Strömungstechnik

Dominik Denker

Gradient Trajectory Analysis of Reacting Turbulent Flows



Gradient Trajectory Analysis of Reacting Turbulent Flows

Gradiententrajektorienanalyse von reagierenden turbulenten Strömungen

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

vorgelegt von

Dominik Denker

Berichter: Univ.-Prof. Dr.-Ing. Heinz Günter Pitsch

Asst. Prof. Antonio Attili, Ph.D.

Tag der mündlichen Prüfung: 23. Oktober 2020

Diese Dissertation ist auf den Internetseiten der Universitätsbibliothek online verfügbar.

Berichte aus der Strömungstechnik

Dominik Denker

Gradient Trajectory Analysis of Reacting Turbulent Flows

Shaker Verlag Düren 2020

Bibliografische Information der Deutschen Nationalbibliothek

Die Deutsche Nationalbibliothek verzeichnet diese Publikation in der Deutschen Nationalbibliografie; detaillierte bibliografische Daten sind im Internet über http://dnb.d-nb.de abrufbar.

Zugl.: D 82 (Diss. RWTH Aachen University, 2020)

Copyright Shaker Verlag 2020 Alle Rechte, auch das des auszugsweisen Nachdruckes, der auszugsweisen oder vollständigen Wiedergabe, der Speicherung in Datenverarbeitungsanlagen und der Übersetzung, vorbehalten.

Printed in Germany.

ISBN 978-3-8440-7739-1 ISSN 0945-2230

Shaker Verlag GmbH • Am Langen Graben 15a • 52353 Düren Telefon: 02421 / 99 0 11 - 0 • Telefax: 02421 / 99 0 11 - 9

Internet: www.shaker.de • E-Mail: info@shaker.de

Acknowlegments

The present thesis was completed during my time as a research assistant at the Institute for Combustion Technology, RWTH Aachen University. The research was funded in part from the Deutsche Forschungsgemeinschaft (DFG) under the Project "Regimes in Turbulent Non-Premixed Combustion" as well as from the European Research Counsel (ERC) Advanced Grant "Milestone" (Multi-Scale Description of Non-Universal Behavior in Turbulent Combustion.) The majority of the simulations and the analysis of the results were by conducted on the supercomputers JUQEEN, JURECA and JUWELS of the Forschungszentrum Jülich. I appreciate the sizeable calculation resources provided by the Jülich Aachen Research Alliance (JARA) and the Gauss Centre for Supercomputing (GSC).

I would like to thank my advisor Prof. Heinz Pitsch for his support and guidance as well as for the trust placed in my scientific work which allowed and encouraged me to pursue and develop my own instincts and research interests. The underlying vision and ideas for this work originate from discussions with Prof. Norbert Peters at the very start of my career. Although my time under his guidance was unfortunately cut short, his genius, a seemingly endless enthusiasm and scientific curiosity in combination with his friendly and unassuming nature left a lasting impression on me. I am immensely grateful for the limited time I had the privilege to work with him. Further, I would like to thank my second supervisor Prof. Antonio Attili for the valuable advice and encouragement throughout my research. This thesis benefited greatly from his altruistic commitment and continued dedication in innumerable, highly enjoyable scientific discussions. I am also grateful to Prof. Manfred Wirsum for being the chair of the committee.

I would like to extend my gratitude to my colleagues at the Institute for Combustion Technology for their help, advice and friendship. The unique and amiable environment with a plethora of scientific and also non-scientific discussion topics was largely owed to my dear office mates Jonas Boschung and Fabian Hennig. Further, I would like to especially thank Abhishek Khetan, Stephan Kruse, Kai Niemietz, Metin Korkmaz, Raymond Langer, Bernhard Jochim, Konstantin Kleinheinz and Lukas Berger for the countless memorable moments during discussions, extracurricular activities and conferences.

I am also appreciative for the support I received from the previous gen-

erations of the turbulence group, foremost for the invaluable advice from Michael Gauding and Jens-Henrik Göbbert. Moreover, I would like to thank the student assistants and undergraduate students that worked with me.

