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M. Sc. Jelto Frerichs

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Vorsitz: Prof. Dr.-Ing. Ferit Küçükay
Gutachter: Prof. Dr.-Ing. Peter Eilts
Prof. Dr.-Ing. Michael Bargende

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Preface

The present work was developed during my time as a research assistant at the Institute of Internal Combustion Engines at the Technische Universität Braunschweig. The research leading to this work was conducted during the FVV-project *Propeller Operation with Four-stroke Dual-fuel Engines II*.

My gratitude goes to Prof. Dr.-Ing. Peter Eilts for his interest in my work and for the good working atmosphere. The trust placed in me and the freedom I had in the implementation contributed significantly to the success of the present work. Furthermore, I would like to thank Prof. Dr.-Ing Michael Bargende for his interest in my work and for joining the doctoral committee and Prof. Dr.-Ing. Ferit Küçükay for chairing the doctoral committee.

Also, I would like to thank the working committee of our FVV-project and our chairman Dr.-Ing. Philipp Henschen. In particular I would like to thank our project partner, the Department of Marine Engineering at the Hamburg University of Technology, and especially Mr. Maximilian Schröder who conducted the experimental research, which is used as reference in the present work. Furthermore, I would like to thank MAN Energy Solutions SE for providing engine measurement data during the start of the project and for providing the injection rate measurements of the diesel injector.

If there's one thing I've learned over the last few years, it's that you get through hard times better when you have good companions. I want to thank my former colleagues for the wonderful time at the Institute of Internal Combustion Engines, the fruitful scientific discussions and for the great time we had besides work.

Last but not least, I would like to thank my family and my girlfriend Kalliopi, who have always supported me and thus contributed to the success of this work.

Braunschweig, May 2021

Jelto Frerichs

Abstract

Considering the global sulfur limitation for maritime fuels and the existing IMO Tier III legislation, natural gas as a fuel is getting more important in the shipping sector. One way to use natural gas is the dual-fuel combustion process where a homogeneous lean natural gas mixture is ignited by a micro pilot injection of diesel fuel.

In the present work a predictive combustion model for medium speed dual-fuel engines is developed and implemented in GT-Power. To predict the start of combustion, a detailed physically/chemically based ignition delay model is developed, based on the 1D spray model of Musculus and Kattke. Therefore, detailed correlations for the ignition delay times of the 2-stage ignition process are derived from reaction kinetics calculations. Using these correlations, the reaction progress inside the spray is calculated until ignition. Furthermore, the influence of wall contact of the spray is included in the model, as well as the prolonging effect of overmixing for long ignition delay times.

The spray model results at start of combustion are used to initialize the combustion model. The spray zone and the homogenous natural gas/air mixture are burned with different combustion models, to account for the effect of the inhomogeneous fuel distribution. Due to the implemented state-of-the art sub-models for laminar and turbulent flame speed, a wide range of air-fuel ratios is covered by the combustion model.

To account for the HC emissions two flame quenching models are included and extended with an empirical correlation. NO_x emissions are modelled using a standard Extended Zeldovich Mechanism and for the prediction of knocking combustion a detailed knock model from literature is implemented.

The models are calibrated and validated with measurement data from a single cylinder medium speed dual-fuel engine, except for the ignition delay model which does not require calibration. The start of combustion and the combustion parameters are predicted reasonably for a wide range of injection timings and operation conditions. Furthermore, the included HC models allow for a satisfactory prediction of the engine operation parameters brake specific fuel consumption and indicated mean effective pressure.

Due to the detailed description of the different combustion phases, the influence of the injection timing on the NO_x emission is captured well with the standard NO_x-model. This allows for a proper prediction of the NO_x-limited injection timing over a wide range of boundary conditions. The knock limit is also predicted within an acceptable range for different air-fuel ratios and charge air temperatures.

Kurzfassung

In Anbetracht der weltweiten Schwefelbegrenzung für Schiffskraftstoffe und der bestehenden IMO Tier III-Gesetzgebung gewinnt Erdgas als Kraftstoff zunehmend an Bedeutung. Eine Möglichkeit zur Nutzung von Erdgas ist das Dual-Fuel-Brennverfahren, bei dem ein homogenes, mageres Erdgas/Luft-Gemisch durch eine Piloteinspritzung gezündet wird.

