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► **To cite this version:**

Guilhem Lavabre, Ronan Vicquelin, Olivier Gicquel. Uncertainty quantification for the LES of the H₂ Cabra flame. 10th European Combustion Meeting (2021), Apr 2021, Napoli (virtual), Italy. pp.466–471. hal-03272512

HAL Id: hal-03272512

<https://hal.science/hal-03272512>

Submitted on 28 Jun 2021

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Uncertainty quantification for the LES of the H₂ Cabra flame

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Abstract

High fidelity simulations such as Large Eddy Simulations (LES) are commonly used in combustion research. While turbulence and combustion models become increasingly precise, these simulations still rely on kinetic mechanisms that carry uncertainties that may significantly impact the flame's quantities of interest. In this study, we focus on the lift-off height of the H₂ Cabra flame, which is largely affected by the uncertainty of the operating conditions specifically by the uncertainty of the co-flow temperature. To properly compare experimental and numerical results, one must account for both experimental and numerical uncertainties. A 32-dimensional uncertain space is determined, one dimension corresponding to the co-flow temperature and the others from the uncertain kinetic mechanism. This high-dimensionality means that direct Monte-Carlo or surrogate-based approaches are intractable. A representative physical model of reduced computational cost is used to conduct a global sensitivity analysis. From this, a two-dimensional uncertain space is uncovered, in which most of the variance of the quantity of interest is retrieved, allowing a future uncertainty propagation study in LES of the H₂ Cabra flame.

1. Introduction

In recent years, numerical simulation has taken a growing place in combustion research. High fidelity methods such as Large Eddy Simulation are now commonplace in combustion studies. Still, these simulations are subject to uncertainties coming from the operating conditions, from combustion or turbulent models, or from the chemical kinetic model itself.

Uncertainty quantification (UQ) is a framework that allows accounting for the variability of uncertain inputs, thus allowing to assess the variability of some output quantities of interest. More precisely, this procedure is called forward uncertainty propagation. The classical approach involves a Monte-Carlo estimation of the probability distribution of the quantity of interest (QoI). This, in turns, requires computing a vast number of samples to build a reliable estimate. For high-fidelity combustion simulations, such an approach is intractable. Indeed, each simulation costs tens of thousands of CPU hours and a few thousands of them may be required for a proper Monte-Carlo estimate. Therefore, surrogate models are built using a few carefully chosen samples, and these surrogates are then re-sampled extensively to build the Monte-Carlo estimates of the QoI. Still, surrogate models are challenging to build in high dimensional spaces such as the one spanned by the uncertain chemistry. Ergo, global sensitivity analysis is needed to reduce the uncertain dimension beforehand.

The purpose of this paper is to put forward an uncertain dimension reduction suitable for conducting a forward uncertainty propagation for the lift-off height of the H₂ Cabra flame, accounting for the uncertainty of the co-flow temperature and of the kinetic mechanism.

2. The H₂ Cabra flame

The H₂ Cabra flame is a diffusion flame auto-igniting in a vitiated co-flow. The co-flow is a mixture of hot dioxygen and water vapour, whereas the jet is composed of hydrogen diluted in nitrogen at room temperature. The experimental

setup of the H₂ Cabra flame is presented in Figure 1. The flame's quantity of interest is its lift-off height, that is, the distance between the burner's lips and the bottom of the flame front. The nominal operating conditions of the flame are given in Table 1.

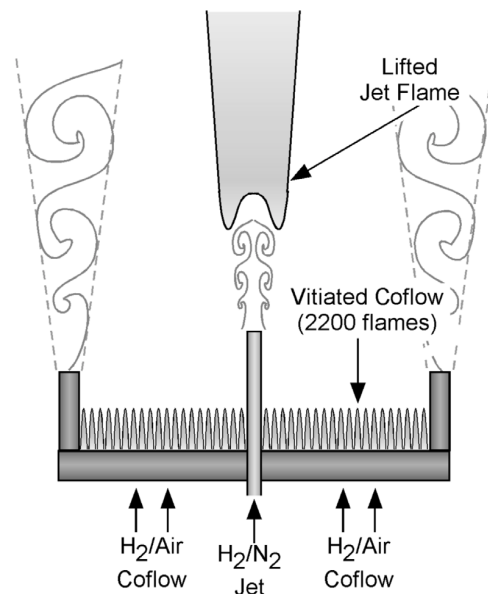


Figure 1: Experimental set up of the Cabra H₂ flame [1]

3. Large Eddy Simulation of lifted diffusion flames

The flame is simulated using an LES approach with tabulated chemistry using the solver AVBP developed by CERFACS [3]. Subgrid-scale quantities are modelled with the so-called Sigma model [4]. Tabulated chemistry is used to handle chemical reactions. More precisely, since the flame is a diffusion flame and is auto-igniting [5], the Unsteady Flamelet Progress Variable approach with a presumed PDF closure model is used, as described by Ihme and See [6]. This approach essentially consists of the tabulation of non-premixed auto-igniting flamelets.

