TU DARMSTADT: INSTITUTE FOR SIMULATION OF REACTIVE THERMO-FLUID SYSTEMS

MODELING OF TURBULENT HYDROGEN COMBUSTION

Vinzenz Schuh

TECHNISCHE UNIVERSITÄT DARMSTADT

STFS

CFD4H2

OpenFOAM

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AGENDA

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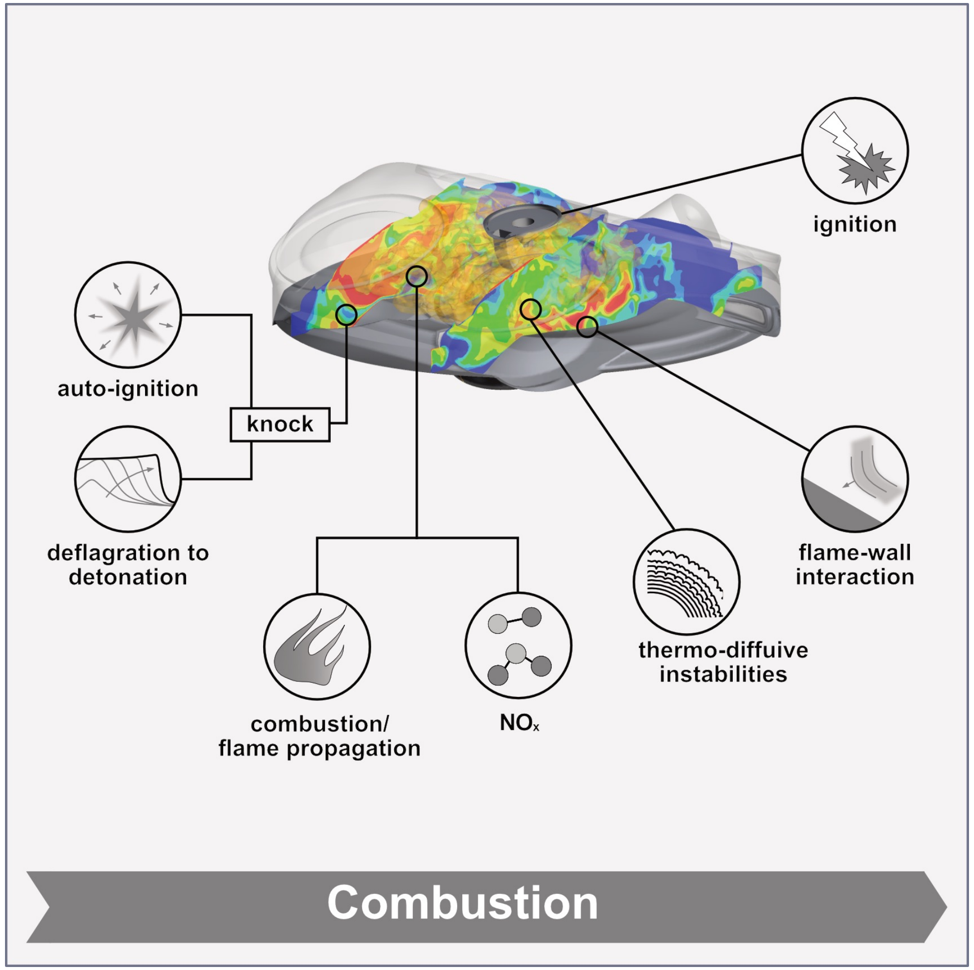
1 Challenges in modeling H2 combustion

2 Chemistry modeling

3 Turbulence-chemistry interaction



HYDROGEN COMBUSTION

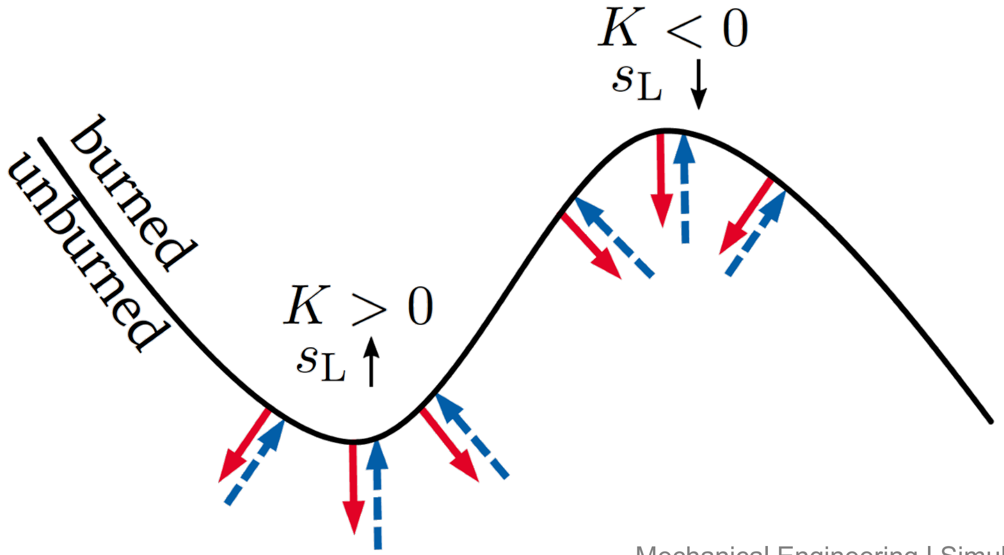
Thermodiffusive instability

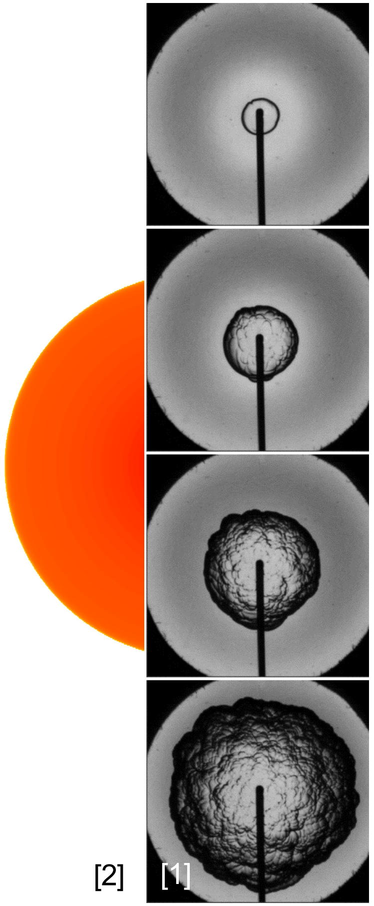
[1] Beeckmann, ITV, RWTH Aachen, Germany
[2] Wen et al., STFS, TU Darmstadt, Germany

