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Large Eddy Simulation of bluff-body flame approaching blow-off: A sensitivity study

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Abstract

As almost all combustion processes of practical interest take place in the presence of turbulence, the development of the increasingly refined turbulence-chemistry interaction (TCI) models has led to highly sophisticated approaches. Nearly all of the studies comparing different models focus on stable premixed/non-premixed flame configurations. In this work, the focus is on well-documented, lean premixed bluff-body stabilized flames approaching blow-off and on the blow-off sequence itself. Large Eddy Simulations (LES) have been used to capture the time-dependent, three-dimensional flow-field using Transported Probability Density Function (TPDF), Partially Stirred Reactor Model (PaSR) and Implicit LES (ILES) models. Furthermore, the influence of finite-rate chemistry and different chemical mechanisms is evaluated to determine the limitation and capability of the different TCI approaches for modelling flames just prior to and during the transient blow-off process. While the average flow-fields do not reveal any significant differences between modelling approaches, detailed analysis of the flame reveals that there are differences in the predicted flame thickness and composition. The ability of the considered TCI models to predict local as well as full flame extinction during the blow-off is investigated as well. It is demonstrated that such a blow-off sequence is not always governed by complex chemistry.

Keywords: Bluff-body, Blow off (BO), Large Eddy Simulation (LES), turbulence-chemistry interaction (TCI), Transported Probability Density Function (TPDF), Partially Stirred Reactor Model (PaSR), Implicit LES (ILES)

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1. Introduction

Maintaining a stable flame in circumstances where the flame speed is several orders of magnitude smaller than the flow velocity is difficult, typically requiring a flame holding device. With increasing interest in lower NOx systems, the problem of keeping the flame anchored and maintaining stable burning conditions becomes even more challenging due to the lean premixed combustion conditions with lower temperatures. While swirl-stabilization is used in most gas turbine burners, bluff-body stabilization is found in a wide range of environments, such as ram-jets, scram-jets and turbojet afterburners, as well as in laboratory set-ups for fundamental studies (Chaudhuri et al. (2011)). The idea is to create a recirculation zone (RZ) behind the bluff-body where the hot burnt gases are recirculated, acting as a heat source and igniting the incoming mixture.

Traditionally, the focus has been on predicting the conditions where blow-off occurs, identifying critical parameters such as blockage ratio, type of fuel, equivalence ratio, temperature, and velocity (Longwell et al. (1949, 1953); Russi et al. (1953); Wright (1959); Spalding (1953); Zukoski and Marble (1956)). Most of the early studies focused on deriving physics-based correlations most often based on time-averaged characteristics, (Williams et al. (1949); Williams and Shipman (1953), Longwell et al. (1949, 1953)). Bluff-body flames under non-premixed conditions have also been studied during the *TNF-workshops-series*, (Sandia (1998)). Shanbhogue et al. (2009) present a review of bluff-body flames focusing on recent advances in understanding the influence of the mixture properties on the spatiotemporal dynamics of the flow-field. Both Shanbhogue et al. (2009) and Chaudhuri and Cetegen (2009); Chaudhuri et al. (2010, 2011, 2012) discuss different theories on bluff-body blow-off ***but very few studies focus on numerically predicting blow-off and flashback (Ma et al. (2018); Kim et al. (2018); Hodzic et al. (2018)).***

One of the more commonly investigated bluff-body setups is the so-called Volvo-rig, involving a triangular wedge-shaped bluff-body (Sjunnesson et al. (1992); Bai and Fuchs (1994); Fureby and Löfström (1994); Kim and Pope (2014); Erickson and Soteriou (2011)). The case has also been used for comparison of different combustion models by Ma et al. (2013), evaluating different TCI models and numerical schemes by Rochette et al. (2018) and chemical reaction mechanisms by Zettervall et al. (2017). Despite the triangular bluff-body shape, the three-dimensional effects were proven to be significant, Fureby and Löfström (1994). While some studies have been performed considering transient blow-off and flashback (Sommerer et al. (2004)), the experimental focus is usually on the stable flame configuration. In a recent work by Wang et al. (2013), the authors introduce a benchmark case where the flame is subjected to a pulse of inflow velocity resulting in local extinction and re-ignition. While a significant body of work focusing on transient processes using LES exists, there are very few focusing on the blow-off process itself. Sommerer et al. (2004), for example, showed that LES was capable of correctly predicting flashback and blow-off limits for a partially-premixed swirled burner. Tyliczszak et al. (2014) correctly predicted the blow-off limit for swirling spray flames. In previous

studies by Hodzic et al. (2013, 2017b,a), the three-dimensional bluff-body flame holder corresponding to the experimental investigation of Kariuki et al. (2012) was used as a test-case *owing to the* extensive experimental database containing both flow and flame data for stable flames and flames very close to blow-off. A significant shift in the large-scale structures was identified, as well as the possible causes of the shift and their impact on the flame fragmentation. Evaluation of the different theories and proposal on the sequence of events leading to blow-off was presented by Hodzic et al. (2017b). Similar results are seen in a recent experimental study by Chowdhury and Cetegen (2018). In the *present study*, the focus is on the sensitivity of the predicted flame to different TCI models, the choice of chemical mechanisms, and *on the performance* of different TCI models in predicting the transient blow-off of the bluff-body case.

Large eddy simulations (LES) have been performed for capturing the unsteady characteristics and dynamics of the flames under consideration. LES involves explicitly computing large-scale structures and modeling the effect of the small, unresolved scales below a certain filter size. However, LES still encounters difficulty in resolving the combustion which most often occurs below the filter size. Even though a variety of combustion models have been proposed (Pitsch (2005); Poinso and Veynante (2000); Cant and Mastorakos (2007)), there are still significant challenges in numerically predicting the interaction between the turbulent flow, mixing and chemistry. Most combustion models are derived from the RANS models (Pope (2004)) and usually classified with respect to flame-turbulence interaction and chemistry description (Fiorina et al. (2015)). These are categorized by Fiorina et al. (2015) as the geometrical (or topological approaches), statistical approaches and mixing approaches. Alternative classifications do exist, for instance those of Fureby (2007, 2012) which categorizes in infinite/finite-rate chemistry and flamelet models.

