

TNF target flame: Lean premixed turbulent H₂/air slot-jet flames at high pressure and temperature.

Authors

Sofiane Al Kassar^a, Antonio Attili^a

Affiliations

^a School of Engineering, Institute for Multiscale Thermofluids, University of Edinburgh, Edinburgh EH9 3FD, United Kingdom

Introduction

The influence of elevated pressure and temperature on premixed lean hydrogen flames is investigated using Direct Numerical Simulations (DNS), with a focus on the interplay between turbulence, thermodiffusive instabilities, and differential diffusion effects. The combined increase of temperature and pressure is investigated since these two variables are usually linked in applications such as gas turbines and internal combustion engines. Three DNS of turbulent premixed lean hydrogen/air flames are compared: one at ambient conditions (1 atm, 298 K), another at gas-turbine conditions (20 atm, 700 K), and one at intermediate conditions (5 atm, 472 K), all featuring a jet Reynolds number of $Re = 11,200$ and Karlovitz number of $Ka \approx 90$. Since pressure and temperature have opposing influences on thermodiffusive instability and thermodiffusive effects in general, their combined action leads to negligible variations in one- and two-dimensional laminar flames. In contrast, turbulent jet flames exhibit pronounced differences despite the minimal changes observed in laminar conditions.

DNS configuration and methods

The reactive, unsteady Navier-Stokes equations are solved under the low Mach number approximation, with the mixture assumed to follow the ideal gas equation of state. A finite-rate multistep chemistry model involving 9 species [1] is employed to solve the species and temperature equations, as described in [2]. Transport properties are computed using a mixture-averaged model [2]. The thermodiffusion (Soret) effect is included using the model proposed by Schlup and Blanquart [3].

The governing equations are solved using a semi-implicit finite difference method [4], which has been extensively applied in various configurations [2, 5–7]. Spatial derivatives are discretised using second-order finite differences for the momentum equation and scalar diffusive terms, while a third-order weighted essentially non-oscillatory (WENO) scheme [8] is employed for the convective terms in the scalar equations. The chemical source term is treated using Strang's operator splitting [9], with integration performed by the stiff ordinary differential equation (ODE) solver CVODE [10].

Operation conditions

The flame configuration considered is a slot turbulent premixed jet flame surrounded by a

coflow of burnt gases. The jet consists of a hydrogen/air mixture with an equivalence ratio $\Phi = 0.4$. Three cases are considered, corresponding to typical ambient conditions ($p = 1$ atm and $T_u = 298$ K), gas-turbine conditions ($p = 20$ atm and $T_u = 700$ K), and intermediate conditions (5 atm, 472 K).

For all cases, the Reynolds number $Re = UH/\nu$ is 11,200. The inlet velocities, jet widths, and laminar flame speeds yield a nominal Karlovitz number $Ka = \delta_f^2/\eta^2$ approximately equal for all cases, where δ_f is the thermal flame thickness and η is the Kolmogorov scale. The thermal flame thickness is defined as $\delta_f = (T_b - T_u)/\|\nabla T\|_{\max}$. The Kolmogorov scale is defined as $\eta = (\bar{\nu}^3/\bar{\epsilon})^{1/4}$, where $\bar{\epsilon}$ is the Favre averaged energy dissipation and $\bar{\nu} = \overline{\mu/\rho}$ is the ensemble averaged viscosity. While the Ka number is nominally the same in the three cases, the different attenuation of turbulence across the three flame leads to different actual Ka in the flame in the three cases, see Tab. 1.

The domain is periodic in spanwise direction (z), with open boundary conditions prescribed at the outlet in the streamwise direction (x), and slip conditions imposed at the lateral boundaries (y). The inlet velocity field is generated from an auxiliary simulation of a fully developed turbulent channel flow. A uniform mesh is used in all three directions, with a grid resolution Δ satisfying $\Delta/\eta \approx 1$ and $\delta_f/\Delta \approx 10$. The total number of grid points is about 1.4 billion in all simulations.

Table 1: Conditions, one-dimensional characteristics, simulation parameters and turbulent characteristics of the three DNS cases.