Finally, I wish to thank my family on both sides of the Atlantic for their encouragement and interest. Most of all I am beholden to my wife, Amy, for her unlimited love, support and patience.

Zusammenfassung

In dieser Arbeit werden reagierende turbulente Strömungen mit der Dissipations Element (DE) Analyse untersucht. Dies ist eine Gradiententrajektorien basierte Methode zur Unterteilung turbulenter Felder in raumfüllende Unterregionen, in denen sich Skalare monoton verhalten. Im Kontext der Verbrennung ist diese Eigenschaft wichtig, da DEs somit lokal und eindeutig das maximale Ausmaß aufzeigen, welches eine von diffusivem Transport dominierte Struktur, wie z.B. eine Flamme, in einer turbulenten Strömung potentiell einnehmen kann.

Zuerst wird die DE-Analyse auf das Mischungsbruchfeld Z aus direkten numerischen Simulationen (DNS) von nicht vorgemischten Freistrahlflammen angewandt. Es wird gezeigt, dass sich die normierte DE-Parameterstatistik sowie die charakteristischen Skalierungen der jeweiligen Mittelwertgrößen nicht von innerten turbulenten Strömungen unterscheiden. Zusätzlich wird gezeigt, dass die skalare Dissipationsrate χ mit dem Gradienten der größeren lokalen Strömungstopologie, dem DE-Gradienten g, in Beziehung gesetzt werden kann. Ein DE-Parameter basiertes Regimediagramm für nicht vorgemischte Verbrennung wird eingeführt und verifiziert.

Des weiteren werden nicht-lokale Effekte in DNS von vorgemischten Freistrahlflammen untersucht. Die DE Analyse wird auf die Temperaturfelder T angewendet, welche jedoch im Gegensatz zu Z einen chemischen Quellterm besitzen. Die Selbstähnlichkeit der normierten DE-Längenverteilung bleibt bestehen, jedoch zeigt die Statistik der skalaren Differenz ΔT einen deutlichen Einfluss der Flammenstruktur. In der Flammenstrukturanalyse wird gezeigt, dass die Einführung von Extrempunkten nahe der Flammenfront zu einer signifikanten Verdickung der Vorwärm- und Reaktionszone führt. Dieser Effekt wird quantifiziert und mit der Brenngeschwindigkeit in Beziehung gesetzt.

Abschließend werden die gewonnenen Erkenntnisse bei der Modellierung der Verbrennung genutzt. Die Skalierung und Selbstähnlichkeit der DE-Parameterstatistik werden in einer Methodik für die Vorhersage von Verbrennungsregimen bei nicht vorgemischter Verbrennung verwendet. Diese Methodik wird in Reynolds-gemittelten Navier-Stokes-Simulationen eines PKW-Dieselmotors angewendet. Weiterhin wird ein Modell für die Wahrscheinlichkeitsdichtefunktion von Z eingeführt, welches Effekte von laminaren Bereichen und externer Intermittenz berücksichtigt.

Abstract

In this thesis, reacting turbulent flows are analyzed from a structural point of view using Dissipation Element (DE) analysis, which is a gradient trajectory (GT) based method for compartmentalizing turbulent fields into space filling sub-regions in which scalars behave monotonically. In the context of combustion, this property is important, as DEs locally and unambiguously indicate the maximum extent a diffusive transport dominated structure, such as a flame, can potentially occupy in a turbulent flow.

First, DE analysis is applied to the mixture fraction field Z of a series of direct numerical simulations (DNS) of non-premixed jet flames. In a statistical investigation, it is shown that the normalized DE parameter statistics as well as the characteristic scalings of the respective mean quantities do not differ from non-reacting turbulent flows and are therefore unaffected by the heat release. Additionally, it is demonstrated that the scalar dissipation rate χ can be related to the gradient of the larger local flow topology as represented by the DE gradient g. The DE parameters are then used in the construction of a regime diagram for non-premixed combustion which is verified by the DNS results.