The geometrical or topological approaches assume that the turbulent flame may be represented as distribution of reaction zones (flamelets), each assumed to be a local laminar flame at the local conditions. These include *Flame Surface Density* (FSD) (Boger et al. (1998)) or wrinkling models (Hawkes and Cant (2001); Weller (1993); Tabor and Weller (2004)), the G-equation (Kerstein et al. (1988)) and the *Thickened Flame model* (TFM) (Butler and O'Rourke (1977)). They have been successfully implemented in a number of different conditions (Peters (1999); Nogenmyr et al. (2009)) including flash-back/blow-off and ignition studies (Selle et al. (2004); Sommerer et al. (2004); Schmitt et al. (2007); Boileau et al. (2008)).

The statistical approaches are based on probability density functions (PDF) of the thermo-chemical variables with or without velocity. Approaches based on PDF provide compelling advantages in modeling reactive flows due to an effective resolution of the closure problem arising from averaging or filtering the chemical reaction rates term (Pope (2000)). It was initially proposed by Givi (1989) and the filtered probability function (FDF) formulation *was developed* by Pope (1990). The two different PDF-based methods are presumed PDF, referred to as FDF in the context of LES, and transported PDF approaches (Haworth (2010)) and have been used under a range of flame configurations (Mustata et al. (2006); Jones et al. (2007); Jones and Navarro-Martinez (2007); Jones and Prasad (2010); Jones et al. (2012); Bulat et al. (2013)).

Mixing approaches are often based on extension of previous RANS models, e.g. the Eddy-Break-Up model (EBU) (Spalding (1977)) or the Eddy-Dissipation-Concept (EDC). Combustion is thus treated as a mixing problem rather than a reaction problem. The chemical reaction-rates are assumed to be controlled by mixing, proportional to the inverse of mixing time (Fiorina et al. (2015)). The partially stirred reactors model (PaSR) of Chomiak and Karlsson (1996) follows the same concept of introducing a fractal description of the turbulence. The computational cell is divided into two different fractions, the reacting volume fraction and the surrounding fluid. Inside the reacting zone, a perfectly stirred reactor (PSR) assumption is made in which all reactants are perfectly mixed with each other. The implicit LES (ILES) in combustion, sometimes referred to as Monotonically Integrated LES (MILES) model, is one of the simplest models, computing the reaction-rates directly through the Arrhenius law assuming thus that each cell is a perfectly stirred reactor (Fureby (2007); Grinstein and Kailasanath (1995); Duwig and Fuchs (2008); Duwig et al. (2011); Hodzic et al. (2017a)).

Here the ILES, PaSR and filtered probability density function (PDF) model is used for predicting ignition/extinction and pollutant formation for flames close to and during the blow-off event after a thorough analysis of the chemical mechanisms' performance.

The rest of the paper is organized as follows. First, the *computational case* setup is described in Section 2. Then the models and methods are given in Section 3, including a description of the LES method and the TCI models used. Finally, the results are presented in Section 4, with salient conclusions presented in Section 5.

2. Case set-up

The burner used in the current numerical study was originally developed by Balachandran et al. (2005) and is shown in Fig. 1, together with the computational domain and an example of the shape and position of the flame. The bluff-body consists of a 45deg half-angle cone mounted on a cylindrical rod. The computational domain itself is bounded by a large expanding rectangular box, where a small co-flow ($0.2m/s$) is added around the burner for improved numerical stability. Premixed air and methane are injected into the burner approximately $2D$ upstream of the bluff-body, D being the outer diameter of the burner.

The set-up is based on that presented by Kariuki et al. (2012, 2015), replicating three cases presented in Kariuki et al. (2012); *an isothermal case*, one with a stable flame, one with a leaner flame close to blow-off and one matching the blow-off limit itself, outlined in Table 1. Approximately the same velocity is used in all three reacting cases, giving a Reynolds number based on the bluff-body diameter of around $2 \cdot 10^5$. The velocity is set at the inlet boundary with 5% artificial turbulence in the X and Y -direction, 10% in the Z -direction for the main inlet and zero artificial turbulence in the co-flow. The gas temperature is 300 K and species mass fractions are set at the inlet, replicating the equivalence ratio as specified in the experimental

study. A zero-gradient boundary condition is adopted for the pressure. At the outlet, the pressure is set to a constant value of 101.325 kPa with zero-gradient boundary conditions for all other variables. On the burner walls, a no-slip velocity boundary condition is used with a temperature of 300 K (588 K at the upper burner wall).

The grid consists of approximately 90% cubes and prisms, and polyhedrons for the rest with a total of 1.5 million cells. It is locally refined around the flame zone and the smallest cells have a size of $l/d = 0.026$, where d is the diameter of the bluff-body. A time-step of $\Delta t = 10^{-6}$ s is used, giving a maximum Courant-Fredrich-Levy number ($CFL = U\Delta t/\Delta x$) of 0.3 for all cases. The non-reacting case was computed for 2s of physical time and later used to initialize the reacting cases, where the ignition was started by placing burnt products in the RZ. These reacting cases were later computed for approximately 1s, disregarding the transients during the ignition.

3. Models and Methods

Simulating turbulent combustion involves solving a fluid dynamics problem and a chemical problem which are coupled in a highly non-linear manner. In order to capture complex flame-flow dynamics and interaction phenomena, LES is used in combination with different TCI and finite-rate chemistry models.

3.1. Large Eddy Simulations

The governing equations in LES are filtered in space, resolving the dynamics of the large scale structures (larger than the filter cut-off wavelength) and modeling only the small, unresolved scales. The filtering is performed with a spatial filter applied to the equations of motion. The filter of a function $f = f(\mathbf{x}, t)$ is defined as its convolution with a filter function G according to:

$$\bar{f}(\mathbf{x}, t) = \int_{\Omega} f(\mathbf{x}', t) G(\mathbf{x} - \mathbf{x}'; \Delta(\mathbf{x})) d\mathbf{x}' \quad (1)$$

defined over the entire flow domain Ω having a characteristic width Δ , which may vary. In reacting flows with strong density gradients, the introduction of density-weighted, or Favre-filtered quantities is often made, $\tilde{f} = \overline{\rho f}/\bar{\rho}$, where ρ is the density. Applying the filtering operation according to Eq. (1) to the conservation equations of mass, momentum and enthalpy, the LES equations can be written as:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i}{\partial x_i} = 0, \quad (2)$$

$$\frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i \tilde{u}_j}{\partial x_j} + \frac{\partial \bar{p}}{\partial x_i} = \frac{\partial}{\partial x_j} \left(\mu \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) + \bar{\rho} \tilde{u}_i \tilde{u}_j - \overline{\rho u_i u_j} \right), \quad (3)$$

