approach implies maintaining the encountered values of the reactive scalar ϕ in previous time steps. If a new result is found, the old value gets simply overwritten by the new one. The persistence approach aids with minimizing the effect of the scaling method, namely bringing $\sum_{j \in N(c)} P_c(c_j)$ and $\sum_{i \in N(z)} P_z(z_i)$ closer to unity, especially at the start of the simulation where the solution tables are still empty. Different variations for scaling and persisting the turbulent scalars were tested and presented in the results section.

4 Results and Discussions

4.1 Numerical Setup

The selected case for validating the model is a single-cylinder metal research engine with a 15.8:1 compression ratio corresponding to a Volvo 13L six-cylinder heavy-duty truck engine. It has previously been investigated in [16], where n-dodecane is injected at high pressure in the combustion chamber. Table 4.1 summarizes the operating conditions. The simulation is a part load injection case using both RILEM and WSR. The chemical

Initial pressure (bar)				1.69
Initial temperature (K)				395
Initial composition	O2	N2	CO2	H2O
% Mass	16.5	75.3	5.97	2.26
IMEP (bar)				7.08
Engine speed (RPM)				1200
Start of injection				3.1° bTDC
End of injection				3.3° aTDC
Injected mass (mg)				13

Table 4.1: Operating conditions for the engine case

mechanism utilized in this case is a reduced n-dodecane mechanism with 54 species proposed by Yao et al. in [39]. The findings are also compared to experimental data and the CFD results obtained with the WSR model.

4.2 SSALEM

Figure 4.1 represents snapshots of a single Spherical Stand-Alone LEM (SSALEM) simulation using the driving parameters extracted from a WSR reacting case. The physical presentation of the LEM was possible by plotting the positions of the LEM cells centers. In addition, the representation of the LEM scalars, such as temperature, mixture fraction, or mass fraction for a specific species, was also possible. It is essential to highlight that the evolution of the LEM line represented by the presented figures will vary if a different eddy sequence is utilized due to the stochastic behavior of the small eddies.

The right side of figure 4.1 displays the ignition process on the LEM, where high temperatures appear in the regions where the fuel was consumed after passing by the stoichiometric mixture fractions. The intermediate species CO is following the development of the flame, leaving only a tiny amount of fuel on the edges of the line to be consumed. The fuel mass fraction is nearly entirely consumed in the right side of figure 4.1, and the CO mass fraction is still present on the line but should disappear after some time since it is an intermediate species. Another observation is the two distinct flames existing on

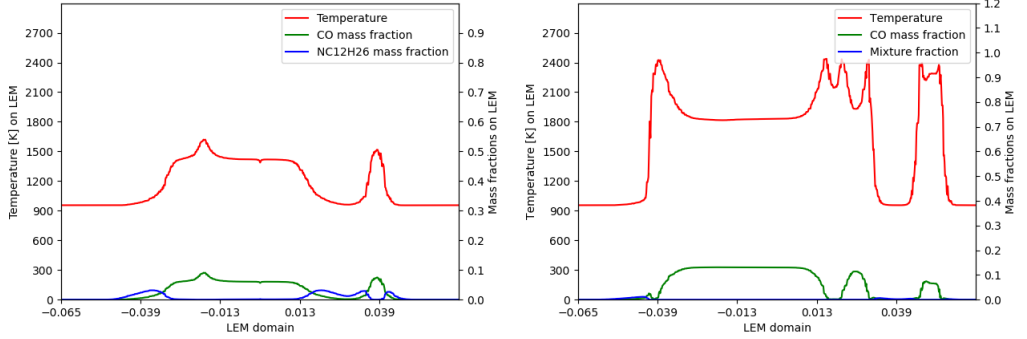


Figure 4.1: *Physical representation of Ignition on the LEM line*

the LEM that can clearly be observed on the right side of the figure due to a large-scale vortex that distributed the fuel from the center of the line to a different region. It was also possible to run multiple SSALEMs with different eddy sequences. The results of this process will be shown in the mRILEMs section since they describe the same purpose.

4.3 RILEM

As highlighted in the previous section, the LEM line's development is associated with the implemented eddy sequence. This correlation can generate empty bins in the solution tables since the latter are constructed based on the LEM distribution of the turbulent scalar. Running two RILEM simulations with different LEM eddy sequences can lead to different results since the mean values on the CFD are calculated based on two different solution tables. This matter can be considered an artifact of the RILEM method, which will be improved using the mRILEMs approach. There are several options to initialize and fill the table in Z and c spaces during a simulation which are explained in the following section.

4.3.1 Unburnt Composition Initialization

The first investigated approach utilizes the unburnt state to initialize the solutions across both Z and c spaces. This method, combined with the persistence approach, will ensure that no holes are present in the solution tables, which will help the solver reach the end of the simulation without crashing. All CFD cells will have a total enthalpy value and a species mass fraction composition to iterate the temperature. However, this method leads to unrealistic low-temperature values and missing ignition processes. This is because the fuel-air mixtures favorable for fast ignition process ($Z \approx 0.05$) can only be created in a short time by turbulent mixing, i.e., by eddies hitting the fuel injection zone. With just one LEM line, it cannot be guaranteed that the sequence of turbulent eddies can always create these favorable conditions for ignition. As a result, this initialization approach

with just one LEM does not allow for ignition in a robust way.

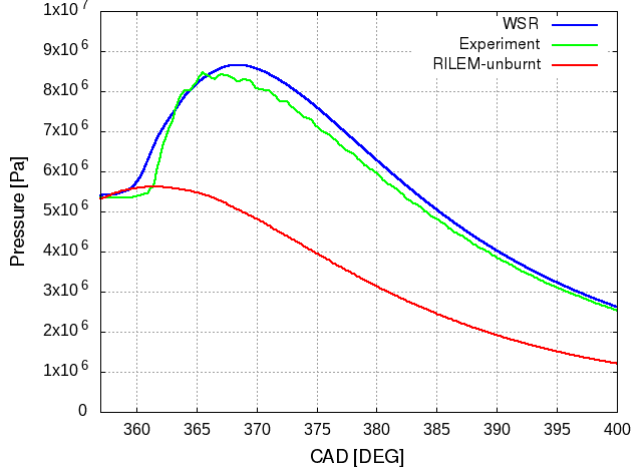


Figure 4.2: *Pressure trace of the unburnt initialized RILEM solution*

4.3.2 Interpolation between unburnt and equilibrium initialization

One of the straightforward solutions to get meaningful solutions for high values of c is to utilize the equilibrium solution. The solution tables are initialized based on a linear interpolation between the unburnt and the equilibrium state. This method gives different results depending on which strategy is utilized for the $\dot{c}$ solution table.