Secondly, non-local effects in DNS of premixed combustion are investigated in a series of spatially evolving jet flames. DE analysis is applied to the temperature fields T which, contrary to Z, possess a chemical source term. The self-similarity of the normalized DE length distribution is retained, but the statistics of the scalar difference ΔT show a clear influence of the flame structure. In the consecutive GT based flame structure analysis, it is shown that the introduction of extremal points close to the flame front leads to a significant thickening of both the preheating and inner reaction zone. This effect is quantified and related to the turbulent burning velocity.

Finally, the insights gained are used in combustion modelling. The scaling and self-similarity of the DE parameter statistics are used in a framework for the prediction of combustion regimes in non-premixed combustion. This framework is applied in the Reynolds averaged Navier-Stokes simulation of a passenger car diesel engine. Further, a novel model for the probability density function of Z is presented, which considers effects of laminar regions and external intermittency.

Publications

This thesis is mainly based on the following publications in scientific journals and a book chapter.

- D. Denker et al. "Dissipation element analysis of premixed jet flames". In: *Comb. Sci. Tech.* 191.9 (2019), pp. 1677–1683.
- D. Denker, A. Attili, and H. Pitsch. "Dissipation Element Analysis of Inert and Reacting Turbulent Flows". In: *Data Analysis for Direct Numerical Simulations of Turbulent Combustion*. Ed. by H. Pitsch and A. Attili. Springer International Publishing, 2020. Chap. 2, pp. 19–41.
- D. Denker et al. "A New Modeling Approach for Mixture Fraction Statistics Based on Dissipation Elements". In: *Proc. Comb. Inst* (2020).
- D. Denker et al. "Gradient Trajectory Analysis of the Burning Rate in Turbulent Premixed Jet Flames". In: *Comb. Sc. and Tech.* 192.11 (2020), pp. 2189–2207.
- D. Denker et al. "Dissipation Element Analysis of Non-premixed Jet Flames". In: *J. Fluid Mech.* 905 (2020), A4.

Additionally, the following journal publications were contributed during my time at the Institute for Combustion Technology:

- J. Boschung et al. "Finite Reynolds number corrections to the 4/5-law for decaying turbulence". In: *Phys. Rev. Fluids* 1.064403 (2016).
- J. Boschung et al. "Analysis of structure function equations up to the seventh order". In: *J. Turbul.* (2017), pp. 1–32.
- A. Schnorr et al. "Feature Tracking by Two-Step Optimization". In: *IEEE Transactions on Visualization and Computer Graphics* (2018).
- M. Bode et al. "Using Physics-Informed Super-Resolution Generative Adversarial Networks for Subgrid Modeling in Turbulent Reactive Flows".
 In: Proc. Comb. Inst. (2020).

- M. Gauding et al. "On the combined effect of internal and external intermittency in turbulent non-premixed jet flames". In: *Proc. Comb. Inst.* (2020).
- A. Attili et al. "Turbulent flame speed and reaction layer thickening in premixed jet flames at constant Karlovitz and increasing Reynolds numbers". In: *Proc. Comb. Institute* (2020).

Contents

A	cknov	vlegm	ents	iii
Zι	ısam	menfa	ssung	v
\mathbf{A}	bstra	ct		vii
Pι	ublica	ations		ix
\mathbf{C}_{0}	onter	ıts		xi
Li	st of	Figur	es	xv
Li	st of	Table	S	xix
1	Intr	oducti	ion and Motivation	1
2	Intr	oducti	ion to Reacting Turbulent Flows	3
	2.1	Theor	etical Concepts of Turbulence	3
		2.1.1	Governing Equations of Fluid Motion	3
		2.1.2	Characteristics of Turbulent Flows	5
		2.1.3	Scales in Turbulent Flows	6
		2.1.4	Geometries in Turbulent Flows	9
	2.2	Introd	luction to Turbulent Combustion	10
		2.2.1	Non-dimensional Numbers in Turbulent Combustion .	11
		2.2.2	Models for Turbulent Combustion	13
	2.3	Outlin	ne of the Thesis	15
3	Intr		ion to Dissipation Element Analysis	19
	3.1	Introd	luction to Dissipation Elements	19
		3.1.1	Definition of Dissipation Elements	19
		3.1.2	Physical and Numerical Considerations	24
	3.2		tics of Dissipation Element Parameters	27
		3.2.1	Marginal Statistics and Scaling of mean DE Parameters	
		$3 \ 2 \ 2$	Joint Statistics	28