$$\frac{\partial \bar{\rho} \tilde{Y}_k}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i \tilde{Y}_k}{\partial x_i} = \frac{\partial}{\partial x_i} \left(-\overline{\rho u_i Y_k} + \bar{\rho} \tilde{u}_i \tilde{Y}_k + \frac{\mu}{\sigma} \frac{\partial \tilde{Y}_k}{\partial x_i} \right) + \bar{\rho} \tilde{\dot{\omega}}_k, \quad (4)$$

$$\frac{\partial \bar{\rho} \tilde{h}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i \tilde{h}}{\partial x_i} = \frac{\partial}{\partial x_i} \left(-\overline{\rho u_i h} + \bar{\rho} \tilde{u}_i \tilde{h} + \frac{\mu}{\sigma} \frac{\partial \tilde{h}}{\partial x_i} \right), \quad (5)$$

where u_i is the velocity component i ; Y_k , $\dot{\omega}_k$, p and μ are the mass fraction, reaction-rate of species $k = 1 \dots N$, pressure and viscosity, respectively; and the mass and heat fluxes have been approximated by Fick's and Fourier's law. This is in line with previous work in the field (Mustata et al. (2006); Jones and Navarro-Martinez (2007); Jones and Prasad (2010); Jones et al. (2012)) where the assumption of equal turbulent Schmidt and Prandtl numbers (σ) has been used, as is the case in this study. The **SGS**-stress tensor, appearing from the filtering, i.e. $(\tau_{SGS} = \bar{\rho} \tilde{u}_i \tilde{\varphi} - \bar{\rho} \widetilde{u_i \varphi})$, is modeled with the standard Smagorinsky model (Smagorinsky (1963)).

3.2. Turbulence chemistry interaction models

Three different TCI models are considered in this study; Partially Stirred Reactor (PaSR), Implicit LES (ILES) approach and the Transported PDF model, explained below.

3.2.1. Partially Stirred Reactor (PaSR) model

In the PaSR model (Chomiak and Karlsson (1996)), the computational cell is divided into two different fractions, the reacting volume fraction and the surrounding fluid. Inside the reacting zone of the cell, a perfectly stirred reactor (PSR) assumption is made in which all reactants are perfectly mixed with each other. Fluctuations of the chemical source terms are therefore neglected. The model assumes that this fraction of the reactor in the cell is proportional to the ratio of the chemical reaction time, τ_c , to the total conversion time in the reactor:

$$\kappa_k = \frac{\tau_c}{\tau_c + \tau_{mix}}, \quad (6)$$

where τ_{mix} is characterizing the exchange process between the reactant mixture and the unburnt mixture and τ_c the chemical reaction time calculated from the concentration rate of the product species. Even though there are multiple ways to define τ_{mix} , the most common definition is:

$$\tau_{mix} = C_{mix} \sqrt{\frac{\mu_{eff}}{\rho \epsilon}}, \quad (7)$$

where the mixing rate constant (C_{mix}) has been set to unity **with $\mu_{eff}/\rho\epsilon$ representing the ratio of effective viscosity and the dissipation rate.**

3.2.2. Implicit LES (ILES)

In the implicit LES (ILES) approach, the filtered reaction-rates in Eq. 4 are directly computed through:

$$\tilde{\dot{\omega}}_k = \dot{\omega}_k(\tilde{Y}_k, \tilde{T}), \quad (8)$$

where $\dot{\omega}_k(\tilde{Y}_k, \tilde{T})$ is **calculated using** the Arrhenius expression based on the filtered temperature and species mass fractions, usually for reduced chemical mechanism **in the same manner as in the PaSR model.** The approach assumes that the flame is relatively well resolved so that each grid cell can be seen as a

well-stirred reactor. This approach has been shown to perform well for higher Karlowitz number (Ka) cases (Duwig et al. (2011)) and is sometimes referred to as quasi-laminar chemistry (QLC) approach. It is the numerical diffusion that results in an artificial thickening of the flame and the approach has been succesful in a number of studies (Eberle et al. (2018); Edwards et al. (2012); Lourier et al. (2015); ?); Potturi and Edwards (2015); Ranjan et al. (2016); Strakey and Eggenpieler (2010); Zhang et al. (2010); Hodzic et al. (2017a)), in most studies, due to the relatively fine resolution. Furthermore, since the flame is stabilized by the recirculating hot gases, the most important chemical parameters are the ignition time and the temperature, which are believed to be well captured by the finite-rate chemistry.

3.2.3. Transported PDF method (TPDF)

In the PDF method, a joint subgrid PDF is obtained from a solution of a modeled evolution equation. A filtered PDF for the N_s (number of the species considered plus the enthalpy) scalar quantities necessary for description of the reaction (chemical source term in Eq.(4)) can be defined as:

$$P_{SGS}(\underline{\psi}; \mathbf{x}, t) = \int_{\Omega} \mathcal{F}(\underline{\psi}; \mathbf{x}', t) G(\mathbf{x} - \mathbf{x}'; \Delta(\mathbf{x})) d\mathbf{x}' \quad (9)$$

where $\mathcal{F}(\underline{\psi}; \mathbf{x}', t) = \prod_{k=1}^{N_s} \delta(\psi_k - \phi_k(\mathbf{x}', t))$ is the fine-grained PDF and ψ is representing the phase or sample space of the scalar quantities ϕ_k , with δ representing the Dirac delta function. P_{SGS} is the probability of observing the scalar variable $\psi = \phi$ within the filter volume, defined in Eq.(1). Based on the conservation equations, an exact evolution of the density-weighted PDF ($\tilde{P}_{SGS}$) can be derived (Gao et al. (1993); Colucci et al. (1998); Jaber et al. (1999)), resulting in:

$$\begin{aligned} & \bar{\rho} \frac{\partial \tilde{P}_{SGS}(\underline{\psi})}{\partial t} + \bar{\rho} \tilde{u}_j \frac{\partial \tilde{P}_{SGS}(\underline{\psi})}{\partial x_j} + \sum_{k=1}^{N_s} \frac{\partial}{\partial \psi_k} \left[\bar{\rho} \tilde{\omega}_k(\underline{\psi}) \tilde{P}_{SGS}(\underline{\psi}) \right] \\ & = - \frac{\partial}{\partial x_j} \left[\overline{\rho(\underline{\psi}) \mathcal{F}(\underline{\psi}) u_j} - \bar{\rho} \tilde{u}_j \tilde{P}_{SGS} \right] - \sum_{k=1}^{N_s} \frac{\partial}{\partial \psi_k} \left(\overline{\frac{\mu}{\sigma} \frac{\partial^2 \phi_k}{\partial x_i \partial x_i} \mathcal{F}(\underline{\psi})} \right) \end{aligned} \quad (10)$$

