Pareto-efficient combustion modeling for improved CO-emission prediction in LES of a piloted turbulent dimethyl ether jet flame

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Abstract

This study extends the Pareto-efficient combustion (PEC) framework to adaptive LES combustion simulations of turbulent flames. With the focus on improving predictions of CO emissions, PEC is employed to augment a flamelet/progress variable (FPV) model through local sub-model assignment of a finite-rate chemistry (FRC) model. A series of LES-PEC calculations are performed on a piloted partially-premixed dimethyl ether flame (DME-D), using a combination of FPV and FRC models. The drift term is utilized in the PEC framework to estimate the model error for quantities of interest. The PEC approach is demonstrated to be capable of significantly improving the prediction of CO emissions compared to a monolithic FPV simulation. The improved accuracy is achieved by enriching the FPV model with FRC in regions where the low-order model is determined insufficient through the evaluation of the drift term. The computational cost is reduced by a factor of two in comparison to the full finite-rate calculation, while maintaining the same level of accuracy for CO predictions.

Keywords: Pareto-efficient combustion framework; Adaptive combustion modeling; Dimethyl ether; Large-eddy simulation; Turbulent combustion

1. Introduction

Turbulent reacting flows involve complex physico-chemical processes that cover a wide range of time and length scales. The chemical conversion of a large number of species together with the rich flow structures pose significant challenges to numerical modeling and simulations. Several combustion modeling approaches have been developed to avoid the direct evaluation of the detailed reaction chemistry by using low-dimensional manifold representations [1]. Through these models, the high-dimensional thermo-chemical state space can be parameterized by a reduced set of scalars.

Based on the manifold abstraction, the Pareto-efficient combustion (PEC) framework [2] was developed, which allows the usage of detailed
description of the combustion chemistry in limited regions where it is necessary, while avoiding the concomitant overhead in regions where low-cost approaches, such as flamelet-type models [3–5], are deemed sufficient. PEC is formulated to require minimal user input, consisting of (i) a set of candidate combustion models that can be described by the manifold abstraction, (ii) a set of quantities of interest (QoI), denoted by \( Q \), such as emissions of CO, and (iii) a weighting coefficient, denoted by \( \lambda \), to balance computational cost and desirable model accuracy. The PEC approach differs from the dynamic adaptive chemistry (DAC) [6–8] in its more general adaptation capability beyond the extent of chemical manifolds. Thus, PEC has the potential to effectively reduce the number of active transport equations in addition to the complexity associated with chemical kinetics.

The PEC approach utilizes a so-called drift term that is formulated to identify the deficiency of these low-order models. Specifically, the drift term examines the compliance of a particular combustion model with respect to the underlying flow-field representation [9]. By locally enriching the low-order flamelet models using models of higher physical fidelity, the PEC approach was demonstrated to improve the prediction of emissions while incurring lower cost compared with simulations in which finite-rate chemistry is applied uniformly.

While the PEC framework was proposed to address the modeling challenges in simulating complex flames, it has only been applied, in its entirety, to a series of small-scale simulations of steady-state or slowly varying tribrachial flames [2]. Although the key component of PEC, the so-called drift term, was extended to LES formulations and studied in detail as a stand-alone tool for examining the compliance of a particular combustion model with respect to the underlying turbulent flow-field representation [9], the effectiveness of PEC in adapting the dynamic assignment of combustion models in unsteady turbulent environments is yet to be demonstrated. Other issues to be addressed are the computational efficiency and dynamic load-balancing of this method when applied to massively parallel computations.

The objective of this work is to extend the application of PEC to LES of turbulent flames with the specific goal of efficiently improving the prediction of CO emissions. To facilitate a cost-effective realization of the local model adaptation for large-scale 3D calculations, efficient computational strategies are developed for solving finite-rate chemistry, evaluating the drift term for error estimation, and scalable parallelization. The combined framework is applied to LES of a piloted turbulent dimethyl ether (DME) jet flame using a combination of the flamelet/progress variable approach (FPV) [5] and finite-rate chemistry (FRC). The predictive capability and computational efficiency of the PEC framework are analyzed in comparison to monolithic, nonadaptive simulations using only FPV or FRC models.