		3.2.3 DE analysis of Reacting Flows	32
4	Dir	ect Numerical Simulations of Turbulent Reacting Flows	37
	4.1	Introduction to Direct Numerical Simulations	37
	4.2	Numerical Methods and Algorithms	40
		4.2.1 Numerical Methods of the Non-Reacting Cases	42
	4.3	Configurations and Case Descriptions	43
	4.4	Turbulent Flame Analysis	46
5	Dis	sipation Element Based Flame Analysis of Non-Premixed	
		mes	51
	5.1	Dissipation Element Analysis	53
		5.1.1 Marginal Dissipation Element Parameter Statistics	55
		5.1.2 Joint Dissipation Element Parameter Statistics	58
	5.2	Regimes in Turbulent Non-Premixed Combustion	63
		5.2.1 Local Flame Analysis	73
		5.2.2 Temporal Evolution of the Combustion Regimes	76
6	Dis	sipation Element Analysis of Turbulent Premixed Com-	
	bus	tion	7 9
		6.0.1 Configurations	79
	6.1	DE Analysis of the Temperature Fields in Premixed Jet Flames	82
		6.1.1 Marginal Statistics	82
		6.1.2 Joint Statistics	88
	6.2	Gradient Trajectory Analysis of the Burning Rate	96
		6.2.1 Flame Structure Analysis	98
		6.2.2 Correlation between Reacting Scalars and DE Parameters 1	.03
		6.2.3 Integral Statistics	108
7	Gra	ndient Trajectory Statistics Based Modelling Applications1	.13
	7.1	Prediction of Non-Premixed Combustion Regimes	13
		7.1.1 Modelling Framework	14
		7.1.2 Engine Simulations	19
		7.1.3 Modelling Results	121
	7.2	A New Modeling Approach for Mixture Fraction Statistics 1	124
		7.2.1 Gradient Trajectory Analysis	28
		7.2.2 Modeling The Mixture Fraction Structure 1	29
		7.2.3 DE Based Modeling Approach	131
		7.2.4 Model Validation and Discussion	134

8 Summary and Conclusion

137

List of Figures

3.1	Schematic representation of a DE and its parameters in one-
	dimensional space
3.2	Schematic representation of gradient trajectories connecting
	the same extremal points in three dimensional space
3.3	A DE in the mixture fraction field Z in a DNS of non-premixed
	temporally evolving jet flame
3.4	Schematic representation of the potential methods of obtaining
	spatial statistics in the DE decomposed space
3.5	PDF of the normalized DE length ℓ/ℓ_m
3.6	Ratio of the Kolmogorov micro scale η to the mean DE length
	$\ell_{\rm m}$ for various inert and reacting cases
3.7	JPDFS of the normalized DE length and DE scalar difference
	for various fields in different flow configurations
3.8	Mean DE scalar difference conditioned on the DE length for
	various flow configurations
3.9	a): Mixture fraction Z profile in physical space obtained from a
	counterflow configuration and schematic DEs. b): Correspond-
	ing stationary flamelet solution of the normalized heat release
	$\dot{\omega}_T$ in mixture fraction space. c) and d): Mean stoichiometric
	temperature $\langle T_{\rm st} \rangle$ in a DNS of planar non-premixed jet flame
	conditioned on the stoichiometric scalar dissipation rate $\chi_{\rm st}.$.
4 4	
4.1	General setup of the non-premixed DNS investigated in this
	thesis.
4.2	Starting profiles of the stream-wise mean velocity component
	and scalars.
4.3	Mixture fraction Z in the x-y center plane at time steps $t^* = 10$
	and $t^* = 20$
4.4	Normalized temperature T^* in the x - y center plane at time
	steps $t^* = 10$ and $t^* = 20$
4.5	Temporal evolution of the normalized Favre averaged scalar
	dissipation rate and temporal evolution of the normalized area
	of the iso surface of the stoichiometric mixture fraction

