

# Mind the gap: turbulent combustion model validation and future needs

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## Abstract

This overview collects a range of well characterized experiments used in the step-wise validation of turbulent combustion models, from gas phase non-premixed jet flames to spray flames, and from simple symmetric jets to real device geometries, focusing primarily on statistically steady state experiments. We discuss how the experiments and models are constructed, approaches to modelling, and the tradeoffs between the level of detail and computational demands. The review highlights a number of experiments used for benchmarking models, selecting a few examples where models have clearly succeeded, as well as some areas where there are clear needs in the experimental database. In particular, the areas of turbulent spray combustion and soot prediction, as well as combustion under high pressures appear as the least developed and present the clearest gaps for both models and experiments. Based on the successful application of advanced methods of uncertainty quantification to a number of problems in reacting flows, we suggest that these methods might be used to advantage in the design of experiments. This would enable an upfront examination of the extent to which comparisons between measurable scalars and velocities allow clear distinction between model features.

*Keywords:* turbulent combustion, diagnostics, model validation

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## 1. Introduction

The general objective in the design of devices using turbulent combustion is to produce clean hot gases in a stable manner over a wide range of conditions, either for the direct, efficient conversion into mechanical power in engines and turbines, or for the indirect use of enthalpy for heat exchange with some other fluid, for purposes of heating or power generation. This apparently simple mission stumbles into inherent tradeoffs between stability and the production of undesirable pollutant byproducts. Enormous progress has been made in numerical modelling of reacting and non-reacting flows, yet one cannot always make accurate predictions about the pollutant emissions, instability or reaction limits of new devices without building them. This state of affairs results from the incomplete knowledge of some of the fundamental kinetics (particularly in the case of large hydrocarbons and soot), as well as from inherent difficulties in predicting the behavior of highly non-linear turbulent flow systems.

In this paper, we take a very broad view of the state of turbulent model validation over the past decade, and set the stage for a discussion of what may be opportunities for developing more efficient validation strategies for turbulent combustion models. There is only so much room in a topical review (and panel discussion) to cover such a broad topic. The present paper provides an entry point by collecting information on validation targets and methods, and identifies some of the directions for research and methods. For conciseness, we only consider stabilized flames as a target, excluding the growing database of unsteady experiments in combustion vessels, rapid compression machines, and engines.

The paper is structured as follows: a brief review of the issues in turbulent combustion is presented, describing the key difficulties in modelling and measurements, followed by a discussion of the process of validation, existing databases, and the state of the art in model comparisons. The review leads to a reflection on the gaps in the database, and finally, to questions about how current models can be used to improve the development of validation experiments.

## 2. Turbulent Combustion Models and Closures

### 2.1. Multiscales and Multiscalars

There are three main challenges associated with modelling turbulent reacting flows, as discussed in many distinguished reviews and books [1–4]: (a) the vast range of temporal and spatial scales, from device spatial scales of the order of meters down to micrometer scales

where mixing and viscous dissipation take place; (b) the range of species reacting at different time scales; (c) the highly non-linear behavior of chemical reactions with the highly variable local temperature. For the modeller, this means that not all scales and not all species may be accurately reproduced, and a compromise between fidelity and computational resources must be made. For the experimentalist, these demands challenge the dynamic range and resolution capability of any technique. The mesh resolution in practical CFD calculations cannot span the range of scales, and some spatial averaging or filtering must be done: subgrid models must therefore account for the non-linear contributions of the unresolved fluctuations.

The ratio of the largest length scale  $\ell_T$  to the molecular diffusion length scale  $\ell_K$  can be approximated based on the hypothesis of scale-invariant dissipation rate [5, 6],  $\left(\frac{\ell_T}{\ell_K}\right) = \text{Re}^{\frac{3}{4}} = \left(\frac{u_T \ell_T}{\nu}\right)^{\frac{3}{4}}$ , where  $u_T$  is the integral turbulent velocity,  $\nu$  the fluid viscosity, and  $\text{Re}$  the corresponding turbulent Reynolds number. Correspondingly, integral time scales vary according to  $\left(\frac{\tau_T}{\tau_K}\right) = \text{Re}^{\frac{1}{2}}$ . At the high pressures and flows rates associated with high specific power in gas turbines and engines,  $\text{Re}$  can be of order  $10^3$  to  $10^5$ , so that two to three orders of magnitude in time or space need to be resolved. Whilst this lies in the realm of petascale direct numerical simulations, it is clearly beyond the reach of repeated design calculations. The turbulent time scales are compared to the corresponding chemical (and chemical-diffusive) scales  $\tau_c$ , generating the Damköhler number,  $\text{Da} = \tau_T/\tau_c$  and Karlovitz number,  $\text{Ka} = \tau_c/\tau_K$  [7, 8], and the two numbers are related by  $\text{Da Ka} = \tau_T/\tau_K = \text{Re}^{1/2}$ .

Flame-like structures are associated with short chemical time scales, with  $\text{Da}$  in the hundreds, and these tend to exist as wrinkled or intermittently extinguished flames up to  $\text{Ka}$  of the order of thousands [9, 10]. Under autoignition processes taking place at the initiation of combustion in compression-ignition engines, time scales can be large, with low  $\text{Da}$ , and reactions take place in a more spatially distributed mode. High power density demands higher  $\text{Re}$  and  $\text{Ka}$  numbers, and the job of the designer becomes to understand the limits of turbulent mixing and reactions for a particular objective.

The focus of a large number of experimental and modelling studies has been to investigate how well models of turbulent diffusion and premixed flames are able to represent the observed species or flame propagation characteristics, and to some extent the limits of stable combustion under these conditions. These studies, and the philosophy governing the experimental efforts de-

signed to validate these models (or not), are described in some detail in the next section. But first, let us take a look at the equations that govern scalar reactions, which are the source of the difficulties.

## 2.2. Governing equations

Turbulent combustion models use differential conservation equations, typically in an Eulerian framework, to make predictions about the evolution of the relevant scalars and velocity fields. At the simplest level, what makes combustion special in comparison to non-reacting turbulent flows is the evolution of the scalar species and release of thermal energy, which leads to density changes, and thereby a coupling with momentum. In practice, the key scalars are species which represent progress of reaction or heat release (often a sum of CO, CO<sub>2</sub>, and H<sub>2</sub>O), temperature, and a total mixture fraction  $Z$ , usually a normalised linear combination of species representing the total original atomic abundance in the reacting streams. If we consider only gas phase species, in the low Mach number limit for many situations, the conservation equation for a scalar  $\psi$  reads, in the approximation of Fickian diffusion:

$$\frac{D\rho\psi}{Dt} = \frac{\partial\rho\psi}{\partial t} + \nabla \cdot (\rho\mathbf{u}\psi) = \nabla \cdot (\rho D_\psi \nabla\psi) + \dot{\omega}_\psi \quad (1)$$

where radiative heat losses are not considered in the case of the energy equation. Equation 1 can be filtered or time-averaged [2, 3, 11] to yield an equation of form:

$$\frac{\partial\bar{\rho}\tilde{\psi}}{\partial t} + \nabla \cdot (\bar{\rho}\tilde{\mathbf{u}}\tilde{\psi}) = \nabla \cdot \mathbf{T}_\psi^u - \nabla \cdot \mathbf{T}_\psi^D + \bar{\omega}_\psi \quad (2)$$

where the flux terms for convection with velocity  $\mathbf{u}$  and density  $\rho$ ,  $\mathbf{T}_\psi^u = \bar{\rho}(\tilde{\mathbf{u}}\tilde{\psi} - \mathbf{u}\psi)$ , molecular diffusion,  $\mathbf{T}_\psi^D = \rho D_\psi \nabla\psi$  and reaction  $\bar{\omega}_\psi$  require modelling. The averaged or filtered terms do not in general correspond to the values of the operators evaluated at averaged or filtered conditions: departures from the averaged temperature create significant deviations in the reaction rates of most scalars, which depend exponentially on the local temperature. Extensions and variations of these models are required, for example, for systems involving multiple phases, such as spray or particle reactions, which require additional source terms for the scalars, which couple with the liquid or solid phase. The following discussion concerns closure models and experiments for scalars primarily in the gas phase.