2. PEC framework

As discussed in Section 1, the PEC-framework aims to improve the cost and accuracy of combustion simulations by applying a spatially heterogeneous sub-model assignment that is dynamically adapted during unsteady LES calculations. Three key components of PEC are discussed in this section: (i) the model assignment based on the balance between efficiency and fidelity of combustion models, (ii) the drift term used to estimate the model error without prior information of a reference solution, and (iii) the coupling of scalar transport equations among different models. The interested reader is referred to [2] for a detailed description of the PEC formulation.

2.1. Governing equations

The system of the fully compressible Navier-Stokes equations is considered in this work. The Favre-filtered conservation laws of mass, momentum, total energy, and reactive scalars take the following form:

\[
\partial_t \tilde{\rho} + \nabla \cdot (\tilde{\rho} \tilde{u}) = 0, \tag{1a}
\]

\[
\partial_t (\tilde{\rho} \tilde{u}) + \nabla \cdot (\tilde{\rho} \tilde{u} \tilde{u} + \tilde{p} I) = \nabla \cdot (\tilde{\tau} + \tau_{\text{sgs}}), \tag{1b}
\]

\[
\partial_t (\tilde{\rho} \tilde{E}) + \nabla \cdot [\tilde{\rho} \tilde{u} (\tilde{\rho} \tilde{E} + \tilde{p})]
= \nabla \cdot [(\tilde{\tau} + \tau_{\text{sgs}}) \cdot \tilde{u} - (\tilde{\rho} + q_{\text{sgs}})], \tag{1c}
\]

\[
\partial_t (\tilde{\rho} \tilde{\phi}) + \nabla \cdot (\tilde{\rho} \tilde{u} \tilde{\phi}) = -\nabla \cdot (\tilde{j} + j_{\text{sgs}}) + \tilde{S}_\phi, \tag{1d}
\]

where \( \tilde{\tau} \) is the stress tensor, \( q \) is the heat flux, and \( p \) is the pressure obtained from the equation of state.

For the scalar equation in Eq. (1d), \( \tilde{\phi} \) is defined to be the concatenation of manifold-describing variables of candidate models: \( \tilde{\phi} = [\tilde{\phi}_{m_1}, \ldots, \tilde{\phi}_{m_N}] \), with the set of candidate models being \( M = \{m_1, \ldots, m_N\} \). The manifold-describing variables are used to evaluate the filtered chemical source term, denoted by \( \tilde{S}_\phi \), as well as the reconstructed species mass fractions.

Pressure, temperature, and thermo-physical properties are obtained from density, internal energy, and species mass fractions that are reconstructed from the chosen manifold. Note that for the FPV model, the thermodynamic state is determined by the reconstructed species mass fractions together with the transported density and total energy. As such, the equation of state and thermodynamics are modeled consistently for
all sub-models considered. Such treatment of the thermodynamic state was previously considered for applying flamelet models to compressible flows [10,11].

2.2. Pareto-efficient model assignment

The model assignment, which is represented by the mapping $M : \Omega \rightarrow M$, determines the model of choice at any point in the computational domain $\Omega$. This assignment is obtained in the PEC framework by minimizing the weighted sum of estimated error ($e$) and cost ($c$):

$$
\min_{M : \Omega \rightarrow M} \left( \int_{\Omega} e(M(x), x) dx + \lambda \int_{\Omega} c(M(x), x) dx \right),
$$

(2)

The coefficient $\lambda$ is a user-input parameter, expressing the preference in the balance between efficiency and fidelity. As such, model assignment of lower cost but higher error will be chosen with an increased value of $\lambda$. The estimated local cost ($c$) is a model-specific constant. In the present case, the cost is evaluated as the number of transported scalars of the combustion model, since the computational cost is made to scale linearly with the number of scalars in the computational approach discussed in Section 3.

