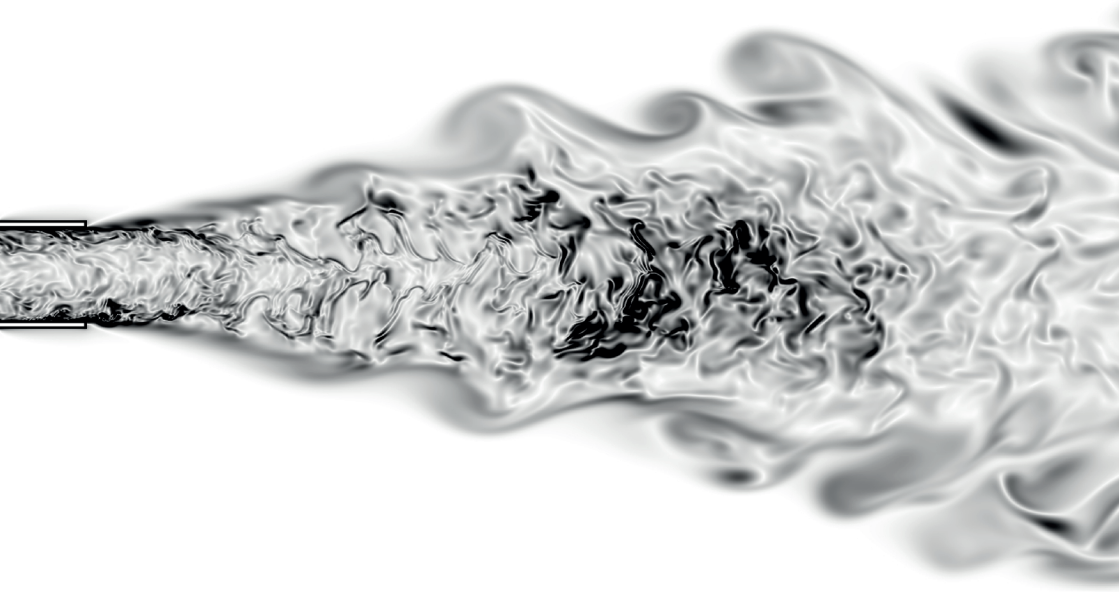
# Numerical Study on Thermodiffusive Instabilities in Laminar and Turbulent Hydrogen Flames

Lukas Berger



# Numerical Study on Thermodiffusive Instabilities in Laminar and Turbulent Hydrogen Flames

# Numerische Untersuchung von thermodiffusiven Instabilitäten in laminaren und turbulenten Wasserstoffflammen

Von der Fakultät für Maschinenwesen der Rheinisch-Westfälischen Technischen Hochschule Aachen zur Erlangung des akademischen Grades eines Doktors der Ingenieurwissenschaften genehmigte Dissertation

vorgelegt von

Lukas Konstantin Willi Berger

Berichter: Univ.-Prof. Dr.-Ing. Heinz Günter Pitsch
Assoc. Prof. Michael Edward Mueller, Ph.D.

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Berichte aus der Energietechnik

**Lukas Berger**

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*To my dear parents.*

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Aachen, in June 2022 Lukas Berger

# Zusammenfassung

Die Verwendung von Wassserstoff stellt eine vielversprechende Möglichkeit zur Dekarbonisierung thermochemischer Energiewandlungsprozesse dar. Allerdings ist dies mit zahlreichen wissenschaftlichen und technologischen Herausforderungen verbunden. Beispielsweise neigen magere Wasserstoff/Luft-Flammen zu thermodiffusiven Verbrennungsinstabilitäten. In der vorliegenden Arbeit wird ihr Einfluss anhand von Direkten Numerischen Simulationen (DNS) untersucht. Es wird gezeigt, dass sie einen wesentlichen Einfluss auf die Flammendynamik haben können und die Flammenausbreitungsgeschwindigkeit um ein Vielfaches erhöhen können. Eine Analyse der Faltungen der Flammenfront in laminaren Strömungen zeigt die Existenz einer kleinsten und einer größten Flammen-intrinsischen Längenskala auf. Die kleinste Längenskala resultiert aus der Bildung zellulärer Strukturen entlang der Flammenfront. Im Gegensatz zu Flammen, die keine thermodiffusiven Instabilitäten ausbilden, kann zudem eine größte Längenskala unabhängig von der Größe des Simulationsgebietes identifiziert werden. Beide Längenskalen können der thermodiffusiven Instabilität zugeordnet werden und resultieren nicht aus einer Interaktion der thermodiffusiven und ebenfalls vorhandenen hydrodynamischen Instabilität. Weiterhin wird gezeigt, dass theoretische Modelle nicht in der Lage sind, die Ausbreitung thermodiffusiv instabiler Flammen hinreichend genau zu beschreiben, weshalb die Neigung laminarer magerer Wasserstoff/Luft-Flammen, thermodiffusive Instabilitäten zu entwickeln, bei verschiedenen Brennstoff-Luft-Verhältnissen, Temperaturen und Drücken untersucht wird. Für eine umfassende Bewertung werden hierzu das charakteristische lineare und nicht-lineare Regime der Flammenausbreitung untersucht. Um die Interaktion zwischen thermodiffusiven Instabilitäten und Turbulenz zu untersuchen, wurden großskalige DNS turbulenter Wasserstoff/Luft-Flammen in einer Schlitzbrennerkonfiguration durchgeführt. Es zeigt sich, dass thermodiffusive Instabilitäten die turbulente Flammengeschwindigkeit durch Generierung von Flammenoberfläche und Variationen der lokalen Reaktionsraten erheblich beeinflussen. Insbesondere wird durch die größere Krümmung der Flammenfront und die positive Streckungsrate in der turbulenten Strömung eine Verstärkung der Effekte der differentiellen Diffusion in der turbulenten Flamme beobachtet. Dies zeigt, dass thermodiffusive Instabilitäten in turbulenten Strömungen aufrechterhalten und sogar verstärkt werden können.