where the assumption of equal diffusivities has been used and the spatio-temporal dependency of the PDF has been dropped. The three terms on the LHS represent *respectively; the rate of change of the PDF in the physical space, the convection of the PDF in the physical space, and the chemical source production in the sample space*. An exact and closed form chemical source term now appears, i.e. in terms of $\underline{\psi}$ and $\tilde{P}_{SGS}(\underline{\psi})$. The two terms on the RHS in Eq.(10) represent the **SGS**-transport and mixing of the PDF, are unknown and must be modeled. The first term on the RHS is approximated by a simple gradient closure:

$$\overline{\rho(\underline{\psi}) \mathcal{F}(\underline{\psi}) u_j} - \bar{\rho} \tilde{u}_j \tilde{P}_{SGS} = - \frac{\mu^{SGS}}{\sigma^{SGS}} \frac{\partial \tilde{P}_{SGS}}{\partial x_j} \quad (11)$$

where σ^{SGS} is a constant turbulent Schmidt/Prandtl number assigned the value of unity (Jones and Prasad (2010); Mustata et al. (2006)). The second term representing the mixing of the PDF can be expressed as:

$$\begin{aligned} - \sum_{k=1}^{N_s} \frac{\partial}{\partial \psi_k} \left(\frac{\mu}{\sigma} \frac{\partial^2 \phi_k}{\partial x_i \partial x_i} \mathcal{F}(\underline{\psi}) \right) &= \frac{\partial}{\partial x_i} \left(\frac{\mu}{\sigma} \frac{\partial P_{SGS}(\underline{\psi})}{\partial x_i} \right) \\ &- \sum_{k=1}^{N_s} \sum_{\beta=1}^{N_s} \frac{\partial^2}{\partial \psi_k \partial \psi_\beta} \left\{ \left(\frac{\mu}{\sigma} \frac{\partial \phi_k}{\partial x_i} \frac{\partial \phi_\beta}{\partial x_i} \mid \phi = \underline{\psi} \right) P_{SGS}(\underline{\psi}) \right\} \end{aligned} \quad (12)$$

the term now represents the **SGS**-scale mixing as well as the effect of the molecular diffusion on the **PDF**. The unclosed term in Eq.(12) is modeled using the Linear Mean Square Estimation (LMSE) closure (Nordmeyer-Massner et al. (2009); Dopazo (1975)), also sometimes referred to as Interaction by Exchange with the Mean (IEM) method (Mustata et al. (2006); Jones and Navarro-Martinez (2007); Jones et al. (2012); Bulat et al. (2013)). The final term in Eq.(12) is thus replaced by:

$$\frac{1}{\tau_{SGS}} \sum_{k=1}^{N_s} \frac{\partial}{\partial \psi_k} \left[(\psi_k - \tilde{\phi}_k(\mathbf{x}, t)) \bar{\rho} \tilde{P}_{SGS}(\underline{\psi}) \right]. \quad (13)$$

The joint pdf equation is finally expressed as:

$$\begin{aligned} \bar{\rho} \frac{\partial \tilde{P}_{SGS}(\underline{\psi})}{\partial t} + \bar{\rho} \tilde{u}_j \frac{\partial \tilde{P}_{SGS}(\underline{\psi})}{\partial x_j} + \sum_{k=1}^{N_s} \frac{\partial}{\partial \psi_k} \left[\bar{\rho} \dot{\omega}_k(\underline{\psi}) \tilde{P}_{SGS}(\underline{\psi}) \right] \\ = \frac{\partial}{\partial x_j} \left[\left(\frac{\mu}{\sigma} + \frac{\mu_{SGS}}{\sigma_{SGS}} \right) \frac{\partial \tilde{P}_{SGS}(\underline{\psi})}{\partial x_j} \right] - \frac{1}{\tau_{SGS}} \sum_{k=1}^{N_s} \frac{\partial}{\partial \psi_k} \left[(\psi_k - \tilde{\phi}_k(\mathbf{x}, t)) \bar{\rho} \tilde{P}_{SGS}(\underline{\psi}) \right] \end{aligned} \quad (14)$$

where the time-scale of the sub-grid mixing is assumed to be given by:

$$\frac{1}{\tau_{SGS}} = C_d \frac{\mu + \mu_{SGS}}{\bar{\rho} \Delta^2}. \quad (15)$$

The **SGS**-mixing constant *is set to* $C_d = 2$ (Jones and Kakhi (1998); Bulat et al. (2013); Jones and Prasad (2010)). In the **Eulerian Monte Carlo (EMC)**-method used here, a system of stochastic differential equations (SDE) equivalent to the PDF equation is derived Eq.(14). This equation is estimated by an ensemble of N stochastic fields $\xi_k^n(\mathbf{x}, t)$ for each of the scalars accounting for N_s number of chemical species as well as the enthalpy transport equation, which is then solved with the Monte Carlo method (Valiño (1998)). The evolution of the n^{th} stochastic field is expressed as:

$$\begin{aligned} \bar{\rho} d\xi_k^n &= -\bar{\rho} \tilde{u}_i \frac{\partial \xi_k^n}{\partial x_i} dt + \frac{\partial}{\partial x_i} \left[\Gamma_t \frac{\partial \xi_k^n}{\partial x_i} \right] dt + \bar{\rho} \sqrt{2 \frac{\Gamma_t}{\bar{\rho}}} \frac{\partial \xi_k^n}{\partial x_i} d\mathbf{W}_i^n \\ &- \frac{\bar{\rho}}{2\tau_{SGS}} (\xi_k^n - \tilde{\phi}_k) dt + \bar{\rho} \dot{\omega}_k(\underline{\xi}^n) dt \end{aligned} \quad (16)$$

with $1 \leq k \leq N_s$ and $1 \leq n \leq N$ where the Ito formulation was used. The term $\Gamma_t = \frac{\mu}{\sigma} + \frac{\mu_{SGS}}{\sigma_{SGS}}$ is the molecular plus the sub-grid scale diffusion coefficient while the $d\mathbf{W}_i^{(n)}$ is representing the increments of

a vector Wiener process. The $d\mathbf{W}_i^{(n)}$ is approximated by the time-step increment $\eta_i^n \sqrt{dt}$ where η_i^n is a $\{-1, +1\}$ dichotomic random vector in line with Valiño (1998). All of the one-point moments arising from solution of the SDE's will be identical satisfying thus both the mass conservation and boundedness of the modeled PDF equation.