	Case 1	Case 2	Case 3
p [atm]	1	5	20
T [K]	298	472	700
ϕ [-]	0.4	0.4	0.4
s_L [m/s]	0.186	0.314	0.555
δ_F [μm]	707	136	31.5
σ	4.44	3.10	2.35
Le_{eff}	0.34	0.34	0.34
Ze	11.5	12.0	11.4
H [mm]	7.82	1.55	0.36
U_{bulk} [m/s]	25.8	57.0	120.3
U_{coflow} [m/s]	5.17	11.4	24.1
Re_{jet}	11200	11200	11200
Δ [μm]	65	13.0	3.0
δ_F/Δ	10.9	10.5	10.5
η_{min}/Δ	0.6	0.6	0.6
Re_λ	9-20	16-26	26-40
$\eta/H \cdot 1000$	12-20	9-15	7-10
Ka	20-40	40-70	70-100

Exemplary results

Figure 1 shows the normalised temperature and turbulent kinetic energy for the three cases.

Figure 2 shows the turbulent flame speed, flame area, and stretch factor.

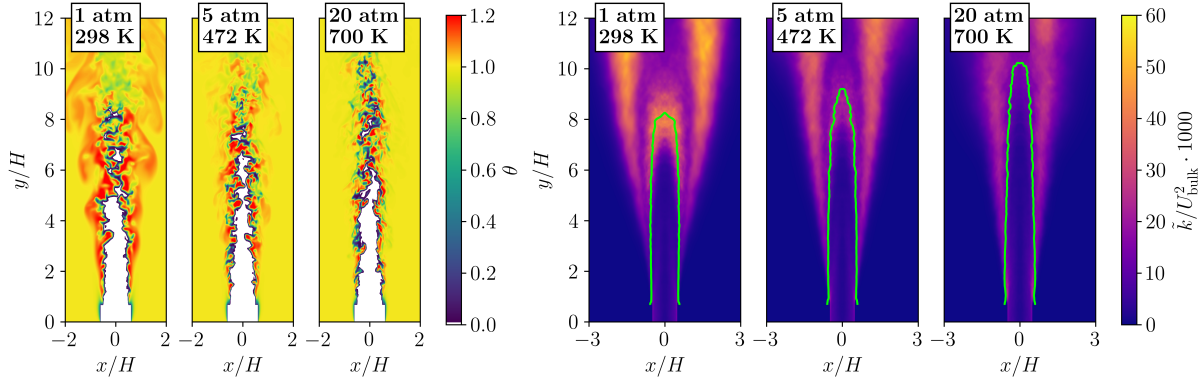


Figure 1: Two-dimensional slices of the turbulent flames for the three cases: Progress variable based on temperature θ (left), turbulent kinetic energy \tilde{k} normalised with the bulk velocity U_{bulk} (right). Isocontours of the progress variable based on hydrogen $C_{\text{H}_2} = 0.93$, corresponding to the peak reaction rate, are represented on top of \tilde{k} to help locate the flame.