H_2 combustion includes complex physical phenomena

- Differential diffusion ($\mathrm{Le} \neq 1$)
- Intrinsic instabilities

Thermo-diffusive instabilities
Highly corrugated flame front + cellular structures
Significantly increased flame surface and flame propagation



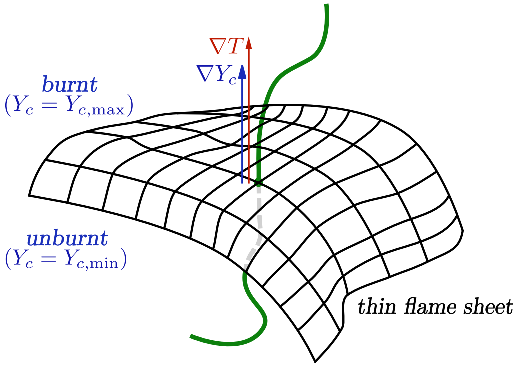


HYDROGEN COMBUSTION

Challenges in modeling H_2 combustion

Chemistry modeling

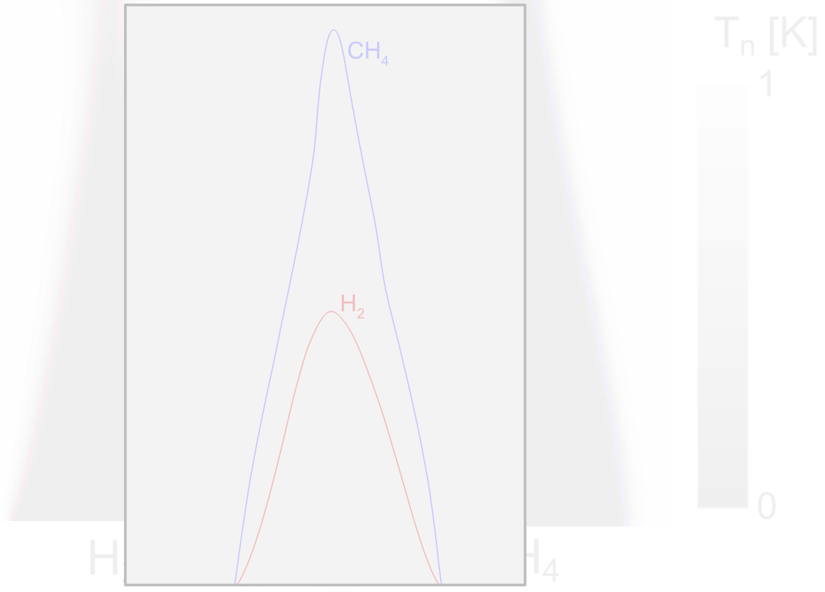
Prediction of differential diffusion effects?
Manifold generated from planar unstretched premixed flames?



How do flamelet models perform for thermo-diffusively unstable hydrogen/air flames?

Turbulence flame interaction

Same laminar flame speed, but different turbulent flame speed



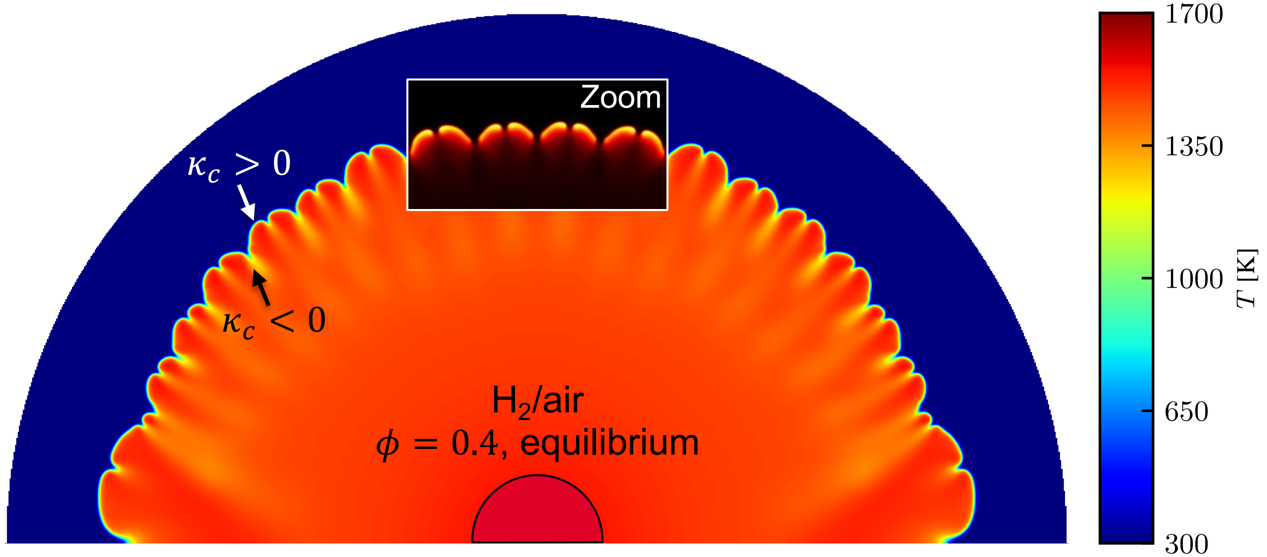
Thermo-diffusive instabilities amplify turbulent flame speed significantly!
No model can capture these effects