## 2.3. Combustion closures

Closures are traditionally grouped into a choice of how the subgrid or fluctuating model handles diffusional

and reaction terms in Eq. 2. There are excellent recent reviews on the details of the many models and their usage, as detailed below; a guide to best practices to the use of these models has also recently appeared [12]. The next subsections briefly describe flamelet and PDF/micromixing models.

### 2.3.1. Flamelet models

Flamelet models assume that the time scales associated with chemical reaction are smaller those associated with turbulence. The conservation equations then allow the diffusion and reaction terms to be combined into a single entity, the flamelet, which can be transported convectively by the turbulent flow. Closure of the reaction term typically invokes a presumed PDF model, tied to conservation equations for the variance of the progress variable and mixture fraction, which gives rise to a term involving the subgrid scalar dissipation rate  $\overline{\chi_\psi} = \overline{D_\psi |\nabla\psi|^2}$ . The latter is finally related to the filtered or grid scale  $\Delta$ , a local turbulent viscosity (or reciprocal time scale  $\tau_\Delta$ ) and a scalar variance, often via an algebraic closure, or modelled with corrections for reactive scalars. Flamelet models offer great simplification, by tying most scalars to a single progress variable  $c$ , which is transported by turbulence, and a local representation of the conserved atomic scalar in the form of a mixture fraction,  $Z$ . Reviews of models for premixed and non-premixed flamelets and variations thereof explain in greater detail how the progress of reaction is connected to other scalars via pre-calculated and tabulated flamelets [4, 7, 13–15]. The key disadvantage of the method is of course associated with the assumption of the existence of a flamelet, which may not hold in situations such as autoignition, multiple streams or for scalars for which reacting time scales are larger than turbulent time scales. Even in these cases, however, extensions have allowed continuation where the model assumptions are broken, by using additional progress variables, in the case of slowly varying soot [16–18] or NO [19], or by using switching variables to capture the behavior of partially premixed flames [20, 21], or autoignition in lifted flames [22].

### 2.3.2. Micromixing models

Micromixing models, which encompass transported-PDF models, make no assumption regarding the ratio of time scales of reaction relative to turbulence time scales, are therefore applicable over any range of Damköhler or Karlovitz numbers. Simple micromixing models assume full or partial mixing within the subgrid scale, accompanied by reaction [1, 23]. Full transported

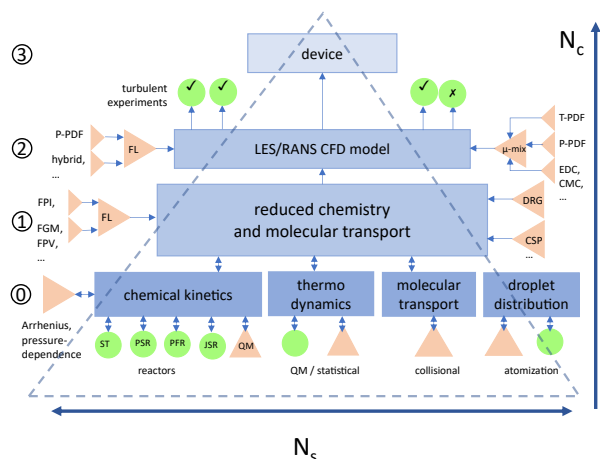


Figure 1: Hierarchy of model validation. Tan triangles: sub-models; green circles: experiments. Numbered circles (left): validation tier levels. Arrows: direction of information.  $N_c$ : number of cells;  $N_s$ : number of scalars. Acronyms indicated are for the many devices and methods used. Tier 0: PSR, PFR, JSR: perfectly stirred, plug flow and jet-stirred reactors; ST: shock tube; QM: quantum mechanical calculations. Tier 1: Example chemical reduction methods, including, FL: flamelet, FGM: flamelet generated manifold, FPV: flamelet-progress variable; FPI: flamelet-progress indicator; DRG: directed relation graphs; CSP: computational singular perturbation. Tier 2: large classes of flamelet (FL) or micromixing ( $\mu$ -mix) models, for example: PDF: probability distribution function, T-PDF, P-PDF: transported/presumed PDF; CMC: conditional moment closure, EDC: eddy dissipation closure.

PDF approaches integrate equations for the evolution of the multivariable, single point PDF, but require models for closing the mixing term. The latter must resolve molecular diffusion at the smallest scales, a difficult task which can be achieved only by including efficient models of diffusion across the multidimensional space [1, 4, 24, 25]). A number of simplified variants of PDF and stochastic models significantly reduce the dimensions across which diffusion occurs, for example one-dimensional turbulence [26], conditional or multiple mapping closures [27, 28], which lower the dimensionality of systems by projecting the dependence of species onto a small number of variables.

The need to control computational costs associated with these complex multiscale, multiscale calculations generates a hierarchy of model validation, as discussed in the following sections.

### 3. Hierarchical model validation

Turbulent combustion models include models for chemistry and molecular transport, the associated heat release, and turbulent transport, as outlined in Fig. 1. The size of the computational problem or system  $N_s$  is approximately proportional to the product of the num-

ber of cells in the system  $N_c$ , and the number of scalars involved in the system,  $N_s$ , defining the total computational time. There is therefore an inherent tradeoff between the achievable level of detail in the model, represented by  $N_s$  and the geometric extent or detail ( $N_c$ ) for a given total duration of the simulations. In order to accomplish a simulation given a total available computational resource, higher order models are simplified to a smaller number of scalars (or cells), requiring validation at each level moving up in the hierarchy. Validation starts from comparisons of chemical kinetic and thermodynamic models against fundamental experiments or quantum mechanical calculations (Tier-0), moving onto the generation of reduced chemical and transport models (Tier-1). At the lowest Tier, chemical and transport models can be very detailed, whereas the flow setup may be simple, such as a fully mixed device. A validation strategy between reduced order models against their more detailed counterparts with a larger number of scalars (*e.g.* using techniques for systematically reducing mechanisms) or a smaller number of cells (*e.g.* models for the PDFs of unresolved quantities, such as presumed or transported PDFs), ensures that the next step in the hierarchy can be taken with some assurance. The focus of the present paper is specifically on the validation of turbulent combustion models in (Tier-2), but it is useful to consider parallels and distinctions between the process of validation of chemical kinetics to the validation of turbulent combustion models.

#### 3.1. Tier 0 - Chemical kinetics, transport and thermodynamics

Simulations and validation experiments often start by selecting the appropriate level of detail for the problem, from equilibrium to single-step reactions, to multi-step reactions. There is a vast literature dedicated to the subject for a variety of fuels, and well established methods for composing and extracting chemical kinetic models from data emerging from shock tubes, jet stirred and plug flow reactors, as well as theoretical models [29, 30]. Periodic reviews of the available information are codified into comprehensively validated models for hydrocarbon oxidation for a variety of hydrocarbon fuels over a wide range of temperatures and pressures. Examples of well understood oxidation mechanisms are (a) the GRI mechanism for methane [31], (b) mechanisms for syngas oxidation [32], and (c) mechanisms for hydrocarbon autoignition [33–35]. However, reaction mechanisms and their rates are continually revised, with an optimal set of reactions and their constants produced in a feedback loop between experiments and models,

246 informed by sensitivity analysis and uncertainty quan- 296  
247 tification, to extract optimum parameters in the sense 297  
248 of a feasible optimum set [30, 36]. Both the chemistry 298  
249 and the thermodynamics for liquid and solid fuels are 299  
250 less well studied than that of smaller hydrocarbons, al- 300  
251 though there are a number of well established surrogate 301  
252 models for diesel and gasoline surrogates used both for 302  
253 flames and autoignition. Mechanisms for soot forma- 303  
254 tion are significantly more complex, involving sectional 304  
255 (size dependent) models, yet validation datasets for soot 305  
256 are rarer than for hydrocarbons. Models for soot are al- 306  
257 ways a low order model, representing the thousands of 307  
258 species or classes thereof [37, 38]. Model reduction is 308  
259 often necessary prior to incorporating into combustion 309  
260 models, yet one must keep in mind how these models 310  
261 were originally obtained, as well as simplified, lest they 311  
262 be used beyond their validation range. The final tar- 312  
263 get of a turbulent combustion simulation may or may 313  
264 not be sensitive to the uncertainties in the chemical ki- 314  
265 netic mechanism or thermodynamic model, yet system- 315  
266 atic uncertainty quantification is rarely incorporated into 316  
267 routine validation exercises.