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Table 1: H₂ Cabra flame experimental conditions [2]

Central jet		Co flow	
Q_{H_2} (slm)	25	Q_{H_2} (slm)	225
Q_{N_2} (slm)	75	Q_{air} (slm)	2100
T_{jet} (K)	305	T_{coflow} (K)	1045
V_{jet} (m/s)	107	V_{coflow} (m/s)	3.5
Re_{jet}	23600	Re_{coflow}	18600
d_{jet} (mm)	4.57	d_{coflow} (mm)	210
X_{H_2}	0.25	X_{H_2O}	0.1
X_{N_2}	0.75	X_{O_2}	0.15
		X_{N_2}	0.75

Q: volumetric flow rate; X: mole fraction;
Re: Reynolds number; d: diameter

Following Cabra’s definition [1], lift-off height is located where the Favre-averaged field of OH mass fraction $\overline{Y_{OH}}$ first reaches 600 ppm.

Each simulation costs about 100k CPU-hours on the Irene KNL supercomputer with Intel Xeon Phi 7250 (KNL) @ 1.4 GHz cores.

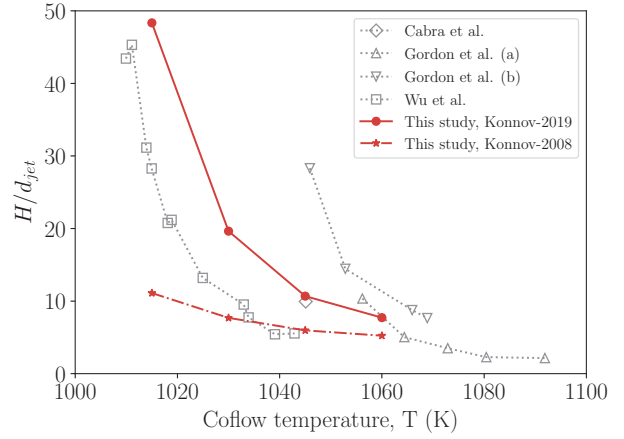
4. Sensitivity to T_{coflow} and the kinetic mechanism

Several LES runs were carried out to explore the Cabra flame’s sensitivity to parameters that affect its lift-off height. Figure 2 shows plots of normalized lift-off height against the co-flow temperature (measured in experiments, prescribed in simulations) for this study, compared to the literature.

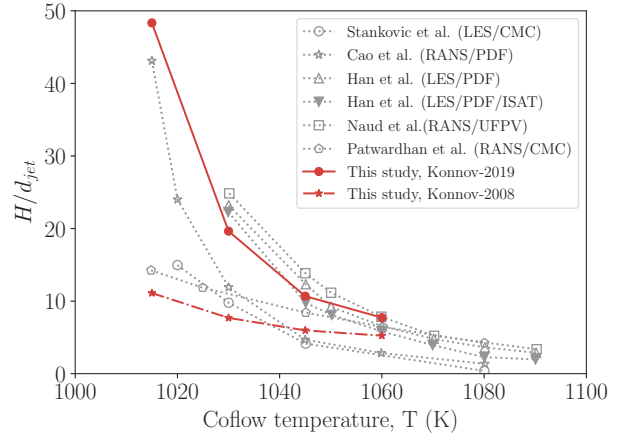
On the one hand, the lift-off height’s sensitivity to the co-flow temperature was already well known [13]. Figure 2 (a) shows a comparison between our preliminary LES simulations and experimental data. When focusing on experimental data, a zone of significant sensitivity to temperature is spotted for low co-flow temperatures, while an asymptotic regime seems to take place for higher temperatures. Furthermore, large horizontal discrepancies are observed between all these measurements, suggesting substantial experimental uncertainties.

