DNS-Based Analysis of Flame Dynamics in Turbulent H_2-CO-Air Mixtures

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Motivation

- Formation of flammable gas mixtures due to the release of H_2/CO into contained environments following accidents in:
  - nuclear power plants: H_2/CO produced during a meltdown
  - process engineering: Leakage of $H_2/CO/air$ (syngas) mixtures which represent an important intermediate product, e.g. in the field of renewable energies (Haber-Bosch)
- Demand to characterize the combustion of syngas mixtures at different fuel compositions (α) and equivalence ratios (ϕ)
- Particular attention given to transient flame dynamics, influenced by turbulence and intrinsic flame instabilities

Numerical Method

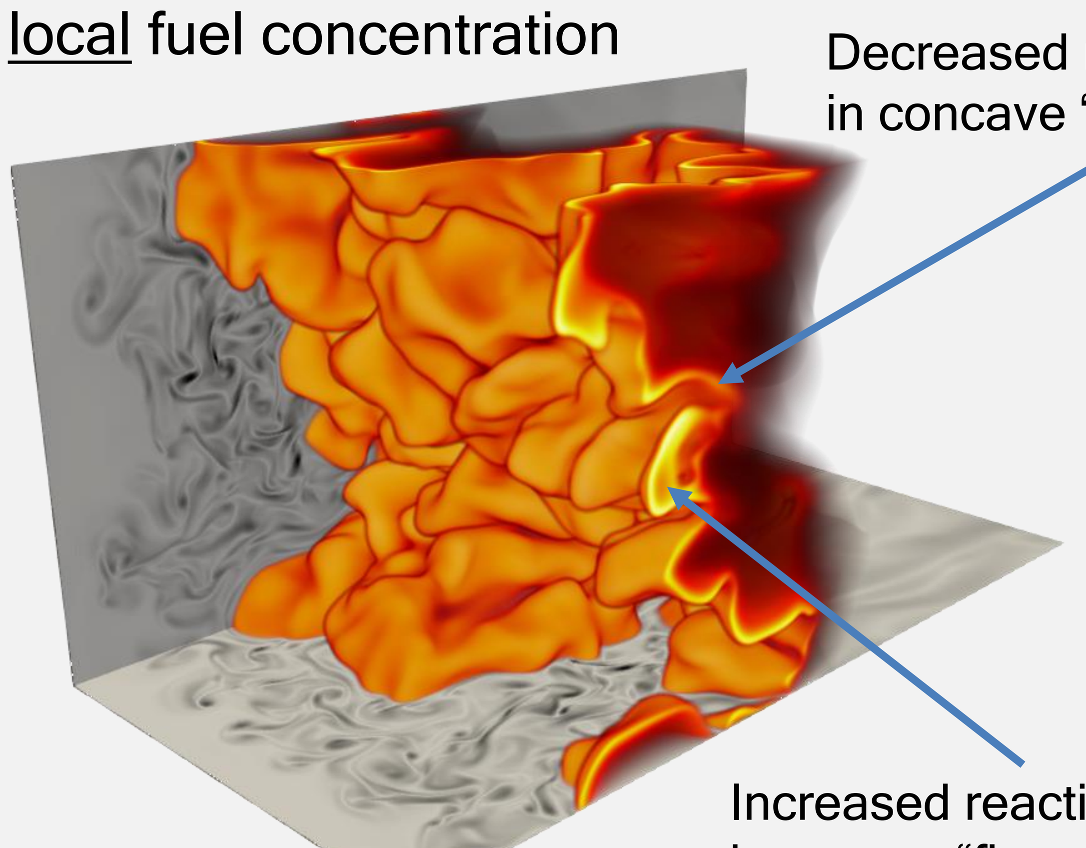
- SENGA2 DNS Solver by Cant (2015)
- Fully compressible Navier-Stokes equations, 10th-order central finite-difference scheme for spatial discretization
- Explicit time advancement is accomplished using a fourth-order, low-storage Runge-Kutta method
- Detailed multi-step chemistry using a syngas-optimized chemical mechanism by Davis et al. (2005), containing
  - 14 species
  - 34 elementary reactions
- Mixture-averaged transport approach

Simulation Setup

- Cuboidal computational domain, discretized by a uniform Cartesian grid with $1024 \times 512 \times 512$ equidistant points, parallelized on 8192 cores
- Spatial resolution results in a domain size of $\sim 3 \times 1.5 \times 1.5\ cm^3$
- Flame initialized using an 1D flame profile, turbulence is imposed via decaying turbulent flow fields (Batchelor-Townsend)
- Simulations are conducted over a simulation duration of three eddy turnover times $\tau_{et} \equiv L_{11}/u'$
- DNS study considers several syngas mixtures (varying ϕ and α), chosen to investigate impact of CO on transient, possibly instability-driven flame behavior