The following scenario clarifies the rationale behind combustion occurring for this approach: It is understood that ignition occurs if a CFD cell has the combination of a mixture fraction close to stoichiometry in a high-pressure, high-temperature environment. For the CFD to calculate the mass fractions corresponding to an ignition scenario, it will extract mass fractions from the solution table with a specific Z, c combination. The solution tables were either empty or initialized with the unburnt composition in the previous methods; additionally, the sequence of turbulent eddies of one LEM cannot guarantee the creation of ignitable air-fuel mixtures. The combination that the CFD requires is fulfilled by the information originating from the initialized solution table. It is worth stressing that the calculated mean value did not originate from the LEM but from the initial values of the solution tables. This strategy will create a feedback loop between the CFD and the LEM that will be described in the following: A high-temperature region on the CFD will increase the number of turbulent eddies on the line, this increase will lead to more turbulence, expanding the possibility of creating ignitable regions on the line. The high CFD pressure is enforced on the LEM due to the pressure coupling technique, which will lead to even more effortless ignition on the line.

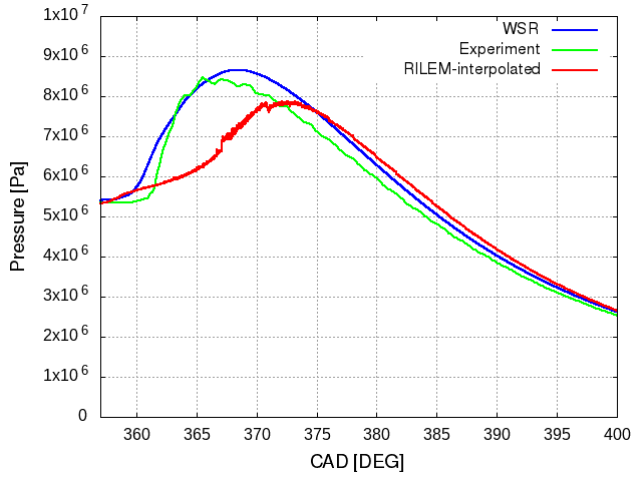


Figure 4.3: *Pressure trace of the interpolated initialized RILEM solution between the unburnt and equilibrium solutions without scaling the PDFs for $\dot{c}$*

Despite the results of the pressure trace being relatively satisfying, a fundamental problem can be pointed out with this method. The issue lies in the interpolation approach. Applying this approach to species mass fractions is not entirely correct due to the unrealistic representation of $T(Z, c)$ and $Y_s(Z, c)$ by a simple linear interpolation, which are highly non-linear functions of Z and c . A reliable functioning combustion model should give the correct composition at each time step. Using this method, the absent intermediate species in both the unburnt and the burnt compositions will lead to missing values for these species on the CFD. The only values that will appear are the ones originating from the LEM. This problem will lead to wrong temperatures in the intermediate stages of combustion since it results from a composition that lacks the complete spectrum of intermediate species mass fractions. An initialization using the homogeneous reactor with a prescribed volume can solve the problem that the interpolation method was causing. A homogeneous reactor initialization will ensure that the solution table of species mass fractions has the intermediate species information. However, the homogeneous reactor approach will completely neglect the turbulence-chemistry interaction that is important for predicting pollutant formation. The expectancy is that the LEM will overwrite the solution table in the middle of the simulation to account for the turbulence-chemistry interactions. An alternative solution is to develop a method where the use of LEM is maximized and the simulation time is reduced.

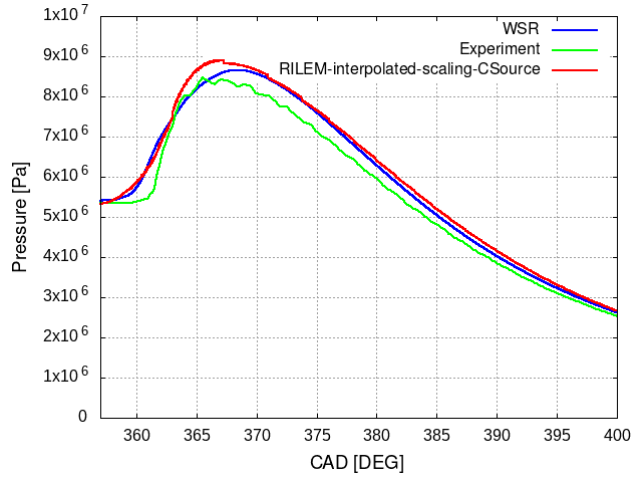


Figure 4.4: *Pressure trace of the interpolated initialized RILEM solution between the unburnt and equilibrium solutions with scaling the PDFs for $\dot{c}$*

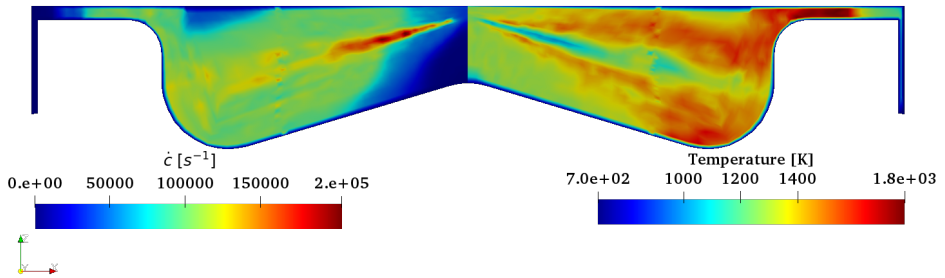


Figure 4.5: *RILEM interpolated species with scaling the PDF of $\dot{c}$ results for CAD = 363.00 $\dot{c}$ distribution on the left and temperature on the right.*

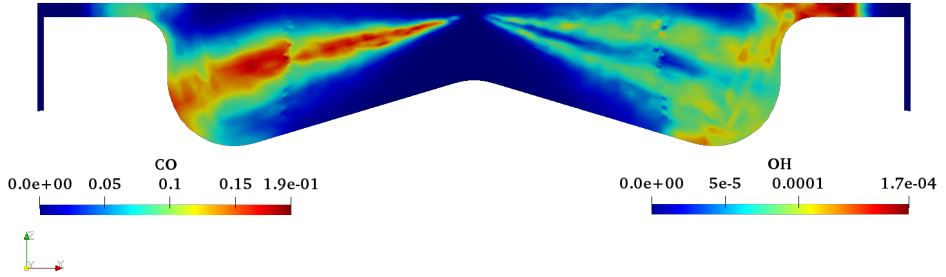


Figure 4.6: *RILEM* interpolated with scaling the PDF of $\dot{c}$ results for $CAD = 363.00$. *CO* mass fraction on the left and *OH* mass fraction on the right.