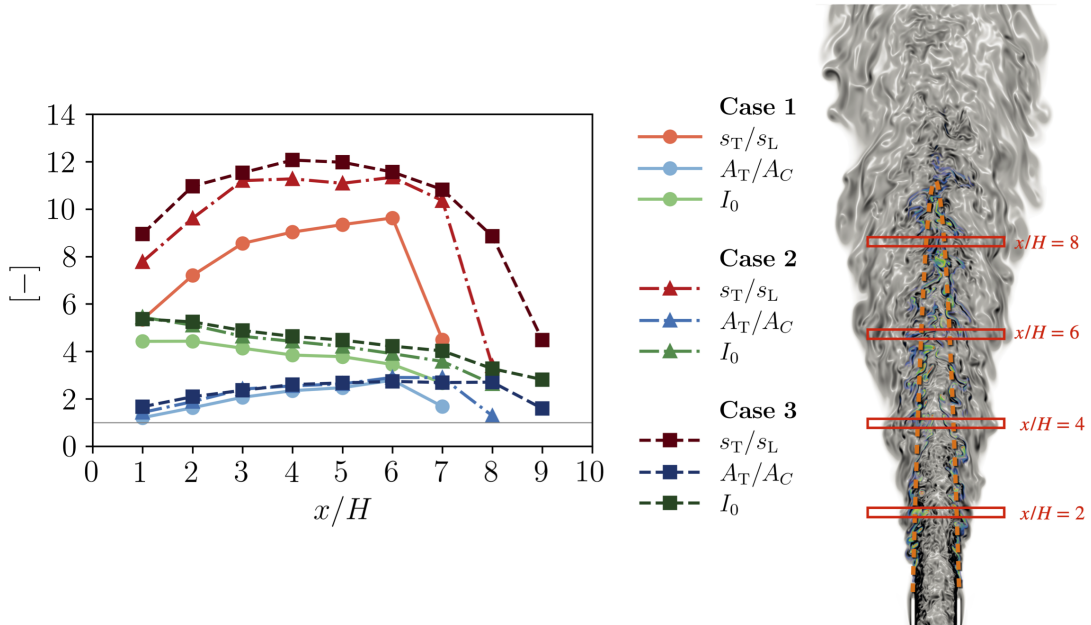


Figure 2: Evolution of the turbulent flame speed s_T , flame surface area A_T and stretch factor I_0 along the flame. s_T and A_T are respectively normalised with the laminar flame speed s_L , and the reference flame surface A_C obtained from an isocontour of mean progress variable.

How to get access to the data

Upon request. Contact Antonio Attili (antonio.attili@ed.ac.uk)

References

- [1] Michael P Burke, Marcos Chaos, Yiguang Ju, Frederick L Dryer, and Stephen J Klippenstein. Comprehensive h₂/o₂ kinetic model for high-pressure combustion. *Int. J. Chem. Kinet.*, 44 (7):444 – 474, 2012.
- [2] A. Attili, F. Bisetti, M. E. Mueller, and H. Pitsch. Effects of non-unity lewis number of gas-phase species in turbulent nonpremixed sooting flames. *Combust. Flame*, 166:192–202, 2016.
- [3] Jason Schlup and Guillaume Blanquart. A reduced thermal diffusion model for H and H₂. *Combustion and Flame*, 191:1–8, 2018. doi: 10.1016/j.combustflame.2017.12.022.
- [4] O. Desjardins, G. Blanquart, G. Balarac, and H. Pitsch. High order conservative finite difference scheme for variable density low mach number turbulent flows. *J. Comput. Phys.*, 227:7125–7159, 2008.
- [5] L. Berger, K. Kleinheinz, A. Attili, and H. Pitsch. Characteristic patterns of thermodiffusively unstable premixed lean hydrogen flames. *Proc. Combust. Inst.*, 37(2):1879–1886, 2019.
- [6] Antonio Attili, Stefano Luca, Dominik Denker, Fabrizio Bisetti, and Heinz Pitsch. Turbulent flame speed and reaction layer thickening in premixed jet flames at constant Karlovitz and increasing Reynolds numbers. *Proc. Combust. Inst.*, 38(2):2939–2947, 2021. doi: 10.1016/j.proci.2020.06.210.
- [7] L. Berger, A. Attili, and H. Pitsch. Synergistic interactions of thermodiffusive instabilities and turbulence in lean hydrogen flames. *Combust. Flame*, 244:112254, 2022.
- [8] X.D. Liu, S. Osher, and T. Chan. Weighted essentially non-oscillatory schemes. *J. Comput. Phys.*, 115(1):200–212, 1994.
- [9] Gilbert Strang. On the construction and comparison of difference schemes. *SIAM journal on numerical analysis*, 5(3):506–517, 1968.
- [10] A.C. Hindmarsh, P.N. Brown, K.E. Grant, S.L. Lee, R. Serban, D.E. Shumaker, and C.S. Woodward. Sundials: Suite of nonlinear and differential/algebraic equation solvers. *ACM Trans. Math. Softw.*, 31(3):363–396, 2005.