

A Comparative Study of the Simulation of Turbulent Ethanol Spray Flames

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Abstract Experimental data for a series of spray flames is utilized to perform analysis of validation studies conducted by multiple contributors. In this multiphase context, various choices for boundary conditions as well as modeling frameworks and formulations are evaluated. Both large eddy simulation (LES) and Reynolds-averaged Navier-Stokes (RANS) approaches showed the ability to capture droplet evolution with regards to mean and fluctuating velocities. This accuracy is contingent on the proper specification of both droplet and gas phase velocities at the jet exit. The combined effect of combustion and evaporation model choices impacts the downstream volume flux of droplets and resulting gas phase temperature. Further investigation is required to isolate individual model effects for high-temperature spray-laden environments. Proposed solutions involve the simulation of a wider array of flow conditions or lowerlevel experiments to remove the effects of model coupling.

1 Introduction

The simulation of turbulent spray combustion is inherently complex due to the multi-scale interactions between the turbulent flow, the combustion process, and spray droplet dispersion. While several models have been proposed, their validity has not been extensively tested using standard and canonical flame experiments. Establishing model validity is a difficult task, but is primarily attained by comparison with meaningful experimental configurations. In this sense, measurements made in flows that bear resemblance to the final problem of interest, say aircraft engines, is important. The focus of this work is such a validation exercise carried out using the so-called Sydney spray flame [23], which includes a set of experiments of a spray jet flame performed at a range of inflow conditions.

In this effort, we are guided by the success of the Turbulent Non-premixed Flames (TNF) workshop [9], where a similar validation exercise aimed at gas phase

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turbulent combustion was developed. That program, in our opinion, led to a number of advances in the way research is conducted in the area of turbulent flames. First, it provided common ground for experimentalists and modelers to discuss the state-of-the-art in their respective areas, and to use this expertise to advance the goal of predictive modeling. The experimentalists became aware of the specific computational requirements, including well-characterized boundary conditions, which dramatically altered the quality of validation data. Similarly, modelers understood the intricate complexities in measurement science, which enabled better use of data and inference even with limited number of measurements. This workshop changed the modeling and validation perspective in a unique and positive way.

The Turbulent Combustion of Sprays (TCS) workshops have a similar mission but deal with the increased complexities arising from spray-based fuel injection. As we will discuss below, this presence of the liquid phase dramatically alters the level of information required for simulations, creating a tougher environment for developing well-characterized measurements. In particular, the inflow conditions require more detailed characterization than that envisioned in gas phase flames. The purpose of this article is twofold: (1) Provide a summary of the validation exercise conducted as part of the TCS2 and TCS3 workshops, and (2) discuss the key information needed to fully characterize and inform the simulations.

2 Experimental Configuration

In this section, the experimental configuration and a discussion of the validation data from the perspective of the simulations are provided.

The Sydney spray flame were conducted at University of Sydney by Masri and co-workers [5, 11, 23]. From a modeling perspective, this is one of the very few experiments that contain sufficient characterization of the configuration that allows for advanced modeling tools such as large eddy simulation (LES) to be used. The geometry of the burner is shown in Fig. 1. The burner consists of a round central jet, supplying atomized liquid fuel carried by air, a pilot flame and an outer air coflow. The burner is mounted vertically with a co-flow wind tunnel velocity of 4.5 m/s. The outer diameter of the burner annulus is 25 mm with a lip thickness of 0.2 mm. The pilot flame consists of a stoichiometric mixture of hydrogen, acetylene and air. The liquid spray is initially introduced 215 mm upstream of the nozzle exit plane. Previous spray flame experiments have used this burner, and additional details on the configuration can be found in [23, 37].

The series of experiments varied both liquid fuel and air mass flow rates in the core jet. Figure 2 shows the parameter space for the flame series, which lie well within the stability limits for ethanol fuels (shown by solid lines in Fig. 2). From within this extensive database, three flames were selected for further modelling studies, namely cases 2, 6 and 7 for either of acetone and ethanol fuels (i.e. Cases EtF2, EtF6, EtF7 and AcF2, AcF6, AcF7). In this initial work, only two flames are selected for further analysis, specifically the ethanol fuel cases EtF2 and EtF6. Flow parameters for these flames are seen in Table 1.

