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

Super-grid Linear Eddy Model (SG-LEM)

Efficient mode- and regime-independent combustion closure for Large Eddy Simulation (LES)

ABHILASH M. MENON

Department of Mechanics and Maritime Sciences
Division of Combustion and Propulsion Systems
CHALMERS UNIVERSITY OF TECHNOLOGY

Gothenburg, Sweden 2022

Super-grid Linear Eddy Model (SG-LEM)
Efficient mode- and regime-independent combustion closure for Large Eddy Simulation (LES)
ABHILASH M. MENON

Department of Mechanics and Maritime Sciences
Division of Combustion and Propulsion Systems
Chalmers University of Technology
SE-412 96 Gothenburg
Sweden
Telephone: +46 (0)31-772 1419

Chalmers Reproservice
Gothenburg, Sweden 2022

Abstract

Next-generation combustion technology such as 'lean burn' and HCCI (Homogeneous Charge Compression Ignition) present new challenges for combustion modelling. The presence of locally varying combustion modes (premixed vs. non-premixed) and regimes (fast/non-fast chemistry vs. turbulent time scales) belie a need for combustion models that make few assumptions of the underlying combustion process and can also incorporate turbulent stirring. Lean burn for gas-turbines introduce complex ignition sequences and phenomena like blowout which requires both a finite-rate chemistry description as well as turbulence-chemistry-interaction for accurate modelling. Auto-ignition and differential-diffusion capabilities are also desirable features for modelling HCCI and hydrogen combustion, respectively. The Linear Eddy Model (LEM) is a mode- and regime-independent sub-grid combustion closure for Large Eddy Simulation (LES). LEM resolves, along a one-dimensional line, all spatial and temporal scales, provides on-the-fly local turbulent flame statistics, captures finite rate chemistry effects, and directly incorporates turbulence-chemistry interaction using stochastic processes. In LES-LEM an LEM-line is advanced in each LES cell which makes the approach computationally rather expensive.

In this thesis, a novel closure approach is presented using LEM which involves coarse-graining of the LES mesh to generate a coarse 'super-grid' comprised of 'super-cells'. Each super-cell, instead of each LES cell, then contains a single LEM line which advances the combined reaction-diffusion equations and also provides binned statistics for thermochemical scalars such as species mass fractions, the method is hence termed 'super-grid LES-LEM' or simply, 'SG-LEM'. Local LES filtered states are then obtained by probability-density-function (PDF) weighted integration of binned scalars, akin to standard presumed PDF approaches for reactive LES. The thesis also introduces a new 'splicing' scheme for the super-grid formulation where LES resolved flow information is accounted for via Lagrangian transport of LEM fragments between adjacent domains.

A pressure based solver was developed using the OpenFOAM library to test the proposed model with a premixed ethylene flame stabilized over a backward facing step, a setup for which DNS data is available for validation. The new model is able to produce LES-resolved flame structures and species mass fractions at a significantly lower cost than standard LES-LEM. Comparison with time-averaged reaction rates show good agreement with DNS data where the model is able to correctly capture regions of net production and consumption of highly sensitive OH. In general, SG-LEM is able to provide high fidelity reaction rate statistics with the compute efficiency of a mapping-type closure. The encouraging results and performance of SG-LEM indicate its suitability for industrial reacting simulations once full validation is complete. While it is yet unclear how the presented mapping strategy will cope with transient phenomena like extinction, it retains desirable features of LES-LEM and is able to report thermochemical scalars averaged over individual LEM domains for diagnosis.

Keywords: Large Eddy Simulation; Linear Eddy Model; Mapping-closure; Lagrangian splicing; Mesh coarse-graining

List of publications

This thesis consists of an extended summary and the following paper:

Paper 1 A. Menon, M. Oevermann, A. R. Kerstein "A super-grid approach for LES combustion closure using the Linear Eddy Model", submitted to *Combustion Theory and Modelling, Taylor & Francis.*

Acknowledgements

Firstly, I'd like to thank my supervisor Michael Oevermann for giving me this opportunity, his sincere and careful guidance contributed greatly to this work and allowed me to grow both professionally and academically during this time. A special thanks to Alan Kerstein for the spirited discussions we've had, for sharing his seemingly limitless ideas with our research group and for driving us to innovate and seek higher goals.

I couldn't ask for nicer colleagues than the ones the at the ECaPS division at Chalmers led by Lucien Koopmans, you all make this a great place to work indeed. Thank you, Nidal Doubiani for being a fantastic office-mate and for the many brainstorming sessions we've had by the whiteboard. Special thanks also to Henrik Ström who brought much needed perspective to our projects during our weekly meetings.

Funding for the project from the Swedish Research Council is gratefully acknowledged as is the compute resources provided by the Swedish National Infrastructure for Computing (SNIC).

Lastly, I'd like to thank my family for their unwavering support and encouragement, especially my mother Sushama who has been my rock through the best and worst of times. Life in Gothenburg is made immeasurably better by friends like Dani, Nick, Irena and Elin. Last but not least, thank you, Hanna for being my closest friend and an amazing partner.

