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The Role of Thermodiffusion and Dimensionality in the Formation of Cellular Instabilities in Hydrogen Flames

T. Zirwes[1], F. Zhang[2], T.L. Kaiser[3], K. Oberleithner[3], O.T. Stein[4], H. Bockhorn[4], A. Kronenburg[1]

1) Institute for Combustion Technology (ITV), University of Stuttgart

2) Institute for Technical Chemistry, Karlsruhe Institute of Technology

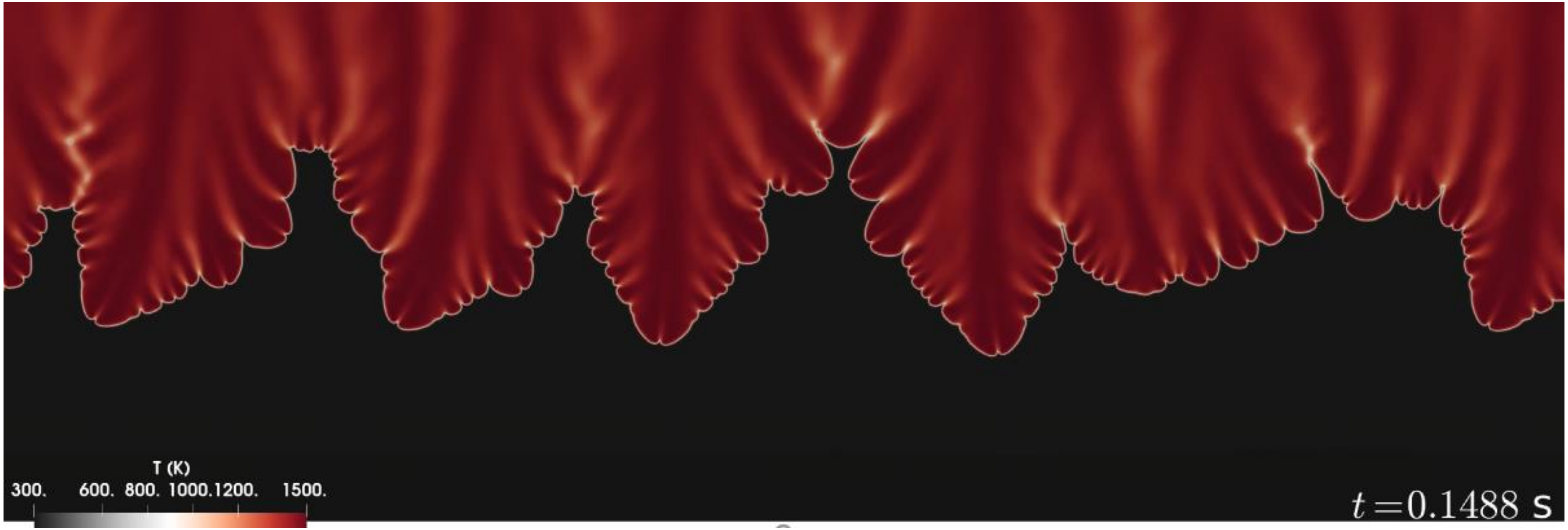
3) Laboratory for Flow Instabilities and Dynamics, Technische Universität Berlin

4) Engler-Bunte Institute, Karlsruhe Institute of Technology

Motivation

Thermodiffusive instabilities

- A common numerical approach to study thermodiffusive instabilities in laminar flame propagation until flame fingers form



- Hydrogen − air at $\phi = 0.4$ and atmospheric conditions

Thermodiffusive instabilities

- The previous simulations were all performed in 2D
- Motivation of this work:
  - What is the impact on cell formation when simulations are performed in 3D?
  - What is the impact of thermodiffusion (Soret effect)?
- Aspects of these were studied by other authors before:
  - Theoretical work by Matalon
  - Grcar et al. (2017): https://doi.org/10.1016/j.proci.2008.06.075
  - Schlup & Blanquart (2017): https://doi.org/10.1080/13647830.2017.1398350
  - X. Wen et al. (2024): https://doi.org/10.1016/j.combustflame.2024.113497
  - ….