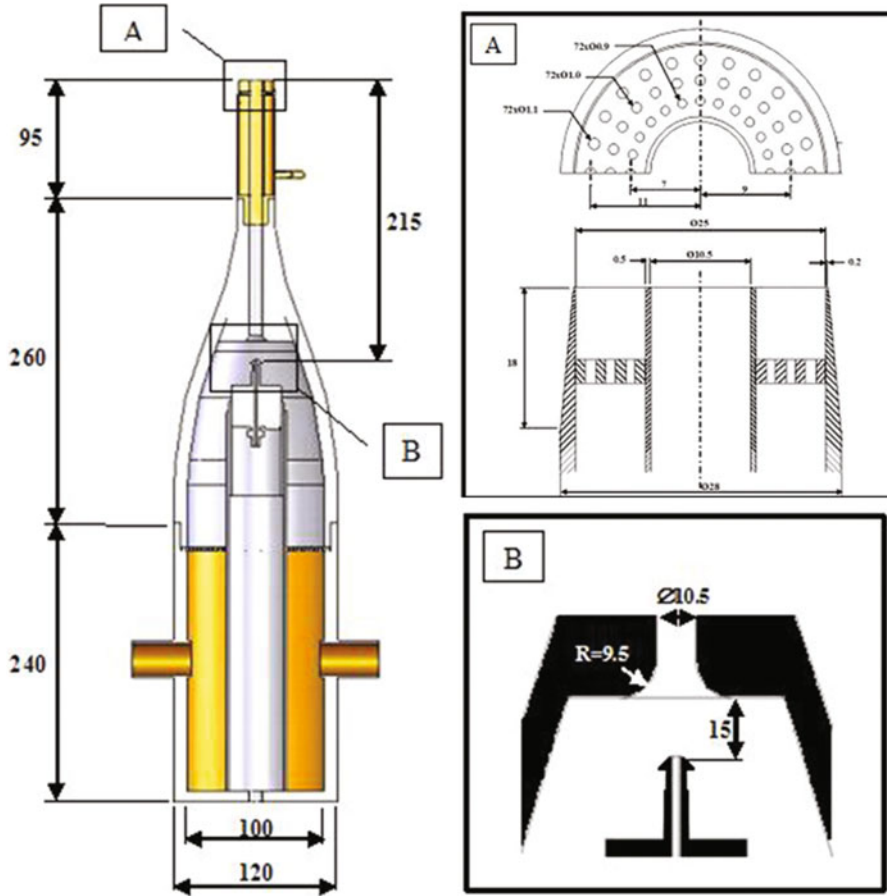


Fig. 1 Sydney burner configuration. Inset views show the pilot burner outflow (*top*) and nebulizer contour (*bottom*)

2.1 Inflow Conditions

As mentioned in Sect. 1, inflow conditions play a crucial role in the validation tests for spray flames. In aircraft engines, liquid jets are atomized before entering the main combustion region. In such flows, the description of the atomization process controls the spray number density function, as well as the spatial penetration of the fuel jet. Accurate characterization of the atomization process remains a challenging problem to model [10]. However, the focus of this work is on the interaction of atomized droplets with the turbulent flame, allowing for the use of simpler inflow conditions. In the experiments, a nebulizer is used to generate low-momentum droplets, which are then carried downstream by the surrounding flow. The droplet-air mixture passes through the 215 mm pipe, where both the gas phase turbulence and droplet velocities

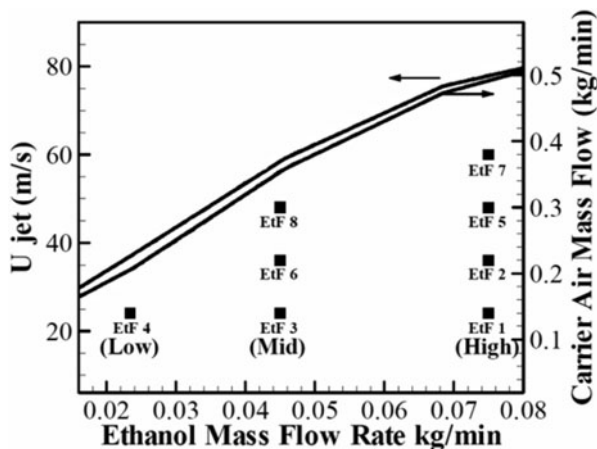


Fig. 2 Ethanol flame series air and fuel mass flow rate. Ethanol flame stability limits denoted by solid lines

Table 1 Selected flame conditions

	EtF2	EtF6
Bulk velocity (m/s)	36	36
Liquid fuel injection rate (g/min)	75	45
Measured liq. flow at jet exit (g/min)	66.3	41.1
Vapor fuel flow rate at jet exit (g/min)	8.7	3.9
Equivalence ratio at jet exit	0.3	0.2
Jet Reynolds number	30,500	27,400
Flame length (cm)	72	53

develop. Due to the relatively high volatility of ethanol, significant evaporation occurs in the pipe. This evaporation rate increases with fuel loading, and EtF2 exhibits much higher liquid-phase loss compared to EtF6 (Table 1).