Contents

Abstract i

List of publications iii

Acknowledgements v

I Extended Summary 1

1 Introduction 3
1.1 Reactive CFD . . . 3
1.1.1 Flow simulation . . . 3
1.1.2 Combustion modelling . . . 4
1.2 Challenges and motivation . . . 5
1.3 Objective . . . 6
1.4 Thesis outline . . . 6

2 Theory 7
2.1 The Linear Eddy Model (LEM) . . . 7
2.2 LEM as combustion model for LES . . . 8
2.3 Super-Grid LES-LEM . . . 9

3 Methodology and main findings 11

4 Concluding remarks 15
4.0.1 Future work . . . 15

Bibliography 17

II Appended papers 21

Part I
Extended Summary

1 Introduction

Humanity has harnessed combustion since time immemorial, it powers the modern world and finds use in sectors ranging from large-scale power generation, aviation and shipping to surface transport and domestic cooking. The use of fossil-fuel-driven combustion technology has, over time, had knock-on detrimental effects to human health and nature. These come by way of pollutants and climate change led by greenhouse gases such as CO_2 and has prompted a global response from governments to try and shift the socio-technical landscape of these activities to cleaner and safer standards. Emission norms for automobiles grow ever stricter on the limits for pollutants like CO and NO_x while there is increasing competition from electric cars. Similar trends are seen in aviation and shipping. These factors pressure traditional combustion technologies to continually innovate to remain competitive and in step with global sustainability commitments. In this vein, enormous research effort goes into improving fuel quality, after-treatment systems and design methodology for devices such as ICEs (Internal Combustion Engines) and gas-turbines. Combustion devices are often complex, requiring several years of design and testing by a highly a skilled workforce before entering production. Over the years, simulation methods have emerged as an invaluable tool in the design cycles for these devices. One such is reactive flow simulations using Computational Fluid Dynamics (CFD) and forms the background area of interest for this work. In a general sense, reactive CFD can be seen as a coupling of flow simulation with numerical chemistry computation. It allows engineers to design and test several aspects of a combustion device e.g. flow geometry that promotes mixing of air and fuel, the effect of various fuel blends on pollutant formation, flame instabilities and pressure rise due to combustion, to name a few.

1.1 Reactive CFD

1.1.1 Flow simulation

Simulation of turbulent flows entails the time-advancement of the Navier-Stokes equations on a computational mesh. These are essentially the conservation principles of mass and momentum written in an *Eulerian* framework. In addition to these, reactive CFD requires transport equations for energy as well as chemical species to be advanced. Direct Numerical Simulation (DNS) of Navier-Stokes requires resolving of the full range of turbulent scales and thus needs ultra-fine mesh- and time-resolutions. It is computationally intractable but for the simplest, low-Reynolds-number configurations. Practical CFD for engineering flows involves much larger domain sizes and high turbulence levels. Tractability is achieved by either: (1) time-averaging of the turbulent scales, a modelling paradigm known as RANS (Reynolds-averaged Navier-Stokes); or (2) spatial-filtering of the turbulent scales, classified as Large Eddy Simulation or LES. Each approach requires its own, very different, treatment of the unresolved turbulence information, the so called "closure problem". LES is often considered more reliable than RANS because it directly resolves large scale turbulent structures on the computational grid while *turbulence models* for the sub-grid-scale (SGS) closure are well tested in literature. The disadvantage being that LES requires

higher mesh-resolutions and longer computation times than RANS. Hybrid models also exist that utilize LES for wall boundary layers and RANS in the bulk flow.

The utility of reactive CFD within engineering design cycles like depends upon its ability to reliably model major combustion components such as: (1) the evaporation (or devolatilization) of fuels to their gaseous forms; (2) turbulent mixing of air and fuel; (3) molecular diffusion; (4) chemical reactions and heat release; (5) heat exchange between reacting gases and walls; and (6) sub-models that correctly mimic the nature of fuel sprays. The importance of each of these aspects can vary greatly depending on the type of fuel, combustion mode (i.e. premixed or non-premixed), propagation regime (e.g. laminar flames, wrinkled flames etc.), and lastly, on the desired level of output detail. It involves a large separation of scales as chemistry and diffusion (which determine flame structure) are molecular phenomena while turbulent transport is resolved at much larger *continuum* scales. The standard approach to combustion for CFD then involves careful selection of mode- and regime-appropriate combustion models which provide chemistry and flame structure information to the flow solver. Turbulence also plays a significant role in the combustion process and, via turbulence-chemistry interaction (TCI), creates transient behaviour like extinction and re-ignition. For ICEs, investigations have shown that the predictive capability of reactive CFD depends strongly on the handling of these nuanced interactions (see [1, 2]). LES has been found to be suitable for ICE simulations due the importance of large-scale flow structures and transient phenomena [3]. It is necessary also to model unsteady phenomena like blow-out or re-ignition in a gas turbine combustor (see [4, 5]) since RANS-based methods are more suited to mean stationary flows.

1.1.2 Combustion modelling

Combustion models determine *chemical closure* in reactive flow simulation i.e. they handle the chemical reactions and heat release at scales unresolved by the flow mesh. Combustion modelling typically starts with assumptions regarding: (1) chemical and turbulent time-scales, (2) the treatment of TCI, and (3) the combustion mode (premixed vs. non-premixed). Simple models like the Eddy Break-up Model (EBU) [6] assume *fast chemistry* and describes the combustion process purely by turbulent mixing. The turbulent mixing term utilizes a 'tuned' coefficient which is set using experimental or DNS data, it might also vary case-by-case depending on the experience of the simulation engineer/researcher. This approach cannot predict pollutants like CO which is an intermediate specie that requires a more complete *finite-rate* chemical description. In contrast, WSR (Well-stirred Reactor) neglects (sub-grid) turbulent mixing but describes finite-rate chemistry with as complex chemical reaction mechanisms as needed or as can be afforded computationally. It is often called a "no model" approach and cannot capture TCI unless used with a very fine mesh resolution leading to DNS in the limit of resolving all scales with the mesh. Finite-rate models require numerical integration of highly non-linear reaction rates over a given time-advancement, this can be a major compute expense depending on the level of detail used in the chemistry model, i.e. the number of chemical species and reactions. Those that can account for turbulent mixing, e.g. PaSR (Partially-stirred Reactor) [7] and EDC (Eddy Dissipation Concept) [8], also require tuned model coefficients to do so. More sophisticated models utilize a statistical description of turbulent reacting flow