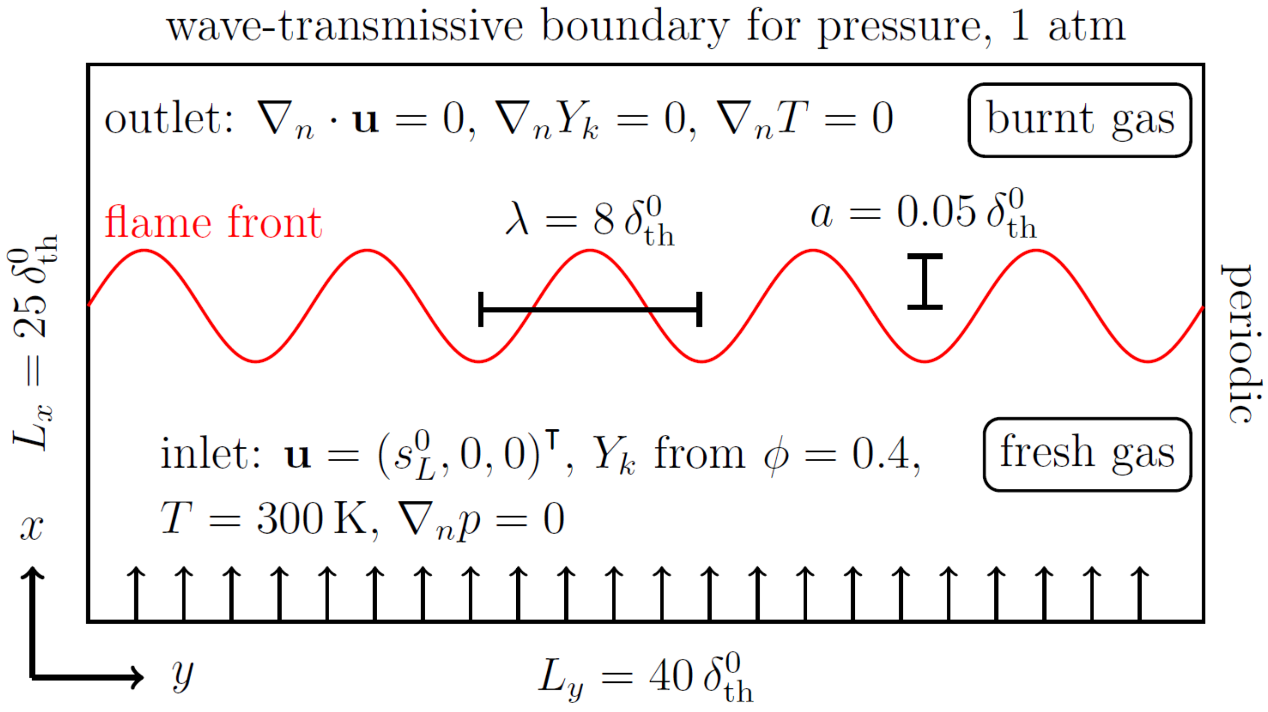
Numerical Setup

Numerical Setup

- Hydrogen-air at $\phi = 0.4$ and atmospheric conditions
- Laminar inflow
- Initial perturbation of the flame front
- Simulation done in 2D/3D & with/without Soret diffusion
- Mechanism by Li et al. with 9 species and 19 reactions