4.4 mRILEMs

4.4.1 mRILEMs with unburnt matrices initialization

In this approach, the solution tables for mRILEMs were initialized based on the unburnt composition, which means that the LEMs need to provide chemical closure for ignitable fuel-air mixtures on the CFD without the assistance of interpolation or a homogeneous reactor. 16 LEM lines were utilized for this simulation. Figure 4.7 demonstrates that

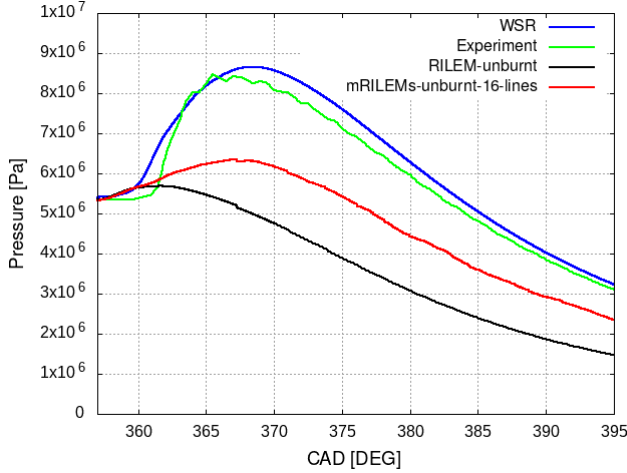


Figure 4.7: *Pressure trace of the scaled and persisted 16 mRILEMs empty initialized solution*

utilizing mRILEMs provided a more pronounced pressure peak than the output provided by unburnt RILEM. This observation indicates that the utilization of multiple LEMs with different turbulent eddy sequences indeed helps create more ignitable cells on the LEM lines. The first evident approach is to maximize the number of LEM lines utilized to cover the solution tables completely.

4.4.2 mRILEMs with scaling and persistence

Based on the previous result, the LEM lines struggle to update the CFD state accurately due to incomplete solution tables for PDF integration. As described in the previous chapter, two approaches are possible to solve this issue: A large number of LEM realizations to update the entire set of solution tables at each time step or realizing fewer LEM runs with scaling the PDFs and persisting the LEM time history. In this section, we use the second approach combined with 16 LEM realizations.

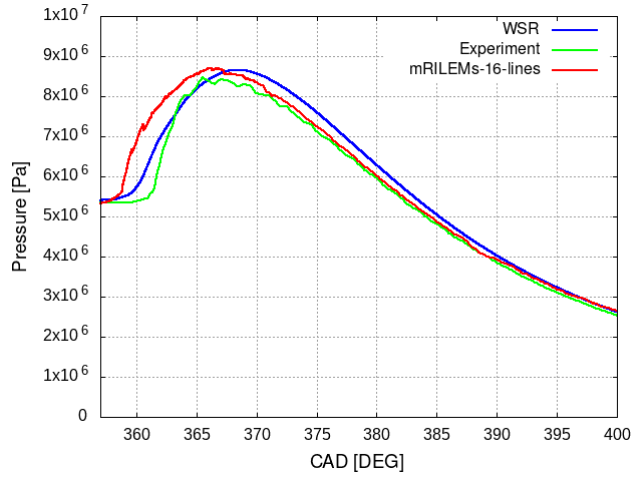


Figure 4.8: *Pressure trace of the scaled and persisted 16 mRILEMs empty initialized solution*

The LEM lines are initialized empty for this simulation, which signifies that all solutions observed from the CFD result from the data discovered on the LEM lines. Figures 4.9 and 4.10 clearly show that utilizing more LEM lines results in the acquiring more data, which motivates the utilization of multiple LEM lines. However, empty bins can still be observed, which signifies that PDF scaling and persisting the LEM solutions is required for all turbulent scalars. Figure 4.8 show a pressure trace that follows the expected trend and successfully predicts the peak and the tail of the pressure trace. LEM is working as a pure combustion model in this case, since the the chemical state is updated exclusively from the LEM advancement and not from the initialization of the solution table.

Figure 4.11 shows the results of the ignition point $CAD \approx 359$, where on the temperature field is displayed right side. A high temperature can be noticed around the stocheometric region of the spray which corresponds to what is expected. On the left side, the progress variable source term is shown