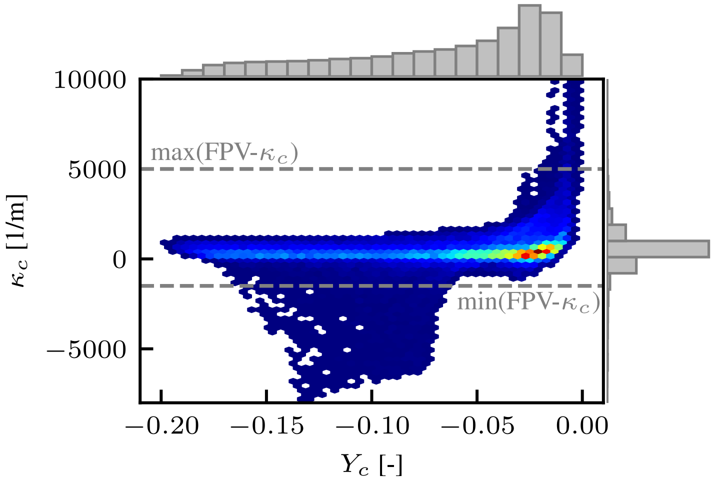
SPHERICAL EXPANDING FLAME[1,2]

[1] Wen et al., Combust. Flame (2021)
[2] Böttler et al., PROCI (2022)

NUMERICAL SETUP

- Mixture averaged diffusion
- Transport equation solved for all 12 species and sensible enthalpy
- H_2-air
- $\phi = 0.4$
- $T_0 = 300$ K
- $p = 1$ atm
- $Y_c = Y_{H_2O} - Y_{H_2} - Y_{O_2}$
- $\approx$ 8 Mio. Cells
- OpenFOAM

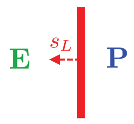


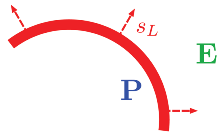


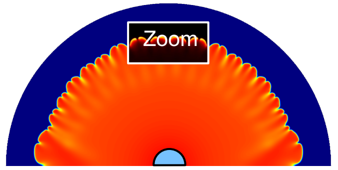
HYDROGEN COMBUSTION

Assessment of the thermo-chemical state[1]

[1] Böttler et al., PROCI (2022)

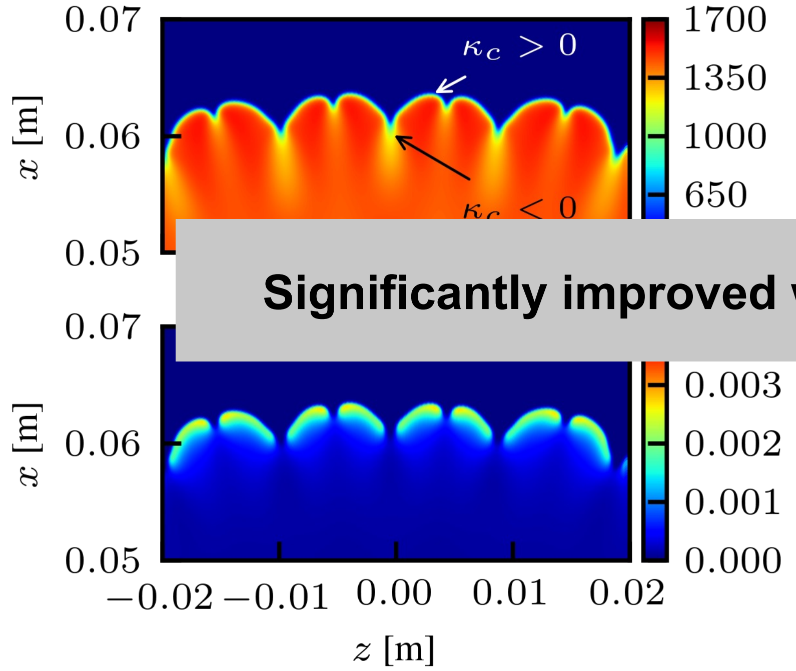






$$\epsilon_i = \frac{(i_{\mathrm{DNS}} - i_{\mathrm{FPV}})}{\max(i_{\mathrm{DNS}})}$$

DNS
- Reference model
- $\psi(T, p, Y_k)$



Significantly improved when including curvature effects into the Flamelet model

FULLY RESOLVED SIMULATION

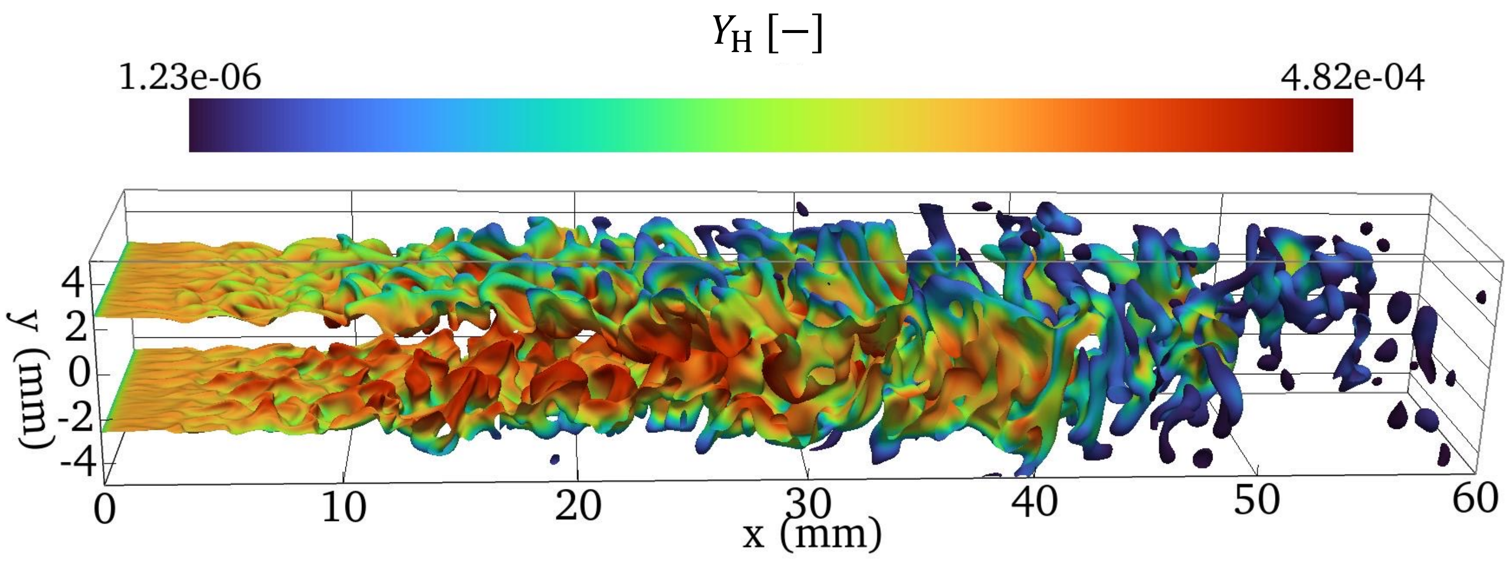
Premixed Turbulent H_2-air Slot Flame[1]