In der vorliegenden Arbeit wird ein prädiktives Verbrennungsmodell für mittelschnell laufende Dual-Fuel-Motoren entwickelt und in GT-Power implementiert. Zur Vorhersage des Verbrennungsbeginns wird ein detailliertes physikalisch/chemisch basiertes Zündverzugsmodell entwickelt, das auf dem 1D-Spray-Modell von Musculus und Kattke aufbaut. Dazu werden aus reaktionskinetischen Berechnungen detaillierte Korrelationen für die Zündverzugszeiten der 2-stufigen Selbstzündung abgeleitet. Mit Hilfe dieser Korrelationen wird der Reaktionsverlauf innerhalb des Sprays bis zur Zündung berechnet. Außerdem wird der Kontakt des Sprays mit der Brennraumwand berücksichtigt, ebenso wie der verzögernde Einfluss von starker Abmagerung des Sprays auf den Zündverzug.

Die Ergebnisse des Spraymodells zum Zündzeitpunkt werden zur Initialisierung des Verbrennungsmodells verwendet. Die Sprayzone und das homogene Erdgas/Luft-Gemisch werden mit unterschiedlichen Verbrennungsmodellen verbrannt, um den Effekt der inhomogenen Brennstoffverteilung zu berücksichtigen. Durch die Verwendung von Submodellen für die laminare und turbulente Flammengeschwindigkeit, die dem aktuellen Stand der Technik entsprechen, kann eine große Bandbreite an Kraftstoff/Luft-Verhältnissen von dem Modell abgedeckt werden.

Zur Modellierung der HC-Emissionen werden zwei Flammenlöschungsmodelle einbezogen und mit einer empirischen Korrelation erweitert. Die NO_x-Emissionen werden mit einem Extended Zeldovich Mechanismus modelliert und zur Vorhersage der klopfenden Verbrennung wird ein detailliertes Klopfmodell aus der Literatur implementiert.

Die Modelle werden mit Messdaten eines mittelschnell laufenden Einzylinder Dual-Fuel Motors kalibriert und validiert, mit Ausnahme des Zündverzugsmodells, das keiner Kalibrierung bedarf. Der Beginn der Verbrennung und die Verbrennungsparameter werden für einen weiten Bereich von Einspritzzeitpunkten und Betriebsbedingungen gut vorhergesagt. Darüber hinaus werden unter Berücksichtigung von unverbranntem Kraftstoff auch die Motorbetriebsparameter spezifischer Kraftstoffverbrauch und indizierter Mitteldruck zufriedenstellend vorhergesagt. Aufgrund der detaillierten Beschreibung

der verschiedenen Verbrennungsphasen wird der Einfluss des Einspritzzeitpunkts auf die NO_x-Emissionen mit dem Standard-NO_x-Modell gut erfasst. Es ist außerdem möglich den durch NO_x Emissionen begrenzten spätestmöglichen Einspritzzeitpunkt in zufriedenstellender Genauigkeit vorherzusagen. Die Klopfgrenze kann ebenso für verschiedene Luftverhältnisse und Ladelufttemperaturen zufriedenstellend vorhergesagt werden.

Contents

Abbreviations

0D	Zero-dimensional
1D	One-dimensional
3D	Three-dimensional
AFR	Air-fuel ratio
BMEP	Brake mean effective pressure
BSFC	Brake specific fuel consumption
CA	Crank angle
CAaTDCF	Crank angle after top dead center firing
CFD	Computational fluid dynamic
CH_4	Methane
C_2H_6	Ethane
C_3H_8	Propane
C_4H_{10}	Butane
C_7H_{16}	n-Heptane
CCV	Cycle-to-cycle variabilities
CV	Control volume
COV_{IMEP}	Coefficient of variance of the indicated mean effective pressure
DOE	Duration of energizing
EGR	Exhaust gas recirculation
FVV	Research Association for Combustion Engines e. V.
H_2	Hydrogen
HC	Hydrocarbons
IMEP	Indicated mean effective pressure
HCCI	Homogeneous charge compression ignition
HIL	Hardware in the loop
IMO	International Maritime Organization