through the use of probability density functions (PDFs). PDFs can be presumed to follow well described mathematical functions, as in the case of flamelet-based methods [9] or Conditional Moment Closure (CMC) [10]. A more involved alternative is to advance transport equations for the PDFs (termed TPDF) [11, 12] which has the advantage of an exact treatment of the chemical *source* term; turbulent mixing as well as diffusion, however, constitutes a significant modelling challenge [13] and TPDF is is computationally expensive as a whole. Linear Eddy Model (LEM) [14] is a stochastic sub-grid mixing and combustion closure which directly resolves flame structures in one-dimensional (1D) space. The models described so far can handle both premixed and non-premixed flames. Several models specialise to one or the other e.g. Bray-Moss-Libby (BML) [15] for premixed flames and RIF (Representative Interactive Flamelets) [16] for non-premixed.

Combustion models can be of a 'reaction-rate' or 'mapping' type. In the former, transport equations are advanced for every chemical specie with chemical source terms determined by reaction-rate models. EBU, EDC, WSR and PaSR fall in this category. The latter involves advancing transport equations for primitive scalars like *mixture fraction* (instead of each chemical species) from which thermochemical scalars are computed and 'mapped' onto the compute mesh. TPDF and RIF are examples of mapping-type closures. LEM has been implemented in both manners.

1.2 Challenges and motivation

The emergence of newer technologies like HCCI (Homogeneous Charge Compression Ignition), "lean burn" and MILD (Moderate or Intense Low-oxygen Dilution) combustion brings new modelling challenges. They can operate either in the "middle-ground" of partially-premixed conditions, and/or across a wide range of propagation regime, sometimes combined with *auto-ignition*. Hydrogen is now being explored as a fossil-fuel alternative for transport and in steel production which brings its own modelling challenges. Its high diffusivity, via differential diffusion effects, contributes to, e.g., elevated burning temperatures, combustion instabilities and the formation of NO_x, a temperature-sensitive pollutant. Given this background, an ideal combustion model for next-generation devices can be imagined as having the qualities of: (1) mode-independence i.e. it does not assume a premixed or non-premixed nature of the flame; (2) propagation-regime-independence i.e. it does not require assumptions on the chemical time scales relative to turbulent time scales; (3) differential diffusion capability for fuels like H_2; and (4) computationally efficiency for use in industrial simulations.

These combined goals are not straightforward to achieve. Of the models listed above, LEM and TPDF make fewer assumptions combustion process and is quite general in nature. Notably, LEM is the most mode- and regime-independent of the available approaches. Both approaches use stochastic processes for turbulent micro-mixing. In TPDF, transport equations for high-dimensional PDFs are recast as stochastic differential equations for notional particles for tractability. Stochastic micro-mixing models like Modified Curl [17] and Euclidean Minimum Spanning Tree [18] work on these virtual particles unlike LEM which resolves the flame structure (spatially and temporally) in 1D-space and directly incorporates turbulent micro-mixing. The formulation of LEM, which will be discussed in

Part II, represents micro-mixing as a series of length-scale-breakdown operations governed by established scaling laws for isotropic turbulence. It does not need tuned coefficients to reflect the flame-propagation regime. A key difference between LEM and standard PDF models is that molecular diffusion is *not* modelled and LEM and is instead resolved in physical 1D space. This allows a straightforward consideration of differential diffusion for fuels like H_2. However, three dimensional combustion phenomena, e.g. driven by curvature effects, are not captured by LEM and would require additional modeling on the one-dimensional line.

1.3 Objective

LEM forms the backbone of this work. It has been used previously as combustion closure for LES[19–22], a strategy termed LES-LEM, where each LES cell contains a highly resolved 1D LEM-line that independently evolves reaction-diffusion equations. It is, however, an expensive model for reasons which shall be discussed in section 2.2. We present a novel closure LES-LEM method which uses coarse-meshing procedures applied to the CFD mesh in order to implement a multi-scale combustion closure. The coarse-level mesh, or 'super-grid', led to this method being called 'super-grid LES-LEM' or simply, 'SG-LEM'. The primary goal of SG-LEM is computational speed-up of LES-LEM while preserving the benefits of LEM (i.e. mode- and regime-independence; fully resolved flame-structures, diffusion and turbulent mixing) while also preserving the 'in situ' nature of LES-LEM closure derived from 'splicing', a key component that communicates advection information between the LEM and LES levels (c.f. section 2.2) . Apart from computational speed-up, SG-LEM is generally guided by the dual goals of: (1) accurate, LES-resolved flame structures production; and (2) predictive thermochemical statistics.

The objective of this work is then to describe, implement and test the SG-LEM methodology for turbulent combustion using LES.

1.4 Thesis outline

This thesis consists of two parts: Part I is an extended summary of the concepts that contextualize the appended paper in Part II, which then contains the full mathematical description of SG-LEM and also presents results for a premixed ethylene-air flame test case along with comparisons made to DNS data for the same.