Visualization of Instabilities

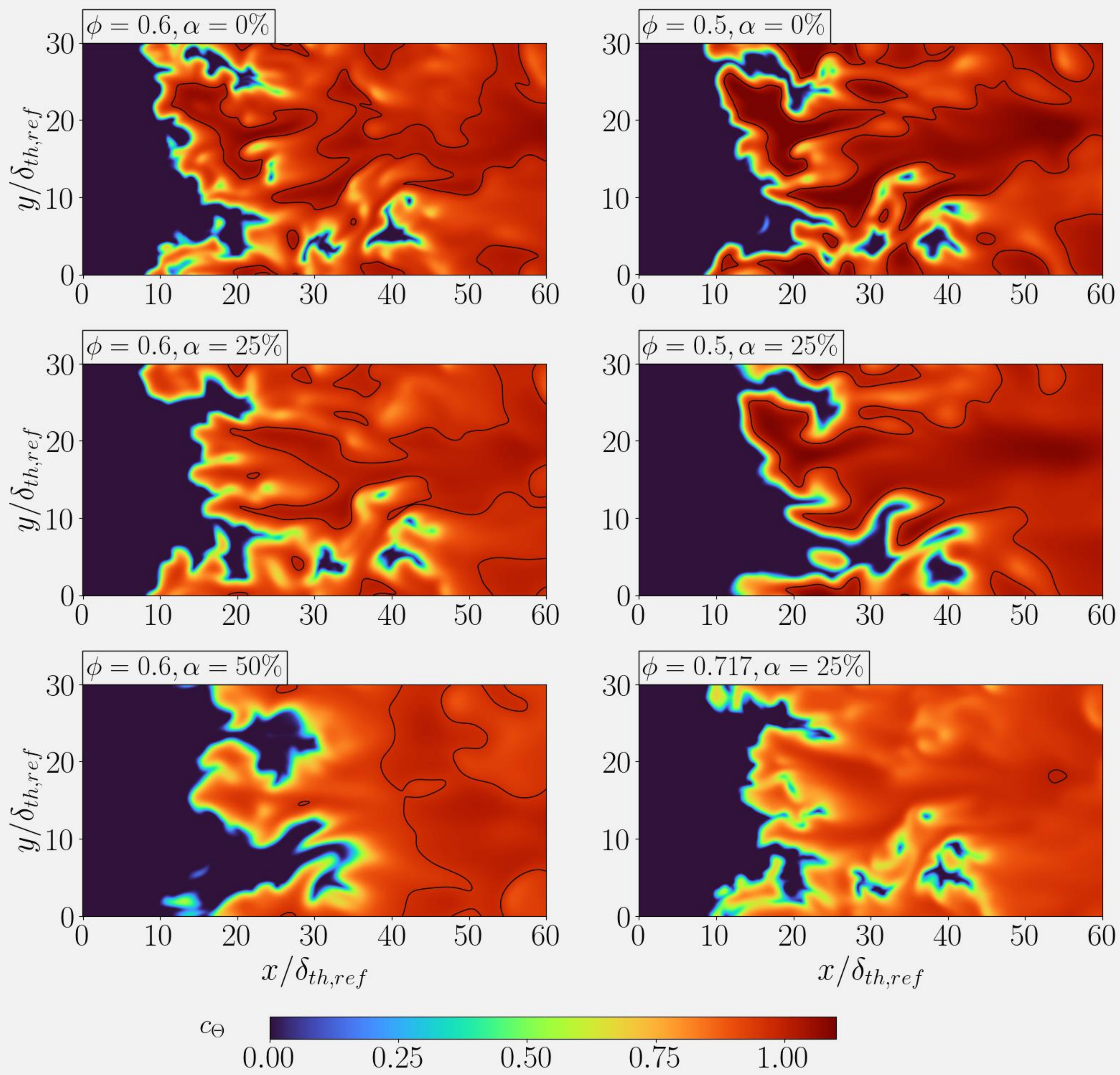
- If the fuel molecules' mass diffusivity exceeds the thermal diffusivity of the entire mixture ($Le \equiv D_{th}/D_{fuel} \ll 1$), there is increased diffusion of fuel into convex parts of the flame
- For lean ($\phi < 1$) mixtures, this results in regions with:
  - Increased local fuel concentration, leading to elevated chemical consumption and thus to local flame acceleration
  - Lower local fuel concentration