The evaporation and the presence of the long pipe produce flow anisotropies, the impact of which are difficult to assess due to the lack of detailed measurements. First, due to significant droplet inertia, especially for the larger particles, it is reasonable to expect a change in the droplet size distribution as a function of the axial distance traversed in the pipe. Moreover, the presence of the walls could lead to additional issues including condensation and potential droplet-droplet interactions (although the bulk loading is still in the dilute regime). Second, evaporation inside the pipe leads to fuel release in the gas phase, which then mixes with the carrier fluid downstream of the nebulizer. Since the droplet evaporation itself is spatially inhomogeneous, gas phase fuel concentration is also expected to be inhomogeneous. Depending on the level of turbulence in the pipe, there could be incomplete mixing by the end of the pipe leading to a non-uniform spatially and temporally varying fuel inflow condition. At this point, the experiments do not have the information necessary to characterize the scalar distribution. Rather, any such discrepancy from the uniform inflow conditions has to be inferred from flame behavior downstream.

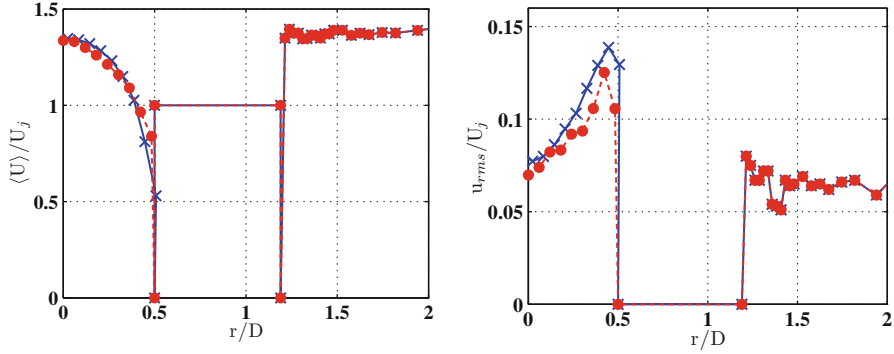


Fig. 3 Experimental gas phase streamwise mean (*left*) and RMS (*right*) velocities at $x/D = 0.3$ for cases EtF2 ($\times$) and EtF6 ($\bullet$)

The experimental data closest to the inflow consists of measurements taken at $0.3D$, where D denotes the diameter of the central jet. In order to validate simulation inflow conditions, experimental results at this most upstream location report radial profiles of two components of velocity for both the gas and dispersed phase, as well as droplet volume flux and probability density functions of droplet diameter. Figure 3 shows the streamwise mean and RMS velocities measured for the air/fuel mixture. Despite a significant difference in droplet mass loading between the two cases, the normalized mean gas velocities and relative turbulent intensities are similar. It should be noted that neither case is fully turbulent at the jet exit due to presence of droplets slowing the development of the near-wall turbulent structures.

From the simulation viewpoint, inflow conditions are required for both gas phase and droplet phase. While the gas phase properties are inferred based on the discussion above, specifying the inflow conditions for the droplet is more difficult. For the models used here, the droplet size distribution as well as the velocity distribution are required. The experimental data consists of droplet class-specific velocity component statistics at axial distance of $0.3D$ (Fig. 4). Clearly, there is appreciable variation in the velocity depending on the size, indicating that droplet residence time in the pipe will vary with diameter, thus causing droplets to be differentially evaporated. Smaller droplets will evaporate faster, leaving larger droplets behind as the spray traverses the pipe. This will result in a higher SMD further downstream with a distribution that is skewed towards larger droplets and an increase in D_{10} as is observed experimentally. Additionally, the slip velocity at the exit plane is not zero and larger droplets are slower than the gas phase, thus increasing their residence time. The impact of the skewed distribution and the slip velocities on the calculations is not known and needs to be ascertained.

Figure 5 shows the droplet size distribution function, normalized by the total number density. As expected the near-wall distribution contains more of the larger droplets, indicating that these droplets enter the boundary layer close to the pipe wall. This indicates that the number density function is nonuniform across the inlet.