[1] Böttler & Kaddar et al., Int. J. Hydrog. Energy (2023)

Burned products

Fresh mixture

Burned products



NUMERICAL SETUP

- H_2-air
- $\phi = 0.5$
- $T_0 = 300$ K
- $p = 1$ atm
- Re = 10.000
- ≈ 350 Mio. Cells
- 19200 Cores
- OpenFOAM

Which phenomena need to be included into our combustion models?

ANALYSIS OF PHYSICAL PHENOMENA

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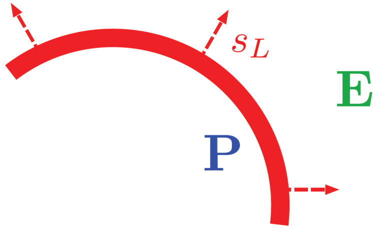
[1] Böttler & Kaddar et al., Int. J. Hydrog. Energy (2023)

THERMOCHEMICAL STATES

- Conditional mean of potential control variable

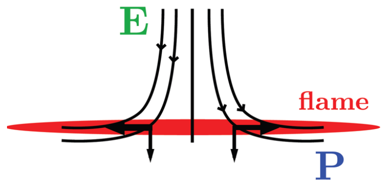
EFFECT OF CURVATURE

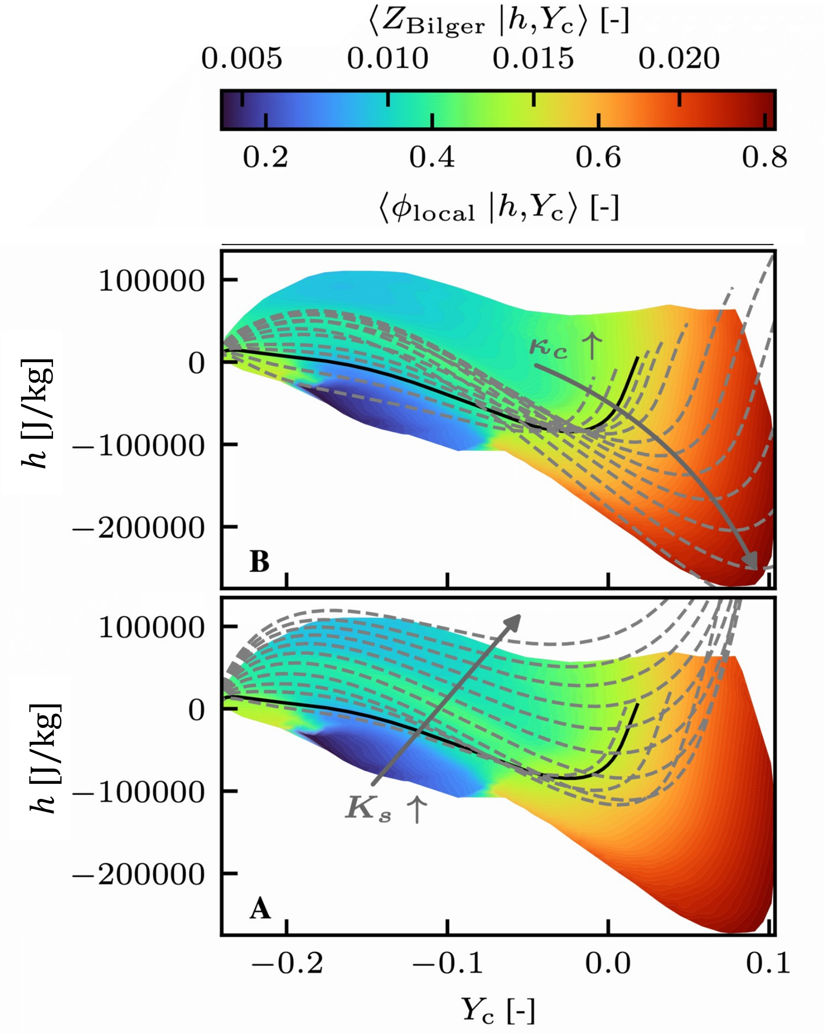
- CSM solutions with $K_s = 0, -500\ \mathrm{m}^{-1} \leq \kappa_c \leq 8000\ \mathrm{m}^{-1}$
- Significantly richer mixtures
- Lower enthalpy levels



EFFECT OF STRAIN

- CSM solutions with $\kappa_c = 0, -100\ \mathrm{s}^{-1} \leq K_s \leq 28000\ \mathrm{s}^{-1}$
- Insignificant shift in local composition
- Increased enthalpy values





CHEMISTRY MODELING OF H_2 COMBUSTION

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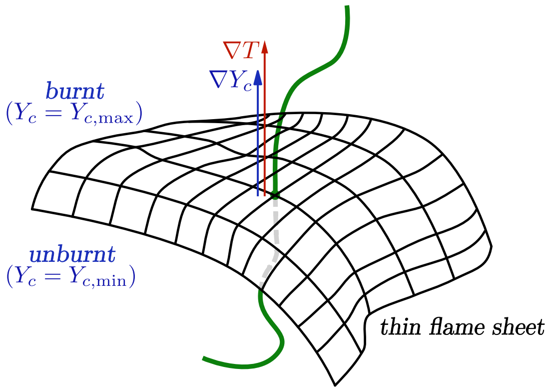
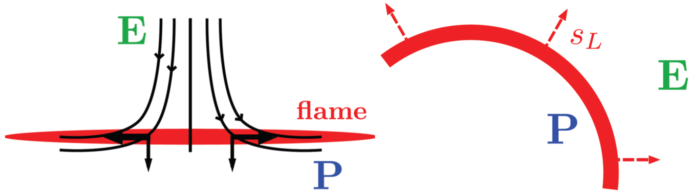


