

# Interpolation Error of FGM Tabulation in an Unnormalised Progress Variable Subspace



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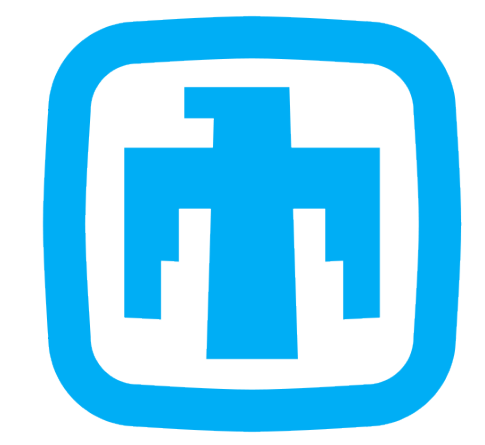
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## 1. INTRODUCTION

- When considering preferential diffusion effects in tabulation of thermochemical states employed in the flamelet-generated manifold (FGM) method, tables are stored by lookup of various control variables. These control variables typically include mixture fraction,  $Z$  and normalised progress variable,  $PV$ .
- If preferential diffusion effects are considered, mixture fraction is not constant for each flamelet, and insufficient data to define the progress variable boundaries leads to many studies undertaking interpolation in the unnormalised progress variable space, [1-3].
- This causes flamelet lengths to vary in the unnormalised progress variable subspace (relative to other nearby flamelets), causing interpolation and extrapolation to be undertaken across incorrect values (Fig 1.)
- Various types of FGM errors have been previously quantified, including error due to steep thermochemical value gradients and non-monotonic progress variable definitions. However, to best knowledge, no work highlights the very significant errors arising from interpolation in an unnormalised progress variable subspace.