On the other hand, the flame’s numerical simulation is also sensitive to the kinetic mechanism used to model chemistry. To our knowledge, this sensitivity has only been studied once for the H₂ Cabra flame [14]. Figure 2 (b) shows the results of different numerical studies of the H₂ Cabra flame. For the most part, they accurately display the dependency between lift-off height and co-flow temperature. Still, significant discrepancies remain between these studies. The problem is that all of them use different kinetic mechanism, mesh, turbulence and combustion models. Therefore, no conclusion can be drawn from them as to which choice significantly impacts the QoI.

In our study, in red on Figure 2, we simulate the Cabra flame with two different mechanisms from Konnov, published ten years apart: Refs [15] and [16]. We demonstrate that all other things being equal, using different kinetic mechanisms can significantly change the lift-off height. As a matter of fact, the Konnov (2019) mechanism is able to



(a)



(b)

Figure 2: Normalized lift-off height of the Cabra flame plotted against the temperature co-flow. (a): Comparison with experimental data [2, 5, 7], (b): Comparison with other numerical studies [8–12]

showcase the zone of acute sensitivity in the correct range of temperatures, while the 2008 mechanism does not. This highlights the fact that the numerical simulation of the flame is highly sensitive to the kinetic mechanism, to the point that two mechanisms of the same lineage can bring about very different behaviours.

5. Accounting for the input uncertainties

As shown in Section 4, both the co-flow temperature and the kinetic mechanism significantly impact the lift-off height of simulated H₂ Cabra flames. Both of them are uncertain, and the following will focus on assessing their impact on the uncertainty of the flame’s lift-off height. Therefore, in this study, the focus is given to these uncertain variables.

5.1. Co-flow temperature

As stated in the original publication by Cabra [2], the co-flow temperature can be measured with an uncertainty of about 3%, which corresponds to $\pm 30K$. As we can see from Figure 2, such uncertainty on co-flow temperature introduces significant variability in the lift-off height. There-



fore, it must be taken into account to compare simulations with the experimental results.

As far as we are aware, no more information is available about this uncertainty. The least-informative probability distribution - the uniform distribution between $T_{\text{Min}} = 1015$ K and $T_{\text{Max}} = 1075$ K - is consequently chosen for the co-flow temperature.

$$T_{\text{co-flow}} \sim \mathcal{U}(T_{\text{Min}}, T_{\text{Max}}) \quad (1)$$

5.2. Kinetic mechanism

Konnov published in 2008 a complete combustion mechanism for H_2 containing information about reaction rate uncertainties [15]. In this mechanism, they are represented as Arrhenius pre-exponential factors following log-normal distributions, while the other parameters remain constant.

$$k_j = A_j T^{\beta_j} \exp\left(\frac{-Ea_j}{RT}\right) \quad (2)$$

$$\xi_j = \frac{\log(A_j/A_j^0)}{\frac{1}{3}\log(UF_j)} \sim \mathcal{N}(0, 1) \quad (3)$$

With k_j being the rate constant of reaction j , A_j the pre-exponential factor, A_j^0 its nominal value and UF_j its uncertainty factor.

In this study, we choose to work with the updated Konnov mechanism published in 2019 [16]. As shown in Figure 2, it yields better agreement with other simulations and experimental data than Konnov (2008) for our case, mainly concerning the co-flow temperature sensitivity.

Konnov's 2019 mechanism contains many species and reactions not useful in our case, namely the excited species and the reactions that involve them. While useful to predict species used in experimental diagnostics, this extra complexity only leads to more expensive computations without changing much the evolution of predominant species [16]. Therefore, we boiled down the kinetic mechanism to retain only non-excited species and the reactions involving them. Figure 3 shows no significant discrepancy in the probability distribution of the auto-ignition delay time between the original mechanism and the reduced one in our operating window.

Finally, the reduced mechanism contains 31 reactions, and therefore 31 uncertain pre-exponential factors.

In total, 32 random variables are accounted for, including the co-flow temperature. This relatively high dimensionality means that the forward uncertainty propagation problem is intractable directly, even with the help of surrogate models, as these are very expensive to build in high dimension.

6. Uncertain dimension reduction

Because LES runs are costly and because building a surrogate in high dimension requires many samples, accounting for all input uncertainties is not affordable. Therefore, a priori uncertain dimension reduction is mandatory. To this end, a global sensitivity analysis has to be performed to sort out important variables from less important ones, that is, to highlight the variables whose uncertainty lead to the greatest uncertainty in the quantity of interest.