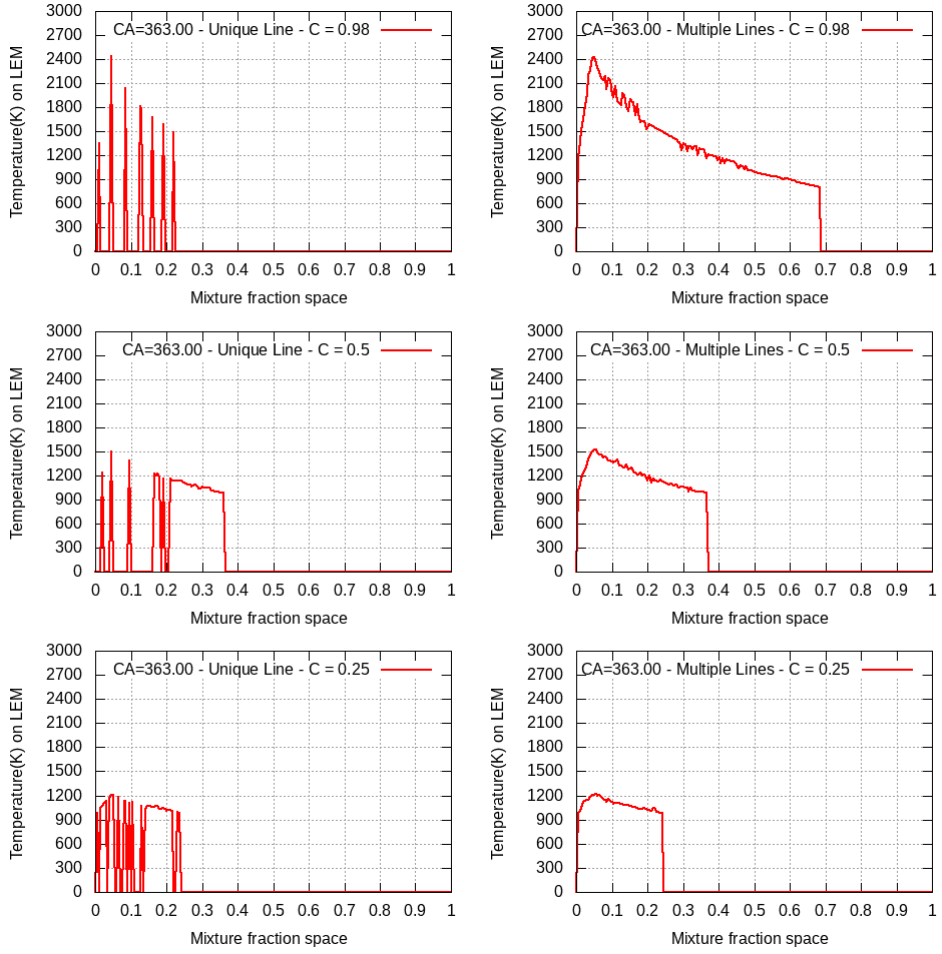


Figure 4.9: Representation of temperature statistics for 1 line on the left and 16 lines on the right for different c values

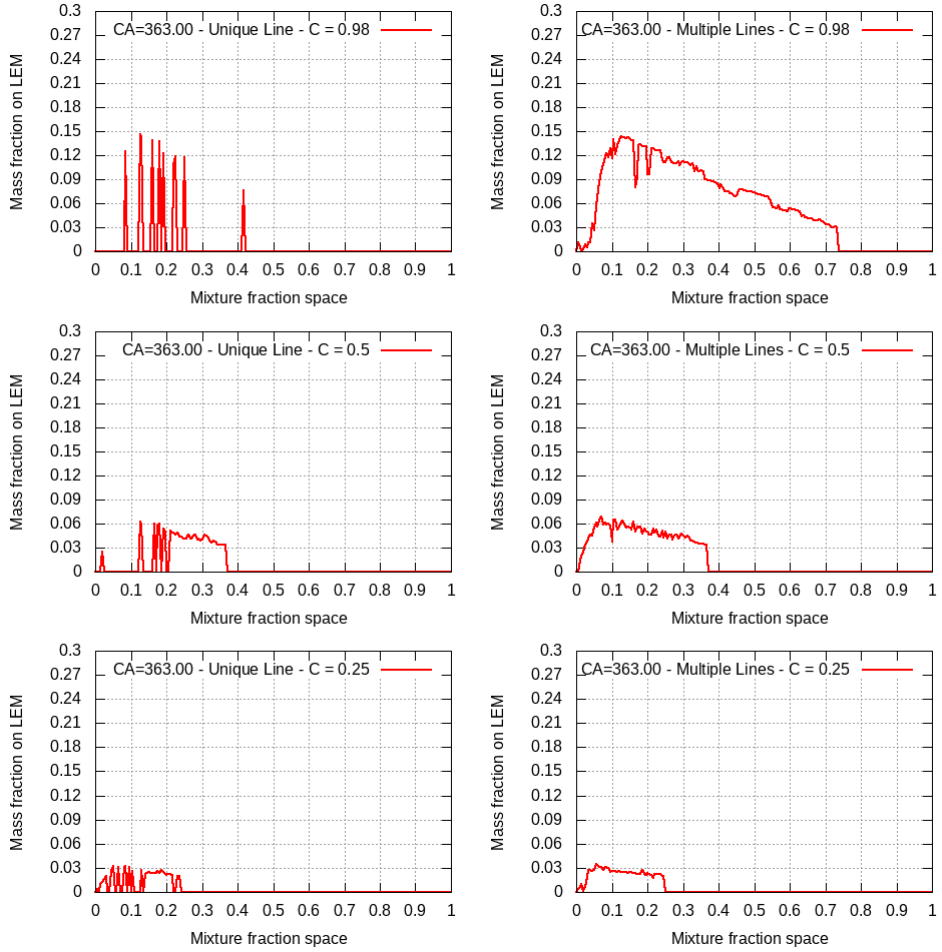


Figure 4.10: Representation of CO mass fraction statistics for 1 line on the left and 16 lines on the right for different c values

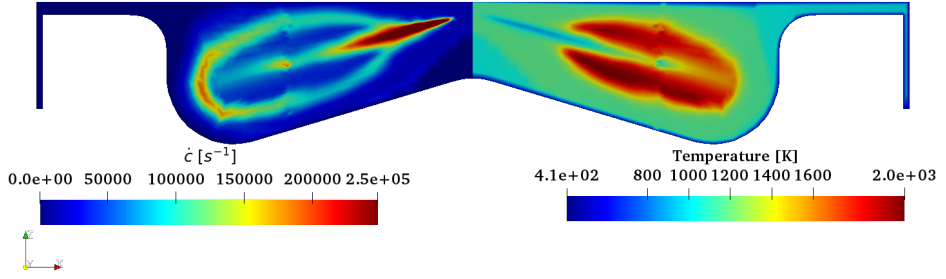


Figure 4.11: *mRILEMs* results with scaling all PDFs for $CAD = 359.00$. $\dot{c}$ term on the left and temperature on the right