TABULATION METHOD

- Relevant physics need to be captured in manifold

HYDROGEN CHARACTERISTICS

- When introducing curvature as controlling variable, laminar flame characteristics can be reproduced
- In turbulent flame curvature (mixture stratification) and strain are crucial phenomena

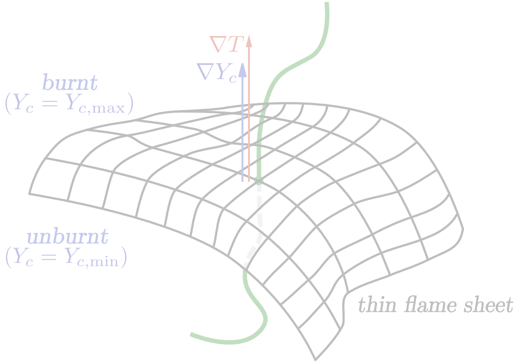


HYDROGEN COMBUSTION

Challenges in modeling H_2 combustion

Chemistry modeling

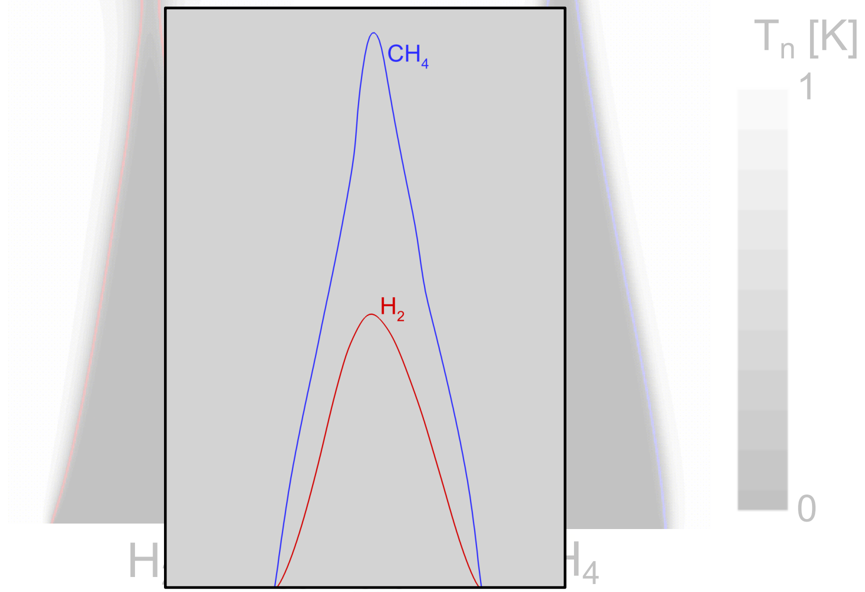
Prediction of differential diffusion effects?
Manifold generated from planar unstretched premixed flames?



How do flamelet models perform for thermo-diffusively unstable hydrogen/air flames?

Turbulence flame interaction

Same laminar flame speed, but different turbulent flame speed



Thermo-diffusive instabilities amplify turbulent flame speed significantly!
No model can capture these effects

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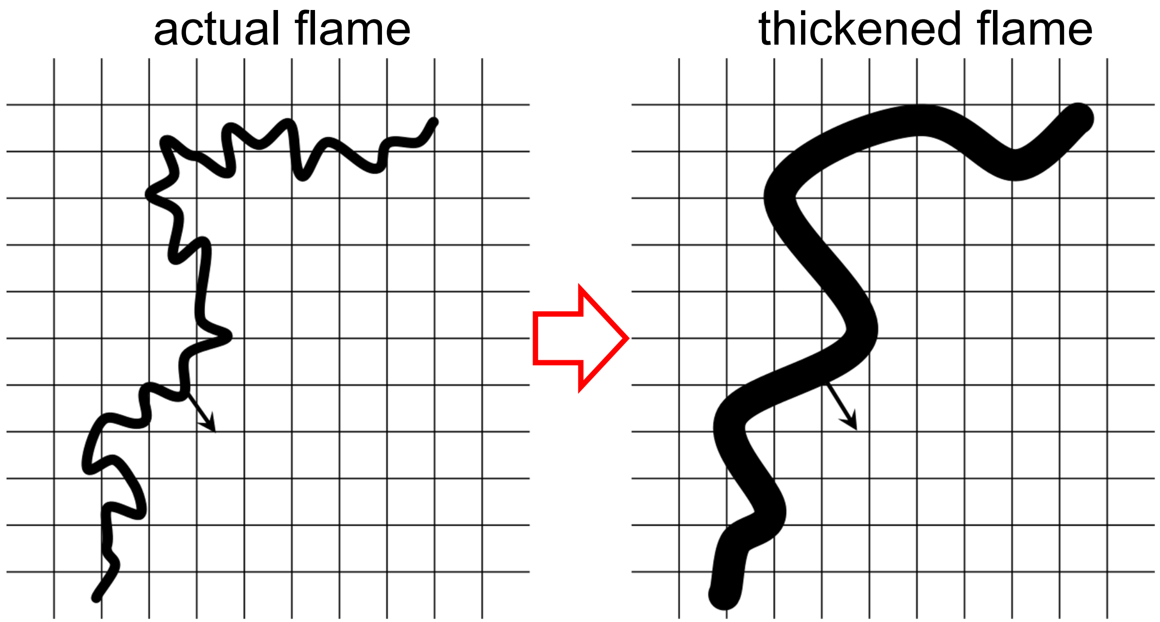
ARTIFICIAL THICKENED FLAME