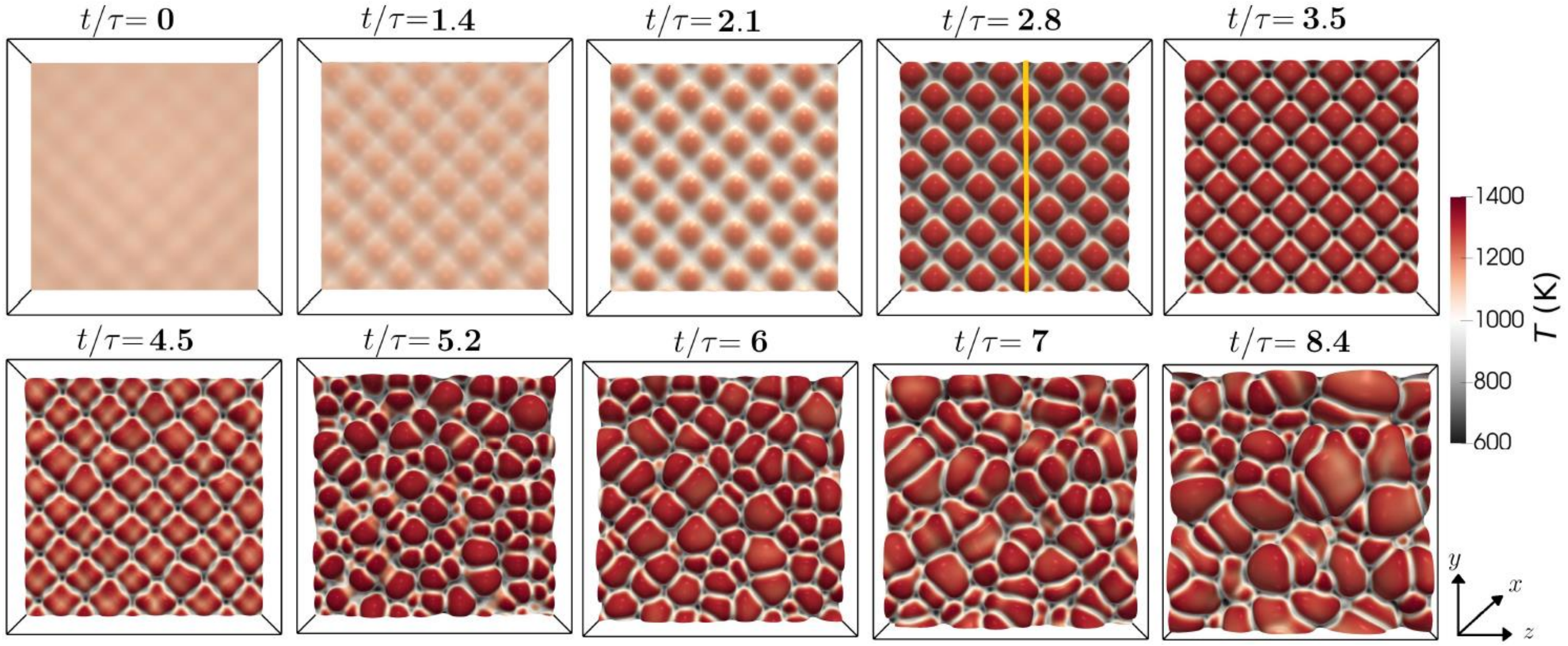
Table 1: Properties of reference laminar 1D flames.

ϕ	Soret	s_L^0 (m/s)	δ_{th}^0 (mm)	τ (ms)	$Y_{\mathrm{H_2,iso}}$
0.4	no	0.239	0.599	2.510	0.00138
0.4	yes	0.227	0.613	2.703	0.00128



Cell formation

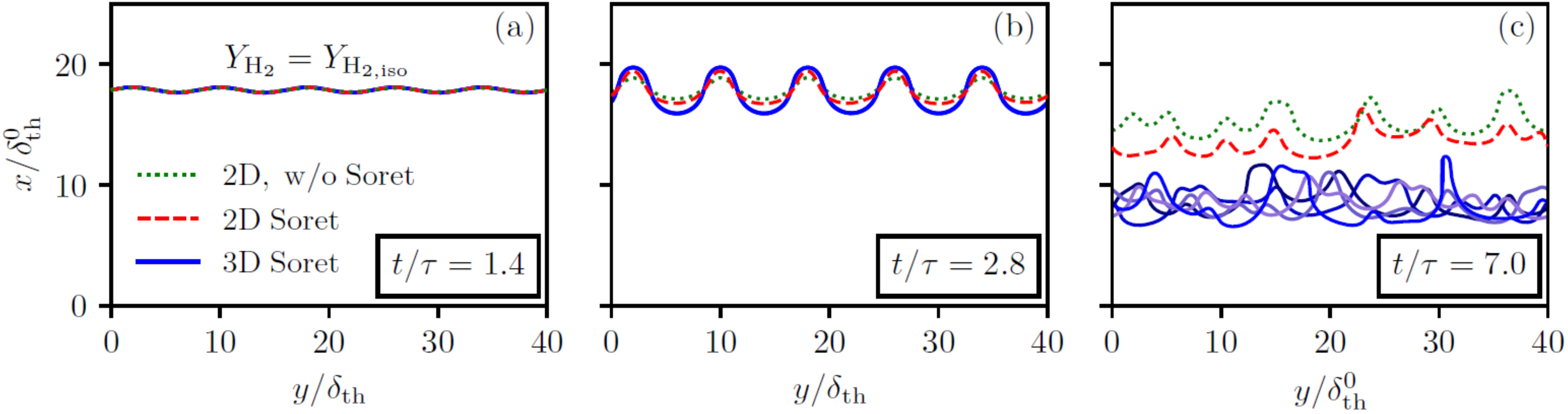
- First, linear growth regime, then decay into secondary structures (non-linear regime)



- 3D Simulation with Soret diffusion. Iso-surface of $Y_{H_{2,iso}}$ colored by temperature.