2 Theory

2.1 The Linear Eddy Model (LEM)

From the theory of turbulent flows comes the idea of *Homogeneous isotropic turbulence* (HIT), an ideal state where turbulent fluctuations are statistically uniform in all directions. This is a useful assumption in turbulence modelling wherein HIT is assumed within every CFD finite volume (or cell). It stands to reason then that turbulent mixing of a passive scalar, say a dye, within each cell would also lead to a statistically uniform distribution of said scalar i.e. the distributions along any line-of-sight is statistically independent of its orientation. This is the justification for the Linear Eddy Model (LEM) which was first introduced as a 1D mixing model for non-reactive scalars [14] and then later extended to reacting mixtures [23]. Owing to its 1D nature, a 'DNS-like' resolution can be used to advance reaction-diffusion equations affordably. The 1D domain used for this is called an 'LEM line' consisting of 'LEM cells' or 'wafers'. The effect of turbulent mixing is approximated using stochastic re-arrangements called 'triplet maps', each of which mimic the effect of a turbulent eddy on the 1D line, illustrated in Fig. 2.1. An eddy interval is represented by its lower boundary x_0 and its length l. The position, size and timing of triplet maps are stochastic in nature. Here, x_0 is sampled from a uniform distribution i.e. it can occur anywhere within the bounds of the LEM line, while l is sampled from a size distribution (or PDF) which is derived from established inertial range scaling laws of three dimensional turbulence [24, 25]. The timing of the eddy event is sampled from a *Poisson* process with a mean value that reflects the turbulent Reynolds number Re_t.

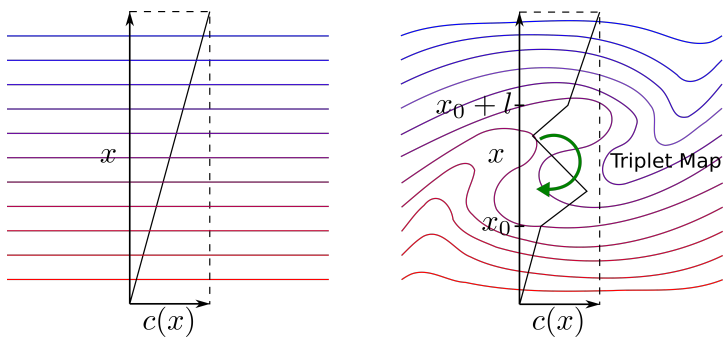

Figure 2.1: *Triplet map approximates the stirring effect of a single turnover of an isotropic turbulent eddy; the coloured lines are concentration isopleths for a scalar; the figure on the left represents a scalar gradient where the straight line shows concentration.*

Stochastic triplet maps are how LEM incorporates TCI into its formulation. Consider the 1D premixed flame in Fig. 2.2 which propagates from right to left. Reaction-diffusion advancement without turbulence gives a laminar flame (dashed blue curves) while the stirring action of turbulence, effected by triplet maps, mimics a turbulent flame front (black curves). Mixing increases scalar gradients and promotes diffusion of species as well

as temperature. This increases flame speeds while also decreasing peak flame temperature and affects chemical advancement in complex ways. Reaction-diffusion advance is usually implemented in segregated manner. In this work, a second order finite difference scheme with implicit time marching is used to advance diffusion. An LEM cell effectively acts as an individual reactor capable of finite-rate chemistry which, as mentioned before, requires the use numerical integration of reaction-rates over each LEM advancement - for *every* LEM cell. Hence, LEM can be an expensive method for CFD combustion closure.

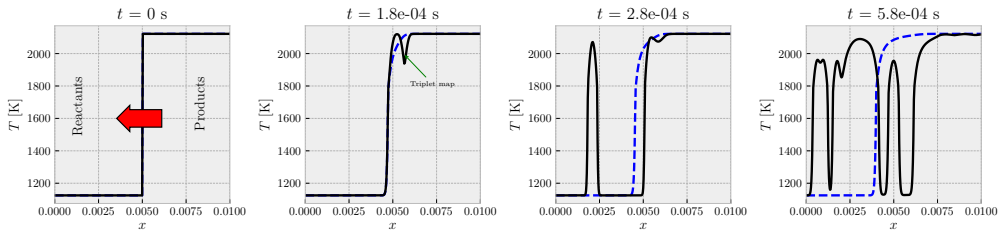

Figure 2.2: *LEM advancement of a premixed flame. Dashed blue curves: laminar flame; black curves:* $Re_t = 500$.

2.2 LEM as combustion model for LES

As mentioned before, in LES-LEM, each LES cell contains a highly resolved 1D LEM-line that independently evolves reaction-diffusion equations. Coupling procedures relay flame information between the LEM and LES levels i.e. LEM lines provide *on-the-fly* chemical closure for each LES cell. The advection (or geometry-driven flow) information is communicated to the LEM level through a Lagrangian splicing algorithm, this promotes a locally-relevant, *in-situ*, nature to the closure. Splicing involves transporting LEM fragments from one LEM line to another in a manner that reflects the fluxes resolved by the LES mesh: the lengths of spliced fragments are determined by the flux magnitude and so is the order. Splicing order is guided by the principle that LEM fragments corresponding to higher fluxes must be displaced by greater amounts for a given time step. Fig. 2.3 demonstrates flux ordered splicing, it shows four LEM lines within their respective finite volumes before and after splicing. Note that partial LEM cells can also be spliced, contrary to what might be indicated in the figure. This splicing step is applied after each CFD flow advancement.