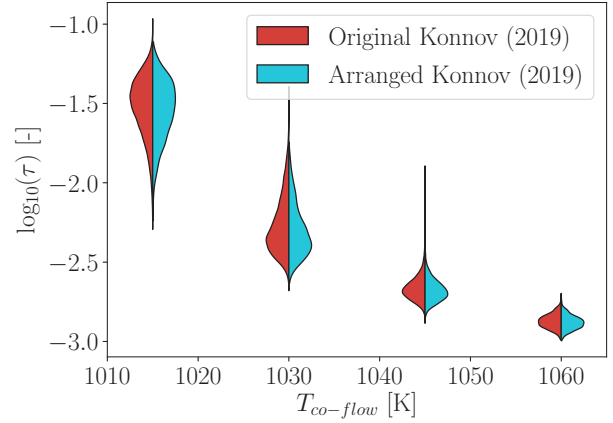


Figure 3: Violin plots of the auto-ignition delay τ in the conditions of the Cabra flame for different co-flow temperatures for the original and boiled down Konnov 2019 mechanisms

Again, global sensitivity analysis cannot be implemented directly on the 3D flame lift-off height for tractability reasons. Instead, a representative physical problem of much reduced computational cost has to be used.

6.1. A representative reduced physical problem

Auto-ignition being the dominant stabilisation mechanism for the Cabra flame in most of the operating conditions [5], it can be assumed that the lift-off height of the flame is first-order dependent on the auto-ignition delay (IDT) of the most reactive mixture in the jet [14]. In Figure 4, we compare the normalised auto-ignition delay time of the most reactive mixture to the normalised lift-off height for different co-flow temperatures, with different nominal kinetic mechanisms. The auto-ignition is detected in the same way as lift-off is detected in the 3D flame, i.e. when $Y_{\text{OH}} = 600$ ppm. The nominal initial conditions of the reactor are given in Table 2. Figure 4 shows a very similar response to inputs impacting the auto-ignition delay between 0D auto-ignition delay and the Cabra lift-off height. The only notable discrepancy occurs at low co-flow temperature, only for the 2019 mechanism, which predicts a very long ignition delay, which should lead to a large lift-off height. However, in this case, a different stabilisation mechanism, namely premixed propagation, becomes dominant [5]. This may lead to an overestimation of the impact of the uncertainty of the co-flow temperature. While this has to be kept in mind, it is not critical because the analysis of Section 4 shows that this uncertain parameter has to be taken into account anyhow.

0D auto-ignition simulations are, therefore, a representative physical problem for most of the Cabra flame's operating conditions. Furthermore, each 0D simulation costs about 0.1 CPU-second, making them suitable for a Monte-Carlo-based sensitivity analysis.

A Monte-Carlo study is conducted to account for the uncertainties of the co-flow temperature and the kinetic mechanism on the 0D auto-ignition delay. Table 3 records some statistics of this study. The uncertainty on the QoI is con-



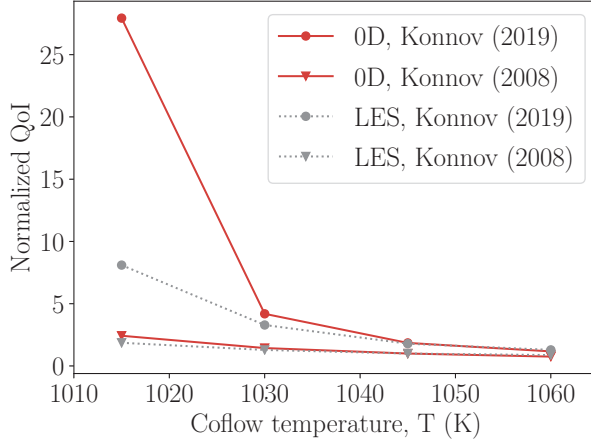


Figure 4: Comparison of the evolution of IDT (0D) to lift-off height (LES) for 2 kinetic mechanisms. All auto-ignition delays are normalised by the IDT at a co-flow of 1045K with the Konnov (2008) mechanism. All lift-off heights are normalised by the lift-off height at a co-flow of 1045K with the Konnov (2008) mechanism.