### 268 3.2. Tier 1 - Reduced models

269 The purpose of validation at *Tier 1* is to reduce the 320  
270 number of scalars that need to be carried to the next 321  
271 level, while still reproducing key results from the exper- 322  
272 iments in *Tier 0*, for example autoignition times, or from 323  
273 experiments in *Tier 1*, such as premixed flame speeds, 324  
274 extinction or ignition. Systematic methods of reduc- 325  
275 tion and tabulation of chemical kinetic mechanisms, ei- 326  
276 ther with or without molecular diffusion effects [14, 39–  
277 41], produce reduced reaction mechanisms, or generate  
278 look-up tables as a function of the smaller set of scalars. 327  
279 There are many methods of mechanism reduction, and 328  
280 many variants thereof, denoted by acronyms in Fig. 1.  
281 A succinct review of their features and merits is available 329  
282 in Ref. [42]. Reduced mechanisms for use in turbulent 330  
283 flow calculations are usually of order of tens of species 331  
284 for realistic geometries. However, a very large class of 332  
285 LES or RANS simulations for practical combustors re- 333  
286 lies on only one or two scalars – a progress of reaction 334  
287 and a mixture fraction, very successfully for the simu- 335  
288 lation of flame species behavior. Extensions to incorpo- 336  
289 rate the simulation of the slower species such as NO and 337  
290 CO are routinely included in the reduction mechanism 338  
291 or tabulation [39, 43, 44].

### 292 3.3. Tier 2 - Turbulent combustion measurements and 293 model validation

294 In Tier 0 and 1, the objective of the model valida- 343  
295 tion exercise is to obtain a minimum set of chemical 344

kinetic parameters compatible with the existing thermo-  
dynamics and experimental datasets and their uncertain-  
ties. In Tier 2 validation, the objective is different. In  
general, one wishes to benchmark an existing physical  
representation of turbulent combustion against a set of  
conditions of interest, and demonstrate that the target  
measurands agree with the predictions within accept-  
able bounds. However, the feedback loop between the  
error found and required changes to the model is not  
necessarily obvious. A robust model should have a *min-*  
*imum* and *transparent* number of adjustable constants,  
and be validated against target experiments over a suffi-  
ciently wide range of conditions. These constants are  
generally associated with the subgrid models, ei-  
ther directly as parameters in the adjustment of scalar  
dissipation or turbulent viscosities, apparent turbulent  
Schmidt numbers or other factors. If model parameters  
need to be changed depending on the conditions or the  
model chosen, its broader utility is lost.

Researchers have used benchmark experiments to re-  
examine model assumptions and alter them, relaxing  
strong assumptions, reviewing correlations or consider-  
ing originally neglected terms in equations. Given the  
variety of assumptions used for subgrid models, the par-  
ticular adjustments made can easily get lost in compar-  
isons that may have different simulation details, such as  
mesh distribution. Published model validations almost  
invariably claim acceptable agreement with the experi-  
ments, yet the value of comparisons lies in understand-  
ing the modes of failure, and creating methods for dy-  
namically determining an optimum model choice.

## 328 4. A brief history of validation experiments for tur- 329 bulent reacting flows

330 Validation experiments for combustion have a long  
331 and distinguished history. This review considers sam-  
332 ples of experimental datasets over the past 20 years  
333 which have served as beacons for modelling efforts.  
334 Given the need for statistical information for the mod-  
335 els, time and space resolved measurements are re-  
336 quired, particularly regarding correlations between the  
337 state space of temperature and species. Pope [45] sug-  
338 gested in a 1985 review that the experimental techniques  
339 of laser-Doppler-anemometry (LDA) and Raman spec-  
340 troscopy were approaching the stage where simultane-  
341 ous measurements of local instantaneous velocities and  
342 scalars would soon be possible, allowing probability  
343 models to be directly validated. As ever, one tends to  
344 overestimate the coming speed of technical change, yet  
there are promising developments afoot.

345 A vast set of measurements have been produced for 395  
346 turbulent flames, but only a subset of those is suffi- 396  
347 ciently detailed to address some of the questions re- 397  
348 garding the suitability of the turbulence-chemistry and 398  
349 turbulence-diffusion model. One of the purposes of ex- 399  
350 periments at this level is to provide data to test the hy- 400  
351 potheses set out in models, or at least the results of the 401  
352 hypotheses. In particular, assumptions in the models 402  
353 posit inherent conditional relationships between scalars, 403  
354 particularly between temperature and species. Whereas 404  
355 it is always possible to test models *a posteriori* based 405  
356 on the final mean or fluctuation measurements, the 406  
357 power of detailed, single shot experiments which pro- 407  
358 vide species-temperature and/or velocity-species statis- 408  
359 tics lies in the ability to test out *assumptions* in the 409  
360 model-based correlations between scalars under a range 410  
361 of conditions. Table 1 provides a non-exhaustive col- 411  
362 lection of experiments produced for model validation, 412  
363 including a variety of flame types, but focusing on sets 413  
364 that are sufficiently complete to be useful, thus provid- 414  
365 ing a broad sample of validation datasets that explore 415  
366 the variety of flame structures. A number of experi- 416  
367 ments on stratified flames listed on Table 1 also extend 417  
368 into purely premixed flames, but a much larger set of 418  
369 *premixed* experiments exists for a variety of configu- 419  
370 rations of steady and unsteady premixed flames, as re- 420  
371 viewed by [46], and in ongoing workshops on premixed 421  
372 flame model verification and validation (*e.g.* [47]). 422

#### 373 4.1. Tools of the trade 423

374 The demand for measurements which can generate 425  
375 statistics of instantaneous species mass fractions and 426  
376 temperatures for target gas flames requires specialized 427  
377 Raman, Rayleigh, laser induced fluorescence (LIF) or 428  
378 coherent anti-Stokes Raman scattering (CARS) mea- 429  
379 surements. Unlike the case of velocity measurements, 430  
380 which require significantly less expertise, only three or 431  
381 four well-equipped laboratories around the world have 432  
382 been able to maintain high-end facilities capable of 433  
383 accurate scalar measurements over the past couple of 434  
384 decades. Results are well documented through the TNF 435  
385 Workshop [115]: the work by Barlow and coworkers at 436  
386 Sandia National Laboratories, by Meier and colleagues 437  
387 at DLR Stuttgart, by Bilger and Masri at Sydney, and 438  
388 Dreizler and others at TU Darmstadt, as previously re- 439  
389 viewed in [116, 117]. The collaborative workshop has 440  
390 inspired similar initiatives in engine [118], autoignition 441  
391 [119], and soot research [120]. 442

#### 392 4.2. A smorgarsbord of flames 443

393 Flames investigated at the turn of the 20<sup>th</sup> century 445  
394 were simple diluted turbulent jet diffusion and partially 446

premixed flames with jet Reynolds numbers from 10 to 40  $\times 10^3$ , as shown in the first block of Table 1. The original questions were associated with the ability of variants of flamelet and PDF models to reproduce the flame structure. These experiments offered point measurements with a resolution of hundreds of micrometers, time resolutions of sub-microseconds, and species and temperature accuracies between 1 and 10 percent, which is in general a useful engineering range for model validation.