Due to the heavy computational cost of the ECM method, clustering (Liang et al. (2009)), or agglomeration (Goldin et al. (2009)) is adopted in this study. The method relies on identifying and clustering all cells in all notional fields with similar thermodynamic states into phase-space zones and performing the ODE integration. The mapping of the n^{th} field with composition $\phi^n(Y_1, \dots, Y_{N_S}, h)$ into the discretized phase space can be considered as a mapping between the LES cell-index (LCI) (i, j, k) into the n^{th} zone index in discretized phase space. Reduced descriptions of turbulent reactive flows (for example Ren et al. (2011)) are frequently used where the composition vector $\phi_\alpha^n(Y_1, \dots, Y_{N_S}, h)$ may be described by a reduced number of independent variables $\phi_\alpha^n(Y_1, \dots, Y_{N_R}, h)$ and $N_R < N_S$. Jangi and Bai (2012); Jangi et al. (2013a, 2015) showed, through both DNS and RANS studies under premixed/partially-premixed conditions that computational cells at a given time can be mapped into a phase space $(T, J_H, \nabla J_H \cdot \nabla J_H, Y_{fuel})$. J_H is the mass fraction of hydrogen atom, and $\nabla J_H \cdot \nabla J_H$ is analogous to the scalar dissipation rate. A similar strategy is adopted here; instead of mapping to $\phi_\alpha^n(Y_1, \dots, Y_{N_S}, h)$ or $\phi_\alpha^n(Y_1, \dots, Y_{N_R}, h)$, a mapping is carried out into $(T, \phi, \chi, Y_{fuel})$ space, where ϕ is the equivalence ratio and χ is the scalar dissipation rate. The sensitivity of the results to various extensions of the phase-space dimensionality, e.g., mapping to higher-dimensional $(T, \xi, \chi, Y_1, Y_2, \dots, Y_{N_R})$ spaces can be found in Jangi and Bai (2012); Jangi et al. (2011, 2013b, 2016); Pang et al. (2018).

The laminar flame and ignition delay modeling were performed using the PPREMIX code in CHEMKIN (2013) while the extinction strain rate simulations were performed using CHEMKIN-PRO (2013).

3.3. Chemical kinetic mechanism

One of the key issues with LES using finite-rate chemistry is identifying an adequate reduced chemical mechanism. For example, combustion of methane involves hundreds of species and thousands of reactions and the different reduced mechanisms may have different characteristics. Here, five kinetic mechanisms ranging from 7 to 34 species and 4 to 184 reactions are considered, **listed in Table 2**. A sensitivity analysis of the oxidation scheme on the velocity field for each case considered was performed by Hodzic et al. (2013), and the Warnatz mechanism (Warnatz and Karbach (1997)) was used in Hodzic et al. (2017b). In this work, the laminar flame properties for the different mechanisms are investigated followed by a study of the impact of the mechanism on the heat release rate using the ILES approach. The impact *that* these characteristics have on the capability of the TCI models to predict lean flames close to and during blow-off is also critiqued.

3.4. Numerical Methods

The low-Mach number solver used in this work is based on the OpenFOAM object-oriented library (Weller and Tabor (1998)) using a formally second order accurate finite volume method for the spatial discretization, a second order accurate time-stepping and **Total Variation Diminishing** (TVD) scheme for the convective terms *in the scalar transport equations*. The convective fluxes in the momentum equation are treated with central differencing and pressure-velocity coupling is handled with the Pressure Implicit Splitting of Operators (PISO) method, with a speed-up strategy based on conjugate gradients and multi-grid methods.

4. Sensitivity Study

For the purpose of validation, the results from the simulations have been compared to the experimental data by Kariuki et al. (2012) and Kariuki et al. (2015). **Furthermore**, a grid sensitivity study has been performed for the isothermal case using three different grids with cell-sizes of 0.67mm, 0.44 mm and 1mm at the the shear-layer location, denoted as LES, LES refined and LES coarse, resulting in around 1,500,000, 3,250,000 and 565,000 cells in total, *respectively for the three grids*. Figure 2 shows this comparison between the mean and **RMS**-velocities from the simulations on the three grids and Particle Image Velocimetry (PIV) data by Kariuki et al. (2012). The velocity profiles have been normalized with the bulk-velocity U_{bulk} and the bluff-body diameter $d = 25mm$. Good agreement is observed for all grids compared to the experimental data, with some asymmetry of the experimental data which can be observed close to the bluff-body. The impact of the resolution on the reacting **flow** cases can be found in our previous work (Hodzic et al. (2017b)), together with *the analyses of the* LES quality index (LES_{IQ}) and spectra of the velocity. LES_{IQ} showed that in the entire area of interest, i.e. a few diameters downstream of the bluff-body, the LES_{IQ} exceeds more than 80% indicating a good LES quality (Pope (2000)). Celik et al. (2005) also point out that LES_{IQ} of 75% to 85% can be considered as adequate for most engineering applications typically occurring at high Re numbers. Furthermore, spectral analysis showed that almost two orders of magnitude of the inertial sub-range was resolved. The average and RMS velocity profiles, (Hodzic et al. (2017b)) for both cases A1 and A4 *and the present results shown in Fig. 2* indicate that, disregarding the small asymmetry of the experimental data, *the results from the medium grid are within the uncertainty of the experiments*, i.e. the mass-flow device accuracy of $\pm 3\%$. Based on these results, the medium (LES-grid) has been used for the continued investigation of the flame.

4.1. Laminar flame sensitivity to the chemical reaction mechanism

For finite-rate chemistry computations, it is crucial to assess the chemical reaction scheme. A chemical kinetic model should be able to accurately predict the key flame properties such as the laminar flame speed, ignition delay time and the extinction strain rate. Preferably, the intermediates and radicals in the

flame itself should also be accurately predicted. It is essential to establish whether the reduced chemical mechanism can be used under the very lean, low temperature, atmospheric conditions of interest in the bluff-body stabilized flame considered here.

