

TNF target flame: Turbulent Head-on Quenching H₂/air and CH₄/air flames

Authors

Max Schneider^a, Hendrik Nicolai^a, Thomas Howarth^{b,c}, Andy Aspden^d, Christian Hasse^a

Affiliations

^a Technical University of Darmstadt, Department of Mechanical Engineering, Simulation of reactive Thermo-Fluid Systems, Otto-Berndt-Str. 2, 64287 Darmstadt, Germany

^b Department of Aeronautical and Automotive Engineering, Loughborough University, Loughborough, LE11 3TU, UK

^c Institute for Combustion Technology, RWTH Aachen University, Templergraben 64, 52056 Aachen, Germany

^d School of Engineering, Newcastle University, Newcastle-Upon-Tyne, NE1 7RU, UK

Introduction

Direct numerical simulations (DNS) of turbulent head-on quenching (HOQ) of premixed lean H₂/air flames ($\phi = 0.4$, $T_u = 300$, K, $p = 1$, bar) and, for reference, CH₄/air flames ($\phi = 0.7$, $T_u = 300$, K, $p = 1$, bar) were conducted over a range of turbulence conditions (varying Karlovitz (Ka) and Damköhler (Da) numbers) in homogeneous and isotropic turbulence (HIT). The objective of the simulations and the resulting dataset is to investigate the flame–wall interaction (FWI) of thermodynamically unstable flames under turbulent conditions and to assess how an enhanced thermodynamically response induced by turbulence [1, 2] influences the quenching process.

The presented dataset includes snapshots of the full thermochemical state for a large number of time steps before and during the quenching process, up to complete flame extinction, as well as the corresponding simulation setups.

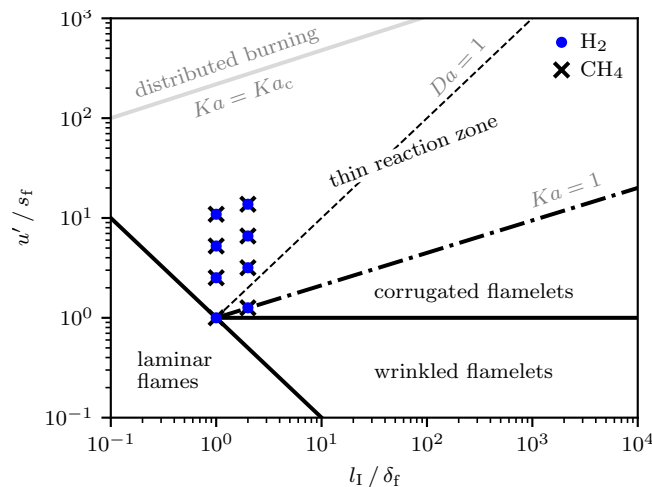


Figure 1: Turbulent regime diagram

Table 1: Reactant (left) and turbulence (right) conditions. All turbulence conditions are applied to both fuels.

Fuel	ϕ	$s_f / \text{m/s}$	$\delta_f / \mu\text{m}$	Λ_f	Υ_f	Ka_f	Da_f
H ₂	0.4	0.38	490	1	1.0	1	1.0
					2.520	4	0.397
					5.241	12	0.191
					10.903	36	0.092
CH ₄	0.7	0.193	595	2	1.260	1	1.587
					3.175	4	0.630
					6.604	12	0.303
					13.737	36	0.146

DNS configuration and methods

The DNS were performed using PeleLMEx [3, 4], a DNS solver with finite-rate chemistry that solves the low-Mach-number formulation of the reacting Navier–Stokes equations, treating the fluid as a mixture of ideal gases. A mixture-averaged model is employed for species diffusion, and thermal diffusion is accounted for using the model described in [5]. The discretization couples a multi-implicit spectral deferred correction scheme for integrating the mass, species, and energy equations with a density-weighted approximate projection method, which enforces a spatially constant thermodynamic pressure through a velocity divergence constraint.

Operation conditions

The H₂/air flame simulations were conducted at an equivalence ratio of $\phi = 0.4$, an unburned gas temperature of $T_u = T_w = 300$ K at a pressure of $p = 1$ bar. Chemical kinetics, transport coefficients, and thermodynamic relations were taken from [6].

Simulations for CH₄/air ($\phi = 0.7$, $T_u = 300$ K, $p = 1$ bar) were performed using a reduced GRI Mech 1.2 reaction mechanism (DRM19) [7]. The equivalence ratio was selected such that the 1D laminar flame speed s_1 and thermal flame thickness δ_1 approximately match those of the H₂/air operating condition.

As in flame-in-a-box studies focusing on freely-propagating flames ([1, 8–10]), the strategy of the presented simulations was to consider turbulence–flame–wall interaction in premixed flames within the 2D parameter space Ka_f and Da_f , which represent turbulence–flame interactions at the flame and integral length scales, respectively.

Karlovitz number $Ka_f = \sqrt{\Upsilon_f^3/\Lambda_f}$ and Damköhler number $Da_f = \Lambda_f/\Upsilon_f$ are defined using the freely propagating flame properties (flame thickness δ_f and flame speed s_f) obtained from three-dimensional laminar flame simulations, thus accounting for the thermodiffusive instability, as detailed in [10]. $\Lambda_f = l_1/\delta_f$ and $\Upsilon = u'/s_f$ are the length scale and velocity ratio, respectively, where u' is the rms velocity and l_1 the integral length scale.