The local error, $e$, is defined as the weighted sum of errors estimated for the QoIs:

$$
e(m, x) = \sum_{\psi \in Q} \left( \frac{D^\psi_m}{B^\psi} \right),
$$

(3)

where $m = M(x)$ is the locally applied combustion model; $\psi$ defines a quantity included in the set of QoIs, denoted by $Q$; and $B^\psi$ is the scaling constant. The formulation of the drift term, $D^\psi_m$, will be described in the follow section. A greedy strategy is employed to approximate the solution to Eq. (2) and the detailed algorithm is discussed in [2].

2.3. Drift term

The drift term provides a measure of the compliance of a particular combustion model with respect to the underlying flow-field representation. This drift term is evaluated for each user-specified QoI, $\psi$, and calculates the initial growth-rate of the error if the solution was initialized from a given manifold model. Therefore, the drift term identifies the error induced by the incompatibility between the local flow field and the structure of the combustion model [9]. Specifically, for a given combustion model $m$, the drift term for the QoI $\psi \in Q$ is defined as [9]

$$
D^\psi_m = \bar{\rho} \left( D_t(\psi)\big|_{\psi = \psi_m} - D_t(\tilde{\psi}_m) \right),
$$

(4)

where $D_t$ denotes the substantial derivative and $\tilde{\psi}_m$ is the QoI determined from the manifold of model $m$. The first term, $D_t(\psi)\big|_{\psi = \psi_m}$, represents the evolution of $\psi$ following the transport equations, if it were initialized by the manifold determined value $\psi_m$. The second term, $D_t(\tilde{\psi}_m)$, represents the change of $\tilde{\psi}_m$ following the evolution of the manifold-describing variables, which can be evaluated via the chain rule as [9]

$$
D_t(\tilde{\psi}_m) = \frac{\partial \tilde{\psi}_m}{\partial \phi_m} \cdot D_t(\phi_m).
$$

(5)

In the present study, the QoIs are chosen to be the mass fractions of selected species. Therefore, all the terms that are present in Eq. (4) can be obtained directly from the simulation using model $m$. As such, the drift term is capable of determining the applicability of a manifold-based combustion model in the absence of prior information from a reference solution.

2.4. Coupling between combustion models

The scalar equations, Eq. (1d), are selectively solved based on the dynamically determined model assignment $M$. As a result, the transport equations for $\phi_m$ are solved only when $M(x) = m$. Coupling between scalar transport equations among sub-domains using different models is achieved via the mechanism of imputing the deactivated manifold-describing variables using those of the activated model. To ensure consistency at the interface of sub-models, the following reconstruction operation is applied before evaluating the right-hand-side of the spatially-discretized governing equations

$$
\tilde{\phi}_m(x) = \phi^R_{m'}(\tilde{\phi}_m(x)) \quad \text{where} \quad M(x) = m,
$$

(6)

for all deactivated models $m' \neq M(x)$. For the FPV and FRC models used in this study, the specific form of the reconstruction operation $\phi^R$ is described in Section 4.3.

The essential conservation properties for mass, momentum, and total energy are preserved during the adaptation procedure since the corresponding conservation equations are universal among sub-domains. The smoothness of the scalar fields is ensured by the combination of the reconstruction operation and the drift term, which detects sharp transitions through the entailed diffusion operator.

3. Computational approach

3.1. Spatial and temporal discretization

LES with PEC-based combustion model adaptation is performed using an unstructured finite-volume solver, CharLES [12]. The fully compressible multi-species Navier-Stokes equations are spatially discretized using a modified
hybrid central-WENO scheme [13,14], which has low numerical dissipation while being stable for discontinuities across contact interfaces. The convection-diffusion and reaction operators of the system are separated by a steady-state preserving 2nd-order operator splitting scheme [15]. The time-stepping of the convection-diffusion part is carried out via a 3rd-order Runge–Kutta (SSP-RK3) method [16]. The spatially independent systems of chemical reactions are integrated using a semi-implicit 4th-order Rosenbrock–Krylov (ROK4E) scheme [15,17]. The stability of the ROK4E scheme is achieved through the approximation of the Jacobian matrix by its low-rank Krylov-subspace projection. As few as three right-hand-side evaluations are performed over four stages. Overall, a minimum of 3.5 source-term evaluations is required per convection-diffusion step, the cost of which is comparable to three evaluations required for a fully-explicit scheme.