Table 2: Initial conditions for the 0D reactor at the most reactive mixture, in the nominal case (corresponding to $T_{\text{coflow}} = 1045 \text{ K}$)

P (Pa)	101325	Y_{O_2}	0.1669	$Y_{\text{H}_2\text{O}}$	0.0626
T (K)	1011.3	Y_{H_2}	0.0009	Y_{N_2}	0.7696

T : Temperature; P : Pressure; Y : Mass fraction

siderable, as shown by the 95% confidence interval, which spans an entire order of magnitude. Moreover, the important discrepancy between the mean of the distribution and the nominal case suggest substantial non-linearities in the underlying physical phenomenon.

Table 3: Statistics of the Monte-Carlo study on the auto-ignition delay 0D reactor

Auto-ignition delay time (ms)			
mean	median	nominal	95% confidence interval
5.10	2.07	2.04	[0.99 , 21.9]

6.2. Global sensitivity analysis

A powerful metric for sensitivity analysis is the set of Sobol indices [17]. Each index represents the portion of the variance of the QoI explained by the associated variable or group of variables, which is exactly what we need to discriminate uncertainties of consequence.

The indices are defined by transforming the QoI into its unique Sobol-Hoeffding (S-H) decomposition:

$$F(\xi) = \sum_{i \subseteq \mathcal{D}} F_i(\xi_i) \quad (4)$$

With F the QoI, ξ the vector of its uncertain inputs and \mathcal{D} the set of indices of the components of ξ , i a subset of \mathcal{D} , ξ_i

the corresponding input vector, and F_i the associated S-H functional.

The Sobol indices are defined for each group of variables i as:

$$S_i = \frac{\mathbb{V}[F_i]}{\mathbb{V}[F]} \quad (5)$$

Where $\mathbb{V}[X]$ is the variance of X .

In most practical cases, neither the S-H decomposition nor the Sobol indices are accessible analytically, and several ways co-exist to approximate them numerically.

In this study, we chose to approximate S-H functionals as truncated Polynomial Chaos (PC) terms, that is:

$$F_i(\xi_i) \approx \sum_{\alpha \in \mathcal{A}_i} \psi_\alpha(\xi_i) F_\alpha \quad (6)$$

Where ψ_α is the α -th basis polynomial, F_α its weight in the PC expansion of F , and \mathcal{A}_i the set of indices of PC basis polynomials that involve the group of variables i . Using the orthonormality of the PC basis, we can then approximate the Sobol indices as:

$$S_i(F) \approx \frac{\sum_{\alpha \in \mathcal{A}_i} F_\alpha^2 \langle \psi_\alpha, \psi_\alpha \rangle}{\sum_{\alpha \in \mathcal{A}} F_\alpha^2 \langle \psi_\alpha, \psi_\alpha \rangle} \quad (7)$$

The PCE is determined using least square regression with 10-fold cross-validation using 100k Monte-Carlo samples. To reduce the computational cost of determining the PCE weights, the PC basis is truncated at a maximum order of 3 and first-order interactions. A summary plot of the PCE is given in Figure 5 as a means of visual validation.

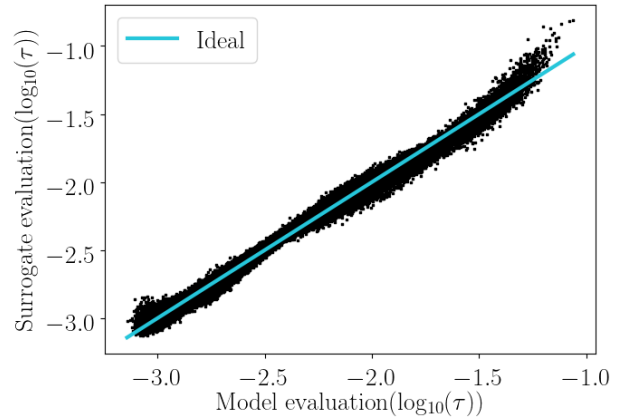


Figure 5: Summary plot of the PCE used to compute the Sobol indices

The Sobol indices, plotted in Figure 6, highlight the dominance of two uncertainties in the problem:

- The co-flow temperature: As already exposed in Section 4, the QoI is highly sensitive to the co-flow temperature. The large uncertainty range associated with this variable makes it the most impacting uncertainty in this configuration.

