

Abhishek Y. Deshmukh

Physics-based Reduced-order Modeling of Fuel Injection and Combustion Processes in Internal Combustion Engines

Physics-based Reduced-order Modeling of Fuel Injection and Combustion Processes in Internal Combustion Engines

Physikbasierte Modelle reduzierter Ordnung für die Kraftstoffeinspritzung und Verbrennungsprozesse in Verbrennungsmotoren

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

vorgelegt von

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“Essentially all models are wrong, but some are useful.”

— George E. P. Box

Preface

The present dissertation has materialized through my work as a research assistant at the Institute for Combustion Technology (ITV) at the RWTH Aachen University. The work on direct gas injection was performed within the Ford-RWTH Aachen Research Alliance Project FA-0099 funded by the Ford Motor Company. The support and computing resources for simulations were provided by the JARA-HPC partition of the RWTH Compute Cluster under projects JARA0117 and thes0382. Cascade Technologies Inc. provided licenses for their compressible flow solver CHRIS, while Convergent Science Inc. provided licenses for CONVERGE simulation software. The experimental data for validation were provided by Delphi Technologies. The work on liquid fuel injection was funded in part by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany's Excellence Strategy – Exzellenzcluster 2186 “The Fuel Science Center” ID: 390919832. Furthermore, part of the work was funded by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program (grant agreement no. 695747). The simulations of this part were conducted using the computing time granted by the JARA Vergabegremium and provided on the JARA Partition part of the supercomputer CLAIX at RWTH Aachen University (project no. JARA0212).

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Aachen, November 2, 2021

Abhishek Y. Deshmukh

Abstract

Despite developments in electric propulsion systems for the transport sector, internal combustion engines, due to their high energy density, will remain the primary propulsion technology in the near future. To reduce their environmental impact, emerging technologies, such as direct-injected (DI) compressed natural gas (CNG) engines and so-called bio-hybrid fuels from renewable electricity and bio-based carbon sources, offer potentially high thermal efficiency and low pollutant emissions. Furthermore, bio-hybrid fuels offer a huge greenhouse gas reduction potential compared to conventional fuels due to the closed carbon cycle.

Gaseous fuel injection with supersonic flows has a strong influence on in-cylinder turbulence, mixing, and combustion. Numerical simulations can help to characterize the high-speed gas jets and use them advantageously in the design of DI-CNG engines. However, such simulations are numerically challenging and compute-intensive due to the presence of shocks as well as small time and length scales. On the other hand, the design of low-carbon liquid fuels for a combustion process requires rapid and repeated evaluation of new candidates over a wide range of conditions, which is not always possible due to several reasons, e.g., limited availability of fuels, adaptation required in combustion systems, or compute-intensive three-dimensional (3D) simulations.

To this end, this dissertation focuses on the development of reduced-order models (ROMs) that enable faster simulations of DI-CNG engines and rapid screening of the novel fuel candidates for compression ignition engines. The first part of the dissertation is devoted to the fundamental understanding of gas injection using resolved simulations and the subsequent development of ROMs for the fuel injection in engine simulations. The second part presents a *cross-sectionally averaged reactive turbulent spray* (CARTS) model for transient inert and reactive sprays in compression ignition engines.

The ROMs for the gas injection have been able to reduce the simulation times by about a factor of five, preserving the associated physics and also enable DI engine simulations to investigate in-cylinder flow, mixing, and their potential impact on combustion. On the other hand, the CARTS model is faster by more than one order of magnitude compared to high-fidelity 3D simulation methods and provides characteristic parameters of mixing, combustion, and pollutant formation with acceptable accuracy for fuel screening as well as other applications, e.g., closed-loop engine control.

Zusammenfassung

Trotz der Weiterentwicklung elektrischer Antriebe werden Verbrennungsmotoren aufgrund ihrer hohen Energiedichte in naher Zukunft die primäre Antriebstechnologie im Transportsektor bleiben. Um die Umweltbelastung zu reduzieren, bieten neue Technologien, wie z. B. direkt-einspritzende (DI) Erdgasmotoren (CNG) und sogenannte Bio-Hybrid Fuels, welche auf erneuerbarer Elektrizität und Biomasse basieren, einen potenziell hohen thermischen Wirkungsgrad bei geringen Schadstoffemissionen. Zusätzlich bieten Bio-Hybrid Fuels durch den geschlossenen Kohlenstoffzyklus ein enormes Treibhausgasreduktionspotenzial gegenüber konventionellen Kraftstoffen.