KF	Knock frequency
KI	Knock integral
LHV	Lower heating value
LLNL	Lawrence Livermore National Laboratories
LNG	Liquified natural gas
LTHR	Low temperature heat release
MFB02	Crank angle when 2% of the fuel is burned
MFB50	Crank angle when 50% of the fuel is burned
MWM	Motorenwerke Mannheim
NG	Natural gas
NUI	National University of Ireland
NO	Nitrogen monoxide
NO_2	Nitrogen dioxide
NO_x	Nitrogen oxide
R^2	Coefficient of determination
RANS	Reynolds-averaged Navier–Stokes
SI	Spark ignited
SOC	Start of combustion
SOE	Start of energizing
SOI	Start of injection
TDC	Top dead center

Symbols

Subscripts

0	Start value
1...9	Numbering
a	Ambient gas
avail	Available
b	Burned; break up
bu	Burn up
calc	Calculated
Ceil	Ceiling temperature for LTHR
Ch	Charge air
cl	Centerline
comb	Combustion
Cyl	Cylinder
D	Diesel (Pilot fuel)
e	Entrained into the flame front
EGR	Exhaust gas
FF	Flame front
flame	Flame (thickness)
high	High temperature ignition
i	Allocation to control volume, spray model
int	Integral (length scale)
j	Timestep, spray model
k	Allocation to combustion chamber wall (head, piston, liner)
l	Liquid fuel
low	Low temperature ignition

max	Maximum
mix	Mixture
mr	Most reactive
NG	Natural gas
overmixing	Change due to overmixing
pilot	Pilot zone
pot	Potentially
prem	Premixed
Q	Quench
reac	Change due to chemical reactions
Ref	Reference value
SOC	Start of combustion
trans	Transition
u	Unburned
w, wall	Combustion chamber walls (head+piston+liner)

Latin symbols

A	Coefficient, knock model
B	Coefficient, temperature increase due to LTHR
$BasisPG$	Background noise of the cylinder pressure signal (knock detection)
c	Progress variable
c_m	Mean piston speed
c_p	Specific heat capacity (constant pressure)
C_{bu}	Model parameter, turbulent entrainment model
C_{ign}	Model parameter, ignition delay
$C_{overmixing}$	Model parameter, ignition delay

C_{prem}	Model parameter, combustion of premixed pilot fuel
C_{quench}	Model parameter, quench layer thickness
C_{Spray}	Model parameter, spray angle
C_{ST}	Model parameter, turbulent entrainment model
d	Thickness
D	Diffusion coefficient; cylinder bore
$e1$	Model parameter, knock model
E_A	Activation energy
F	Coefficient, laminar flame speed and NO_x model
$f_1 \ldots f_4$	Model parameters, laminar flame speed (n-heptane)
f_{trans}	Transition factor
G	Coefficient, laminar flame speed
h	Specific enthalpy and height
k	Turbulent kinetic energy; reaction rate (NO_x model)
KI	Knock integral
KI_1, KI_2	Integral of the high-pass filtered cylinder pressure in window 1 and 2 (knock detection)
$KRAT$	Knock integral ratio (knock detection)
l	Length
m	Mass and coefficient (laminar flame speed)
M	Momentum
n	Coefficient, laminar flame speed
p	Pressure
$\dot{q}$	Heat flux
r	Inner spray radius; coefficient (laminar flame speed)
R	Outer spray radius; gas constant
S	Spray tip penetration

S_L	Laminar flame speed
S_T	Turbulent flame speed
t	Time
Δt	Timestep
T	Temperature
T^0	Reaction zone temperature, laminar flame speed
ΔT	Temperature increase due to low temperature heat release
u	Velocity
u'	Mean turbulent velocity
V	Volume
x	Distance from injector nozzle
X	Volumetric fraction
Y	Mass fraction

Greek symbols

α_0	Coefficient, package model
α	Coefficient, Abramovich profile and knock model
β	Coefficient, spray model and knock model
γ	Coefficient, knock model
$\delta_1 \dots \delta_9$	Coefficient, mixing temperature
Δ	Difference
Θ	Spray cone angle
λ	Air-fuel equivalence ratio and thermal conductivity
ν	Kinematic viscosity
ξ	Dimensionless radius
ρ	Density

τ	Time scale, ignition delay and eddy burn up
$\upsilon_1 \ldots \upsilon_4$	Exponents of the ignition delay correlation
φ_{df}	Dual-fuel fraction
Φ	Equivalence ratio
ω_c	Source term of progress variable c

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