LES assumes HIT-conditions at the sub-grid level and hence there is a consistency in the modelling assumptions of LES-LEM between the grid and sub-grid levels. The benefits of using LEM as sub-grid closure for LES come with some drawbacks, the chief of which is computation time. This stems from three main factors:

1. Chemistry has to be advanced for each LEM cell individually, typically this means 5 to 10 chemistry integrations per LES cell as each one provides a finite-rate description of the combustion process.

2. Each triplet-map requires chemistry integration to be interrupted, each re-start of the numerical integrator is a computational overhead. This means that high Reynold's number flows (i.e. more frequent triplet maps) can quickly become cumbersome to simulate with LES-LEM.

3. Lagrangian splicing overheads can be a significant, especially when LEM fragments have to be sent across processor domains when computing with an HPC (High Performance Cluster). Splicing also introduces artefacts in the form of sharp discontinuities on the LEM line, frequent splicing implies that it could become the dominant mode of turbulent mixing over triplet-maps. This effect, however, has not been quantified in previous studies.

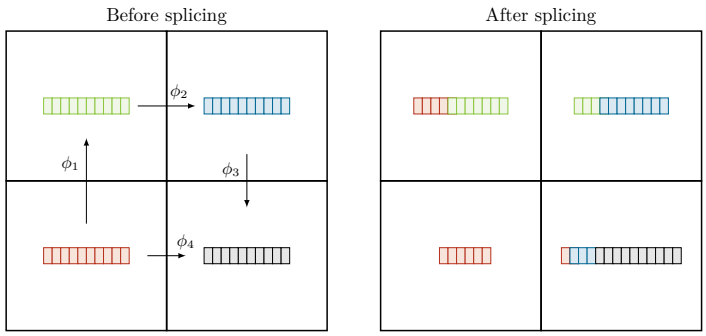

Figure 2.3: *Schematic showing flux ordered splicing; arrows of different length indicate unequal fluxes between finite volumes.*

2.3 Super-Grid LES-LEM

This work explores a novel approach to LES-LEM combustion closure which addresses the points above. A key innovation being the use of mesh coarse-graining procedures applied to the LES mesh. The super-grid consists of cell-clusters, each of which contains a single LEM line (instead of each LES cell) and hence leading to a scaling down of the total number of LEM lines in the computational domain. The new approach, SG-LEM, requires an updated splicing algorithm to accommodate cell-clustering.
The coupling between the LEM and LES tiers has to be modified as well - in standard LES-LEM, coupling is done by averaging thermochemical information over individual LEM lines within each LES cell whereas for the new variant, a method which can distribute combustion information among the cells of each super-cell is needed. A mapping type-closure was developed based on RILEM (Representative Interactive Linear Eddy Model) [26, 27] was developed to achieve this. Here, each LEM line (for each super-cell) provides conditionally averaged flame statistics to determine thermochemical scalars for individual LES cells via PDF weighted integration, akin to standard flamelet-based models or RIF. Fig. 2.5 shows mass fractions conditioned on reaction progress variable c for the 1D flame

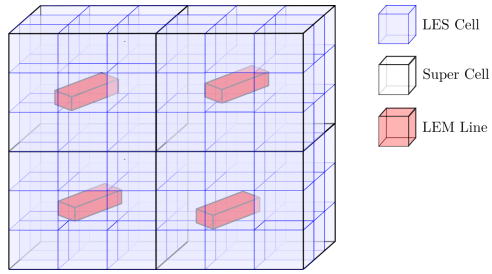

Figure 2.4: *Schematic representation of SG-LEM.*

shown above. Conditioning variables in the original RILEM closure [26] include mixture fraction Z as well as reaction progress variable c, as it was intended for non-premixed flames in ICE simulation. Presumed β- and δ-PDFs are used for Z and c respectively, again similar to RIF or flamelet-based models. This approach is modified for premixed flames by omitting Z altogether and opting for β-PDFs for c.

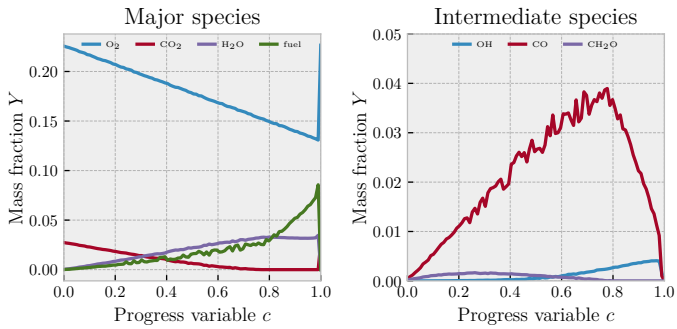

Figure 2.5: *Mass fractions conditionally averaged on progress variable c, from LEM advancement shown in Fig. 2.2.*

The PDF shapes are determined by the first and second moments of Z and/or c at each CFD cell. The first moment (mean i.e. $\widetilde{Z}$ and/or $\widetilde{c}$) is arrived at by advancing its transport equation whereas an algebraic method can be used for the second moment (variance i.e. $\widetilde{Z''^2}$ and/or $\widetilde{c''^2}$). These moments vary from CFD cell to cell whereas the LEM-derived binned statistics vary at the super-grid level. Combined, these lead to an LEM-driven local combustion closure that is local, *on-the-fly* and more efficient than standard LES-LEM. It is important to note that the SG-LEM does not lead to a loss of resolution on the LEM level - they still resolve all scales.