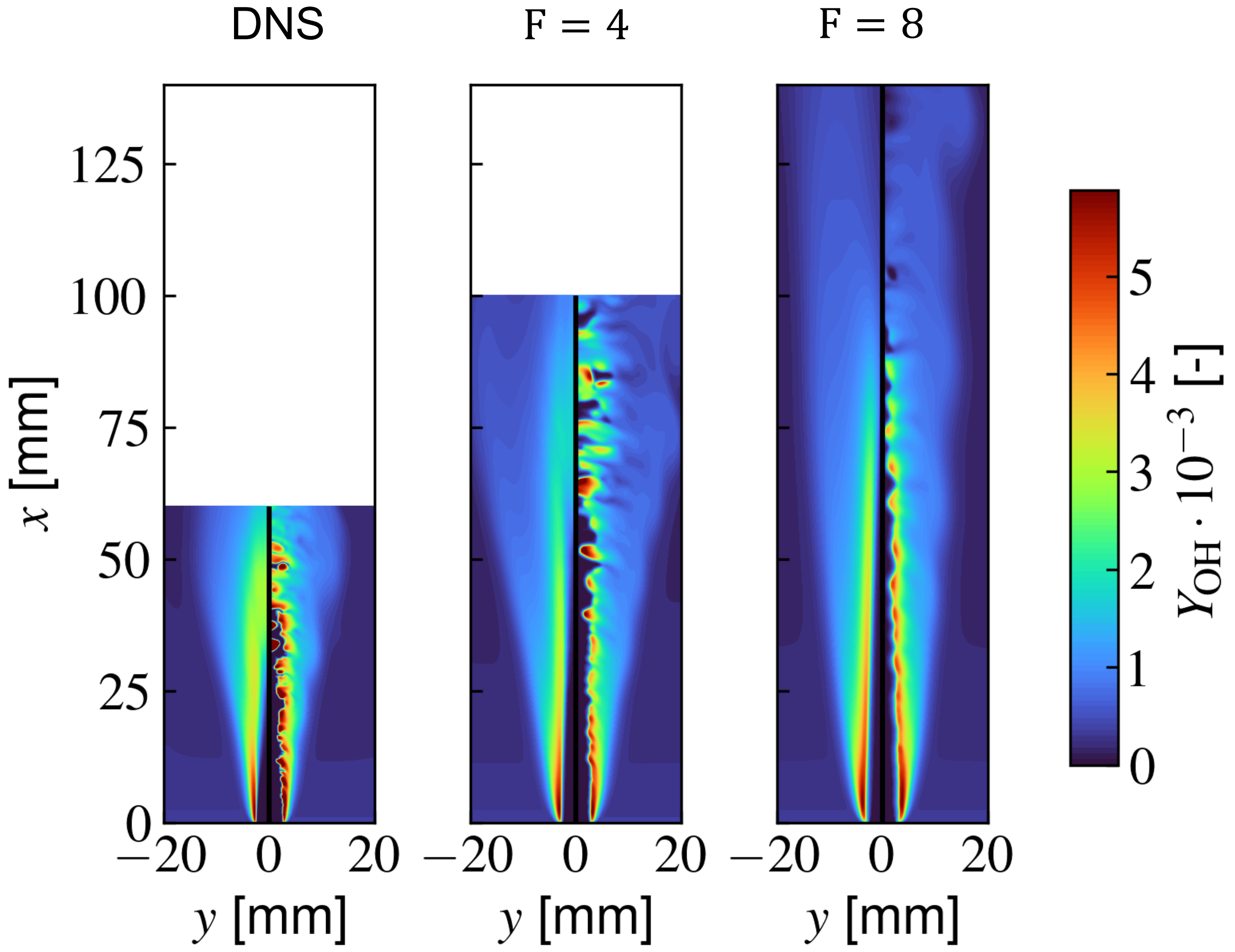
- Thicker flame is less responsive to flame wrinkling
- Fuel consumption $s_c^{ATF} \neq s_c^0$
- Efficiency function E ensures same fuel consumption: $s_c^{ATF} \overset{!}{=} s_c^0$

$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial \rho u_i Y_k}{\partial x_i} = \frac{\partial}{\partial x_i}\left(F E \rho Y_k V_{k,i}\right) + \frac{E \dot{\omega}_k}{F}$$



Efficiency functions E does not consider thermo-diffusive instabilities & turbulence-chemistry interaction

ATF IN SLOT FLAME



ASSESSMENT

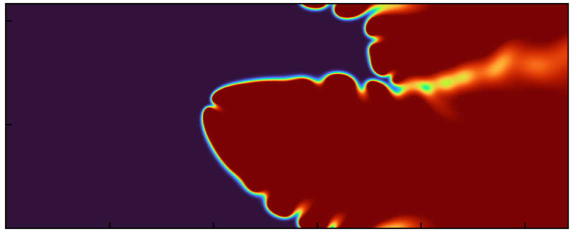
- Thickened flames show less turbulent fluctuations
  → large modeling effort
- Synergistic effects of turbulence and TD instabilities not captured by current models (including efficiency function)
  → consumption speed underestimated
  → wrong prediction of flame length

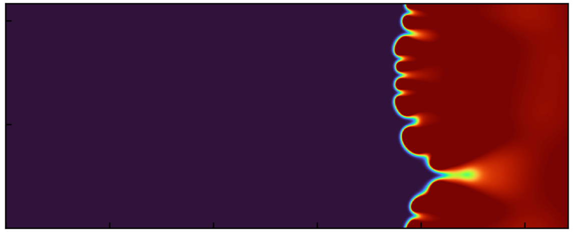
Current TCI models cannot predict correct consumption speed of hydrogen combustion