Flame propagation

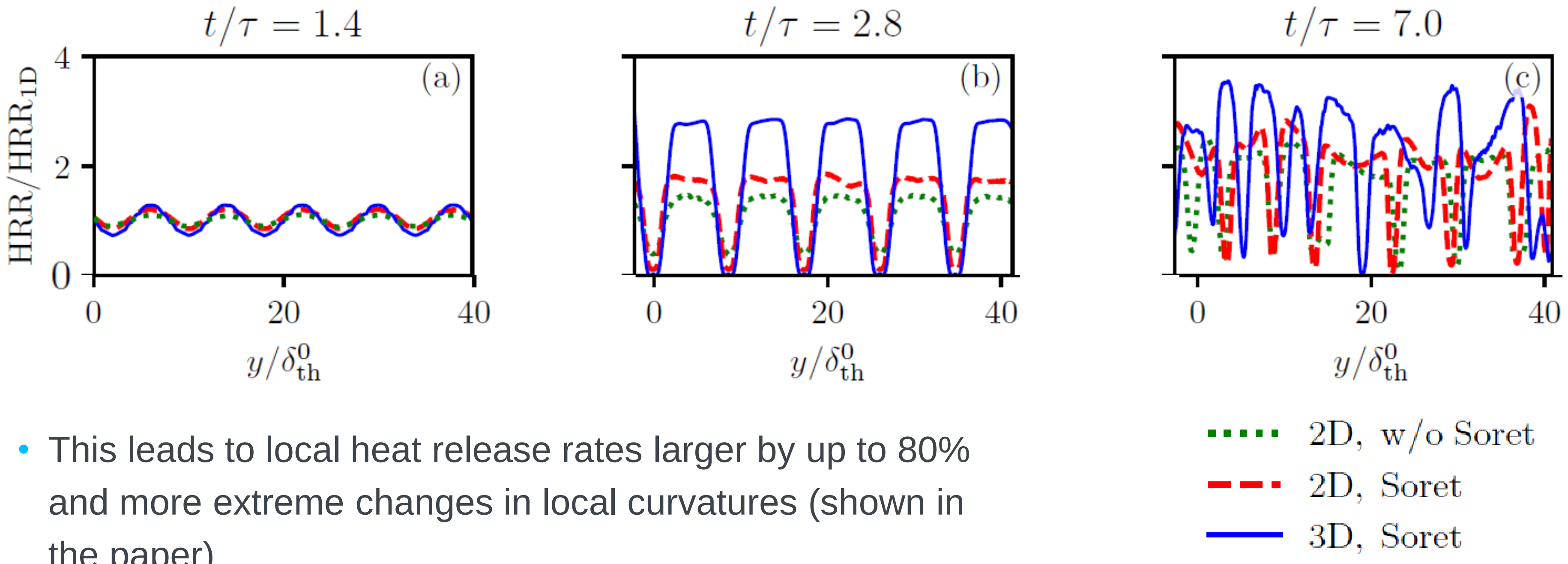
- Flame propagation in 2D/3D and with/without Soret diffusion



- Faster propagation in 3D, and also faster propagation with Soret diffusion

Effect on flame structure

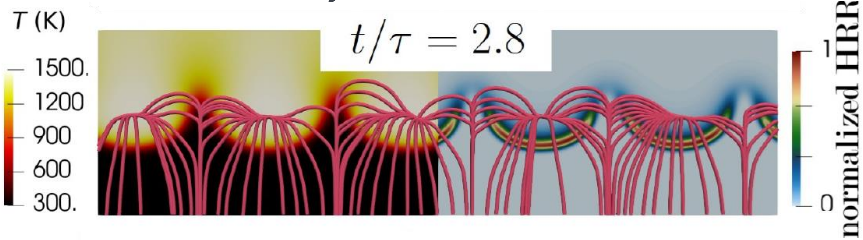
- In 3D, curvatures are higher, leading to a stronger focusing/defocusing of diffusion fluxes

