



## Comparison of full multicomponent transport and mixture-averaged approximation in a forced, time-dependent, methane-air coflow diffusion flame

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The CFD solver `laminarSMOKE++` [1], designed for laminar reacting flows with detailed kinetic mechanisms, is used to compare two different approaches for modelling multicomponent diffusion including Soret effects in a forced, time-dependent laminar lifted  $\text{CH}_4/\text{N}_2$  flame in air. On the one hand, the mixture-averaged approximation is used, and on the other hand full multicomponent transport derived from the Kinetic Theory of Gases is considered using the efficient  $1+M$  formulation [2, 3] recently implemented in `laminarSMOKE++` [4]. The time-dependent oscillating flame considered, corresponding to the experiment reported in [5], allows to compare the lift-off heights and time responses in the different calculations depending on the diffusion flux treatment.

### References

- [1] Cuoci A et al. Numerical Modeling of Laminar Flames with Detailed Kinetics Based on the Operator-Splitting Method. *Energy and Fuels*. 2013;27:7730-7753.
- [2] Arias-Zugasti M et al. Efficient calculation of multicomponent diffusion fluxes based on kinetic theory. *Combustion and Flame*. 2016;163:540-556.
- [3] Naud B et al. Accurate heat (Fourier) and mass (Fick and thermodiffusion) multicomponent transport at similar cost as mixture-averaged approximation. *Combustion and Flame*. 2023;249:112599.
- [4] Naud B et al. Complete multicomponent versus mixture-averaged calculations of a laminar  $\text{H}_2/\text{N}_2$  diffusion flame including heat transfer at the burner and Soret effects. *International Journal of Hydrogen Energy*. 2025;In Press.
- [5] Dworkin SB et al. Computational and experimental study of a forced, time-dependent, methane–air coflow diffusion flame. *Proc. Combust. Inst.* 2007;31:971-978.