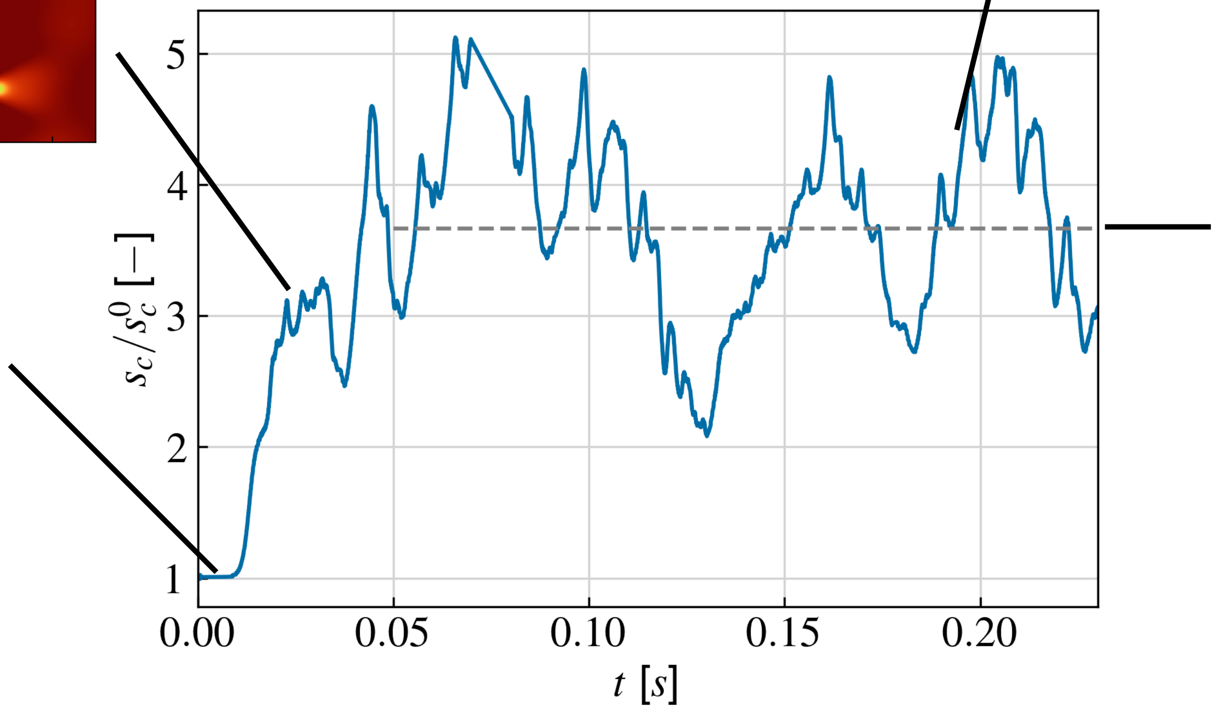
TD = Thermodiffusive
TCI = Turbulence chemistry interaction

INTRINSIC INSTABILITIES

2D freely propagating flame







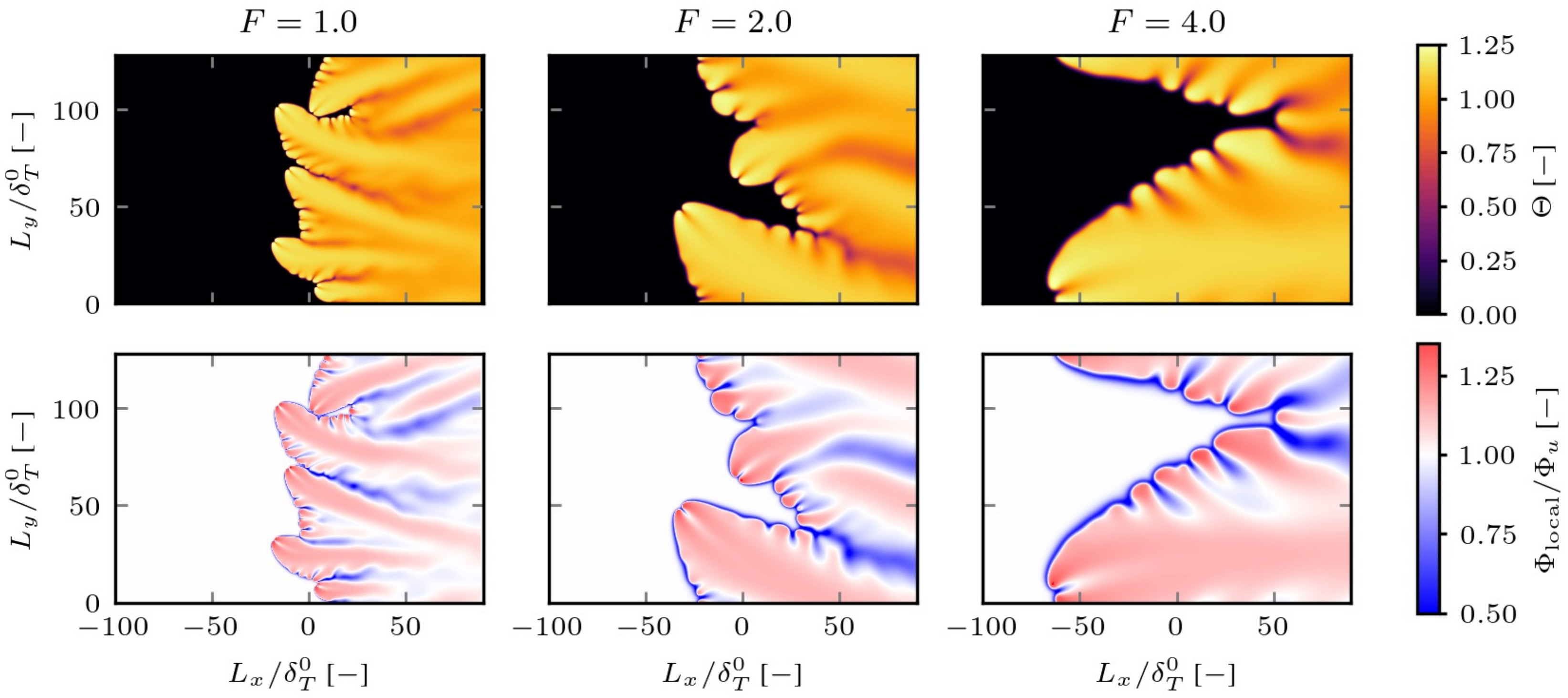
Average increase of consumption speed due to instabilities

Thermo-diffusive instabilities lead to a significant increase of average fuel consumption

INSTABILITIES IN THICKENED FLAMES

SCALING WITH THICKENING

- Thickened flames show similar instabilities
- Characteristic length scales of flame scaled by F