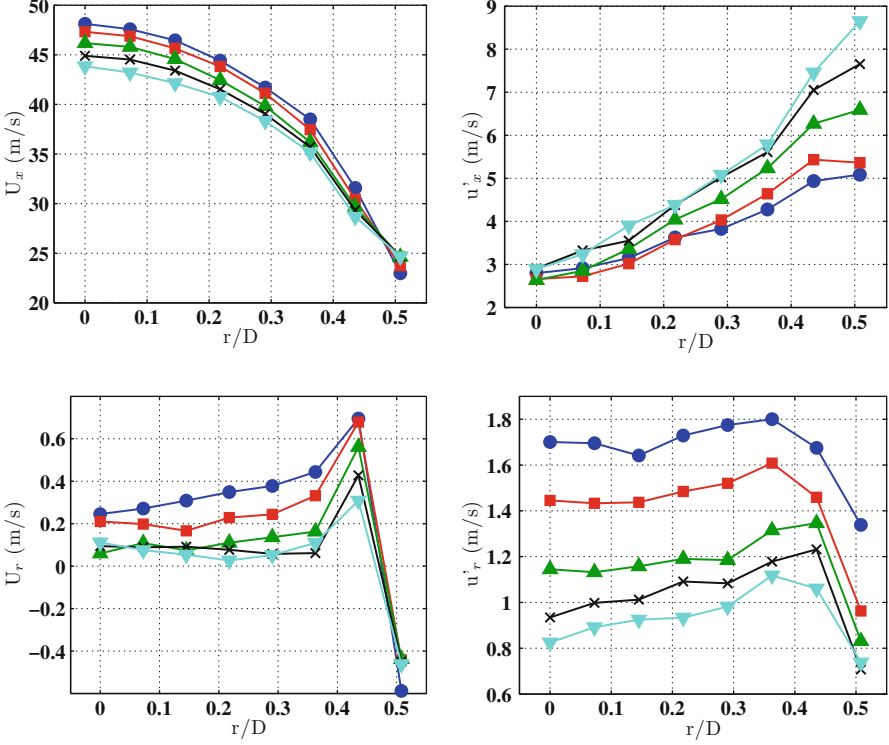


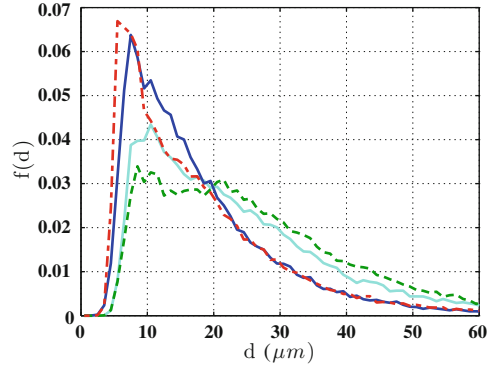
Fig. 4 Experimental droplet velocities from EtF2 at $x/D = 0.3$, including streamwise mean (*top left*), streamwise rms (*top right*), radial mean (*bottom left*), and radial rms (*bottom right*). Droplet diameter subranges are given by 0–10 μm (—●—), 10–20 μm (—■—), 20–30 μm (—▲—), 30–40 μm (—×—), and 40–50 μm (—▼—)

The lack of a fully developed gas phase flow velocity (inferred from the smallest droplets) is likely due to the presence of these large droplets that attenuate the turbulent fluctuations.

2.2 Validation Data

In addition to the measurements at the nozzle exit, measurements were collected downstream in order to validate the unconstrained droplet mixing and evaporation processes. The available data includes radial profiles of the following time-averaged quantities: (1) Two component mean and RMS droplet velocities, (2) corresponding Reynolds stresses, (3) droplet volume flux, (4) D_{10} and D_{32} moments of the droplet diameter distribution, and (5) gas phase temperature. For these flames, gas phase temperature data is available at streamwise positions of $x/D = 10, 20$, and 30 ,

Fig. 5 Experimentally measured droplet diameter PDF at $x/D = 0.3$ at centerline for EtF2 (—) and EtF6 (---) and again near nozzle wall for EtF2 (—) and EtF6 (---)



while all other quantities are available up to $x/D = 30$ in increments of five jet diameters.

3 Simulation Data from Multiple Contributing Groups

As part of the TCS3 workshop, four different groups contributed to the comparisons. The simulation approaches, inflow conditions, and combustion models run the gamut providing a rich set of simulation results for comparison. In this section, the individual contributions and the simulation techniques are discussed.