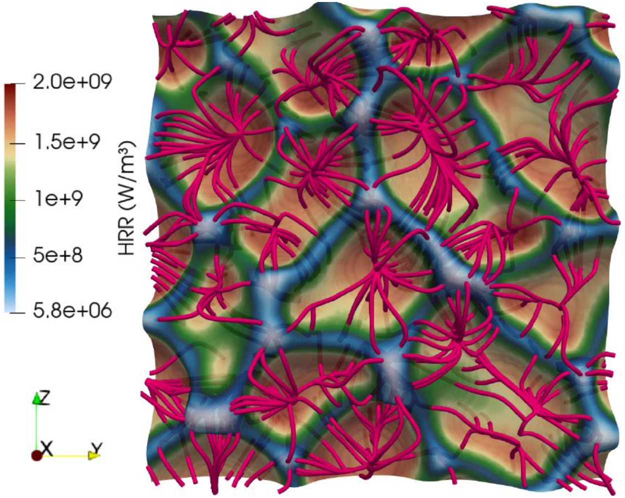


- This leads to local heat release rates larger by up to 80% and more extreme changes in local curvatures (shown in the paper)

Trajectories of progress variable c = Y_{H_2O}

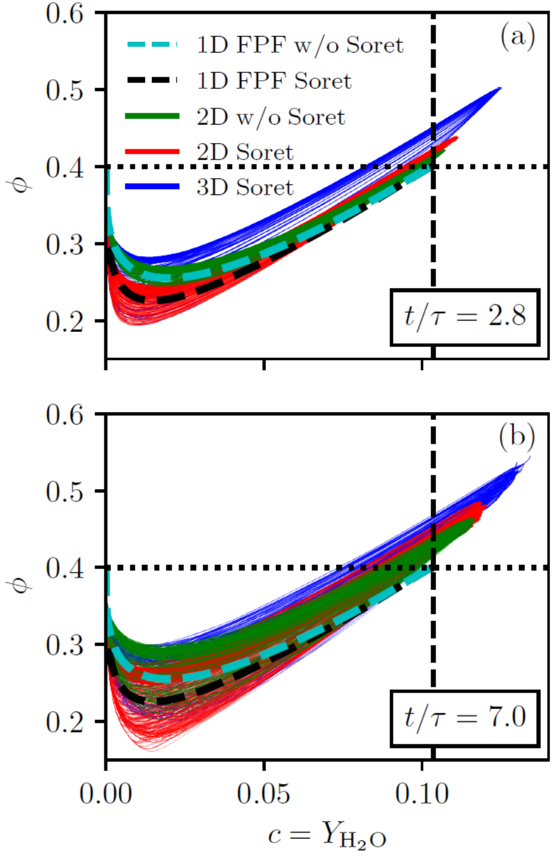
Trajectories in 2D





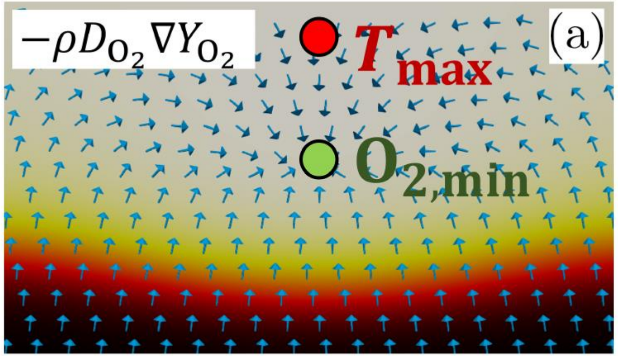
$t/\tau = 7.0$

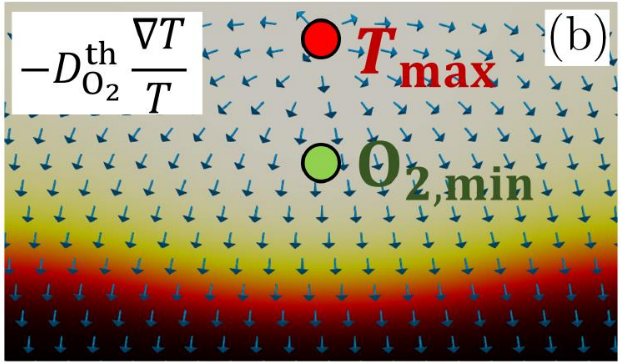
Trajectories in 3D



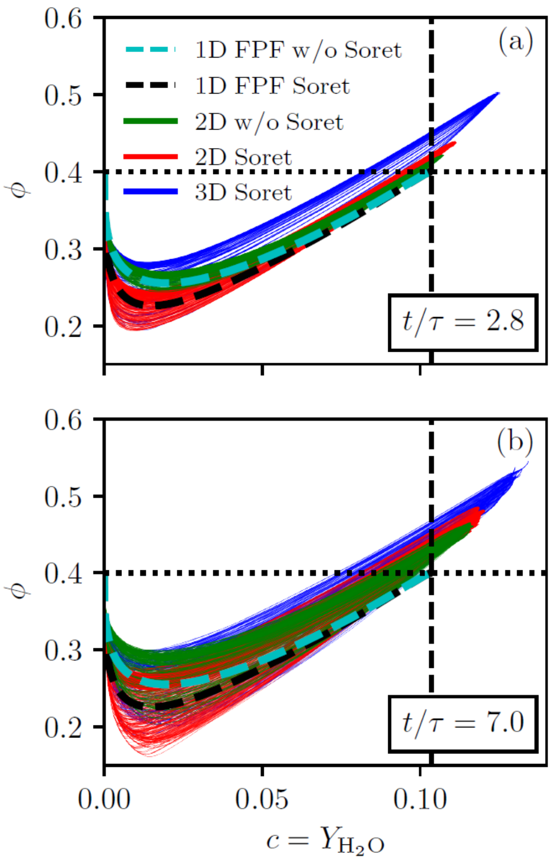
Diffusive fluxes at positively curved flame segments

$$\boldsymbol{j}_k = -\rho D_k \nabla Y_k - D_k^{\mathrm{th}} \frac{\nabla T}{T}$$