A POSTERIORI EVALUATION

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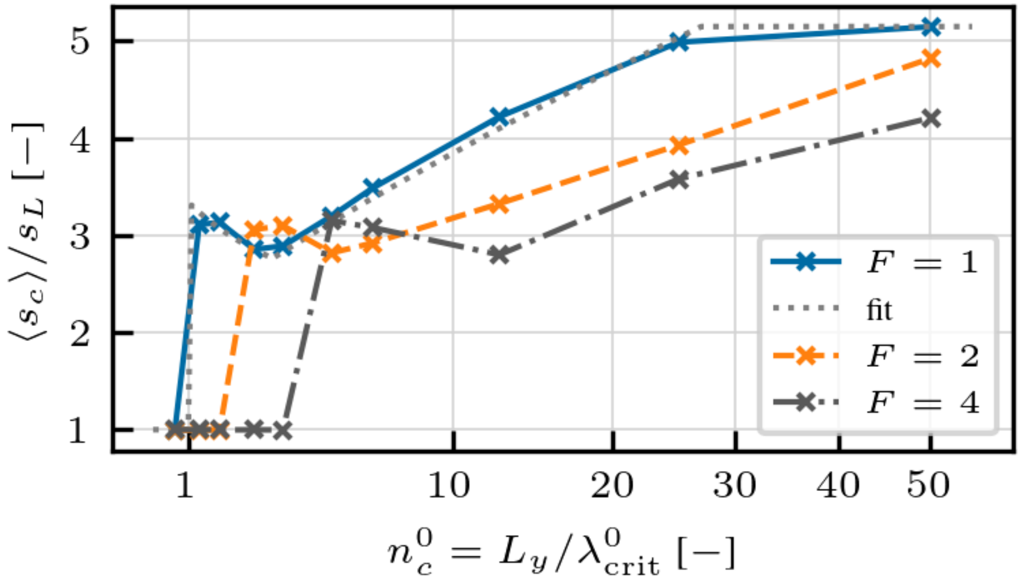
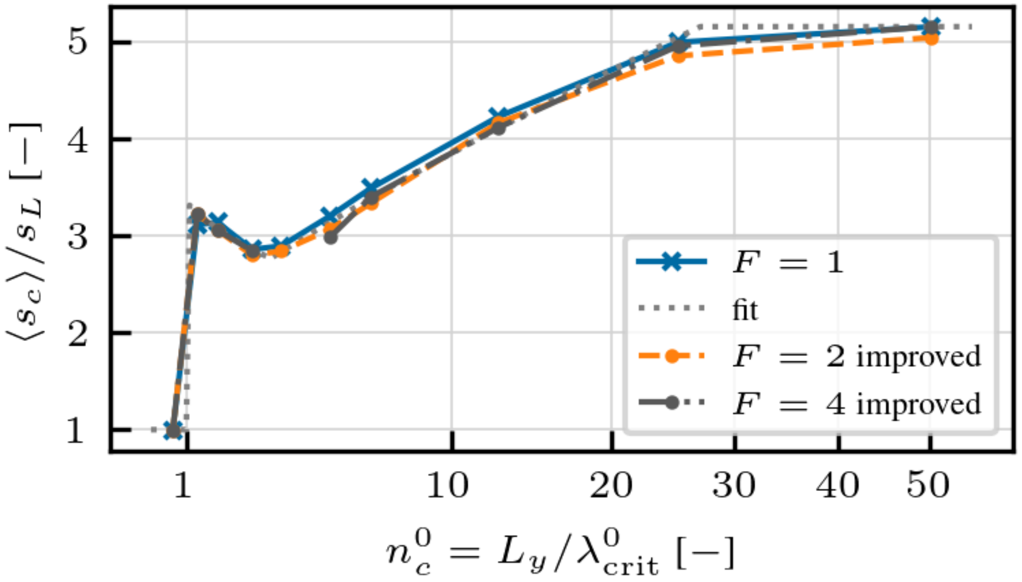
$$E_{TD} = \text{fn}(\Delta, F, \lambda^0_{\text{crit}}, \sigma)$$





Our model predicts the **correct flame propagation speed**.
Flame wrinkling is not captured (not intended)

MODELING OF HYDROGEN COMBUSTION

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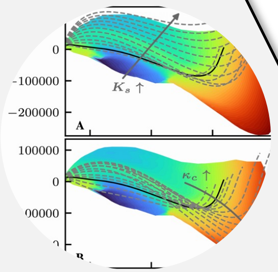
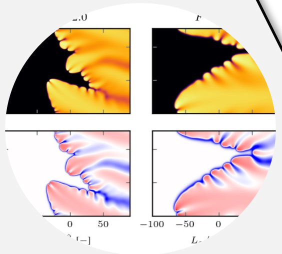


Chemistry modeling

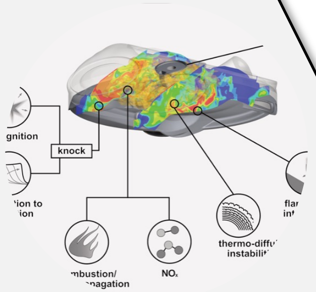
- Flamelet approach including curved and stretched flamelets

OpenFOAM



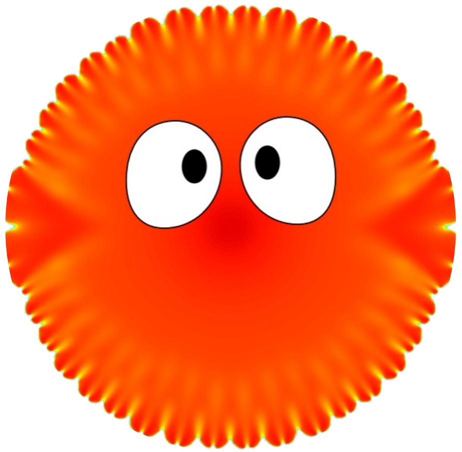
Turbulence chemistry interaction

- Accurately predicts consumption speed



Internal Combustion Engine

- Application of models in LES in Darmstadt Engine



THANK YOU

Vinzenz Schuh, M.Sc.
Simulation of reactive Thermo-Fluid Systems
Technische Universität Darmstadt

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Prof. Dr.-Ing. Christian Hasse

Dr.-Ing. Hendrik Nicolai

Hannes Böttler, Dipl.-Ing.

Driss Kaddar, M.Sc.

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