The investigated reduced reaction schemes are listed Table 2. The laminar flame speeds are shown in Fig. 3 for laminar, steady one-dimensional flames. The detailed chemical scheme Gri-Mech 3.0 and experimental data from Vagelopoulos et al. (1994) have also been added. The JL kinetic model was omitted due to the difficulty of converging below $\phi = 0.75$ conditions even though it performs well under stoichiometric conditions and slightly lean conditions. To the left, the entire range of ϕ values below 1.2 is shown *whereas* to the right, a magnified view of the range $\phi = 0.6 - 0.75$ is shown, i.e. conditions corresponding to cases A1-A5. It is seen that SK30 is almost in perfect agreement with the Gri-Mech 3.0 mechanism, while DRM19 and Warnatz differ. The largest difference is for the Case A1 at $\phi = 0.75$ with approximately 9% for the DRM19 compared to Gri-Mech 3.0. The deviation is smaller for the leaner Case A4, $\phi = 0.64$ with approximately 7% deviation. SK17 shows a different slope as well as lower values for the leaner case when compared to Gri-Mech.

The ignition delay times (IDT) for the *same* chemical schemes are shown in Fig.4. The SK30 results are almost identical to those of the detailed mechanism. DRM19 and Warnatz differ from that of Gri-Mech 3.0, but the largest difference is that of SK17 with increasing deviation for lower temperatures. In general, the *results* show an increase of IDT as the temperature is lowered *as* expected. For easier comparison of the different cases, Fig. 5 shows the IDT for Gri-Mech 3.0 mechanism for all three cases considered. Only a small difference in the ignition delay time can be observed, see Fig. 5, with slightly lower values for the leaner case. As the temperature increases, both cases show almost identical results and the maximum difference is 3% at low temperature. The small difference is not expected to have a notable impact *on* the turbulent flame behaviour.

Flame extinction is an important combustion performance factor in all types of combustors, especially when dealing with very lean, close to blow-off conditions. Here, the ability of the different mechanisms to predict extinction strain rate is considered, as shown in Fig.6 for the Case A1. The extinction *condition*, i.e. the turning point in the graph, shows large discrepancy for the five mechanisms evaluated. It is interesting to note that for SK17, which previously showed the wrong trend, now outperforms both DRM19 and Warnatz.

It can be concluded from the CHEMKIN results that the SK17 scheme performs poorly in the first two tests, while the rest of the schemes are shown to follow the same trend as the detailed mechanism deviating slightly as the blow-off is approached. Based on the laminar flame calculation, we chose DRM19, Warnatz, and SK30 for a detailed turbulent flame sensitivity analysis.

4.2. Turbulent flame sensitivity

Since the heat release (HR) rate is difficult to measure experimentally it is commonly estimated as $HR = CH_2O * OH$ (Kariuki et al. (2015)). In recent work, Hodzic et al. (2017a), a comparison of HR using the ILES approach for validation purpose was presented. Only a minor discrepancy in the HR-*marker* profiles was observed. In order to investigate whether the discrepancy is due to the usage of the estimated HR-*marker* and not the physical HR, the estimated HR-*marker* to the computed HR is evaluated. In Fig. 7, the average calculated HR-*marker* ($HR = CH_2O * OH$) is compared to the actual heat release with the corresponding RMS-results shown in Fig. 8. Both figures show a much bigger difference for the stable case A1. The discrepancy increases further downstream, as shown to the left in Fig. 8. In fact, at $z \approx 0.8d$ downstream, the actual HR is twice the width of the calculated HR-*marker*, both for the average and fluctuating profiles. The peak location, on the other hand, is not significantly affected. The leaner case shows no significant difference in the shear layers although the estimated HR-*marker* underestimates the HR inside the RZ. It is also important mentioning that the estimated HR-*marker* from LES is based on mass fractions and that experimental signal strength may depend on a lot of *other* parameters. The somewhat wider flame predicted by LES can therefore not be explained by the different HR definition using the ILES approach.

For a qualitative comparison of the flames, the mean and RMS of OH were compared to PLIF data *as* presented in the Figs. 9 and 10 for cases A1 and A4 respectively. The mean c-map is based on mass fractions of OH for LES. More precisely, the binarized OH-LES and OH-PLIF images where the regions greater than 50% of the intensity value which correspond to the burned gases are set a value of unity assuming the rest to be regions of unburnt gas. These images were averaged over the complete set of data to obtain the mean progress variable c ranging from 0 to 1. The SK17 *result* is not presented due to the onset of blow-off already at A4 conditions *with this mechanism* whereas the experimental blow-off occurred at even leaner conditions, i.e. $\phi = 0.63$ compared to $\phi = 0.64$ for the case A4. It is evident that all three chemical schemes perform reasonably well, except for the SK17 mechanism which underestimates the flame for the stable case and predicts full blow-off for the A4 condition. Since the *OH* intensity values of the burnt gases were not specified in the experiments, it is difficult to draw any conclusion on the optimal chemical scheme for the current cases. Studying the leaner case, the DRM19 and Warnatz *schemes* certainly look most promising.

For a detailed comparison, the latest simultaneous OH and CH₂O measurements are used (Kariuki et al. (2015)). The estimate of HR-*marker* performed well for estimation of the peak location of HR, but had some discrepancies in the prediction of the width of the HR. Utilizing the ILES approach and all chemical schemes except for SK17, the average and RMS profiles of the HR are shown in Fig. 11 and Fig. 12. Regardless of the chemical scheme used, the HR profile width is slightly underestimated and the location shifted outwards. This shift in the flame position to a larger radial position in the simulation can be partly attributed to the small asymmetry seen in the measurements, Fig. 9, where the measured flame is located

at a smaller radial position at the side where the HR is compared. SK30 fails in predicting the HR inside the RZ whereas the Warnatz scheme performs best. Both the average and RMS profiles show overall good agreement for both stable and just prior to blow-off cases, with some discrepancy in the center of RZ for the leaner case. Overall, the prediction of the radial distribution of the HR is quite good. Based on the results presented in *the* sensitivity study, the DRM19 mechanism is chosen for further simulations due to its *good balance between* performance and computational cost.

4.3. TCI model sensitivity

In Fig. 13 the LES results were obtained for three TCI models: ILES, TPDF, and PaSR, and are compared to PIV data of Kariuki et al. (2012). There is no significant change in the *mean* flow field, regardless of which TCI model was used. A minor difference in the *mean* flow field could be observed between the A1 and A4 cases, as discussed in the experimental study (Kariuki et al. (2012, 2015)). The *mean* length of the RZ and fluctuations in the shear layers are also approximately the same for the two cases (Hodzic et al. (2017b)). The major difference is in the flame migrating into the RZ once blow-off is approached. The flow field on its own is therefore not sufficient for evaluating different combustion models.