The use of jet flames simplifies simulations for two reasons: (a) boundary conditions are simple, (b) the calculations are parabolic, so that the upstream values do not depend on downstream values, allowing calculation domains to be reduced based on computational resources, without prejudice to accuracy [12]. However, unpiloted jet flames cannot be stabilized beyond a critical velocity. Piloting is therefore adopted to support a number of the flames with higher jet velocities without full extinction. The pilot stream temperatures therefore had to be well characterized, and any differences in molecular weights and properties accounted for or tailored to match the main mixture gases.

In particular, a series of lean-pilot, partially premixed jet flame experiments led by Sandia [52, 53, 121] (series D-F) have been simulated by a vast number of researchers. The attraction appeared primarily because these measurements offered not only a full set of scalars, but also quantitative NO and OH measurements. Further, high velocity jets for flames E-F allow testing of models for localized extinction, so these flames continue to be benchmarks for models to this date [43, 122, 123]. A number of additional measurements were made in both the Sandia and DLR flames, including measurements of 2D and 3D fluctuating scalar dissipation of the mixture fraction [53, 121, 124], which allowed an examination of model assumptions and the role of filtering in the comparison of LES and models. A parallel series of flames from the Sydney group were investigated [54–56], with a number of variants on non-premixed jet flames, including bluff-body and swirl-stabilized flames which remained stable up to higher velocities, thus pushing Re and Ka numbers to higher levels and extinction arises. Swirl and bluff-body flames are of course more challenging from the fluid mechanics viewpoint, and can possibly create difficulties with the onset of higher heat transfer at the base. Many of these results are expressed in scatter plots of temperature-mixture fraction, which are useful for limits of diffusion-like flames.

Piloted high velocity non-premixed flames can be pushed to the point where they are lifted. In that case,

Name	Ref.	Description	Fuel	Measurements <sup>a</sup>
<b>Jet non-premixed and partially premixed</b>				
TUD-H3	[48]	diluted non-premixed jet flame	H <sub>2</sub> , N <sub>2</sub>	$T, Y_{NO}, Y_{OH}$
H2-A,B,C	[49, 50]	diluted non-premixed jet flame	H <sub>2</sub> , He	$T, Y_{NO}, Y_{OH}$
DLR-A,B	[51]	piloted non-premixed jet flame	CH <sub>4</sub> /H <sub>2</sub> /N <sub>2</sub>	$T, Y_i, Y_{NO}, Y_{OH}, CH, U, V$
Sandia-C,D,E,F	[52, 53]	lean piloted jet partially premixed flame	CH <sub>4</sub> , air	$T, Y_i, Y_{NO}, Y_{OH}, U, V$
Sydney PF,BF,SM	[54–56]	bluff-body and swirl stabilized flames	CH <sub>4</sub> , CO, H <sub>2</sub> , methanol	$T, Y_i, Y_{NO}, Y_{OH}, U, V$
AJHC	[57]	piloted non-premixed jet flame	CH <sub>4</sub> , H <sub>2</sub>	$T, Y_i, U, V$
DJHC	[58]	piloted non-premixed jet flame	CH <sub>4</sub> (NG)	$T, Y_i, U, V, OH, NO$
<b>Autoigniting/large pilot</b>				
Cabra	[59, 60]	rich piloted partially premixed	H <sub>2</sub> , CH <sub>4</sub>	$T, Y_i, Y_{NO}, Y_{OH}$
PPJB	[61, 62]	lean premixed jet into large pilot	CH <sub>4</sub> and NG	$T, Y_i, Y_{OH}, CH, CH_2O, U, V$
DJHC-2	[63–65]	piloted premixed jet	CH <sub>4</sub> , H <sub>2</sub>	$T, Y_i, Y_{NO}, U, V$
<b>Premixed and stratified</b>				
TUD stratified	[66, 67]	concentric stratified flame, inner pilot	CH <sub>4</sub>	$T, Y_i, U, V$
TUD counterflow	[68]	opposed flow turbulent flame	CH <sub>4</sub>	$T, Y_i, U, V, OH$
Cambridge stratified	[69, 70]	radially stratified flames with/without swirl	CH <sub>4</sub>	$T, Y_i, U, V, OH$
Sydney stratified	[71–75]	piloted burner with variable radial stratification		CH <sub>4</sub> , $T, Y_i, U, V, OH$
<b>Sooting flames</b>				
DLR/Adelaide	[76–78]	lifted non-premixed jet flame	C <sub>2</sub> H <sub>4</sub>	$T, U, V, f_v, d_p$
DLR/Adelaide-2	[55, 79]	bluff-body non-premixed jet flame	C <sub>2</sub> H <sub>4</sub>	$f_v$
Missouri	[80]	non-premixed jet flame (no co-flow)	C <sub>2</sub> H <sub>4</sub>	$f_v$
DJHC-3	[58, 81, 82]	piloted jet flame	NG	$Y_i, U, V, OH, f_v$
DLR/RQL	[83–85]	swirling pressurized flame with secondary air injection	C <sub>2</sub> H <sub>4</sub>	$T, OH, f_v, U, V$
<b>Technical flames</b>				
TECFLAM	[86–88]	model swirling injector, radial vanes, partially premixed burner, operated at high P, T	CH <sub>4</sub>	$T, Y_i, U, V, OH$
GTMC	[89–92]	model swirling injector, radial vanes, partially premixed burner, also operated at pressure and under instabilities	CH <sub>4</sub>	$T, Y_i, U, V, OH, CH$
Siemens SGT-100	[93–95]	Siemens swirling injector, radial vanes, partially premixed burner, operated at high P, T	CH <sub>4</sub> (NG)	$T, Y_i, U, V, OH, NO(ave.)$
NASA LDI	[96]	swirling lean direct injector operated on gas at high P, T	H <sub>2</sub> /CH <sub>4</sub>	$Y_i$
<b>Spray flames</b>				
UC Irvine	[97]	pressure spray hollow cone atomiser flame	methanol	$U_d, V_d, n_d, d_d$
NIST	[98]	pressure spray hollow cone atomiser flame	methanol	$U_d, V_d, n_d$ (dye), $d_d$
CNRS Orleans	[99]	air-assist injector with surrounding co-flow; pilot flame located at variable height from injector	n-heptane	$U_d, V_d, n_d, d_d, U, V$
Yale	[100]	weakly turbulent jet with dilute droplets in co-flow, stabilized at the atomiser tip	methanol	$T, U_d, n_d, d_d$
Sydney	[101, 102]	dilute and dense spray into pilot mixture for autoignition study into piloted co-flow	ethanol, methanol	$U_d, V_d, n_d, U, V$
Sydney-2	[103, 104]	weakly turbulent jet with dilute droplets in co-flow, stabilized at the atomiser tip	acetone, ethanol	$U_d, V_d, n_d, OH$
Cambridge swirl	[105, 106]	swirling confined spray flame	diesel, JP-10, PME, RME	$U_d, V_d, n_d, U, V$
Cambridge jet	[107]	bluff-body stabilized spray flame	n-heptane, n-decane, n-dodecane, jet-A1	CH <sub>2</sub> O, OH, Mie
Cambridge pilot	[108]	piloted bunsen burner with dispersed droplet mist	ethanol	CH <sub>2</sub> O, OH, Mie
CORIA	[109, 110]	confined burner at elevated temperature, non-swirling air flow	ethanol, methanol	$U_d, V_d, n_d, OH$
DHSC	[111, 112]	piloted spray flame into co-flow of air or lean pilot	ethanol	$T, U_d, V_d, n_d, U, V$
DLR	[113, 114]	high pressure and temperature spray flame	$U_d, V_d, n_d$	

<sup>a</sup> Variables indicate single shot measurements of the following variables:  $U, V$ : axial and radial gas velocities,  $U_d, V_d$ : axial and radial gas velocities,  $T$ : gas temperature,  $Y_i$ : stable species concentrations,  $n_d$ : droplet concentration,  $d_d$ : droplet diameter, OH, CH: non-quantitative PLIF,  $f_v$ : soot volume fraction., NG: natural gas.

