TNF target flame: Premixed Turbulent $NH_3/H_2/N_2$-Air Jet Flames at Atmospheric Pressure.

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Introduction

Turbulent premixed precracked $H_2/H_2/N_2$-air jet flames at rich ($\phi = 1.6$) and lean ($\phi = 0.8$) conditions are investigated with a focus on the interaction of turbulence, differential diffusion, stratification and NOx formation in conditions relevant to staged combustion systems. The study investigates four Direct Numerical Simulations (DNS) at atmospheric pressure and ambient jet inlet temperatures. Jet velocities range from 25.0 to 75.0 $\mathrm{m\,s^{-1}}$ resulting in a range of Reynolds numbers of Re = 5900 to 17700. The jet flames are piloted by exhaust gas of a lean H_2/N_2 premixed flame. The conditions are a numerical investigation of experimental TNF target flames in "Premixed turbulent $NH_3/H_2/N_2$-air jet flames at atmospheric pressure" introduced in [1]. The presented data includes temporally averaged fields of key quantities as well as the jet inflow data sampled from the precursor turbulent pipe flow.

DNS configuration and methods

The DNS were conducted using the low Mach number reactive flow solver *nekCRF* [2], which is based on the spectral element method code *nekRS* [3]. The chemical subsystem is solved fully-coupled without splitting of convection, diffusion and reactions using CVODE. The kinetic mechanism of Stagni et al. [4] with 31 species and 203 reactions is used for all simulations. Species diffusion is accounted for by a mixture-averaged transport model excluding the Soret and Dufour effects. 7^{th}-order Lagrange polynomials are used as basis functions for spatial discretization, while a 3^{rd}-order backward differentiation method is used for temporal discretization.

Operation conditions

The flame configuration considered is a cylindrical turbulent premixed jet flame surrounded by a pilot of burnt gases. Geometric dimensions of the burner and computational domain are shown in Fig. 1. The jet consists of a mixture of 40% NH_3, 45% H_2, and 15% H_2 by volume, but varying equivalence ratios. The pilot consists of a lean H_2-air flame at $\phi = 0.57$. Four cases are considered: A variation in jet velocity from 25.0, 50.0, 75.0 $\mathrm{m\,s^{-1}}$ at $\phi = 1.6$ and a variation in equivalence ratio of $\phi = 0.8, 1.6$ at a jet velocity of $50.0\,\mathrm{m\,s^{-1}}$. Across all operating conditions, pressure, jet inlet temperature, pilot composition and pilot exhaust gas velocity are kept constant at $P = 1.0 \times 10^5\,\mathrm{Pa}$, $T_{\mathrm{Jet}} = 300.0\,\mathrm{K}$, $\phi = 0.57$, and $U_{\mathrm{Pilot}} = 11.25\,\mathrm{m\,s^{-1}}$, respectively.

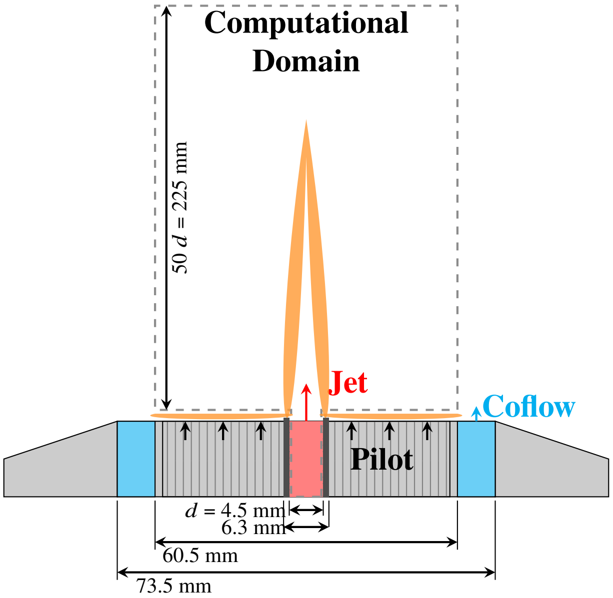

Figure 1: Schematic of the turbulent jet burner. Dashed line indicates the computational domain of the DNS.

The simulation parameters for each operating condition are listed in Tab. 1. The naming scheme specifies the H_2 content (H), the equivalence ratio (P), and the jet velocity (U). Global Karlovitz and Damköhler numbers are defined based on jet inlet values as $\mathrm{Ka}_{\mathrm{Jet}} = \sqrt{(u'^3/l_\mathrm{T})/(s_\mathrm{L}^3/d_\mathrm{L})}$ and $\mathrm{Da}_{\mathrm{Jet}} = (l_\mathrm{T}/u')/(d_\mathrm{L}/s_\mathrm{L})$. Here, the root mean square (RMS) value of the velocity fluctuation is calculated as $u' = 0.075 * U_{\mathrm{Jet}}$, the integral length scale is calculated as $l_\mathrm{T} = 0.2 * d_{\mathrm{Jet}}$, and s_L and d_L are the laminar flame speed and laminar thermal flame thickness, respectively.