3 Methodology and main findings

A pressure based SG-LEM solver was implemented using the *OpenFOAM* library (v. 2.3.1) [28] based on *reactingFoam*, a standard reaction-rate-type solver that had to be modified for the presented model. Validation was performed using a recirculation-stabilized, premixed, ethylene setup for which some DNS data is available. The statistically stationary nature of the flame was beneficial as SG-LEM depends on conditionally averaged data which is gathered over time. At this early stage it is desirable to test the coupling algorithm without the added complication of transient effects like extinction, even though LEM does not have such limitations by itself. The setup for the test case is shown in Fig. 3.1, a premixed ethylene-air mixture with an equivalence ratio 0.42 at 1125 K is introduced into the domain with a bulk velocity of 220 ms^{-1}.

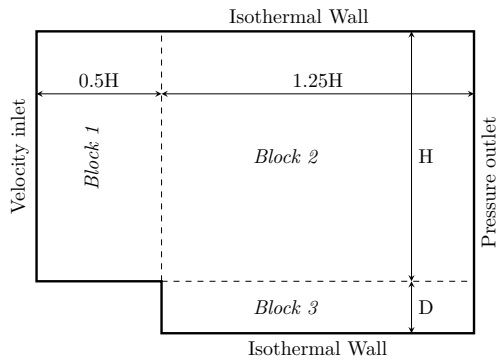

Figure 3.1: *Test case setup.*

The recirculation flow structure and high inlet velocity is also a good test for the splicing algorithm, a feature of this setup is that the flame remains nearly parallel to the step due to the balance of high inlet velocity and dilatation due to combustion. Time averaged DNS data from Aditya et. al. [29] is used to compare results and validate chemistry. The main findings of the investigation w.r.t. the objectives in section 1.3 are listed here:

1. SG-LEM is able to correctly predict the overall flame characteristics of the setup and maintain the recirculation-stabilized structure for several flow through times.

2. RILEM-closure can provide LES resolved flame structures despite binned flame statistics from the coarse level super-grid (see Fig. 3.2). Chemistry output, including production rates of pollutants, can be reported on the super-grid level which and is a direct representation of LEM chemistry advancement.

3. RILEM-closure using presume β-PDFs is able to map major species reasonably well between the LEM and LES levels but radical OH does show some artefacts of the super-grid.

4. Computational speed-up is significant compared to standard LES-LEM (see Fig. 3.3), for the parameters tested in the investigation it can even outperform standard

reaction rate models like PaSR and is likely competitive with other mapping-type closures like RIF. Performance does improve with larger super-grid cell sizes up till a point, beyond this other compute steps like online PDF-generation and flow advancement take precedence.

5. Tests do show some sensitivity to the coarse-graining parameters, for very large super-cell sizes the performance improvement is not proportionate and the reduced resolution of chemistry output is not beneficial. The ideal cluster-size seems to be case dependent, cases with complex features would benefit from smaller super-grid sizes.

6. Comparison with time averaged DNS reaction rates shows strong agreement for regions near the step and far downstream, the transition region between the two is not entirely captured which needs further investigation. Nevertheless SG-LEM is able to provide high fidelity chemical statistics at very low cost compared to standard LES-LEM.

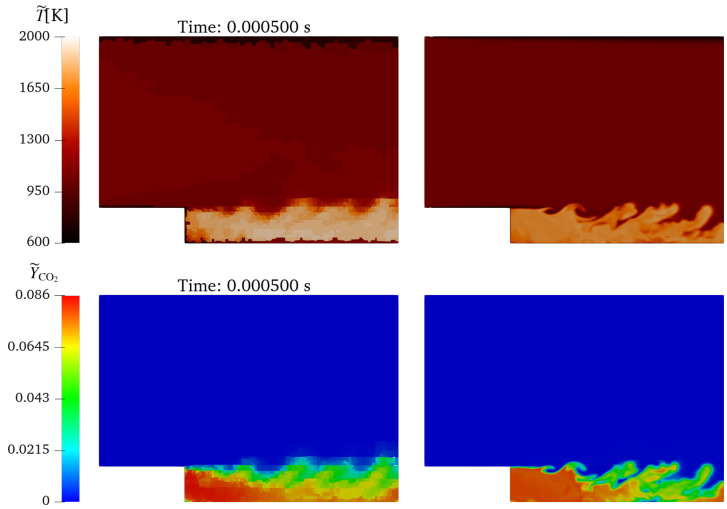

Figure 3.2: *Left: a snapshot of scalars averaged on individual LEM lines; right: LES-filtered results derived from RILEM-closure.*

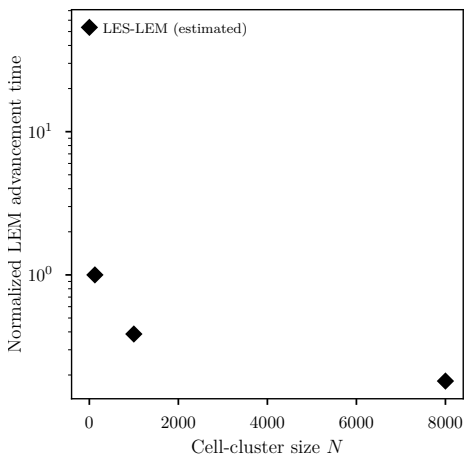

Figure 3.3: *Compute times (normalized) for LEM advancement for the test case - data for the three super-grid simulations was recorded from complete runs while the LES-LEM time was estimated from a partial run.*

4 Concluding remarks

The investigation using a canonical premixed flame test case shows that in an important sense, the main goals of SG-LEM has been achieved. As a mapping-type closure method it is able to fulfill the dual goal of high resolution flame structures as well as thermochemical information. The sparse-level chemistry output in the form of reaction rates is an added bonus. It is able to retain the main benefits of LEM i.e. fully resolved flame structures and diffusion processes with turbulent mixing, all while significantly reducing computational cost w.r.t. standard LES-LEM closure, which makes makes this an attractive combustion model for industry.