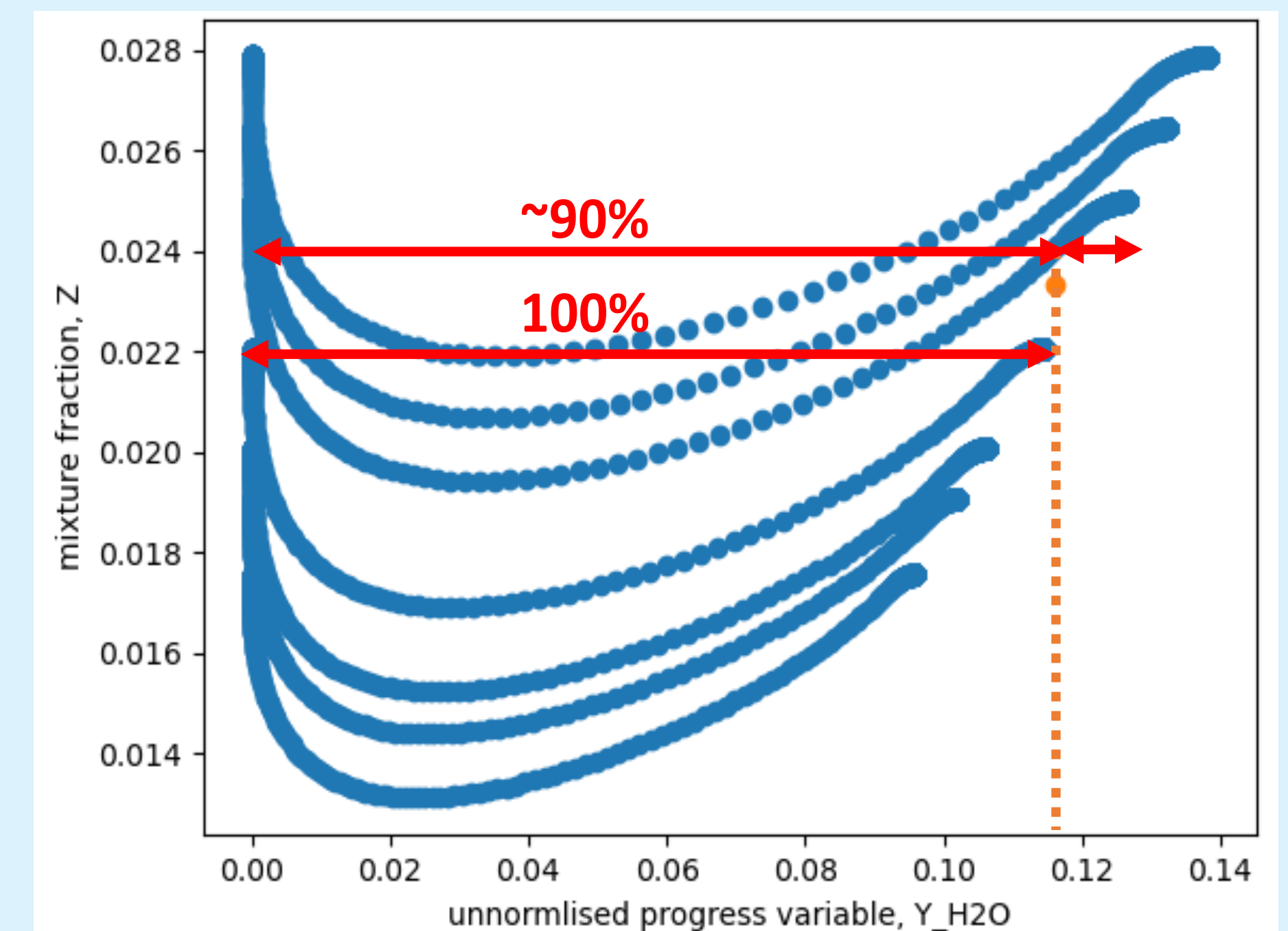


Figure 1 - Schematic of FGM interpolation

## 2. BASELINE PERFORMANCE

- Performance of error reduction methods is analysed by comparing the result interpolated from two flamelets against the original flamelet data.
- The original flamelet data is modelled using 1D FreeFlame model in Cantera software with the following conditions:

**Fuel Blend:** 0.4/0.45/0.15 (mol)  $\text{NH}_3/\text{H}_2/\text{N}_2$

**Oxidiser:** 0.21/0.79  $\text{O}_2/\text{N}_2$  (mol)

**Equivalence ratio:** 0.13 - 0.6; **Inlet Temperature:** 750K

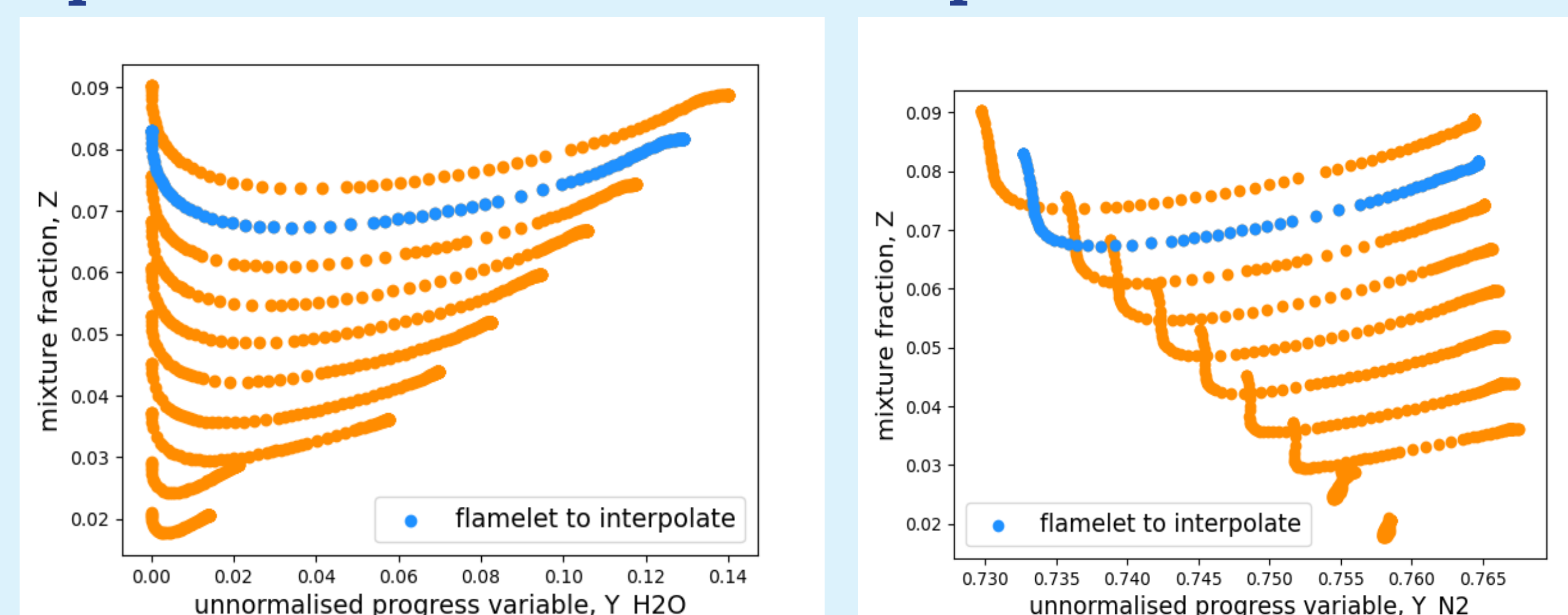


Figure 2 - Z-PV space for two progress variable definitions

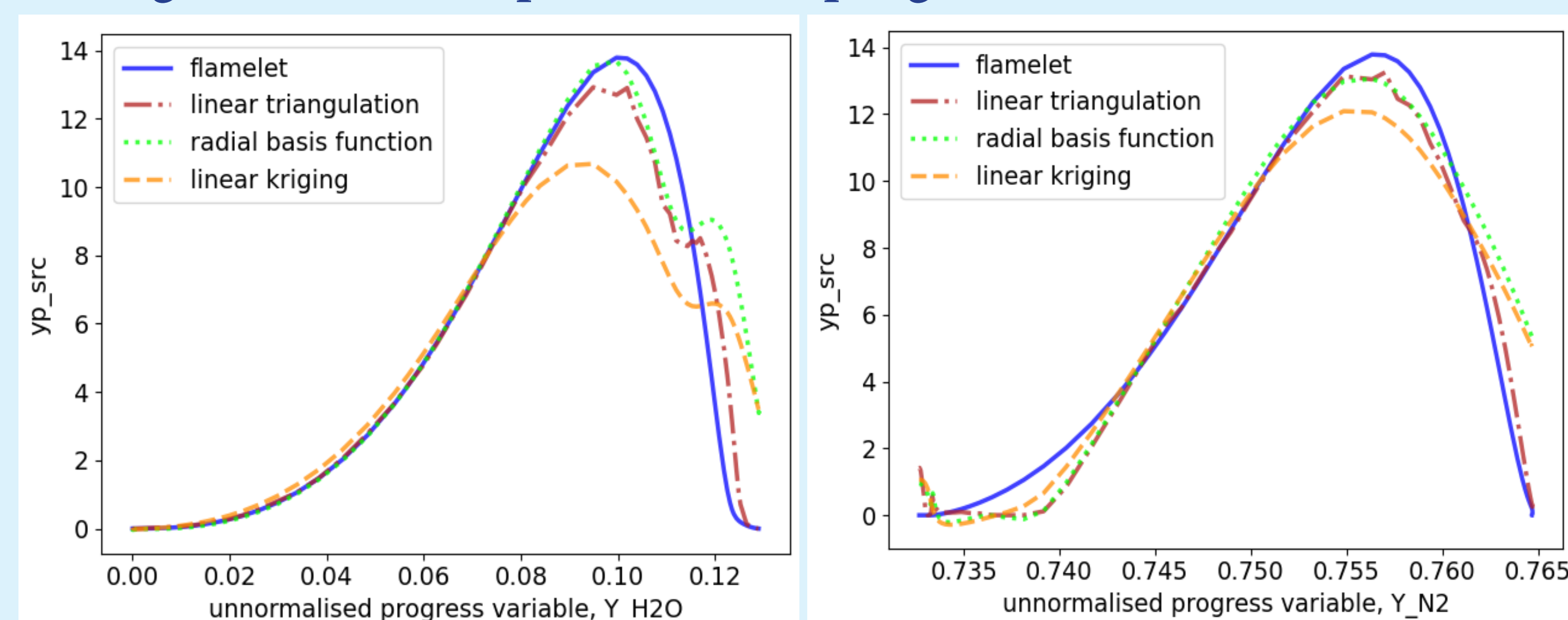


Figure 3 - Source term for flamelet with different interpolation methods vs. original 1D flamelet data ( $Z$  spacing = 0.052)

## 4. CONCLUSION

- Significant interpolation errors can arise from FGM tabulation using an unnormalised progress variable, often undertaken when considering preferential diffusion effects.
- This work provides a comparison of solutions to tackle this error.
- The most accessible solutions are: additional dimension for normalisation and decreasing  $Z$  spacing. However, further  $Z$  spacing reduction below 0.013 was found to have minimal effect.
- Perspective mapping may be viable, but is constrained by a loss of precision based on density of points along  $PV$ .
- For the blend explored in the present study, optimisation of progress variable definition does not produce a viable solution due to the difficulty in balancing monotonic criteria against uniform boundaries on both the burnt and unburnt side of the flamelet.

## 3. COMPARISON OF METHODS

### Additional Parameter for Normalisation

- During interpolation, an additional lookup step is undertaken to find the nearest flamelet and its boundaries for normalisation. Interpolation is then conducted on a normalised progress variable.

### Mixture Fraction Spacing

- Smaller mixture fraction interval during tabulation leads to interpolation between two flamelets that have less variation in length in the  $PV$  subspace.

### Multi-Objective Normalisation of Progress Variable Definition

- A genetic algorithm was utilised to find the progress variable definition that is a compromise between uniform progress variable boundaries and a monotonic definition. No valid solution that meets both monotonic and equal boundaries criteria was found.

### Perspective Transformation Mapping

- In cases where the distribution of data in the  $Z$ - $PV$  space can be captured by a quadrilateral shape, a perspective mapping matrix can be applied to remap the  $Z$ - $PV$  space, allowing normalised progress variable to be used as a control variable.