5.1	A DE in interaction with the flame front in the low Re low dilution case
5.2	DE analysis of the mixture fraction field of the intermediate
0.2	Re case
5.3	Comparison of PDFs of the normalized DE length $\ell/\ell_{\rm m}$
5.4	JPDF of the normalized DE length $\ell^* = \ell/\ell_m$ and normalized scalar difference $\Delta Z^* = \Delta Z/\Delta Z_m$
5.5	Normalized DE scalar difference conditioned on the normalized DE length $\langle \Delta Z^* \ell^* \rangle$ and $\langle \Delta \phi^* \ell^* \rangle$
5.6	Average ratio $C_{\chi} = \langle \chi / \left(2D \langle g^2 \right) \rangle$ in the final time step of the respective simulations
5.7	DE parameter based regime diagram for turbulent non-premixed combustion
5.8	Comparison of the mixture fraction conditioned PDFs $P(T Z)$ of the temperature with the PDF of the temperature averaged within individual DEs $P(\widetilde{T}_{\text{DE}} Z)$
5.9	Heat release rate ω_T for steady state flamelet solutions at quenching scalar dissipation rates and the inner reaction zone approximation by means of a Gaussian profile
5.10	Mean temperature $\langle T \rangle$ conditioned on normalized DE parameters $\Delta Z' = \Delta Z/\delta Z_{\rm r}$ and $g' = g/g_{\rm q}$
5.11	Mean OH-mass fraction $\langle Y_{\text{OH}} \rangle$ conditioned on normalized DE parameters $\Delta Z'$ and g'
5.12	Mean temperature in the minima $\langle T_{\text{DE,min}} \rangle$ and in the maxima $\langle T_{\text{DE,max}} \rangle$ of DEs crossing the stoichiometric iso-surface conditioned on the normalized DE parameter g' and $\Delta Z'$ for the high Re case
5.13	PDF of the temperature conditioned on the stoichiometric mixture fraction and on the individual regimes
5.14	Mass fraction of OH radicals obtained along all gradient trajectories of a single DE.
5.15	Mean DE coefficient of variation of the OH mass fraction $\langle c_{\text{v,OH}}(Z_{\text{st}}) \rangle$ conditioned on the normalized DE parameters g' and $\Delta Z'$
5.16	Temporal evolution of the normalized area of the stoichiometric iso surface attributed to the individual regimes
6.1	Atomic oxygen mass fraction in the $x-y$ center plane of the three DNS of the Bunsen burner configuration

6.2	Upstream $x-y$ center plane of the temperature fields and mirrored corresponding DE analysis of the temperature field.	83
6.3	DE analysis of the passive scalar field in the Inert Isotropic case.	84
6.4	Normalized mean DE length $\ell_{\rm m}/\eta$ and normalized mean DE differences $\Delta\phi_{\rm m}/\Delta\phi_{\rm max}$ and $\Delta T_{\rm m}/\Delta T_{\rm max}$	84
6.5	PDFs of normalized separation length $\ell^* = \ell/\ell_m$	87
6.6	JPDFs of the normalized separation length and normalized scalar difference $P(\Delta \phi^*, \ell^*)$	89
6.7	JPDFs of the normalized separation length $\ell/\delta_{\rm F}$ and the normalized scalar difference $\Delta T/(T_{\rm b}-T_{\rm u})$	91
6.8	Kullback-Leibler divergence of the JPDFs of the normalized DE parameters of the various cases with reference to the JPDF obtained from the Inert Isotropic case	93
6.9	Normalized mean DE scalar difference conditioned on the normalized DE length	95
6.10	The $T=1800{\rm K}$ iso-surface in the stream-wise regions investigated	98
6.11	Mean temperature conditioned on the arc-length distance to the flame surface and the mean temperature additionally con- ditioned on the normalized scalar difference	99
6.12	JPDF of the normalized temperature gradient $\nabla T/\nabla T_{\rm fl}(1800{\rm K})$ and the normalized arc-length distance $s/\delta_{\rm F}$ in the High Re case conditioned on the normalized scalar difference ΔT^*	101
6.13	Schematic illustration of the impact of the scalar structure as indicated by DEs	102
6.14	PDF of the normalized DE parameters ΔT^* and $\ell^* = \ell/\ell_{\rm fl}(\Delta T)$ weighted with the intersection area of the individual DE and the flame surface	104
6.15	Selected mean normalized mass fractions $\langle Y_{\alpha}^{*} \rangle = \langle Y_{\alpha} \rangle / \max Y_{\alpha,\mathrm{fl}}$ and normalized CH ₄ source term $\langle \dot{\omega}_{\mathrm{CH}_4}^{*} \rangle = \langle \dot{\omega}_{\mathrm{CH}_4} \rangle / \min \dot{\omega}_{\mathrm{CH}_4,\mathrm{fl}}$ conditioned on the normalized DE parameters and the temperature of their respective maximum value in the laminar flamelet solution in the High Re case	106
6.16	Mean mass fractions $\langle Y_{\alpha} \rangle$ in the High Re case conditioned on arc-length distance s to the flame surface and conditioned on the normalized scalar difference ΔT^* and the normalized DE length ℓ^*	107