4.0.1 Future work

While the investigation shows promising results for SG-LEM, it is still some ways off from concluding fully validated chemical closure w.r.t. DNS results. The issues seem to stem from deficiencies in the LES setup as the spatial evolution of reaction rates do not exactly match the time averaged DNS results for regions affected by recirculation. Possible fixes may include a more refined mesh, more rigorous treatment of inlet conditions or even the use of wall model for LES. Further investigation is planned for when DNS data is made available so that these issues may be addressed in a follow-up publication. It is also unclear how well RILEM-closure will cope with transient effects like extinction and re-ignition even if such effects are present at the LEM level.

The current and upcoming investigations focus on premixed flames but, since LEM is mode-independent and RILEM-closure was originally developed for non-premixed (or partially-premixed) flames, it stands to reason that SG-LEM must be tested with a canonical non-premixed flame which can be validated against DNS or experimental data. The successful completion of this step would then merit SG-LEM the claim of being a first-of-its-kind high efficiency mapping-type closure for LES which can also provide spatial reaction-rate diagnostics at a sparse mesh level.

Bibliography

[1] J. Janicka and A. Sadiki. "Large eddy simulation of turbulent combustion systems". In: *Proceedings of the Combustion Institute* 30.1 (2005), pp. 537–547. ISSN: 1540-7489. DOI: https://doi.org/10.1016/j.proci.2004.08.279.

[2] Heinz Pitsch. "LARGE-EDDY SIMULATION OF TURBULENT COMBUSTION". In: *Annual Review of Fluid Mechanics* 38.1 (2006), pp. 453–482. DOI: 10.1146/annurev.fluid.38.050304.092133. eprint: https://doi.org/10.1146/annurev.fluid.38.050304.092133. URL: https://doi.org/10.1146/annurev.fluid.38.050304.092133.

[3] C J Rutland. "Large-eddy simulations for internal combustion engines – a review". In: *International Journal of Engine Research* 12.5 (2011), pp. 421–451. DOI: 10.1177/1468087411407248. eprint: https://doi.org/10.1177/1468087411407248. URL: https://doi.org/10.1177/1468087411407248.

[4] M. Boileau et al. "LES of an ignition sequence in a gas turbine engine". In: *Combustion and Flame* 154.1 (2008), pp. 2–22. ISSN: 0010-2180. DOI: https://doi.org/10.1016/j.combustflame.2008.02.006. URL: https://www.sciencedirect.com/science/article/pii/S0010218008000497.

[5] L.Y.M. Gicquel, G. Staffelbach, and T. Poinsot. "Large Eddy Simulations of gaseous flames in gas turbine combustion chambers". In: *Progress in Energy and Combustion Science* 38.6 (2012), pp. 782–817. ISSN: 0360-1285. DOI: https://doi.org/10.1016/j.pecs.2012.04.004. URL: https://www.sciencedirect.com/science/article/pii/S0360128512000366.

[6] D.B. Spalding. "Mixing and chemical reaction in steady confined turbulent flames". In: *Symposium (International) on Combustion* 13.1 (1971). Thirteenth symposium (International) on Combustion, pp. 649–657. ISSN: 0082-0784. DOI: https://doi.org/10.1016/S0082-0784(71)80067-X. URL: https://www.sciencedirect.com/science/article/pii/S008207847180067X.

[7] J Chomiak. *Combustion A Study in theory, fact and application*. Jan. 1990. URL: https://www.osti.gov/biblio/5894595.

[8] B.F. Magnussen and B.H. Hjertager. "On mathematical modeling of turbulent combustion with special emphasis on soot formation and combustion". In: *Symposium (International) on Combustion* 16.1 (1977), pp. 719–729. ISSN: 0082-0784. DOI: https://doi.org/10.1016/S0082-0784(77)80366-4. URL: https://www.sciencedirect.com/science/article/pii/S0082078477803664.

[9] N. Peters. "Laminar diffusion flamelet models in non-premixed turbulent combustion". In: *Progress in Energy and Combustion Science* 10.3 (1984), pp. 319–339. ISSN: 0360-1285. DOI: https://doi.org/10.1016/0360-1285(84)90114-X.

[10] A.Y. Klimenko and R.W. Bilger. "Conditional moment closure for turbulent combustion". In: *Progress in Energy and Combustion Science* 25.6 (1999), pp. 595–687.

ISSN: 0360-1285. DOI: https://doi.org/10.1016/S0360-1285(99)00006-4. URL: https://www.sciencedirect.com/science/article/pii/S0360128599000064.

[11] D.C. Haworth. "Progress in probability density function methods for turbulent reacting flows". In: *Progress in Energy and Combustion Science* 36.2 (2010), pp. 168–259. ISSN: 0360-1285. DOI: https://doi.org/10.1016/j.pecs.2009.09.003. URL: https://www.sciencedirect.com/science/article/pii/S036012850900046X.