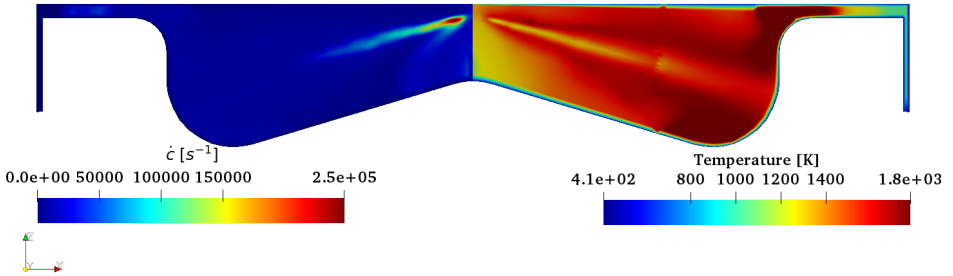


Figure 4.12: *mRILEMs* results with scaling all PDFs for $CAD = 363.00$. $\dot{c}$ term on the left and temperature on the right

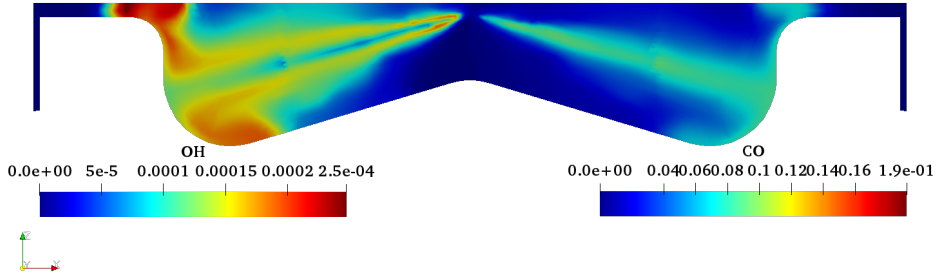


Figure 4.13: *mRILEMs* results with scaling all PDFs for $CAD = 363.00$. *CO* mass fraction on the left and *OH* mass fraction on the right

5 Conclusion and future work

The objective of this work was to use LEM as a mode and regime-independent combustion model for RANS simulations. Transport equations of continuity, momentum, energy, mean and variance of mixture fractions, and mean combustion progress variable are advanced using the open-source solver (OpenFOAM 2.2.5). Driving parameters such as pressure, fuel mass, vapor deposition length, and turbulence statistics are communicated from the CFD to the LEM, where the concurrent process of molecular diffusion, chemical reactions, and turbulence advection occurs. The pressure coupling of CFD-LEM enforces a constant pressure on the line, where maintaining the representative status of LEM in the CFD combustion chamber was ensured by combining the spherical geometry of LEM and the split operator strategy to enforce the CFD pressure while keeping the characteristic length of the line constant. Species mass fractions Y_s and the combustion progress variables source term $\dot{c}$ are conditioned on (Z, c) spaces. The mean values are calculated on the CFD using the probability density functions $\tilde{P}(Z)$ and $\tilde{P}(c)$ for $\tilde{Y}_s$. Temperatures on the CFD are iterated using the calorific equation of state by combining the solution of the total enthalpy equation $\tilde{h}$ and $\tilde{Y}_s$.

The results extracted from RILEM are examined by comparing them with the WSR and the experimental data. It has been noticed that the initialization of the solution tables has a significant impact on the CFD pressure trace, which is mainly due to the stochastic nature of the turbulent eddy events. Different configurations of solutions tables initialization have been analyzed. The approach that had the best result for an individual line was the combination of an interpolated solution table and scaling the PDFs of the progress variable source term while persisting the LEM time history. The recently developed mRILEMs approach using 16 LEM lines, persistence, and scaling of the PDFs has shown promising results with no required initialization of the turbulent scalar solution table. The CFD state was entirely updated from the LEM advancement, which has proven the utility of LEM as an accurate combustion model for ICEs.

Running internal combustion engines on hydrogen is one way to decrease its environmental effect since the emissions are mostly water if pure hydrogen is used as fuel. Running RILEM and mRILEMs on hydrogen can be tested and compared against simulation results of a truck compression ignition engine powered by hydrogen. [40]. The diffusion coefficients used in the LEM equations are mixed averaged, which allows us to detect the different effects of hydrogen as a main fuel due to its fast diffusive nature compared to other species. Investigations of differential diffusion effects are planned to be performed using RILEM and mRILEMs.

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Appended Publications I

Publication I

**Pressure Coupling Of the Spherical Linear Eddy Model
to RANS-CFD for Internal-Combustion Engine Simula-
tion.**

Pressure Coupling Of the Spherical Linear Eddy Model to RANS-CFD for Internal-Combustion Engine Simulation.

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Abstract – As a result of the increase of the use of combustion engines, more restrictive emission standards are applied. New combustion technologies are being constantly developed to enhance the internal combustion engine, this is motivated by overcoming issues that are relevant for both engine efficiency and the environmental aspects. To do that, turbulent combustion modelling is needed.

In this paper, an updated version of the Linear Eddy Model (LEM) will be presented. LEM is capable of simulating premixed, non-premixed and mixed mode combustion, and it is a regime independent model that runs under the assumption of finite-rate chemistry that is sensitive to turbulent chemistry interactions, which makes it suitable for prediction of pollutant formation. A New coupling scheme to the CFD-RANS simulation is proposed, the coupling is based on linking the two models via pressure. The benefits of pressure coupling are that the effects of wall heat losses and latent heat of evaporation that are modelled on the CFD side are an intrinsic part of the pressure term that is linking the two models, in contrast to volume coupling in which these relevant phenomena need supplementary modelling on the LEM side. The pressure coupling results in a radially uniform dilatation of the LEM domain reflecting the combined effects of pressure change, fuel addition, and cylinder volume change during the engine cycle. Consistency of the LEM cone volume and the CFD domain volume is maintained by adopting a split operator strategy involving a volume correction that adjusts the cone angle.

A Spherical Stand-Alone Linear Eddy Model (SSALEM) has been created to conduct relatively fast simplified code development and parameter studies. SSALEM input parameters were drawn from a WSR-RANS simulation and a 1D slider-crank model that calculates the combustion chamber volume that corresponds to a given crank-angle. Model results show the capability to physically track the evolution of several scalars that are solved on the LEM line such as temperature, fuel, and intermediate species in the combustion process.

Keywords: Linear Eddy Model – Pressure coupling – Stand Alone Model – Volume adaption

1. Introduction

Considering the increase in pollutant emissions due to the surge of the use of internal combustion engines, new combustion techniques such as homogeneous charge compression ignition (HCCI), reactivity control combustion ignition (RCCI) and high levels of exhaust gas recirculation (EGR) require further development. Turbulent combustion modelling is considered as a crucial tool for the development of these combustion techniques.