Table 1: Turbulent flame experiments offering quantitative statistics of species and temperature for flame structure validation.

447 entrainment and autoignition at the base of the flame 457  
448 can become a significant mechanism for flame stabiliza- 458  
449 tion. This is a particularly difficult phenomenon to capture 459  
450 with simple flamelet models, and has been a desirable 460  
451 target flame of modellers as a challenge, either as a 461  
452 lifted non-premixed flame (Cabra burner) [59], or a series 462  
453 of lower speed autoigniting piloted flames [57, 58], 463  
454 or stratified-premixed autoigniting jet flames [61, 62]. 464

455 Emerging needs in the validation of premixed and 465  
456 partially premixed flames for practical gas turbine flame 466

models led to a number of investigations, starting from very simple, controlled turbulence stratified flames within flammability limits [66, 67, 69, 70] to piloted rich flames with a more aggressive variance in mixture fraction [71–75].

Demand for accurate data sets on the formation of soot have spurred investigators to adapt previously used turbulent jet flames as benchmarks for soot production [55, 76–82], both at atmospheric pressures and more recently, up to 5 bar [83–85]. In these experiments,

467 flame temperatures are measured using CARS, laser- 517  
468 induced incandescence (LII) and absorption measure- 518  
469 ments are used for determining soot volume fraction. 519  
470 Very high pressure measurements from sprays at well 520  
471 characterized diesel-like conditions are available in the 521  
472 ECN database [118]. There are currently no datasets 522  
473 for steady turbulent soot formation for liquid sprays at 523  
474 high pressures, although it is understood that there are 524  
475 specific datasets for industrial injectors (*e.g.* [125]). 525

476 A small number of flames that are surrogates for real 526  
477 gas turbine flames have been well characterized both at 527  
478 low pressure and high pressure and temperature by the 528  
479 TUD [86, 87] and DLR groups [88–95], as well as more 529  
480 recent experiments at NASA facilities [96]. These very 530  
481 detailed measurements of technically premixed, realis- 531  
482 tic burners demonstrate the state of the art for experi- 532  
483 mental investigations in industrially relevant flames. As 533  
484 discussed further on, realistic simulations of these sys- 534  
485 tems provide a glimpse into what has (or has not) yet 535  
486 been solved for practical problems of this nature. 536

#### 487 4.3. A sprinkle of data

488 Whilst there are many examples of turbulent pre- 538  
489 mixed, partially premixed and non-premixed flames, 539  
490 there is a dearth of good data sets on well-controlled and 540  
491 characterized spray flames, where experimental meth- 541  
492 ods have barely scratched the surface of what is needed 542  
493 and possible. Most of the flames currently used for 543  
494 benchmarking simulations have used pressure atomiz- 544  
495 ers mounted centrally, surrounded by a co-flow, and 545  
496 measurements of droplet sizes and velocities was made 546  
497 using phase-Doppler anemometry (PDA) [97, 98, 105, 547  
498 107, 126]. Some measurements have aimed to decou- 548  
499 ple the spray atomization process from the transport and 549  
500 combustion by producing controlled mists [99, 101– 550  
501 104]. More recently, well-controlled piloted spray mea- 551  
502 surements have also been produced [111, 112]. Only 552  
503 a few of those many experiments provide gas velocity 553  
504 measurements as well as droplet velocities, and only 554  
505 two data sets have produced detailed temperature mea- 555  
506 surements using CARS. The ECN network [118] has 556  
507 been creating a consistent database for diesel-like and 557  
508 gasoline sprays over a range of conditions suitable for 558  
509 validation, and that activity should start to populate the 559  
510 necessary space for robust modelling of these phenom- 560  
511 ena. 561

512 A number of high quality experiments exist as part 562  
513 of a more general database, including a wealth of data 563  
514 on steady and unsteady premixed flames as reviewed 564  
515 in [46], and a growing database of imaging of pre- 565  
516 mixed flames at high Karlovitz numbers [10, 127] which 566

can be modelled directly via DNS [128]. More prac-  
tically, there is also an emerging database on oxy-  
fuel/coal flames [129, 130], and many experiments on  
high frequency visualization of combustion instabilities  
and limit phenomena, for example [131–134], which are  
not addressed in the present review.

From this brief survey, we conclude that there is a  
large variety of test cases offering pointwise scalar and  
velocity information at atmospheric pressure, ranging  
from diffusion to partially premixed flames, with and  
without pilot, and near and away from autoignition. A  
few experiments also have information on relevant pol-  
lutants. There is a much smaller database at high pres-  
sures and temperatures, typically containing informa-  
tion on more practical flames. The detailed database  
on scalars in sprays flames is very small, and almost  
non-existent at pressure. Given the importance of liquid  
phase combustion for practical applications, including  
engines and aeroengines, this state of affairs appears to  
reflect the ingenuity of engineers, who continue to pro-  
duce good products with incomplete information.

#### 5. Minding the gap: the state of the art

Guidelines on model validation [12, 135] in gen-  
eral offer the following advice: (a) validation experi-  
ments should be designed independently, but consid-  
ering input from modellers, (b) boundary conditions  
should be well characterized, and their influence quanti-  
fied, (c) random and systematic experimental uncertain-  
ties should be clearly assessed, (d) a hierarchy of ex-  
perimental measurements of increasing computational  
difficulty and specificity should be created, from glob-  
ally integrated quantities to local quantities, (e) valida-  
tion should be attempted over a wide range of condi-  
tions to which model parameters are sensitive. As a fi-  
nal guideline, not sufficiently emphasized in previous  
studies, (f) validation should be conducted by model-  
ing the quantity directly experimentally measured (say,  
scattered signal or speed of sound), rather than the vari-  
able in the governing equations (*e.g.* temperature). The  
fact that the customer is usually the modeler leads to  
convoluted attempts by experimentalists at inversion of  
the experimental signal, adding to the error in the final  
delivered measurand.

The experiments listed in Table 1 were most fre-  
quently designed by experimentalists, with input from  
modellers, to test robustness of turbulent combustion  
models. However, reality often intervenes to complicate  
what initially seems a simple task to measure boundary  
conditions: effects of heat transfer back to the stabiliza-  
tion point, or the role of boundary layers upstream con-



567 spire to add uncertainty to otherwise well-designed ex-  
 568 periments [136]. Random errors are usually assessed by  
 569 understanding the limitations of the optical diagnostic  
 570 techniques used; yet systematic errors (typically associ-  
 571 ated with flow measurements, instrument calibration or  
 572 asymmetry) are often much more difficult to assess, and  
 573 are only discovered in the rare occasions when an exper-  
 574 iment is duplicated elsewhere. Finally, the measure-  
 575 ment of local rates or terms in balance equation is possi-  
 576 ble only in the simplest of cases – but there is certainly  
 577 room for thoughtful experiment design to target specific  
 578 model features, as highlighted in Section 6. In what fol-  
 579 lows, we consider a few examples of cross comparisons  
 580 between models and experiments, which capture the ad-  
 581 vances in prediction, and suggest a future path.