[12] S.B. Pope. "PDF methods for turbulent reactive flows". In: *Progress in Energy and Combustion Science* 11.2 (1985), pp. 119–192. ISSN: 0360-1285. DOI: https://doi.org/10.1016/0360-1285(85)90002-4. URL: https://www.sciencedirect.com/science/article/pii/0360128585900024.

[13] Alex Krisman et al. "A DNS evaluation of mixing models for transported PDF modelling of turbulent nonpremixed flames". In: *Combustion and Flame* 161.8 (2014), pp. 2085–2106. ISSN: 0010-2180. DOI: https://doi.org/10.1016/j.combustflame.2014.01.009. URL: https://www.sciencedirect.com/science/article/pii/S0010218014000145.

[14] Alan R. Kerstein. "A Linear-Eddy Model of Turbulent Scalar Transport and Mixing". In: *Combustion Science and Technology* 60.4-6 (1988), pp. 391–421.

[15] Kenneth Noel Corbett Bray, Paul A. Libby, and J. B. Moss. "Unified modeling approach for premixed turbulent combustion—Part I: General formulation". In: *Combustion and Flame* 61 (1985), pp. 87–102.

[16] C. Hasse, H. Barths, and N. Peters. "Modelling the effect of split injections in diesel engines using representative interactive flamelets". In: *SAE Technical Papers* (1999). DOI: 10.4271/1999-01-3547.

[17] Rane L Curl. "Dispersed phase mixing: I. Theory and effects in simple reactors". In: *AIChE journal* 9.2 (1963), pp. 175–181.

[18] S. Subramaniam and S.B. Pope. "A mixing model for turbulent reactive flows based on Euclidean minimum spanning trees". In: *Combustion and Flame* 115.4 (1998), pp. 487–514. ISSN: 0010-2180. DOI: https://doi.org/10.1016/S0010-2180(98)00023-6. URL: https://www.sciencedirect.com/science/article/pii/S0010218098000236.

[19] Patrick A McMurthy, Suresh Menon, and Alan R Kerstein. "A linear eddy sub-grid model for turbulent reacting flows: Application to hydrogen-air combustion". In: *Symposium (International) on Combustion*. Vol. 24. 1. Elsevier. 1992, pp. 271–278.

[20] Vaidyanathan Sankaran and Suresh Menon. "Structure of premixed turbulent flames in the thin-reaction-zones regime". In: *Proceedings of the Combustion Institute* 28.1 (2000), pp. 203–209. DOI: 10.1016/S0082-0784(00)80212-X.

[21] Salman Arshad. "Large eddy simulation of combustion using linear-eddy subgrid modeling". PhD thesis. Gothenburg, Sweden: Chalmers Tekniska Högskola, 2019.

[22] Esteban Gonzalez et al. "Effect of the turbulence modeling in large-eddy simulations of nonpremixed flames undergoing extinction and reignition". In: *55th AIAA Aerospace Sciences Meeting*. 2017. DOI: 10.2514/6.2017-0604. eprint: https://arc.aiaa.org/doi/pdf/10.2514/6.2017-0604. URL: https://arc.aiaa.org/doi/abs/10.2514/6.2017-0604.

[23] Alan R. Kerstein. “Linear-Eddy Modeling of turbulent transport. Part 4. Structure of diffusion flames”. In: *Combustion Science and Technology* 81.1-3 (1992), pp. 75–96.

[24] A.R. Kerstein. “Linear-eddy modelling of turbulent transport. Part 6. Microstructure of diffusive scalar mixing fields”. In: *Journal of Fluid Mechanics* 231 (1991). cited By 211, pp. 361–394. DOI: 10.1017/S0022112091003439.

[25] Suresh Menon and Alan R. Kerstein. “The Linear-Eddy Model”. In: *Turbulent Combustion Modeling: Advances, New Trends and Perspectves*. Ed. by Tarek Echekki and Epaminondas Mastorakos. Springer Netherlands, 2011, pp. 221–247. ISBN: 978-94-007-0412-1.

[26] Tim Lackmann et al. “Investigation of turbulence–chemistry interactions in a heavy-duty diesel engine with a representative interactive linear eddy model”. In: *International Journal of Engine Research* 21.8 (Dec. 2018), pp. 1469–1479.

[27] Tim Lackmann, Alan R. Kerstein, and Michael Oevermann. “A representative linear eddy model for simulating spray combustion in engines (RILEM)”. In: *Combustion and Flame* 193 (2018), pp. 1–15. ISSN: 0010-2180.

[28] H. G. Weller et al. “A tensorial approach to computational continuum mechanics using object-oriented techniques”. In: *Computers in Physics* 12.6 (1998), p. 620. DOI: 10.1063/1.168744. URL: https://doi.org/10.1063/1.168744.

[29] Konduri Aditya, Hemanth Kolla, and Jacqueline H Chen. “DNS of a Turbulent Premixed Flame Stabilized over a Backward Facing Step”. In: *11th US National Combustion Meeting*. 2019.

Abbreviations

1D one-dimensional

CFD Computational Fluid Dynamics

DNS Direct Numerical Simulation

EBU Eddy Break-Up (model)

EDC Eddy Dissipation Concept

HCCI Homogeneous Charge Compression Ignition

ICE Internal Combustion Engine

LEM Linear Eddy Model

LES Large Eddy Simulation

PaSR Partially-stirred reactor

RANS Reynolds-Averaged Navier-Stokes

RILEM Representative Interactive Linear Eddy Model

SGS Sub-grid-scale(s)

TCI Turbulence-Chemistry Interaction

TPDF Transported Probability Density Function

WSR Well-Stirred Reactor