3.2. Parallelization and load balancing

For parallel computations on distributed architectures, the unstructured mesh is partitioned into multiple domains. The heterogeneity in the memory layout is accounted for by using a two-layer partitioning strategy [18]. To this end, the inter-node level partition is first performed to determine the control-volumes assigned to each node. The intra-node level partition is then performed to determine the assignment associated with each processor. As such, the locality of the control volumes for processors on the same node is encouraged. During the partitioning processes, the cost of each control-volume is set to be the sum of the local combustion modeling cost, as discussed in Section 2.2, and the fixed cost of solving the compressible Navier–Stokes equations.

In addition to the cost-aware domain decomposition, another level of load balancing is performed for the temporal integration of the chemical reactions where the FRC model is used. The computational task of the time integration is redistributed among processors by exploiting the spatial locality of chemical reactions. The redistribution is conducted via a parallelized rebalancing scheme [19] based on the algorithm of Aggarwal et al. [20].

4. Experimental and computational setup

4.1. Experimental configuration

In the present work, PEC is applied to LES of a turbulent DME jet flame, which was derived from the canonical Sydney/Sandia piloted jet flame series, and was experimentally investigated at Sandia National Laboratories [21,22]. The central fuel jet consists of a mixture of DME and air with an equivalence ratio of $\phi = 3.6$, resulting in a stoichiometric mixture fraction of $Z_{\text{eff}} = 0.353$. The pilot stream consists of a burned mixture of $\text{C}_2\text{H}_5$, $\text{H}_2$, $\text{CO}_2$, and $\text{N}_2$, which is chosen to match a premixed DME flame with $\phi = 0.6$. The fuel jet diameter is $D = 7.45$ mm. The pilot annulus has inner and outer diameters of 8 mm and 18.2 mm, respectively. For this study, the DME-D condition is chosen. The bulk jet velocity is $U_{\text{bulk}} = 49.5$ m/s, which corresponds to a Reynolds number of $Re = 29,300$. The unburned velocity of the pilot stream is 1.1 m/s and the velocity of the air co-flow is 0.9 m/s.

4.2. Numerical setup

The LES is performed on an unstructured mesh with 10.3 million hexahedral elements. The minimal grid spacing at the jet outlet is 0.1 mm. A relatively fine mesh is chosen to reduce the sensitivity on the closure model for the turbulence-chemistry interaction. The velocity inflow profile of the fuel stream is generated using digital filtering [23], with mean and turbulent quantities matching the experimental data. The nozzle wall is considered as non-slip and adiabatic.

For both the FPV and FRC models, the combustion chemistry of the DME-air flame is represented using an 18-species kinetic scheme that was reduced from the 58-species mechanism of Zhao et al. [24], using a combination of skeletal reduction and linear-QSSA [25] method. The detailed description and testing for the reduced mechanism is provided as supplementary material. The molecular diffusion is modeled with species-specific non-unity Lewis numbers assumed constant throughout the flame. The Lewis numbers for the mixture fraction and progress variable are set to be unity. The Lewis numbers for the species are calculated at the equilibrium condition of a stoichiometric mixture of DME and air. The CO-formation is not sensitive to radiation, and radiative heat-loss effects were not considered in the present work. The Vreman model [26] is used to represent the turbulent subgrid stresses. The subgrid-scale turbulent-chemistry interaction is accounted for using the dynamic thickened-flame model (DTF) [27], which has been applied to premixed and non-premixed combustion in conjunction with detailed mechanisms as well as tabulated chemistry [28–30]. By employing identical closure models for the turbulence-chemistry interaction in both FPV and FRC models, the observed difference in the simulation results can be better attributed to variations in the chosen combustion models. A sensitivity study was performed and a maximal thickening factor of 3 was found to be sufficient for the current choice of mesh resolution.

When applied to the 18-species reduced DME mechanism, the efficient integration of the chemical source terms accounts for less than 20% of the overall computational cost in the nonadaptive
FRC simulation, while the computation of the transport equations of the species mass fractions accounts for 65%. Although both components of cost can be reduced via the limited usage of FRC in PEC simulations, reducing the number of transport equations via PEC is critical for obtaining meaningful cost saving.