### 5.1. Rich premixed-diffusion Sandia flame D-F

582 An entire tome could be written on the roughly 400  
 583 comparisons of models and experiments of piloted par-  
 584 tially premixed flames D-F associated with the TNF  
 585 Workshop [115]. These sets have often been selected for  
 586 validation, as they offer not only stable species measure-  
 587 ments, but also NO and OH concentrations. The nature  
 588 of the flame, consisting of a rich stream (25% CH<sub>4</sub>, 75%  
 589 air, for  $\phi = 3.17$ ), surrounded by a lean pilot flame, pro-  
 590 duces a well-controlled environment for the simulation  
 591 of flames exposed to high turbulence levels into near ex-  
 592 tinction. Many LES simulations are able to capture the  
 593 behavior of major species, velocities and temperatures  
 594 with modest spatial resolution, and a range of subgrid  
 595 models. Most LES (and RANS) models are able to cap-  
 596 ture the overall temperature and velocity distributions  
 597 using tabulated or flamelet approaches, although the be-  
 598 havior of the higher velocity flames E-F are more chal-  
 599 lenging for coarser models [43, 137]. Creative solutions  
 600 – for example by the introduction of additional scalars  
 601 with reacting time scales uncoupled to the lead progress  
 602 variable – are used in combination with flamelet models  
 603 to capture extinction behavior, as well as the concentra-  
 604 tions of the slower reacting species CO and NO further  
 605 downstream. A concise review of a number of simu-  
 606 lations of NO in flame D using tabulation and direct  
 607 chemical integration approaches is available in Refs.  
 608 [43, 137]. Figure 2 shows a collection of simulation  
 609 results for NO centerline concentrations, both recent  
 610 and past, using direct integration and extended flamelet  
 611 models. Prediction of NO mass fractions using flamelet  
 612 modes requires inclusion of an additional variable to ac-  
 613 count for disparate time scales as well as accounting for  
 614 subgrid variances, as demonstrated by [44, 138]. In con-  
 615 trast with flamelet models, RANS-PDF models tend to  
 616 be quite successful in representing the chemistry of slow  
 617

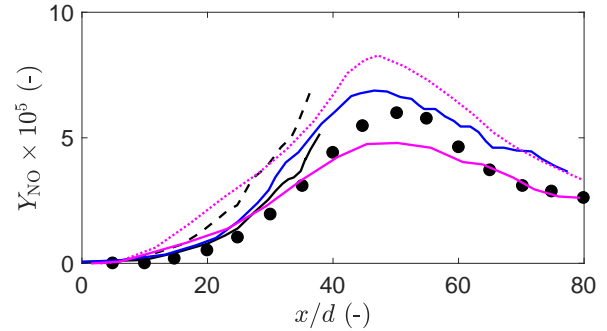


Figure 2: Sample LES simulation and experimental results for Sandia Flame-D using directly integrated chemistry. Symbols are experimental mass averaged mixture fractions along the centerline. Black lines from [43]: Highly resolved ( $2-5 \ell_k$ ) direct integration simulations using GRI2.11 (solid), and GRI3.0 (dashed lines). Blue lines from [140]: ( $40 \mu\text{m}$  grid, tabulated premixed flamelet-PSR model. Magenta lines from [138]: premixed flamelet, coarse grid ( $D/8$ ), with scalar subgrid variance (solid) and with thickened flame model (dash-dotted).

618 reacting species, as shown for example in earlier papers  
 619 by Tang et al. [139], as well as autoigniting flames dis-  
 620 cussed below.

### 5.2. Autoigniting flames

621 Predictions regarding the interaction between high  
 622 velocity reactants and surrounding pilot flames chal-  
 623 lenges simpler models, as the combustion regime be-  
 624 comes a mixture between autoigniting reactants un-  
 625 der partial diffusion control. PDF transport models  
 626 [25, 141] and CMC [142, 143] as well as RANS-PDF  
 627 [144] with reduced chemistry have been used to model  
 628 these systems to predict scalar profiles. Creative ap-  
 629 proaches to modelling these flames by using a switching  
 630 index which can recover either the diffusion, premixing  
 631 or autoigniting regimes, and still use unsteady flamelets  
 632 and tabulation using PFR or PSRs [22, 145, 146]. The  
 633 good performance of flamelet models under these con-  
 634 ditions is perhaps surprising, but as has been noted  
 635 [22, 145], autoignition times are not very sensitive to  
 636 the particular diffusion model used, rendering predic-  
 637 tions rather forgiving of the particular details.

### 5.3. Stratified flames and technically premixed flames

639 The Cambridge and TU Darmstadt stratified flames  
 640 have been the targets of a number of validation ef-  
 641 forts [21, 147–149]. Results on the Darmstadt simu-  
 642 lation results were recently compiled by Fiorina et al.  
 643 [136], showing that stratified flames within the flamma-  
 644 bility limit behave essentially as ensembles of pre-  
 645 mixed flames. The state of the art in understanding  
 646

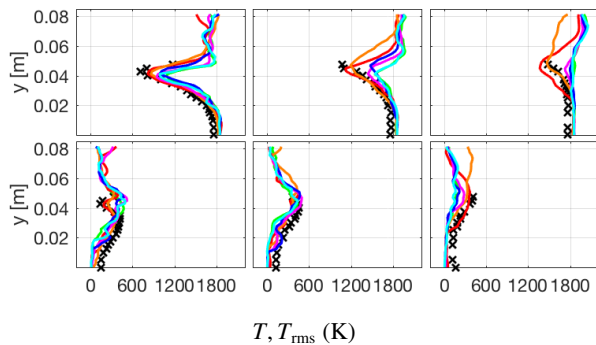


Figure 3: Sample comparison of measured and predicted mean temperature (top) and corresponding RMS fluctuations (bottom) on a 7 Mcell grid model of the SGT-100 burner experiments, for distances from the burner of  $x/D=[1.21, 1.44, 1.66]$ . Legend: (—) LES-PaSR, (—) LES-EDC, (—) LES-FM, (—) LES-TFM, (—) LES-SF, (—) LES-ADM and (+) experimental data from [93–95]. For references to the details of each model, the reader is referred to the original paper [153].

647 of such flames has been recently reviewed and dis-  
 648 cussed in [150]. A recent series of rich-piloted strati-  
 649 fied flames by [71–75] offer an interesting case where  
 650 both premixed and diffusion behavior are simultane-  
 651 ously present, based on the correlation of temperature  
 652 and mixture fraction. A number of papers in this Sym-  
 653 posium address the difficulties in these simulations.

654 Measurements and simulations of technically pre-  
 655 mixed flames under high pressure and temperature have  
 656 been made, mostly on generic gas turbine injectors with  
 657 natural gas, as listed in Table 1, but also on a variety of  
 658 swirl-stabilized burners, as reported in [151, 152] and  
 659 others, where the dataset may not be complete owing  
 660 to proprietary or other reasons. Recent simulations by  
 661 [153–155] of the Siemens SGT-100 burner experiments  
 662 [93–95] have benchmarked a variety of models against a  
 663 whole range of simulations. Fedina et al. [153] analyzed  
 664 the results of six variations of micromixing and flamelet  
 665 models, concluding that the overall error in tempera-  
 666 ture, velocity and major species across the four cross  
 667 sections of the flame were similar for *all* models, as  
 668 shown in Fig. 3. Previous LES results using a simple  
 669 eddy closure model against the same dataset showed an  
 670 overprediction of both outlet NO and CO by a factor  
 671 of about four, whereas more recent predictions of the  
 672 same flame using integration of reduced chemical mech-  
 673 anisms [154, 156] showed results within 25 percent of  
 674 the measured values.