Die Gaseindüsung ist gekennzeichnet von Überschallströmungen und hat einen starken Einfluss auf den Turbulenzgrad und damit auf die Vermischung und die Verbrennung. Numerische Simulationen können dabei helfen diese Hochgeschwindigkeits-Gasstrahlen zu charakterisieren und vorteilhaft für DI-CNG-Motoren auszulegen. Allerdings sind solche Simulationen aufgrund der auftretenden Verdichtungsstöße sowie kleiner Zeit- und Längenskalen numerisch herausfordernd und rechenzeitintensiv. Andererseits erfordert das Design von kohlenstoffarmen Flüssigkraftstoffen die Evaluierung einer Vielzahl von Kandidaten, die aus verschiedenen Gründen nicht immer möglich ist, z. B. wegen begrenzter Verfügbarkeit von Kraftstoffen, erforderlichen Anpassungen in Verbrennungssystemen oder rechenintensiven dreidimensionalen (3D) Simulationen.

Diese Dissertation konzentriert sich auf die Entwicklung von Modellen reduzierter Ordnung (ROMs), die kostengünstigere Simulationen von DI-CNG-Motoren und ein schnelles Screening der Kraftstoffkandidaten für Kompressionszündungsmotoren ermöglichen. Der erste Teil der Dissertation widmet sich dem grundlegenden Verständnis der Gaseindüsung mit Hilfe detaillierter Simulationsmodelle und der anschließenden Entwicklung von ROMs für die Gaseindüsung in Motorsimulationen. Im zweiten Teil wird ein *cross-sectionally averaged reactive turbulent spray* (CARTS) Modell für transiente inerte und reaktive Sprays in Kompressionszündungsmotoren vorgestellt.

Die ROMs für die Gaseindüsung können die Simulationszeiten etwa um den Faktor fünf reduzieren, wobei die zugehörige Physik erhalten bleibt. Dadurch ermöglichen sie DI Motorsimulationen zur Untersuchung der Strömung im Zylinder, der Vermischung und deren möglichen Auswirkungen auf die Verbrennung. Andererseits ist das CARTS-Modell im Vergleich zu hochgenauen 3D Simulationenmethoden um mehr als eine Größenordnung günstiger und liefert charakteristische Parameter der Vermischung, Verbrennung und Schadstoffbildung mit akzeptabler Genauigkeit für das Kraftstoffscreening sowie für andere Anwendungen, wie z. B. in der Motorregelung.

Publications

This dissertation is mainly based on the following peer-reviewed scientific journal publications and a book chapter:

- A.Y. Deshmukh, G. Vishwanathan, M. Bode, H. Pitsch, M. Khosravi, and D. Van Bebbler. Characterization of Hollow Cone Gas Jets in the Context of Direct Gas Injection in Internal Combustion Engines. *SAE Int. J. Fuels Lubr.*, 11, 2018. doi: 10.4271/2018-01-0296
- A.Y. Deshmukh, T. Falkenstein, H. Pitsch, M. Khosravi, D. Van Bebbler, M. Klaas, and W. Schröder. Numerical Investigation of Direct Gas Injection in an Optical Internal Combustion Engine. *SAE Int. J. Engines*, 11, 2018. doi: 10.4271/2018-01-0171
- A.Y. Deshmukh, M. Bode, T. Falkenstein, M. Khosravi, D. van Bebbler, M. Klaas, W. Schröder, and H. Pitsch. Simulation and Modeling of Direct Gas Injection through Poppet-type Outwardly-opening Injectors in Internal Combustion Engines. In K. Srinivasan, A. Agarwal, S. Krishnan, and V. Mulone, editors, *Natural Gas Engines For Transportation and Power Generation*, pages 65–115. Springer, Singapore, energy, en edition, 2019. doi: 10.1007/978-981-13-3307-1_4
- A.Y. Deshmukh, C. Giefer, D. Goeb, M. Khosravi, D. van Bebbler, and H. Pitsch. A quasi-one-dimensional model for an outwardly opening poppet-type direct gas injector for internal combustion engines. *Int. J. Engine Res.*, 21(8), 2019. doi: 10.1177/1468087419871117
- A.Y. Deshmukh, T. Grenga, M. Davidovic, L. Schumacher, J. Palmer, M. Reddemann, R. Kneer, and H. Pitsch. A reduced-order model for multiphase simulation of transient inert sprays in the context of compression ignition engines. *Int. J. Multiph. Flow*, 147, 103872, 2022. doi: 10.1016/j.ijmultiphaseflow.2021.103872
- A.Y. Deshmukh, M. Davidovic, T. Grenga, R. Lakshmanan, L. Cai, and H. Pitsch. A reduced-order model for turbulent reactive sprays in compression ignition engines. *Combust. Flame*, 236, 111751, 2022. doi: 10.1016/j.combustflame.2021.111751

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