Of the four groups of contributors included in this study, three use LES and one uses a RANS approach. All four represent the dispersed phase with a coupled Lagrangian solver applying the point particle assumption [8, 38]. A summary of notable contributor methods are presented in Table 2 with the supplied data specified in Table 3, while additional simulations details and defining characteristics are provided in the following sections.

University of Darmstadt (UDRM) The contributions of M. Chrigui¹, S. Fernando, and A. Sadiki from Technische Universität Darmstadt, designated here as UDRM, included all droplet related quantities of interest for case EtF6. Unique to this simulation amongst all the contributions, the domain extends upstream to the atomizer droplet injection point. The computational domain downstream of the nozzle exit extends 20.4 jet diameters radially and 76.2 jet diameters in the streamwise direction. The structured cylindrical mesh consists of 1.1 million cells. Additional details for analogous simulations have been previously published [6].

With the boundary conditions being specified at the upstream end of the pipe, both gas and droplet phase boundary conditions are relatively simple, allowing for the development of turbulent structures along the 215 mm pre-mixing length before the nozzle exit. The carrier air is introduced at a constant streamwise velocity across

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Table 2 Contributor configuration summary

	Chrigui et al.	Heye and Raman	Prasad et al.	Wunsch et al.
Designation	UDRM	UT-A	USYD	NMCA
Model	LES	LES	LES	RANS
framework				
Inflow location	Nebulizer exit	Nozzle exit	Nozzle exit	Nozzle exit
Grid size	1.1 million cylindrical cells	384 x 192 x 64 cylindrical	200 x 100 x 100 Cartesian	250 x 75 x 2
Gas phase inflow velocity	Bulk velocity	Fully turbulent pipe flow	Synthetic turbulent to match experimental mean and rms [21]	Prescribed experimental mean and rms
Droplet inflow velocity	Mean matches gas phase with Gaussian rms	Interpolate gas phase velocities to droplet locations	Match experimental mean and rms by diameter class	Match experimental mean and rms by diameter class
Droplet inflow diameter	Discrete MDF to match experimental PDF for droplet diameter classes	Log-normal distribution to match experimental centerline PDF	Nukiyama- Tanasawa distribution matching experimental centerline PDF [27]	Nukiyama- Tanasawa distribution respecting D_{10} and D_{32} for each diameter class [27]
Droplet inflow location	Gaussian random distribution	Uniform random distribution	Random with centerline bias to match experimental flux	Uniform random distribution
Evaporation model	Non- equilibrium [1, 36]	Equilibrium [34]	Equilibrium [1]	Non- equilibrium [25]
Combustion model	FPVA [3]	FPVA [32]	Detailed chemistry	Flamelet
Chemistry mechanism	56 species, 351 reversible step reaction mechanism [22]	50 species, 235 reaction combustion mechanism [4]	Reduced 27 step ethanol mechanism [30]	Ethanol oxidation mechanism [19]
Lagrangian SGS fluctuations	None	None	None	Turbulent dispersion model [24]

the radial profile, with no radial or swirl velocity and no initial turbulence. Droplets are initialized with a matching mean streamwise velocity, while including non-zero radial velocities in an attempt to replicate the nebulizer spray angle, as well as significant turbulent velocities. The droplet inflow diameters were tuned to obtain

Table 3 Summary of case-specific quantities of interest supplied by each contributor.

	Streamwise Vel.	Radial Vel.	D_{10}	Volume Flux	Gas Temp.
UDRM	EtF6	EtF6	EtF6	EtF6	
UT-A	EtF2/6	EtF2/6	EtF2/6		EtF2/6
USYD	EtF2	EtF2			EtF2
NMCA	EtF2/6	EtF2/6	EtF2/6	EtF2/6	EtF2/6

the proper nozzle outflow profiles with locations chosen from a Gaussian distribution to allow for centerline bias.

The continuous phase is solved following an Eulerian approach using a 3D low-Mach number LES code [20, 35, 40]. The solver uses block structured and boundary fitted grids. It is based on the finite volume method in which a co-located grid with a cell-centered variable arrangement is applied. For spatial discretization, specialized central differencing schemes that hold the second order for arbitrary grid cells are used. The convective term in the scalar transport is discretized using non-oscillatory, bounded total variation diminishing (TVD) scheme. For the time stepping, a multiple stage Runge-Kutta scheme with second order accuracy is used. A fractional step formulation is applied and at each stage a momentum correction is carried out in order to satisfy continuity. Hence, a Poisson equation is derived from the continuity equation and solved iteratively with multi-grid and SOR relaxation. The parcels are tracked using a Lagrangian approach, in which the ordinary differential equations describing movement in physical space, the temperature evolution and the evaporation-related mass loss are discretized using Euler first order schemes and solved explicitly.