#### 675 5.4. Sooting flames

676 Simulations of turbulent sooty flames have existed,  
 677 but only recently have reliable detailed comparisons

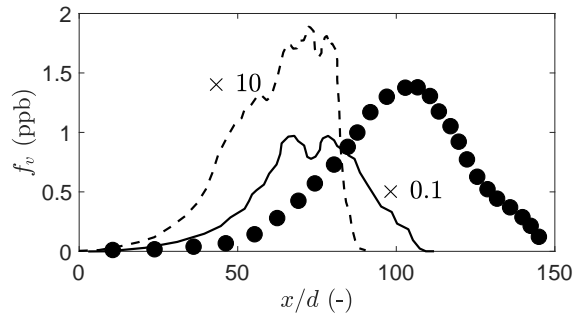


Figure 4: Comparison of experimental measurements of mean soot volume fraction (circles) at the centreline of the flame in [81], simulations [158] and [159] (note different scales for model results).

678 been made between measurements and experiments.  
 679 The DJHC-3 flame [58, 81, 82] has been simulated us-  
 680 ing LES coupled with presumed-PDF methods, with  
 681 additional closures to account for the population bal-  
 682 ance for soot volume and area, and global models for  
 683 PAH growth [157] based on the literature. Donde  
 684 et al. [158] and Sewerin and Rigopoulos [159] used  
 685 a PDF/population balance with stochastic closures to  
 686 model the same flame. In all cases, agreement with  
 687 major species and temperature is good, but estimates of  
 688 soot volume fraction spread over two orders of magni-  
 689 tude, as shown in Fig. 4. Recent comparisons with the  
 690 experimental data from DLR in [83, 84] show encourag-  
 691 ing results for high pressure predictions of soot. Clearly,  
 692 significantly more work is needed in refining models, as  
 693 well as identifying potential measurements which could  
 694 identify the problems. Recent measurements [160] of  
 695 mixture fraction using Kr fluorescence showed an inno-  
 696 vative means of obtaining simultaneous soot and mix-  
 697 ture fraction, for example, and further measurements are  
 698 certainly needed. The emerging measurements from the  
 699 ECN network on soot formation in engines, as well as  
 700 other unsteady measurements [161] of mixture fractions  
 701 in unsteady jets will continue to help improve models  
 702 and their accuracy.

#### 703 5.5. Spray combustion

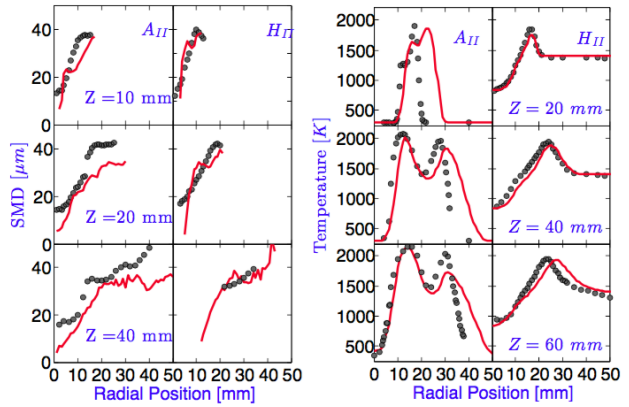
704 A recent review of models for dilute sprays, pro-  
 705 vides an excellent summary of the issues surrounding  
 706 spray simulations, including those of the Delft hot spray  
 707 flame (DHSC) ([111, 112]). The latter experiments  
 708 provide a more complete database than similar stud-  
 709 ies, and several recent studies have tackled the simu-  
 710 lation with good results using flamelet and transported  
 711 PDF [162–164], as well as stochastic methods [165].

712 Sample results for two cases are shown in Fig. 5, one  
 713 with co-flowing air,  $A_{II}$ , and one with co-flowing pilot  
 714 ( $H_{II}$ ). The very interesting and complex structure of  
 715 such flames, which feature multiple reaction zones owing  
 716 to the inner and outer mixing regions, makes them  
 717 a challenging choice, quite apart from the difficulties in  
 718 simulating two-phase flows. Clearly, whereas the structure  
 719 of the piloted spray is reasonably well captured, that  
 720 is not the case for the air co-flow, and this case will  
 721 continue to be the target of model investigations.

722 There have been many simulations of steady spray  
 723 flames, from RANS simulations for practical fuels  
 724 [166], to stochastic-LES simulations [167] of the early  
 725 McDonnell data [97], and CMC models [168] of well-  
 726 controlled pressure-atomized flames [108], as well as  
 727 countless simulations of high velocity, transient au-  
 728 toigniting jets such as those available in the ECN  
 729 database [118]. Yet one of the striking observations  
 730 about the list of steady spray measurements in Table 1  
 731 is that, unlike their gaseous counterparts, none have  
 732 reliable measurements of mixture fraction or species,  
 733 and only few have gas velocities and product temper-  
 734 atures. The main reason for this lack of informa-  
 735 tion is the significant background interference created  
 736 by the highly radiative environment prevalent in soot-  
 737 laden or spray flames, which renders various incoher-  
 738 ent scattering-based techniques impossible to quantify.  
 739 Even robust velocity measurement techniques that rely  
 740 on Mie scatter tend to be affected by background noise  
 741 in highly radiative situations. These difficulties are com-  
 742 pounded at high pressures, as not only does the radi-  
 743 ative background signal increase, but so does the extent  
 744 of signal trapping for measurement techniques such as  
 745 laser induced fluorescence and laser-induced incandescence.  
 746 As a result, the database is limited, and models that  
 747 try to reproduce the features of sooting, particle  
 748 or spray-laden flames can at best reproduce the behav-  
 749 ior of droplet sizes, concentrations and velocities, and  
 750 possibly the location of the flame by comparison with  
 751 OH measurements. Spray and soot combustion mod-  
 752 elling and measurements remain a challenge, and suit-  
 753 able datasets are clearly needed. Coherent optical tech-  
 754 niques offer a sensible way around some of the radiative  
 755 background problems, and the next section discusses  
 756 some emerging diagnostic possibilities.

## 757 6. Experimental needs and opportunities

758 The review of experiments outlined in Section 5 has  
 759 revealed some areas of agreement between models and  
 760 experiments, and some significant gaps. There are, of  
 761 course, as many experimental situations as one cares to



762 Figure 5: Radial profiles of droplet SMD (left), and mean temperature  
 763 (right) at several elevations from the burner, for case  $A_{II}$  (air-spray)  
 764 and  $H_{II}$  (pilot-spray). Line: LES results from [169], symbols: experi-  
 765 mental data from [111]. Left: Sauter mean droplet diameter (SMD);  
 766 right: mean temperatures.

767 invent, so the question is: where should one focus? Be-  
 768 low we list some of the largest gaps, and suggest emerg-  
 769 ing techniques which could be used to address them.

### 770 6.1. Spray and sooting flames

771 Spray flames are luminous and soot-prone, so that  
 772 the workhorse of measurements for temperature and  
 773 species – Raman scattering measurements – does not  
 774 work under these conditions. Ample data are available  
 775 on droplet sizes and velocities, accompanied by occa-  
 776 sional non-quantitative measurements of OH or  $\text{CH}_2\text{O}$ ,  
 777 which are helpful in terms of identifying flame struc-  
 778 tures, but not so useful for quantitative validation. Apart  
 779 from the significant progress highlighted in Sections 5.4  
 780 and 5.5, there is a possible opportunity for new fs/ps-  
 781 CARS techniques in these flames: unlike ns-CARS,  
 782 these techniques have been demonstrated to be insen-  
 783 sitive to both radiative background (since it is a coher-  
 784 ent technique) as well as non-resonant background, and  
 785 work well under sooting conditions [170–174]. Fur-  
 786 ther, their applicability to 1D and 2D-CARS has been  
 787 demonstrated, as well as wideband techniques that can  
 788 extract multiple species [171, 175]. The disadvantage  
 789 of these techniques at the moment is that they require sig-  
 790 nificant specialist expertise, both in setting up the phase-  
 791 sensitive experiments, as well as in processing and in-  
 792 terpreting the information. Modelling efforts need to  
 793 pinpoint what type of information would be most criti-  
 794 cal to differentiate between models, keeping in mind the  
 795 ultimate targets of the validation, whether that be with  
 796 respect to emissions, heat release rate or other param-  
 797 eters.