- Due to non-unity Lewis number/preferential diffusion, locations of species and temperature minima/maxima do not coincide
- At positively curved flame segments, thermodiffusion flux of oxygen opposes that of the Fickian diffusion

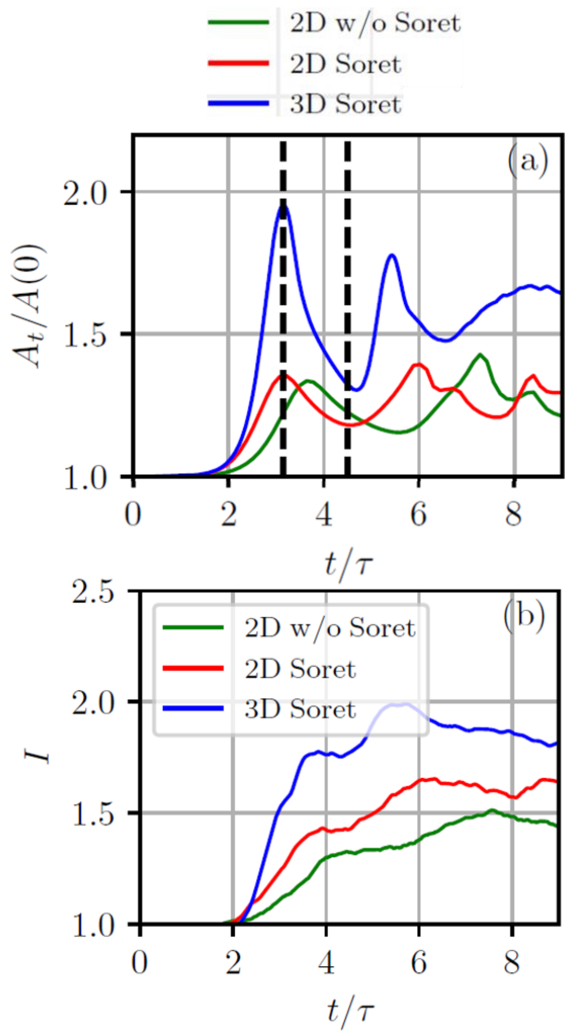


Effect on global flame properties

- For the 3D case, the flame surface area grows more rapidly
- However, the time instance at which transition from primary to secondary structures occurs, is the same as in 2D
- Without Soret diffusion, the transition occurs later
- Higher efficiency factors in 3D and with Soret diffusion
- After secondary structures developed, quasi-steady state (also observed by other authors)