The reactant and turbulence conditions are summarized in Tab. 1, and the corresponding turbulence regimes are shown in Fig. 1 using a premixed regime diagram.

Exemplary results

Figure 2 shows slices of the instantaneous normalized temperature field $\Theta = (T - T_u)/(T_{ad} - T_u)$ at $y = 0$ for different stages of the quenching process, both before and during quenching.

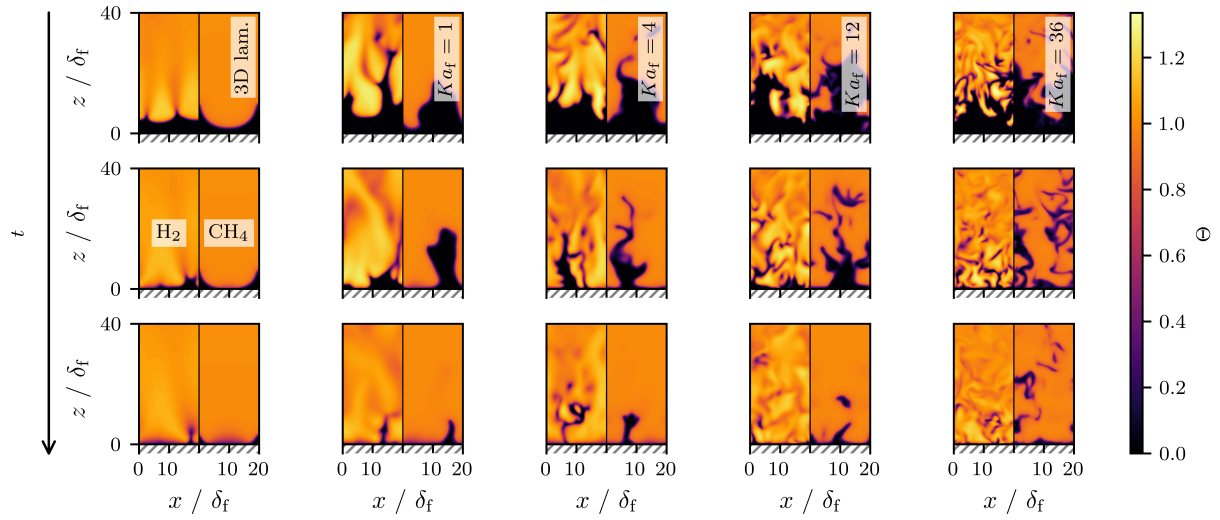


Figure 2: Slices (at $y / \delta_f = 0$) of the normalized temperature Θ for H_2 (left panels) and CH_4 (right panels) for different timesteps of the quenching process.

How to get access to the data

Upon request. Contact Christian Hasse (hasse@stfs.tu-darmstadt.de)

References

- [1] A. J. Aspden, M. S. Day, and J. B. Bell. Turbulence–flame interactions in lean premixed hydrogen: transition to the distributed burning regime. *J. Fluid Mech.*, 680:287–320, 2011. doi: 10.1017/jfm.2011.164.
- [2] L. Berger, A. Attili, and H. Pitsch. Synergistic interactions of thermodiffusive instabilities and turbulence in lean hydrogen flames. *Combust. Flame*, 244:112254, 2022. doi: 10.1016/j.combustflame.2022.112254.
- [3] M. S. Day and J. B. Bell. Numerical simulation of laminar reacting flows with complex chemistry. *Combust. Theory Model.*, 4(4):535–556, 2000. doi: 10.1088/1364-7830/4/4/309.
- [4] L. Esclapez, M. Day, J. Bell, A. Felden, C. Gilet, R. Grout, M. H. de Frahan, E. Motheau, A. Nonaka, L. Owen, B. Perry, J. Rood, N. Wimer, and W. Zhang. PeleLMEx: an AMR Low Mach Number Reactive Flow Simulation Code without level sub-cycling. *J. Open Source Softw.*, 8(90):5450, 2023. doi: 10.21105/joss.05450.
- [5] T. Howarth, M. Day, H. Pitsch, and A. Aspden. Thermal diffusion, exhaust gas recirculation and blending effects on lean premixed hydrogen flames. *Proc. Combust. Inst.*, 40(1–4):105429, 2024. doi: 10.1016/j.proci.2024.105429.
- [6] M. P. Burke, M. Chaos, Y. Ju, F. L. Dryer, and S. J. Klippenstein. Comprehensive H₂/O₂ kinetic model for high-pressure combustion. *Int. J. Chem. Kinet.*, 44(7):444–474, 2011. doi: 10.1002/kin.20603.
- [7] A. Kazakov and M. Frenklach. Reduced Reaction Sets based on GRI-Mech 1.2, 1994. URL <http://combustion.berkeley.edu/drm/>.
- [8] A. Aspden, M. Day, and J. Bell. Turbulence–chemistry interaction in lean premixed hydrogen combustion. *Proc. Combust. Inst.*, 35(2):1321–1329, 2015. doi: 10.1016/j.proci.2014.08.012.
- [9] T. Howarth, E. Hunt, and A. Aspden. Thermodiffusively-unstable lean premixed hydrogen flames: Phenomenology, empirical modelling, and thermal leading points. *Comb. Flame*, 253:112811, 2023. doi: 10.1016/j.combustflame.2023.112811.
- [10] E. Hunt and A. Aspden. Thermodiffusively-unstable lean premixed hydrogen flames: Length scale effects and turbulent burning regimes. *Comb. Flame*, 272:113855, 2025. doi: 10.1016/j.combustflame.2024.113855.