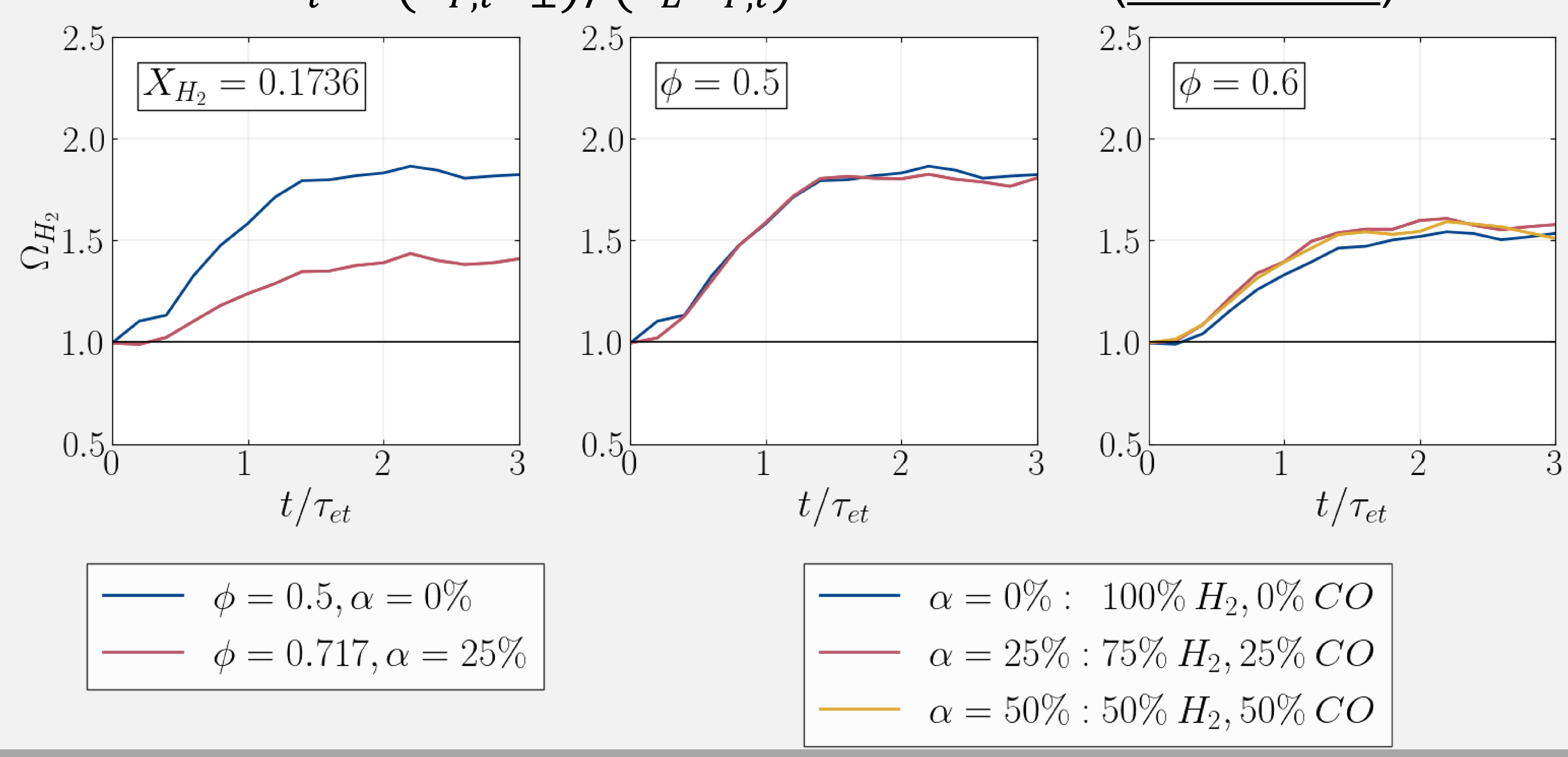
Flame visualized by means of H mass fraction for $\phi = 0.6$ and a fuel comp. of $100\ \%\ H_2$ at $\tau_{et} \approx 3$. Vorticity displayed in the background (Wehrmann 2023)

Results and Discussion

Instantaneous normalized temperature $c_\Theta \equiv (T - T_u)/(T_b - T_u)$ distribution in the $x - z$ midplane for $u'/S_L = 4.0$ cases at $\tau_{et} \approx 3$. Iso-contour for $c_\Theta = 1.0$ (black) encloses super-adiabatic temperature (i.e., $c_\Theta > 1.0$) regions:



- Large super-adiabatic regions - indicating thermo-diffusive instabilities - as well as pronounced wrinkling are observed
- To isolate instability-driven flame acceleration from flame area induced acceleration (wrinkling), the burning rate per unit area of the flame $\Omega_i \equiv (S_{T,i} A_\perp)/(S_L A_{T,i})$ is evaluated (Klein 2020):



Conclusions and Outlook

- Instability-driven flame behavior ($\Omega > 1$) observable for all cases
- Development of Ω indicates the influence of CO on transient flame behavior is:
  - Minor when partially substituted for H_2 (identical ϕ)
  - Notable when added to H_2 (identical X_{H_2}, increased ϕ)
- Valuable database for future subgrid modeling approaches

References

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- Davis et al. (2005), *Proc. of the Combust. Inst.*, 30(1), 15407489
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- Klein et al. (2020), *Flow, Turb. and Combust.*, 104(2), 1386-6184