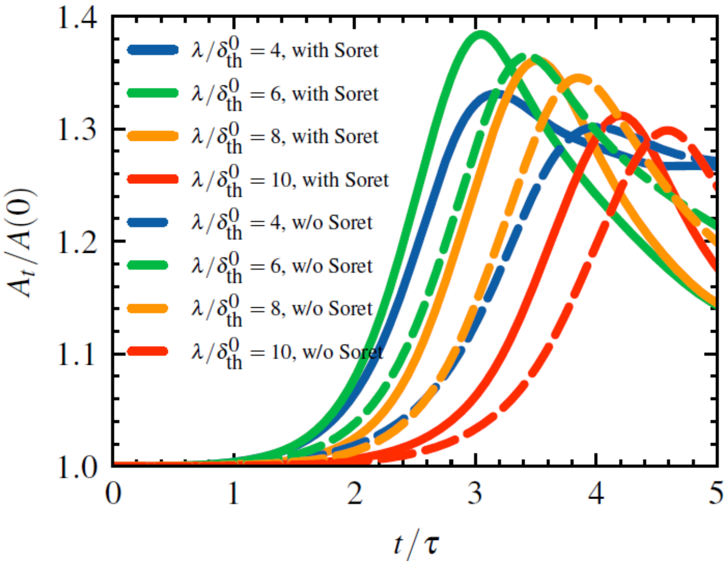
$$I = (s_T/s_L^0)/(A_t/A_0)$$

$$s_T = -\frac{1}{\rho_0 A_0 (Y_{H_2}^0 - Y_{H_2}^b)} \int \dot{\omega}_{H_2} \, dV$$

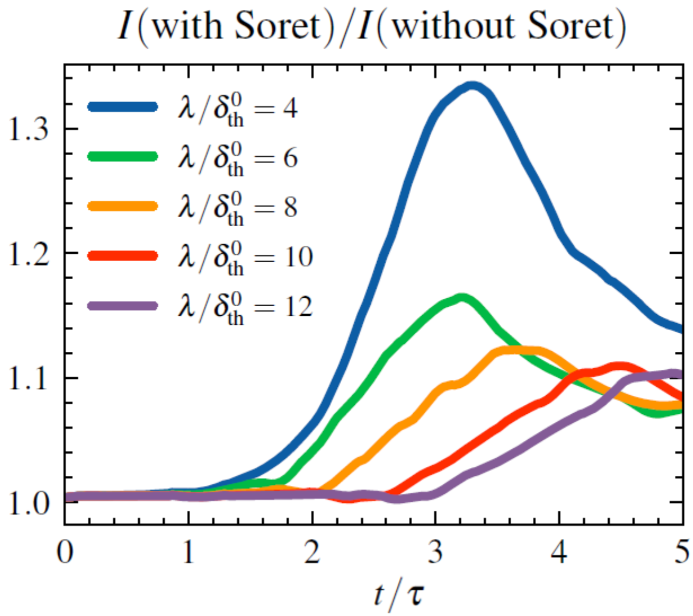


Effect of Soret diffusion as function of perturbation wavelengths

- Cell growth depends on perturbation wavelengths



- Soret diffusion increases efficiency factors depending on initial curvature



Conclusions

- Even at the same cross-section in 2D, a 3D flame exhibits larger curvatures and thus heat release rates exceeding by 80% at the positively curved flame segments, resulting in faster flame propagation
- However, the time instance when the collapse happens is nearly the same
- Soret diffusion leads to lower laminar flame speeds but larger local propagation speeds due to opposed diffusive fluxes at positively curved flame segments
- Collapse into secondary cells occurs later without Soret diffusion
- Effect of Soret diffusion on efficiency factors for early cell formation is a function of perturbation wavelength.

Thank you!

Thorsten Zirwes

e-mail thorsten.zirwes@itv.uni-stuttgart.de
phone +49 (0) 711 685-65637
www.itv.uni-stuttgart.de/institut/team/Zirwes/

University of Stuttgart
Institute for Combustion Technology (ITV)
Pfaffenwaldring 31, 70569 Stuttgart, Germany
Room 03.313