4.3. Pareto-efficient combustion model

The candidate models considered in this study are the FPV and the FRC models. The FPV model is chosen since this flame is largely diffusion-controlled. More complex flames could benefit from using additional sub-models [2,9]. The manifold-describing variables are defined as $\phi = [\tilde{\phi}_{FPV}, \phi_{RC}]^T$.

The choice of using the dynamic thickened-flame model for both FRC and FPV allows for analyzing differences in the prediction of QoIs without the potential complication from the variation of closure models. With the flame being artificially thickened, the FPV manifold is described by the filtered mixture fraction and progress variable, $\tilde{\phi}_{FPV} = [\tilde{Z}, \tilde{C}]^T$, which we note is different from the conventional practice of using a presumed-PDF closure [5,31]. For the FRC model, $\phi_{RC} = [\tilde{Y}_1, \cdots, \tilde{Y}_{N-1}]^T$, leading to an identity mapping between the manifold-describing variables and the filtered species mass fractions. For FPV, the Jacobian-vector multiplication in Eq. (5) can be efficiently calculated by a finite-difference approximation:

$$D_t(\tilde{\psi}_{FPV}) = \frac{\partial \tilde{\psi}_{FPV}}{\partial \tilde{Z}} D_t(\tilde{Z}) + \frac{\partial \tilde{\psi}_{FPV}}{\partial \tilde{C}} D_t(\tilde{C})$$

$$= [\tilde{\psi}_{FPV}(\tilde{Z} + \epsilon D_t(\tilde{Z}), \tilde{C} + \epsilon D_t(\tilde{C})) - \tilde{\psi}_{FPV}(\tilde{Z}, \tilde{C})]/\epsilon,$$

which is first-order accurate with one additional retrieval of the tabulated values and $\epsilon = 1 \times 10^{-9}$ s is chosen in this study.

The progress variable for the FPV model is defined as the sum of mass fractions of H$_2$, H$_2$O, CO, and CO$_2$. Hence, the reconstructed progress variable for FPV, used in Eq. (6), is obtained from $\phi_{RC}$ as $\tilde{C}^\ast = \tilde{Y}_{H_2} + \tilde{Y}_{H_2O} + \tilde{Y}_{CO} + \tilde{Y}_{CO_2}$, while the species mass-fraction for FRC is reconstructed via table reading: $\tilde{Y}^R_k = \tilde{Y}^*_{FPV,k}(\tilde{Z}, \tilde{C})$, where $\tilde{Y}^*_{FPV,k}$ is the tabulated species mass fraction from FPV. The scaling constant $B_y$, shown in Eq. (4), is chosen to be the corresponding species production rates at the equilibrium condition of a stoichiometric DME-air mixture. Due to the consideration of preferential diffusion in the FRC model, the mixture fraction with unity Lewis number cannot be reconstructed from species mass fractions and thus the consistent transport equation for $Z$ is solved throughout the domain.

5. Results and discussion

A series of PEC simulations based on FPV and FRC models are performed. Calculations are carried out for a range of $\lambda$, specifying different levels of efficiency-accuracy preference. Large values of $\lambda$ correspond to preferring the low-order FPV model over the FRC model, which has greater computational complexity but a higher degree of fidelity. The shift toward FPV leads to a decrease in the cost of the simulation and a potential increase in the prediction error. The model assignment is dynamically updated at the beginning of each time step. The quantities of interest specified in the series of LES-PEC calculations are the constitutive species for progress variable: $Q = \{\tilde{Y}_{H_2}, \tilde{Y}_{H_2O}, \tilde{Y}_{CO}, \tilde{Y}_{CO_2}\}$.

We first discuss the calculations at the two limits of the efficiency-accuracy preference, leading to monolithic combustion model model assignments of FPV ($\lambda \rightarrow \infty$) and FRC model ($\lambda \rightarrow 0$). The results obtained from intermediate values of $\lambda$ are then presented, in which the FPV and FRC models are jointly utilized in the LES calculations. Subsequently, aspects of dynamic model assignment and accuracy of CO emissions are addressed. This section is finalized by analyzing the performance and cost savings of the PEC approach.