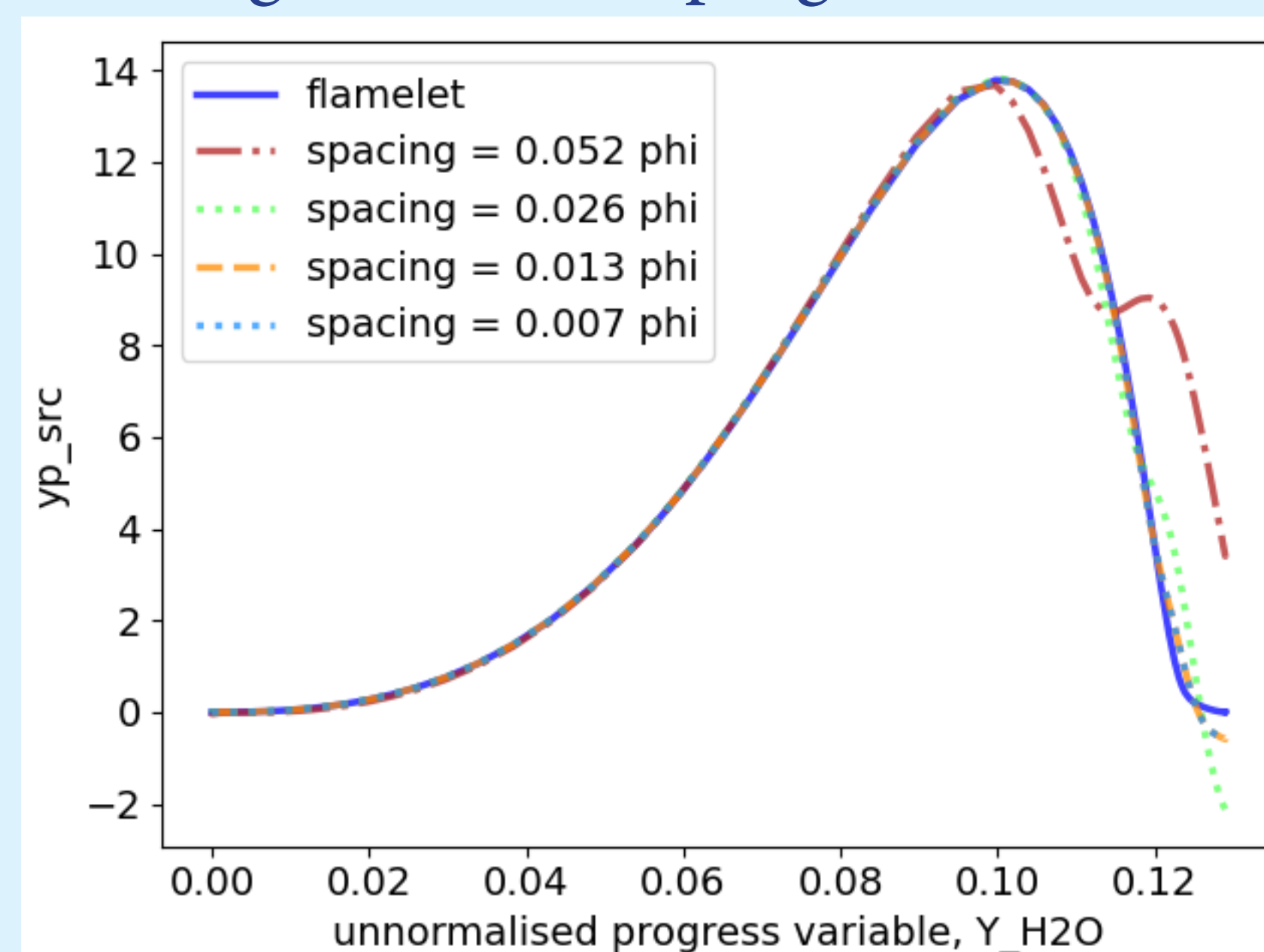


Figure 4 - Impact of mixture fraction spacing on interpolation error

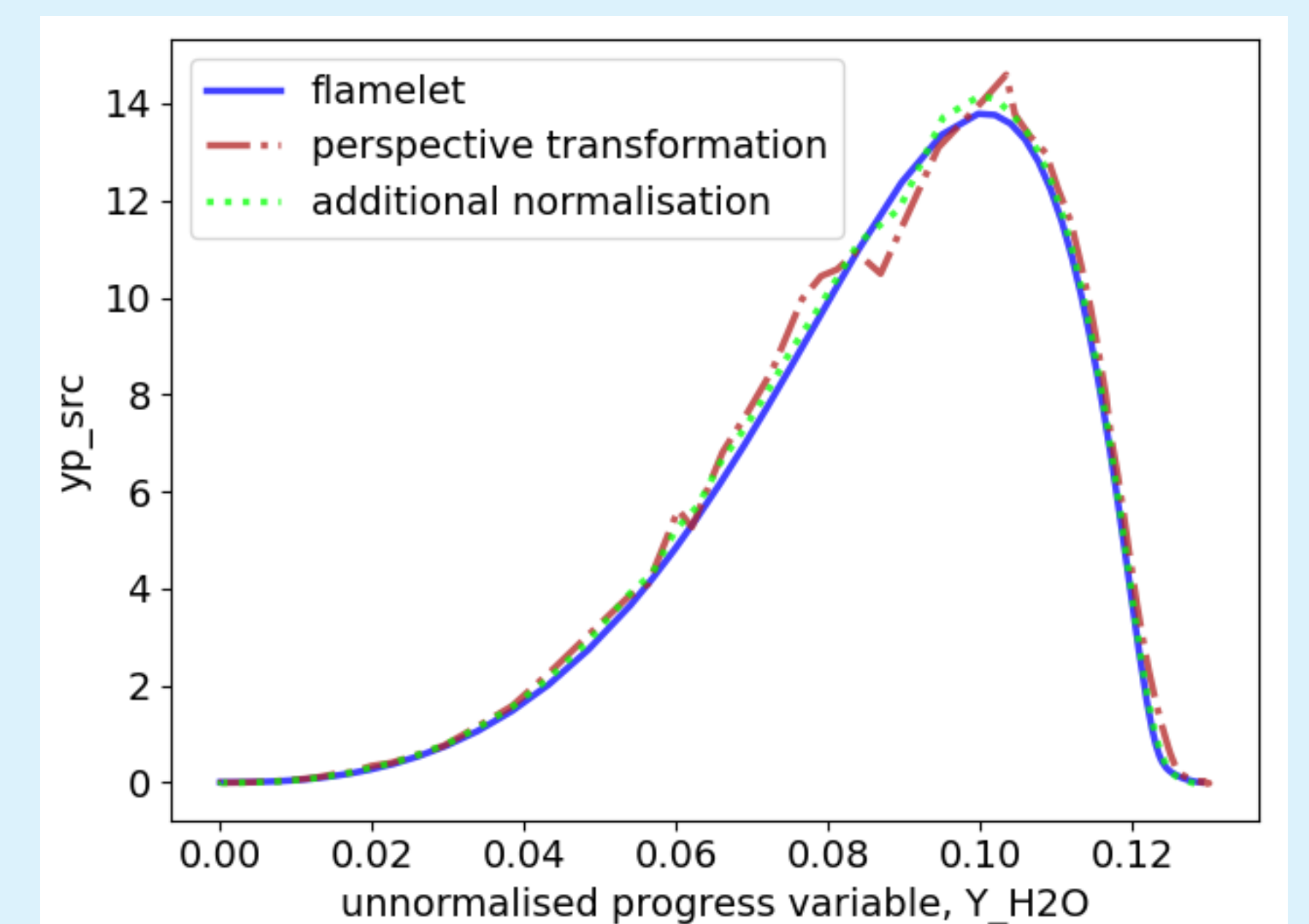


Figure 5 - Impact of other solutions on interpolation error ( $Z$  spacing = 0.052)

## 5. ACKNOWLEDGEMENTS

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## 6. REFERENCES

- [1] K.K.J. Ranga Dinesh, X. Jiang, J.A. van Oijen, R.J.M. Bastiaans, L.P.H. de Goey, Hydrogen-enriched nonpremixed jet flames: Effects of preferential diffusion, *Int. J. Hydrogen Energy*. 38 (2013) 4848–4863.
- [2] L.M. Verhoeven, W.J.S. Ramaekers, J.A. van Oijen, L.P.H. de Goey, Modeling non-premixed laminar co-flow flames using flamelet-generated manifolds, *Combust. Flame*. 159 (2012) 230–241.
- [3] J. Jiang, X. Jiang, M. Zhu, A computational study of preferential diffusion and scalar transport in nonpremixed hydrogen-air flames, *Int. J. Hydrogen Energy*. 40 (2015) 15709–15722.