Droplet evaporation is modeled using the uniform temperature (UT) model of Abramzon et al. [1] and Sirignano [36]. The model describes the evolution of the droplets' temperature and diameter, i.e. evaporation rate and energy flux through the liquid/gas interface. This model is based on the film thickness theory. It does not consider any temperature variation in the interior of the droplets (homogenous temperature). However, the temperature variation is time dependent and accompanied by an unsteady mass transition. Gas phase combustion was modeled using flamelet generated manifold approach [3] that utilizes a 56 species, 351 reaction ethanol combustion mechanism [22].

University of Texas at Austin (UT-A) The LES data collected by C. R. Heye and V. Raman (see [14] for details), further designated by UT-A, included all validation quantities except for droplet volume flux for both EtF2 and EtF6. The simulation inflow is located at the outflow of the jet nozzle, allowing for more direct application of the most upstream experimental measurements. The cylindrical grid is $192 \times 128 \times 64$ cells in the streamwise, radial and azimuthal directions, respectively. The domain captures the entire flame, extending 15 jet diameters in the radial direction and 80 diameters in the streamwise direction.

Gas phase inflow velocities were taken from a separate fully turbulent pipe simulation without spray to provide time-correlated turbulence. Droplet velocities at the inflow were determined by interpolating gas phase velocities to each droplet's location, thus imposing a small Stokes number approximation. The diameter of inflowing droplets was chosen from a log-normal PDF fit to experimental centerline

measurements for each flame. This distribution was assumed to be valid at all radial locations within the core jet. Droplets were uniformly distributed across the jet.

The flows considered here fall in the low-Mach number regime but with variable density induced by boundary conditions and combustion-related energy release. Hence, a low-Mach number fractional time-stepping based LES solver is employed [2, 31, 32]. The essential components of the low-Mach number algorithm are the velocity advancement and pressure-based velocity correction to enforce continuity equation. In order to increase the time-step used, the viscous terms and the convection terms in the radial and azimuthal directions are treated implicitly [7]. To reduce computational expense, an iterative algorithm is used to solve the resulting nonlinear discretized equation [2, 31]. A second-order central scheme is used for spatial discretization in the momentum equations, while a third-order upwinded scheme [13] is used to discretize the nonlinear terms in the scalar transport equations. Further details of the LES algorithm are provided in [7]. The turbulent diffusivity and viscosity terms are modeled using a dynamic Smagorinsky approach [26].

An equilibrium evaporation model was used [34] without accounting for any sub grid turbulent dispersion. In order to improve accuracy in combustion modeling over the commonly used presumed PDF methods while maintaining computational efficiency, a transported joint scalar PDF method for spray laden flows has been developed and applied by the contributors [14]. The joint-PDF of mixture fraction and progress variable is solved using this approach, with the chemical source term for progress variable obtained from a lookup-table. The table itself was constructed based on the flamelet/progress variable approach [32] using a 50 species, 235 reaction mechanism [4].

University of Sydney (USYD) The LES results submitted by V. N. Prasad, S. Navaro-Martinez² and K. H. Luo³, designated henceforth as USYD, contain streamwise droplet velocities and gas phase temperature for EtF2. As with UT-A simulations, the domain inflow is specified at the pipe exit and includes a cross-section of 12 jet diameters in each spanwise direction, with a streamwise extent of 39 jet diameters. The Cartesian grid consists of $100 \times 100 \times 200$ points in the three coordinate directions.

The gas phase inflow velocities utilized the digital inflow generator of di Mare et al. [21] using the experimentally-measured mean and RMS velocities at the pipe exit. Droplet diameters are initialized at each time step through random selection from the reported centerline PDF form [27]. This PDF is presumed accurate across the entire jet cross-section. Each component of the droplet velocity is taken from the experimental measurements, with diameter subrange dependence enforced.

The in-house code BOFFIN [15] developed at Imperial College London was used for the LES simulation. The code is based on a semi-implicit low-Mach number formulation, with all spatial gradients being discretised with energy conserving second order schemes except for the scalar convection, for which a TVD scheme is applied. Following previous studies (e.g. [16, 17]), eight stochastic fields are employed to

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