## 6.2. Real hydrocarbons

Most of the studies discussed above have used methane, as it is the simplest hydrocarbon. Yet the different behavior of higher hydrocarbons is likely to have significant effects, particularly with respect to effective Lewis numbers. Recent DNS work [176, 177] reveals how the complex chemistry of larger hydrocarbon is translated onto the macroscale behavior of turbulent flames. Experimental work using Raman scattering of hydrocarbons becomes more challenging as the the multiplicity of intermediate species creates interferences in the spectral range. Yet detailed information has only started to emerge for turbulent flames containing some of the simpler, soot-free hydrocarbons [178–180].

## 6.3. Realistic densities, realistic $Ka$

The vast majority of experiments have been performed at ambient conditions, yet most combustion devices operate at high pressure and temperature. The barriers are costs (which increase with confinement) and the quality of the measurements, which can suffer due to signal trapping, beam steering, and spectral broadening. Emerging techniques that provide higher signal-to-noise at higher densities (such as laser induced grating spectroscopy [181]) or that are not prone to collisional broadening (ultra-fast techniques) may also help. However, as the discussion in Section 5 and Fig. 3 highlights, it is perhaps surprising that the overall flame structure can be relatively insensitive to the details of the micromixing model in some high turbulence cases. It would be useful to understand how general these findings might be in practical problems.

## 7. Error and uncertainty analysis

The process of model validation is usually considered finished when the error between measurements and simulations is quantified to be within the estimated experimental uncertainty. When discussing highly unsteady phenomena such as turbulent combustion, measures for comparison are typically statistical averages and moments. In the case of instabilities, the quantity of interest may be a characteristic time scale or spectrum. What is an appropriate measure of a validated model? How sensitive is the error to model parameters? And how do we know whether models can be extrapolated beyond the conditions where strict validation was conducted?

The quantification of errors is a general problem associated with probabilistic outcomes in either measurements or models, which has been tackled on the

modelling level via uncertainty quantification (UQ). A number of studies have used statistical methods for error propagation, particularly those associated with the extraction of reaction parameters [182–184], but also thermoacoustic oscillations [185, 186], and are general enough to, in principle, be applicable to any model parameter. Khalil et al. [183] have recently considered the sensitivity of results in a bluff-body flame to a range of model parameters, whilst Mueller and Raman [122] have considered uncertainties in different types of models. Although uncertainties in boundary conditions have been considered by trial and error, the methodology of polynomial expansion in UQ has been used recently for identifying uncertainties due to boundary conditions in spray simulations [187]. Finally, a recent contribution by Ihme and colleagues [188] applies systematic statistical error measurement methods to quantify the overall error for a number of variables in the recently investigated Sydney stratified flame [74, 75], allowing for a quantification of the influence of various predicted intermediate variables on the overall error, as shown in Fig. 6. Clearly, these methods are useful not only to identify the merits of different models, but also to understand the sensitivity of results to measured boundary conditions, to pinpoint cross-correlations, and to guide the models towards better physical representations.

## 8. Designing future experiments

Whereas UQ has been used to quantify the bounds of model uncertainty, and therefore the limits of error between model and experiments, the potential for UQ and error quantification techniques is much more relevant when applied to the *design* of experiments, by attempting to ask the following questions upfront:

1. What is the *target output* of the model? In other words, which predictions are most valuable: CO? NO? Soot? Instability frequency? Rate of combustion? A combination of those with different weights? Over what range of conditions?
2. What qualifies a *good test* of a model or submodel? Changes to the model should yield differentiable outputs: when very different submodels give answers within the accuracy of the experiment, the model is not adequately tested.
3. How *sensitive* are the outputs of the model to the inherent errors in the experiment, for example to details of domain boundary conditions, such as velocity or temperatures?
4. To what extent can the model be confidently *extrapolated* away from validated ranges, given

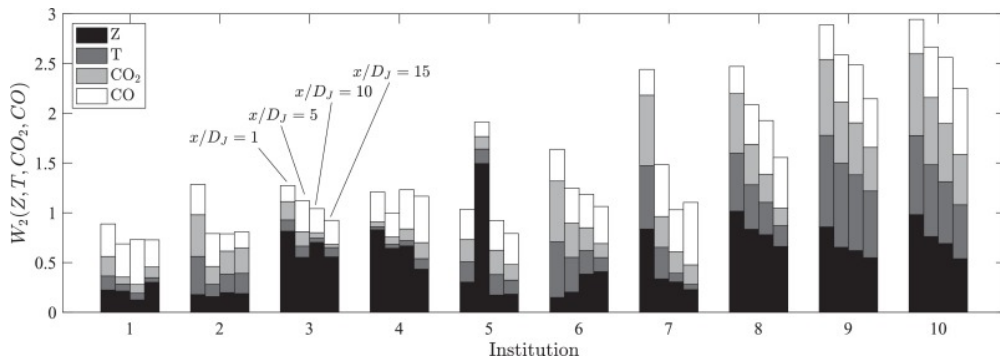


Figure 6: Quantitative comparison of multiscale Wasserstein metric as a measure of global error [188], from ten anonymized LES-calculations, presented at the 13th TNF-workshop [115] for flame conditions FJ-5GP-Lr75-57 in the inhomogenous flame [72–75]. The decomposition of multiscale calculations allows contributions from each variable at each axial location to become visible. The four bar-graphs from each contribution correspond to axial locations of  $x/D_j = [1, 5, 10, 15]$ . Results used in this figure were included with permission from TNF-contributors. Reproduced from [188].

known uncertainties in scaling? For example, if the uncertainties in chemistry due to pressure are well bounded, what are the expected uncertainties of the turbulent predictions at pressure? Can these bounds be used to decide whether experiments are necessary or useful?

These are not technically straightforward questions, but surely worthwhile enterprises given the enormous effort devoted to developing experiments and to acquiring high quality data. Data generated by a validation effort can become significantly more valuable if the targets and sensitivities are clearly understood, and quantified. As well observed by Oberkampf and Trucano [135], decisions about model validation should take into account the various incentives in place for both experimentalists and modellers and their respective institutions, in evaluating the need for (or the results of) a validation exercise. A complex and challenging experiment from the point of view of the diagnostic developers may or may not yield the necessary results for the model. Similarly, complex or computationally-intensive simulations may or not answer the question of whether they are valid over the design range if the output sensitivity is insufficient.

## 9. Summary: a more perfect union

In this brief review, we collect a broad spectrum of validation experiments for turbulent combustion and their respective comparisons, and suggest ways to improve the productivity of validation procedures. Success requires joint work between experimentalists and modellers to understand how to design validation procedures that provide clear answers to well-posed ques-

tions. The most referenced databases have demonstrated the following attributes: (a) well-defined geometries and boundary conditions, (b) accessible data, (c) a sufficient number of independent and complementary scalar and velocity measurements, over a wide enough parameter range, and (d) quantified uncertainties.

Examination of the state of the art in model validation shows that there are clear gaps in validation-quality data in spray, soot, and high pressure combustion. In that vein, there are opportunities for upfront collaboration between modellers and experimentalists to design experimental targets designed with a clear understanding of which model features can actually be tested and distinguished. Further, researchers would benefit from closer exchange in information with industry to better quantify the value of increasing accuracy of predictions for different target variables: how much is a marginal increase in accuracy in NO prediction worth, relatively to other potential quantities? These are challenging questions, yet understanding the value of improvements will help better allocate resources. A panel discussion at this Symposium will hopefully open up the questions raised to enlighten a wider audience.

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