The burner walls are assumed to be adiabatic. At the jet inlet, velocity is prescribed from an auxiliary DNS of a fully developed turbulent pipe flow via overset meshes. An unstructured mesh is used with a grid resolution Δ satisfying $\Delta/\eta \leq 1$ and $d_\mathrm{L}/\Delta \geq 12$. The total number of grid points is about 2.4 billion in all simulations.

Table 1: List of investigated cases with their corresponding naming, and the equivalence ratio, velocity, Reynolds number, Karlovitz number, and Damköhler number of the jet, respectively.

Case	ϕ (−)	$\mathrm{U}_{\mathrm{Jet}}$ ($\mathrm{m\,s^{-1}}$)	$\mathrm{Re}_{\mathrm{Jet}}$ (−)	$\mathrm{Ka}_{\mathrm{Jet}}$ (−)	$\mathrm{Da}_{\mathrm{Jet}}$ (−)
H045P160U025	1.6	25.0	5900	18	0.16
H045P160U050	1.6	50.0	11800	51	0.080
H045P160U075	1.6	75.0	17700	93	0.053
H045P080U050	0.8	50.0	12600	30	0.15

Exemplary results

Figure 2 shows the instantaneous temperature fields in a cutting plane.

Further, the provided data includes:

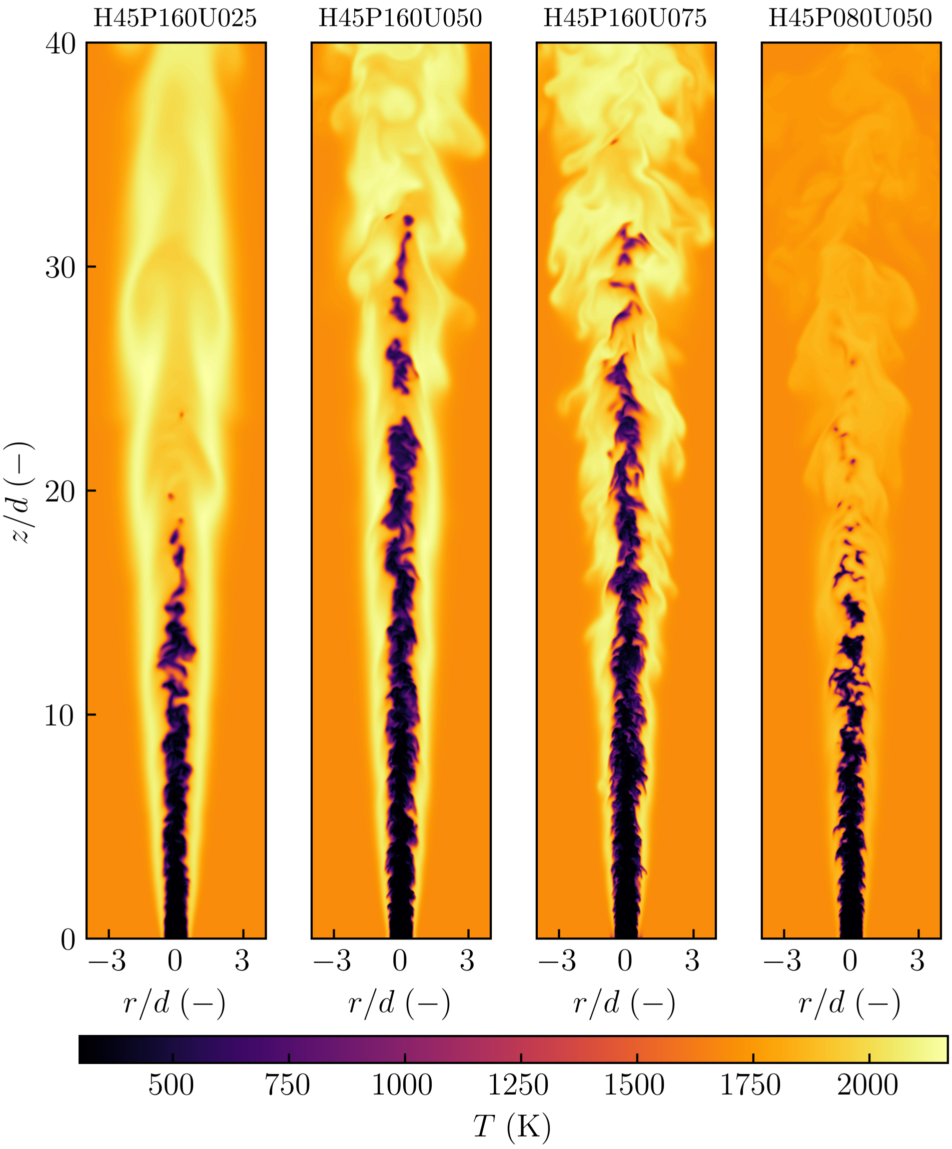

Figure 2: Flame visualization of the cases as instantaneous temperature fields in a cutting plane.

- Mean and RMS values of velocity, temperature, and mass fractions of NH_3, H_2, OH, H_2O_2, NO.
- Turbulent pipe flow: mean and RMS values of velocity.
- Turbulent pipe flow: instantaneous velocities sampled in a plane of the pipe cross section with a frequency of $\Delta t = 10\Delta t_{\mathrm{DNS}}$.

How to get access to the data

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

References

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