Figure 14 shows a comparison of all three models for both of the cases considered. For both cases, the TPDF outperforms the other two models in predicting the peak location of HR-*marker*. The predicted width is slightly larger, especially further downstream. Regarding the leaner flame (A4) to the right, none of the models is able to predict the peak location of HR-*marker*, even though TPDF once again outperforms the other two approaches. The fact that, assuming κ_k (Eq. 6) being equal to unity, i.e. the ILES model, performs better than PaSR model needs a more thorough analysis.

To obtain a clearer indication of the ability of the different models, the normalized individual species concentration (CH_2O and OH) are shown in Figs. 15 and 16 respectively. Focusing on CH_2O , it is clear that the wider profile of CH_2O is the reason for the wider HR-*marker* profiles for case A1. The prediction of the OH level is improved, with the TPDF model performing best. The underestimation of OH inside the RZ causes lower HR in the center of the flame. Overall good agreement is observed for the leaner flame for all models. At approximately $z/d = 0.6$, a deviation is seen in the shear layers *where* the OH levels are overpredicted. It is evident that this discrepancy is larger downstream of the bluff-body which could be due to large-scale instabilities as described in previous work (Hodzic et al. (2017b)) and/or the slightly asymmetric set-up, as mentioned above and shown in Fig. 9.

4.4. Blow-off prediction

The previous subsections have discussed the performance of the model for the two challenging yet stable cases. At the blow-off condition, i.e. $\phi = 0.6$, choosing the same mechanism (DRM19) the TCI models' ability to capture the onset of the blow-off sequence is studied. Once blow-off is approached, only small

changes in the entrainment of the surrounding cold air into the RZ is found, indicating that this is not the main factor influencing blow-off in this unconfined case (Hodzic et al. (2017b)). On the other hand, large concentrations of fuel and intermediate species (CH_2O), as well as strong heat release, appear in the RZ as previously discussed. This is shown in Fig. 17 showing the extremely lean flame with entrainment of CH_2O and unburnt fuel at four time-instances. Even though some fuel is convected downstream, a small amount remains which now moves upstream towards the bluff-body. The iso-contour of OH further demonstrates the complex interaction with CH_2O , i.e. the CH_2O now filling the RZ instead of the OH. Significant amounts of CH_2O are found also at about half of the height of RZ. These pockets of CH_2O and other unburnt and intermediate species enter the RZ, lowering the temperature, and leading to full extinction since the RZ is no longer capable of igniting the incoming mixture. Kariuki et al. (2012) investigated experimentally the duration of the blow-off by varying the blow-off conditions (U_{BO}, ϕ_{BO}), i.e. by either increasing the velocity or decreasing the equivalence ratio. Measurements of the OH^* chemiluminescence were performed during the blow-off event. Here, the blow-off sequence is studied through a sudden decrease of the equivalence ratio from case A4 ($\phi = 0.64$) to $\phi = 0.6$ (Case A5), enforcing blow-off.

A sequence of full blow-off is shown in Fig. 18 showing the gradual decrease in the temperature for the case A5 using TPDF model. The disruption in the shear layers is followed by a decrease in the flame length. Once the temperature in the RZ is too low, the flame is no longer capable of igniting the incoming mixture leading to blow-off. It is important to note that none of the models were able to predict full blow-off at the experimental condition of Kariuki et al. (2012, 2015) ($\phi = 0.63$) using DRM19 scheme. However, all three combustion models predicted blow-off at the A4 conditions using the SK17 scheme. Even though a small uncertainty in the experimental set-up may have a major impact on flame extinction, it is evident that the choice of the chemical scheme is important.

The normalized temperature c is often used for approximating flame thickness, according to:

$$c = \frac{T - T_R}{T_P - T_R}, \quad (17)$$

with T_R and T_P defined as the temperature of the reactants and the products, asserting that flame thickness δ_L is equal to $0.05 < c < 0.95$ or some other, more strict, interval (Cant and Mastorakos (2007)). Mixture fraction on the other hand, is used for quantifying the mixing process, here inside the RZ. Comparison of the three models during the blow-off process is shown in Fig. 19. Here, t_0 is the time-instance at which the mixture at the burner exit attains an equivalence ratio of 0.6 for case A5, a condition at which the flame should extinct. Using the TPDF model, a full extinction of the flame is observed after $\tau_{ext} = 15\text{ms}$. The same time instances are chosen for all three models. The initial state of the blow-off sequence is seen as a relatively thin profile at approximately $Z = 0.035$. The *scatter in mixture fraction is wider* for both PaSR and the TPDF moving towards lower c values, i.e. air entrainment is increasing with lower temperature as a consequence. This is not the case for the ILES model, where the *scatter in mixture*

fraction remains the same but is shifted to lower Z values. Full extinction does not occur using the ILES approach with the current DRM19 chemical model. The PaSR predicts blow-off after $\tau_{ext} = 30ms$ which is, compared to experimental value $\tau_{ext} = 17.5ms$, significantly higher. It is also worth mentioning (Dawson et al. (2011); Kariuki et al. (2012)) that this is a significant time period compared with the characteristic residence time of the burner itself (d/U_b), i.e. $\approx 15d/U_b$. The time-scales involved are thus longer than those of the chemistry and turbulence present here. Just prior to full extinction, seen in Fig. 19 at $\tau = 0.0133s$, the *c-Z scatter plot has a similar shape to its earlier time instances* but shifted downwards towards lower c values. It is important to note that the blow-off at A4 condition using SK17 last approximately the same, i.e. $15ms$, regardless of the model used.

The slightly lifted flame studied here is, as discussed above, stabilized by the hot central recirculation zone. A correct prediction of the diffusion and convection of the radicals within the zone is thus essential for correct prediction of the flame stabilization limits. Comparing the different TCI models shows that both ILES and PaSR are underpredicting the increased local quenching and thus the level of flame fragmentation just prior, and during the blow-off conditions. Despite the fact that the TPDF model slightly overpredicts the blow-off limit, the intensification of the flame fragmentation is accurately captured, shown for example in Fig. 19 and reported and discussed in the experimental study by Kariuki et al. (2015). An alternative view is discussed by Sitte et al. (2016) which focuses on the ignition of the current burner under identical conditions and discusses the quenching and ignition in terms of Karlovitz number (Ka). Sitte et al. (2016) argues that, since neither the u_{rms} nor the length scales L_t differ significantly between the cases, the Ka fields only differ by the factor $1/S_t^2$. However, no strong correlation between the ignition and Ka -number could be identified (Sitte et al. (2016)) but rather a combination of the negative axial velocity and ignition location. The current study also shows that, despite accurately predicting the average flow-flame profiles and the non-dimensional numbers such as Ka -number or Damkohler-number, the complex flame-flow interaction may not always be accurately predicted by the simpler TCI models during the blow-off, despite utilizing identical finite-rate chemistry models.