5.1. Monolithic model assignment

Two baseline simulations are performed, in which FRC and FPV are used as the monolithic combustion model over the entire domain. These calculations are obtained with the weight coefficient of $\lambda = 0.00$ and $\lambda = 0.64$, respectively. The choice of extreme values of $\lambda$ indicates the overwhelming emphasis of efficiency over accuracy or vice versa, and hence the monolithic model assignment. These PEC simulations are labeled as PEC-0 and PEC-64, corresponding to the monolithic utilization of FRC and FPV, respectively. The PEC-64 result is further used to initialized the rest of the calculations to avoid the propagation of information from higher fidelity simulations.

The mean profiles of the monolithic LES results are collected at $x/D = (5, 10, 20, 40)$. The comparison of the computed radial profiles against the experimental measurements is shown in Fig. 1. Overall, Bilger mixture fraction, temperature, and H$_2$O mole fraction are well predicted by both simulations. The level of agreement is comparable to previous LES calculations performed using FPV [32], CMC [33], and PDF [34] approaches. Noticeable deviations from the measurements, however, can be observed for the CO mole fraction of PEC-64 (FPV) at the downstream locations ($x/D = 20, 40$), as the FPV model reduces the chemical time scales of all species to that of the progress variable. Prediction for the CO mole fraction is significantly improved in PEC-0 (FRC) due to the more detailed representation of chemical reactions.
The instantaneous field of the local error estimation for PEC-64 is presented in Fig. 2A. The error estimation is defined as the sum of the normalized drift terms for H₂, H₂O, CO, and CO₂. The value is high on the rich side of the flame and gradually increases along the streamwise direction, marking the regions where FPV shows deficiency. As shown in Fig. 2B, the error estimation agrees well with the comparison of the instantaneous and mean fields of CO mole fraction between PEC-64 (FPV) and PEC-0 (FRC).

5.2. Heterogeneous model assignment

We first focus on the PEC-8 calculation with the weight parameter chosen to be $\lambda = 0.08$. The choice of intermediate values of $\lambda$ results in the adaptive procedure with a mixed usage of the FPV and FRC models, as shown in Fig. 3A. An instantaneous snapshot of this case is displayed in Fig. 3B and C, showing smooth profiles of the temperature and the mole fraction of CO in the presence of heterogeneous model assignments.

The comparison between PEC-8 results and the baseline simulations are shown in Fig. 1, with the color-coded probability of FRC usage in PEC-8. For mean radial profiles that are well predicted by both PEC-64 and PEC-0, such as Bilger mixture fraction, temperature and H₂O mole fraction, the prediction by PEC-8 is expectedly of similar accuracy. The improvement of PEC-8 over PEC-64 can most clearly be observed for CO mole fraction profiles at $x/D = 20$ and 40, which is significantly under-predicted by PEC-64. The deficiency of the FPV model in describing the evolution of CO is correctly detected by the PEC adaptation procedure, resulting in the usage of FRC (marked in red) in regions critical to the correct CO prediction, which accounts for 30.2% of the computational domain. The adaptive usage of FRC in PEC-8 results in the improved prediction of CO emissions as illustrated by the comparison of the instantaneous and mean fields of the CO mole fraction between PEC-64, PEC-8, and PEC-0 in Fig. 2.

The PEC model is further scrutinized by examining simulation results produced with various intermediate values of $\lambda$ ranging from 0.01 to 0.32. The resulting PEC calculations have FRC applied to approximately 10% – 40% of the computational domain. The percentage of the domain modeled
Fig. 2. A: Instantaneous field of local error estimation for PEC-64 (FPV), defined as the sum of the normalized drift terms for H₂, H₂O, CO, and CO₂; B: Comparison of the instantaneous (left) and mean (right) fields of CO mole fraction between PEC-64 (λ = 0.64, FPV), PEC-8 (λ = 0.08), and PEC-0 (λ = 0.00).