Several combustion models have been used and developed during the last years for classical usage such as gasoline combustion (premixed) or diesel combustion (non-premixed). They are typically limited to these two combustions. For example, flamelet models [1] assume the formation of laminar flame structures in a turbulent flow field, resulting in limited interaction between chemistry, molecular transport, and turbulence in the flamelet models because of the parametric coupling that these models are based on. The coupling in flamelet models depends on scalar dissipation rate for non-premixed cases and mean turbulent velocities for the premixed cases.

The Linear Eddy Model has been used a sub-grid model to overcome this limitation. It is a regime and mode independent model that is based on the statistical representation of flow time advancement along a physical line of sight represented by a

one-dimensional computational domain. Because LEM captures direct interactions between turbulent advection, diffusion, and chemical reactions, it can predict highly unsteady effects such as extinction and re-ignition without supplementary modelling. It can be used in different geometries (planar, cylindrical, or spherical) depending on the application case requirements. LEM can be coupled as a sub-grid model in several ways. It has been used in the context of LES simulations in the LES-LEM approach [2] which is a one-dimensional representation of the turbulent combustion process in every LES cell with spatial and temporal resolution comparable to direct numerical simulations. The disadvantage of the LES-LEM model is the computational cost of this high resolution.

In the context of this paper, one LEM line represents the entire combustion chamber, thereby greatly reducing the computational cost. A previous version of this formulation was termed RILEM [3], which stands for the representative interactive linear eddy model. In this model the coupling was done based on a volume constraint, which required supplementary modelling of the heat effects on the LEM side. However, in this paper, LEM will be presented in a one-way-coupled form in which the results of a WSR-RANS simulation supply the pressure time history to LEM but LEM does not provide chemical or other closure information to the CFD.

2. Mathematical Model

The Linear Eddy Model [4, 5] was proposed originally as a scalar mixing model for non-reactive flows. It was later extended to describe reactive flows. It consists of two main processes. The first process is the turbulent transport, represented by a stochastic sequence of independent eddy events. The second process time advances all other effects, which are diffusion, and chemical reactions in the present application. The Linear Eddy Model provides affordable full resolution of spatial and temporal scales by solving the reactive zero-Mach number equations on a one-dimensional line of sight.

2.1. LEM Diffusion and Chemical reactions

The LEM code is based on a pre-existing C++ implementation of One-Dimensional Turbulence (ODT) by David Lignell [4]. The ODT code offers certain features that are adopted in the LEM framework such as grid adaptation and a Lagrangian formulation of the balance equations for species mass fractions Y_s and enthalpy h . The balance equations are the following:

$$\rho \frac{DY_s}{Dt} = -\frac{dj_s}{dx} + M_s \dot{w}_s \quad (1)$$

$$\rho \frac{Dh}{Dt} = -\frac{dp}{dt} - \frac{dq}{dx} - \sum_s j_s \frac{dh_s}{dx} - \sum_s h_s M_s \dot{w}_s \quad (2)$$

ρ is density, j_s the species diffusion flux, M_s the species molar mass, p the pressure, q the heat flux, h_s the enthalpy of species s including the heat formation heat, and $\dot{w}_s$ the chemical source term. The temperature is calculated using the caloric equation of state.

$$h(T) = \Delta h_s^0 + \int_{T_0}^T c_{p,s}(T) dT \quad (3)$$

where Δh_s^0 is the standard heat of formation of species s and c_p , denotes the mass specific heat capacity at constant pressure. The continuity equation in the lagrangian formulation for the one-dimensional line is $\rho \Delta x = \text{const}$. The above-mentioned balance equations are solved using a second- order accurate scheme with central discretization.

of the diffusion terms. The chemistry solver that is used for chemical reactions is the CVODE package using the stiff chemical source integrator an implicit BDF Method. The chemistry is solved in parallel using open MP, where it is possible to specify the number of threads on which the chemistry will be solved.

2.2. LEM Turbulent Transport

The turbulence advection in LEM is represented by stochastic eddy events. An eddy event in the context of LEM is a so-called “Triplet Map.” This operation is a rearrangement of the scalars that constitute the state of each LEM cell. It mimics the effect of turbulent vortices. In addition to the usual LEM representation of the turbulent cascade, triplet maps are also used to represent large-scale fluid motions inside the combustion chamber.

2.2.1. Small Scale Turbulence

The triplet map process follows the presented steps: Once the eddy is decided to be implemented on a certain region of the line, that section of the line will be copied three times, the middle copy gets inverted, the three copies are then connected back with each other and finally the result is compressed back to the original length of the eddy. The described operation increases the gradient within the interval where the eddy happened similarly to the effect generated by the compressive strain in a turbulent flow.

Three quantities are needed to specify an eddy event, size of the eddy l , the eddy’s location and an eddy event time. In the LEM the eddy size is sampled from a prescribed size distribution. Assuming Kolmogorov inertial-range scaling [5], the eddy distribution is

$$f(l) = \frac{5}{3} \frac{l^{-8/3}}{\eta^{-5/3} - l_t^{-5/3}} \quad (4)$$

Using the turbulent Reynolds number

$$Re_t = \frac{u' l_t}{\nu} \quad (5)$$

where ν is the kinematic viscosity and u' is the root mean square velocity fluctuation, l_t the integral length scale, the Kolmogorov length scale η is determined from the inertial scaling law.

$$\eta = N_\eta L Re_t^{-\frac{3}{4}} \quad (6)$$

The mean number of eddy events per unit time per unit length of the 1D domain is

$$\lambda = \frac{54}{5} \frac{\nu Re}{C_\lambda l_t^3} \frac{(l_t/\eta)^{5/3} - 1}{1 - (\eta/l_t)^{4/3}} \quad (7)$$

where $C_\lambda = 15$ and $N_\eta = 10.76$ are model constants with values that can be found in the literature [6]. The turbulent diffusivity on the LEM line corresponds to

$$D_t = u' l_t / C_\lambda \quad (8)$$

Eddy locations, where location is nominally defined as the location of left boundary of an eddy, are randomly sampled from a uniform distribution of eddies over the line and the eddy time is sampled under the assumption of a Poisson process with a mean eddy occurrence time.

$$\Delta\tau_{Eddy} = (\lambda L)^{-1} \quad (9)$$

where L is the domain size. For boundary conditions other than periodic, sampled eddies that extend beyond the right boundary of the domain are not implemented.