5. Conclusions

An LES study was performed on a premixed bluff-body stabilized flame at stable conditions, prior to blow-off and during blow-off by decreasing the equivalence ratio ϕ . The LES results were validated against experimental data of Kariuki et al. (2012) and Kariuki et al. (2015), and were found to be in overall very good agreement. Prior to conducting the reactive case study, sensitivity studies were performed ensuring proper resolution, grid independence, the quality of the LES simulation. Identical numerical solvers were

used for all TCI studies, i.e. second order accuracy in time and space using Smagorinsky model with a constant coefficient as is the case in most LES studies (Haworth (2010)).

While statistically stationary flames remain important targets for model development, they do not take into account transient phenomena like blow-off. A key contribution of this paper is that it reports on the transient blow-off, and most importantly, the influence of the finite-rate chemistry and the combustion model in modeling blow-off. While the velocity profiles showed no significant change when using different TCI models or chemical kinetic *schemes*, some discrepancy was observed when comparing the heat release *rate*. It can partly be attributed to the slightly asymmetrical experimental set-up but the impact of the TCI model was evident in the blow-off case. Conclusions of this work are listed:

- Regarding the chemical mechanisms, the JL mechanism (Jones and Lindstedt (1988)) was not useful for lean cases and SK17 (Sankaran et al. (2007)) showed a trend not seen in experiments or for the other chemical schemes when comparing the laminar flame speed and ignition delay time. On the other hand, SK17 performed well in the extinction strain rate test. None of the laminar flame studies could identify an optimal mechanism for lean flames approaching blow-off.
- The estimated HR-*marker* was sufficient for HR comparison. Further, all chemical schemes provided qualitatively good agreement comparing the binarized OH level and a small discrepancy in the peak location of HR when using ILES model, regardless of the chemical mechanism used.
- Evaluation of the different combustion models showed that TPDF outperforms ILES and PaSR in predicting the peak location of the HR and its width. The accuracy of the prediction is better in the A1 case compared to A4. *This could be due to the fact that both ILES and PaSR approaches assume either fully or partially stirred SGS-mixing which is not always valid, especially when dealing with flames close to and during blow off.*
- Since all three models predicted blow-off using SK17 at A4 conditions, DRM19 was chosen for case A5. The LES results confirm the experimental sequence of blow-off using the TPDF model, at the same time, the sensitivity to the reduced chemical scheme. Neither ILES nor PaSR could correctly predict the blow-off sequence. *This study demonstrates that, utilizing stable flames or flames with some degree of local extinction, may not be sufficient for TCI-model development and validation. While statistical flame behaviour may be correctly predicted the dynamical flame instabilities may not always be accurately captured.*

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Figure 1: Cross-section of the burner to the left, the computational domain in the middle, and an illustration of the flame, showing an instantaneous temperature iso-surface at 1500 K to the right.

Table 1: The bulk velocity at the end of the burner and the equivalence ratio ϕ for the studied cases.

Case	U_{bulk} m/s	ϕ
Isothermal	21.6	
A1	21.6	0.75
A4	21.4	0.64
A5	21.4	0.6

Table 2: Chemical schemes

Case	Nbr. of species	Nbr. of reactions
Warnatz (Warnatz and Karbach (1997))	34	164
DRM19 (Kazakov and Frenklach (2005))	19	84
JL (Jones and Lindstedt (1988))	7	4
SK17 (Sankaran et al. (2007))	17	73
SK30 (Lu and Law (2008))	30	184

Figure 2: Comparison of mean (top) and RMS (bottom) velocity profiles from an isothermal LES on three grids, and PIV data by Kariuki et al. (2012).

Figure 3: Laminar flame speed S_L for the five mechanisms and experimental data from Vagelopoulos et al. (1994) to the left, and magnified view of the special area of interest to the right.

Figure 4: Ignition Delay Time *computed using different* chemical schemes used for the three cases considered, Case A1, A4 and A5.

Figure 5: Ignition Delay Time **computed** using Gri-Mech 3.0 for the three cases considered, Case A1, A4 and A5.

Figure 6: Extinction strain rate *computed using different chemical kinetic schemes* for the stable case A1.

Figure 7: Comparison of the experimentally estimated **mean** heat release ($HR_{avg} - PLIF$), **mean** heat release estimated from LES in the same way as the experiments ($HR_{avg} - LES_{calc}$), and the actual **mean** heat release predicted by LES ($HR_{avg} - LES$).

Figure 8: Comparison of the heat release rate fluctuations using **PLIF** ($HR_{RMS} - PLIF$), **RMS** of the heat release estimated from LES in the same way as the experiments ($HR_{RMS} - LES_{calc}$), and the actual **RMS** heat release predicted by LES ($HR_{RMS} - LES$).

Figure 9: Qualitative comparison of the mean **reaction progress variable** (c-map) for the Case A1.

Figure 10: Qualitative comparison of the mean **reaction progress variable** (c-map) for Case A4.

Figure 11: Comparison of the **mean HR marker** for the two cases using three different chemical schemes.

Figure 12: Comparison of the RMS *HR-marker* for the two cases using three different chemical schemes.

Figure 13: Comparison of the mean velocity profiles at six downstream locations.

Figure 14: *Mean HR-marker* ($\text{CH}_2\text{O}^*\text{OH}$) comparing with *HR-marker* from PLIF for the two cases.

Figure 15: Normalized mean CH_2O *PLIF intensity* and mean CH_2O *mass fractions* from *LES* profiles for the two cases.

(a) *CaseA1*

(b) *CaseA4*

Figure 16: Normalized mean OH *PLIF intensity and mean OH mass fractions from LES* profiles for the two cases.

Figure 17: Instantaneous snapshots OH (dark blue), CH₂O (red) and CH₄ (black) at four time-instances.

Figure 18: Temperature field during the full blow-off sequence for case A5 *simulated* using TPDF.

Figure 19: Scatter plot of the progress variable c and mixture fraction Z during the blow-off sequence.