Fig. 3. Instantaneous fields of (A) model assignment, (B) temperature, and (C) CO mole fraction for PEC-8 (λ = 0.08, left) and PEC-32 (λ = 0.32, right). The regions with FPV and FRC are color coded in blue and red, respectively. The stoichiometric contour of Z_{st} = 0.353 is marked in black lines in (A). The sub-model interface between FPV and FRC is marked in gray lines in (B) and (C).
by FRC is plotted in Fig. 5. The FRC utilization is shown to monotonically decreases with increasing value of \( \lambda \). As discussed in Section 5.1, the monolithic usage of FPV is realized with \( \lambda = 0.64 \). However, it is worth noting that the current adaptation formulation relies on a user-specified value of \( \lambda \). The capability of adjusting \( \lambda \) to satisfy a pre-determined level of cost or accuracy is subject of future study.

In Fig. 4, mean profiles for \( \text{H}_2\text{O} \) and CO mole fractions of PEC-8 are compared with those obtained from PEC-32 (\( \lambda = 0.32 \)) and experiments. At both axial locations, \( x/D = \{10, 20\} \), the accuracy for the mean \( \text{H}_2\text{O} \) and CO profiles is maintained despite a significantly reduced usage of FRC from 26.6% to 8.8%. As shown in Fig. 3, the switch from FRC to FPV occurs, as demanded by the higher value of \( \lambda \), at the up-stream location where

**Fig. 4.** Comparison of the experimental and computed radial profiles of the mean mole fractions of \( \text{H}_2\text{O} \) and CO, from LES-PEC with \( \lambda = \{0.00, 0.08, 0.32, 0.64\} \), at the axial position of \( x/D = 10, 20, 40 \). LES-PEC calculations with \( \lambda = 0.00 \) and 0.64 correspond to baseline FRC and FPV simulations.

**Fig. 5.** Averaged usage of FRC (\% of elements) and normalized cost for LES-PEC with \( \lambda = \{0.01, 0.04, 0.08, 0.16, 0.32, 0.64\} \). The dashed red and blue lines represent the reference cost of nonadaptive FRC and FPV calculations, respectively.
FPV is capable of accurately predicting CO of high strain rate conditions, while the FRC model remains active for the rich mixture downstream as well as regions near the exit plane of the pilot flame.

5.3. Cost analysis

The computational efficiency of the PEC framework is evaluated by measuring the CPU time of PEC simulations for different values of $\lambda$. The computational cost is evaluated for calculations performed on 1000 Ivy Bridge processors. The results are summarized in Fig. 5. The normalized computational cost for the PEC calculations is shown by the solid black line. The red and blue dashed lines represent the reference cost for nonadaptive FRC and FPV calculations, which are different from PEC-64 and PEC-0 in cost due to the absence of overhead associated with PEC.

Significant savings in cost via dynamic combustion model adaptation are achieved, especially considering the high efficiency of the FRC calculation and the compactness of the chosen kinetic scheme. For PEC-32, the cost is reduced to 49.8% of the reference FRC calculation, without having noticeable deviations from the FRC results including CO emissions. The PEC simulation with lowest cost corresponds to PEC-64 with monolithic utilization of FPV. The difference between the cost of PEC-64 and the non-adaptive FPV (dashed blue line) is caused by the overhead of the PEC framework, which can be attributed to the adaptation procedure as well as the consistent but more costly thermodynamic model.

6. Conclusions

In this work, the PEC framework is extended to simulations of turbulent reacting flows and the method is applied to LES of a lifted turbulent DME jet flame. Based on the minimal user-specific inputs for: (i) candidate combustion models, (ii) quantities of interest, and (iii) a weight coefficient representing the balance between efficiency and accuracy, PEC dynamically selects the appropriate local combustion model assignment to best describe the flame under case-specific constraints for accuracy and cost. With the goal to enrich FPV for the improved prediction of CO, a series of LES-PEC simulations is performed with various levels of FRC/FPV usage. The monolithic FPV simulation is shown to be deficient at predicting CO emissions in the down-stream region of the flame. The CO prediction can be significantly improved via the enrichment of FRC occurring at as few as 9% of the domain. The resulting parallel calculation is a factor of two less expensive compared with a highly efficient nonadaptive calculation using finite-rate chemistry uniformly, while not causing noticeable degradation in the predictive accuracy for quantities of interest.

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Supplementary material

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