2.2.2. Large Scale Turbulence

It is possible to implement large scale turbulence effects such as swirl and tumble on the LEM line, like what happens in the context of real engines. These effects are represented by big eddies that are introduced to the LEM line to obtain sufficient dispersion of fuel from the vapor deposition region to other regions of the domain. The big eddies respect a constant size which has been chosen to be equal to the half of the combustion chamber bore. Like the small eddies, big eddies are randomly sampled uniformly along the LEM line. A big-eddy time scale is calculated based on the exit velocity of the fuel v_n and engine cylinder length scale l_c using

$$\tau_{BigEddy} = \theta \frac{v_N}{l_c} \quad (10)$$

where θ is a mixing time constant that accounts for the effect of different geometries and flow conditions on the mixing. Previously and in this study, θ is set equal to unity. The number of the large eddies that would happen in the entire simulation is fixed at the beginning to be the time for one engine cycle divided by the big-eddy time scale and their occurrence times are independently sampled based on a uniform distribution of occurrence time during one engine cycle.

This sampling process of the large eddies is different from one used for the small eddies to avoid excessive cycle to cycle variability of the fuel dispersion process that can be created from significant cycle variability of the number of large eddies.

2.3. LEM Pressure Coupling

LEM and CFD can be coupled in two different ways: i) with volume coupling that was applied in the previous version [3] and ii) via pressure coupling which has been developed and implemented in the current project so far.

In the pressure based CFD-LEM coupling the pressures on the CFD and the LEM match while the volume can (and will) slightly deviate. This is achieved by imposing the CFD pressure on the LEM. The main advantage of the pressure coupling compared to the volume-based coupling is that relevant phenomena such as latent heat of evaporation and wall heat losses, which are modelled in detailed 3D geometry on the CFD side, are implicitly encoded into the pressure. The pressure coupling therefore allows consistent LEM treatment of those effects, which otherwise would require additional modelling on the LEM side.

2.4. Split Operator Strategy

In the pressure-based coupling we enforce a spatially constant LEM pressure matching the spatially averaged time dependent pressure of the CFD. This can be achieved in several different ways, here we adopt the following strategy which we call the split operator strategy:

1. Implementation of physical processes (fuel injection, combustion, diffusion, etc.) as constant volume processes in each LEM cell. This will lead to a change of pressure in each individual LEM cell.
2. Isentropic compression of each LEM cell to the target CFD pressure under the assumption of a fixed composition. This step will alter pressure, temperature, and density within each LEM cell.
3. Calculation of the total volume of the LEM domain.

4. Adjusting the cone-angle of the LEM domain with a prescribed length of the LEM domain to match the volume calculated in step 3.
5. Re-distribution of cell boundaries on the LEM domain.

In the following we describe some of the steps mentioned above in more detail.

2.4.1. LEM Volume Adjustment

As mentioned above, the LEM domain is a double cone. Therefore, the volume of the LEM domain can be adjusted by changing the length of the cone and/or the cone angle. Here we adjust the volume by changing the cone angle and keeping the length fixed. This is motivated by the assumption that the cone is oriented in direction of a spray jet and therefore, under this assumption the length of one LEM cone is limited by the distance between the injector and the cylinder walls.

If D denotes a characteristic length of the cylinder, e.g., the bore or the stroke, the cone angle α is given by:

$$\alpha = \arccos\left(1 - \frac{12V}{\pi D^3}\right) \quad (11)$$

where V_{LEM} is the total volume of the LEM line, which is known after step 3 of the split-operator approach. Since we know the volume of each individual LEM cell, the position of the cell faces on the LEM domain can be re-calculated.

2.4.2. Fuel deposition on the LEM line

Fuel injection is modelled in detail on the CFD side via the spray model. However, evaporated fuel on the CFD domain needs to be added to the LEM line which only represents the gas phase. For this, two main parameters are extracted from the CFD side to be imposed on the LEM to represent the fuel injection process: i) the evaporated fuel mass in one CFD time step and ii) the total volume of cells where fuel has been evaporated. In principle it would be possible to implement a spray model on the LEM line itself, however, it is easier and probably more consistent to use information from the CFD spray model. To have a consistent representation of quantities from the CFD to the LEM, a volume ratio between the CFD and LEM is defined as

$$Q = \frac{V_{LEM}}{V_{CFD}} \quad (12)$$

which is used to scale the vapor deposition volume between the CFD and the LEM.

Evaporated fuel on the LEM line is injected symmetrically relative to the meeting point of the two cones. The current fuel deposition strategy matches the total volume of the cells with and without evaporation on the CFD and the LEM side. On the CFD we evaluate the volume ratio of cells with evaporation to the total volume as

$$\beta = \frac{\sum V_{ev,i}}{V_{CFD}} \quad (13)$$

This ratio defines an initial guess of the volume and the associated radius R_{LEM}^{inj} around the center of the LEM domain over which fuel on the LEM line is injected. The actual fuel mass deposited in each cell depends on its volume based on

$$m_{ev,i}^{LEM} = m_{ev}^{CFD} \cdot Q \cdot \frac{V_{ev,i}^{LEM}}{\sum V_{ev,i}^{LEM}} \quad (14)$$

The implemented fuel deposition method does not guarantee that the fuel vapor mass in each cell stays below the saturation level. However, so far this has not been a problem in the simulations, but it is straightforward to extend the fuel deposition strategy to take local saturation levels into account.