Its index stands alone in this study, dwarfing all effects from other uncertain parameters. This observation has



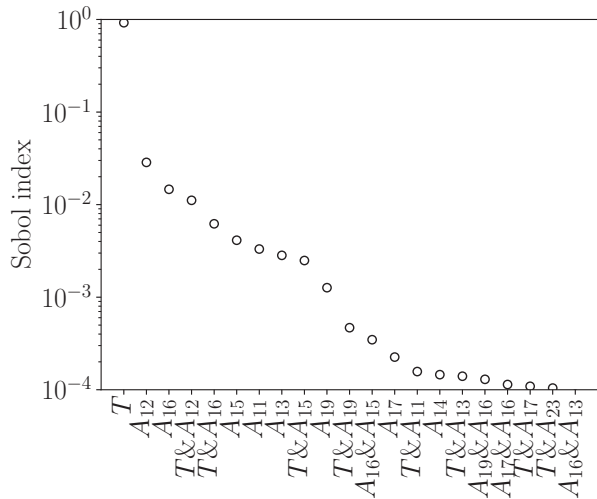


Figure 6: First- and second-order Sobol indices of the auto-ignition delay

to be mitigated with the fact that 0D simulations overestimate the impact of T compared to the real Cabra configuration where premixed propagation is also involved. However, if we restrict the sensitivity analysis to the window where the Cabra lift-off height and the auto-ignition delay have the same behaviour (Fig. 4), the co-flow temperature still comes out on top.

- The pre-exponential constant A_{12} : The 12th reaction, $H + O_2 = OH + O$, has been known for its very high sensitivity for a long time [18]. Because of this, it has since been extensively studied, and as a result, its uncertainty factor (1.1) is the lowest of Konnov’s kinetic mechanism. However, it remains the most impacting uncertain kinetic parameter.

6.3. Dimension reduction

Even if the PCE is truncated, the resulting Sobol indices are sufficient to rank variables and get a rough estimate of the portion of variance explained by each variable or group of variables.

In this study, we choose to truncate the uncertain space to ensure that 95% of the variance of the QoI is retrieved, based on the prediction of the PCE. Only two variables are needed to explain that portion of the variance of the QoI: T and A_{12} .

The reduced uncertain space spanned by these two variables is resampled to validate the truncation. The resulting probability distribution of the QoI is compared to its original distribution in Figure 7. The shape of the distribution is well captured. The peak has both the correct position and the correct amplitude, and the very heavy tail is also reproduced.

Therefore, the uncertainties of the co-flow temperature and of the 12th reaction pre-exponential factor are enough to explain most of the variability of the QoI.

7. Conclusion

In this study, a qualitative sensitivity analysis of the H_2 Cabra flame lift-off height has been performed with LES.

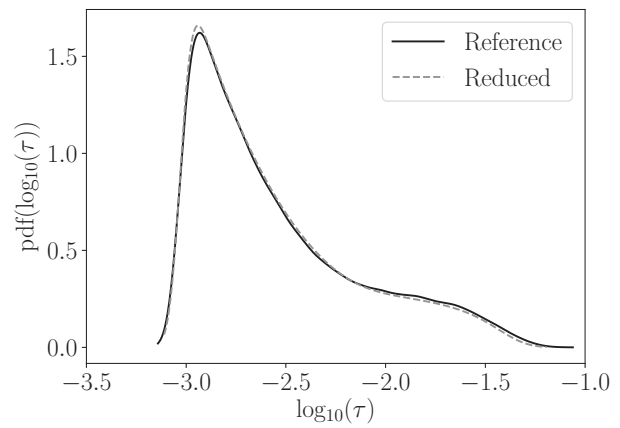


Figure 7: Comparison of auto-ignition delay probability distribution between the initial sampling of the 32D uncertain space and the truncation to the space spanned by T and A_{12}

This analysis has highlighted the importance of performing a rigorous uncertainty propagation of both the co-flow temperature and the kinetic mechanism through numerical simulations of this flame. Uncertain dimension reduction was mandatory to afford such a study. To this end, a representative physical model of much reduced computational cost was put forward to conduct a global sensitivity analysis. This study has revealed a two-dimensional uncertain space where most of the initial problem’s variance is explained.

In this space, surrogate-based forward uncertainty propagation becomes tractable, and this is the focus of ongoing work.

8. Acknowledgements

This work has been funded by a grant from the french Ministère de l’Enseignement Supérieur, de la Recherche et de l’Innovation. Simulations were performed using HPC resources from GENCI-TGCC (Grant A0082B10159) as well as from the “Mésocentre” computing center of Centrale-Supelec and Ecole Normale Supérieure Paris-Saclay supported by CNRS and Région Île-de-France.

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