6.17	Mean CH ₄ source term $\langle \dot{\omega}_{\text{CH}_4} \rangle$ in the High Re case conditioned on arc-length distance s to the flame surface and scalar difference ΔT^*	108
6.18	a): $\langle I_s \rangle$ conditioned on the normalized DE parameters $\ell/\delta_{\rm F}$ and $\Delta T/(T_{\rm b}-T_{\rm b})$ in the High Re case. b): Instantaneous CH ₄ source term $\dot{\omega}_{\rm CH_4}(T)$ for two exemplary DEs and the laminar flamelet solution. c): $\langle I_T \rangle$ conditioned on $\ell/\delta_{\rm F}$ and $\Delta T/(T_{\rm b}-T_{\rm b})$ in the High Re case	110
7.1	PDF of the normalized DE length $\ell^* = \ell/\ell_m$ directly obtained DNS and obtained from the stochastic transport equation	117
7.2	The mean normalized scalar difference conditioned on the normalized DE length ℓ from the high Re case and conditional	
7.3	mean obtained from the stochastic transport equation JPDF of modelled normalized DE parameters at the iso-surface	118
	of $\widetilde{Z}_{\mathrm{st}}$ for three crank angle positions for the baseline case	122
7.4	Mean stoichiometric iso-surface for three different crank angle	
	positions in CFD simulation of the baseline case	123
7.5	Temporal evolution of the stoichiometric iso-surface attributed	
	to the individual regimes	124
7.6	Integrated probability of the "Burning Flamelet" regime $\mathcal{P}_{\mathrm{Flamelet}}$	105
7.7	in all simulated operation points	125
	region (left) and TNTI region (right) in the Inert Jet case	130
7.8	short caption	131
7.9	Modelling results of the zonal PDFs $P_i(Z)$ employing the joint	
	DE statistics obtained from DNS	132
7.10	PDF of the normalized scalar difference $P(\Delta Z^*)$ and normal-	
	ized PDF of the scalar difference conditioned on arithmetic	
	mean $P(\Delta Z^* Z_{\rm m})$ in the Mixing Layer	133
7.11	PDF of the mixture fraction $P(Z)$ for five cross-stream positions	
	$y/h_{1/2}$, with the jet half width $h_{1/2}$, for the Jet Flame and	
	Inert Jet.	135
7.12	Mean density $\overline{\rho}$ obtained from the convolution of $P(Z)$ with a	100
	steady state flamelet solution for the Jet Flame	136

List of Tables

4.1	Numerical and physical initial parameters of the DNS. Where needed, the parameters for the Non-Reacting case II were re-computed with the given values for \overline{U}_0 and H_0	46
6.1	Simulation parameters of the reacting configurations investigated in this chapter. The turbulence statistics are evaluated at the stream-wise position of $x/l_{\rm F}=0.6.$	81
7.1 7.2	Simulated operating points in the CFD of the DI diesel engine. Numerical and physical initial parameters of the DNS	