# Abstract

The deployment of hydrogen represents a unique opportunity to decarbonize thermochemical energy conversion processes, but its utilization involves several scientific and technological challenges as, e.g., lean hydrogen/air flames are prone to thermodiffusive instabilities. In this thesis, a series of direct numerical simulations (DNS) is performed to assess the impact of these instabilities on hydrogen/air flames. Such instabilities are shown to have a leading order effect on the flame propagation, yielding consumption speeds several times higher than the laminar unstretched burning velocity. An analysis of the flame front corrugation in laminar flows reveals the existence of a smallest and a largest flame intrinsic length scale. The former manifests itself by the formation of local cusps along the flame front and it is shown that, in contrast to flames that do not feature thermodiffusive instabilities, a largest flame intrinsic structure that is independent of the simulation domain size exists. Both length scales are shown to be linked solely to the thermodiffusive instability mechanism and not to an interaction of the thermodiffusive and the also prevailing hydrodynamic instability. Theoretical models are shown to be not capable of accurately describing the evolution of such flames, so the propensity of laminar lean hydrogen flames to develop thermodiffusive instabilities is studied at different equivalence ratios, unburned temperatures, and pressures. For a comprehensive assessment of such instabilities, the analysis is performed for the characteristic linear and non-linear regimes of the flame evolution. Finally, to investigate the interactions of thermodiffusive instabilities and turbulence, large-scale DNS of turbulent lean hydrogen/air flames have been performed in a slot burner configuration. Thermodiffusive instabilities are shown to significantly affect the turbulent flame speed, which is not only enhanced by flame wrinkling, but is also greatly increased due to significant variations of the local reaction rates. The effects of differential diffusion are found to be even enhanced in a turbulent flame compared to a laminar flame at the same conditions due to the mean positive strain rate and the higher fluctuations of curvature induced by the turbulent flow. These findings suggest that thermodiffusive instabilities are sustained in turbulent flows and even show synergistic interactions with turbulence.

# Publication List

This thesis is mainly based on the following publications.

- L. Berger, K. Kleinheinz, A. Attili, H. Pitsch. Characteristic patterns of thermodiffusively unstable premixed lean hydrogen flames. *Proc. Comb. Inst.*, 37:1879–1886, 2019.
- L. Berger, A. Attili, H. Pitsch. Intrinsic instabilities in premixed hydrogen flames: Parametric variation of pressure, equivalence ratio, and temperature. Part 1 - Dispersion relations in the linear regime. *Combust. Flame*, 240:11935, 2022.
- L. Berger, A. Attili, H. Pitsch. Intrinsic instabilities in premixed hydrogen flames: Parametric variation of pressure, equivalence ratio, and temperature. Part 2 - Non-linear regime and flame speed enhancement. *Combust. Flame*, 240:11936, 2022.
- L. Berger, A. Attili, H. Pitsch. Synergistic interactions of thermodiffusive instabilities and turbulence in lean hydrogen flames. *Combust. Flame*, 244:112254, 2022.
- L. Berger, M. Grinberg, B. Jürgens, P.E. Lapenna, F. Creta, A. Attili, H. Pitsch. Flame fingers and interactions of hydrodynamic and thermodiffusive instabilities in laminar lean hydrogen flames. *Proc. Combust. Inst.*, 39, 2022 (in press).

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