After vapor deposition new values for density, mass-fractions, and temperature in each affected cell need to be updated applying a simple mixing process at constant volume (the volume of the LEM cell). For the new LEM cell density in cell i we have

$$\rho_{new,i} = \rho_{old,i} + \rho_{Fuel,i} \cdot \frac{V_{Fuel,i}}{V_{LEM,i}} \quad (15)$$

and for the updated mass-fractions

$$Y_{s,new,i} = \frac{Y_{s,old,i} \cdot m_{old} + Y_{s,add,i} \cdot m_{add}}{m_{old} + m_{add}} \quad (16)$$

The temperature of the mixture is calculated with a simplified mixing rule ignoring the difference in specific heats of the added fuel vapor and the mixture within the LEM cell:

$$T_{new} = \frac{T_{old} \cdot m_{old} + T_{Fuel} \cdot m_{Fuel}}{m_{old} + m_{Fuel}} \quad (17)$$

Due to the mixing process LEM cells with fuel injection have changed density, composition and temperature, therefore they have changed pressure as well. To have a constant pressure on the line we correct the pressure and adjust the LEM cell faces and the cone angle according to the split operator approach described above.

3. Spherical Stand-Alone Linear-Eddy Model (SSALEM)

A stand-alone engine LEM model has been created. The stand-alone model offers the following possibilities: simplified code development and validation, faster computation to enable many parameter variations, and modularity for easy coupling to any combustion CFD software.

The time-varying driving parameters for the LEM model (turbulence parameters, cylinder pressure traces and evaporated fuel mass deposition rate and penetration distance) can be provided by simple models or - as done here - with a separate CFD simulation based on the Well Stirred Reactor (WSR) in a pre-processing step. A standard 1D slider-crank model has been added to the stand alone LEM that calculates the volume of the combustion chamber as a function of the engine speed.

4. Results

4.1. Case Description : Volvo Heavy Duty Engine

The investigated case is a single cylinder of a Volvo 13L six-cylinder heavy-duty truck engine. It has a high-pressure fuel injector located in the centre of the top of the combustion chamber and a compression ratio of 15.8:1. The simulation was on a part load configuration with the following operating conditions initial pressure 1.69 bar, initial temperature 395 K, IMEP 7.08 bar, engine speed 1200 RPM, start of injection 3.1° bTDC, end of injection 3.3° aTDC, injected mass 13 mg, and initial gas composition by mass O₂ 16.5%, N₂ 75.3%, CO₂ 5.97%, H₂O 2.26%. The chemical mechanism that was used for this study is a reduced mechanism for n-dodecane combustion which involves 54 species and 256 chemical reactions [7].

4.2. Results

The input parameters for running the SSALEM were created by running a Well Stirred Reactor (WSR) RANS simulation of the case, which is based on Lib-ICE, which is a set of OpenFOAM libraries and solvers for internal combustion engines which is implemented by the ICE group at Politecnico di Milano. Once the inputs are generated, the SSALEM is simulated.

As described before, the stand-alone spherical LEM has been created to investigate different parameters on the LEM line for faster simulations. The possibility to represent the LEM line in physical space has also been added to the code, which

provided the ability to investigate in detail the different processes that modify the LEM physical state and geometrical structure. The aim of this simulation is to observe the output that SSALEM can provide.

To describe the evolution of the LEM line, the temperature and the n-dodecane mass fraction were chosen to represent the different states the LEM line is experiencing. The following two figures display the distribution of temperature, fuel mass fraction, and carbon monoxide mass fraction on the LEM line.

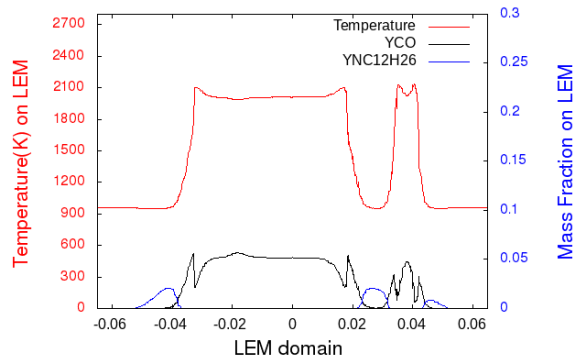


Fig 1: Snapshot of the LEM solution at CAD = 360.34

In Fig 1, the simulation has reached the crank-angle 360.34, It is seen that the LEM line is relatively combusted with the highest temperature on the line reaching $T_{LEM_{Max}} = 2100K$. It also appears that the fuel is decreasing which corresponds to the consumption of the fuel due to combustion.

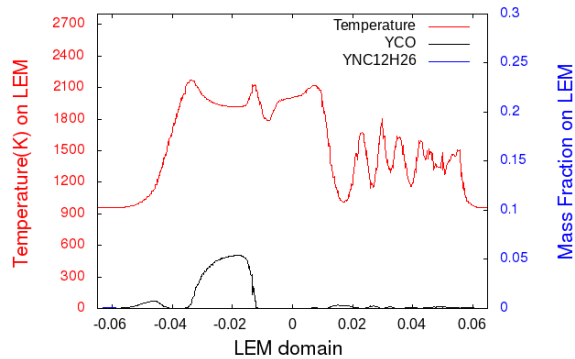


Fig 2: Physical representation of a developed LEM line CAD = 363.85

The combination of the small-scale turbulence, the large-scale turbulence, the diffusion, and the output of the chemistry solver resulted in the state of the LEM line represented above in Fig 2. The LEM representation tool provided the possibility to visually verify the state of the line. The split operator strategy appears to be working by maintaining the LEM length be equal to the combustion chamber bore diameter.

5. Conclusion

Based on the reported results, the pressure-coupled SSALEM can potentially be used as a combustion model by linking it to a CFD-RANS simulation, which is a promising strategy to explore. LEM's sensitivity to turbulence chemistry interactions potentially enables investigation and prediction of pollutant formation.

The development of the SSALEM is an important step in the construction of the pressure-coupled RANS-LEM thanks to its efficiency in code debugging and its clarity in displaying the important steps of the model's framework. It is also useful as a physical representation of the regime evolution along the one-dimensional line during the engine cycle, which can be used for parameter investigation.

LEM is to be coupled with CFD using a pressure constraint. The scalars that are solved on the SSALEM level will be conditionally based on a CFD-level model of the joint PDF of mixture fraction and progress variable. The conditioning will generate outputs that will be mapped to each CFD computational cell. Coupling the LEM with the CFD will result in a different link between the two solvers in terms of pressure than in SSALEM. In the current configuration pressure is pre-calculated using conventional CFD, while in the coupled scheme the pressure will be time advanced at the CFD level after each time interval of LEM advancement, resulting in interesting phenomena that will appear on both the CFD and the LEM sides. These phenomena are to be investigated in future work.

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