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A fast and accurate physics-based model for the NO_x emissions of Diesel engines

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HIGHLIGHTS

- A physical foundation is combined with a simple structure for high execution speed.
- Only few stationary measurements are needed for a fully automatic identification.
- The error during transients is 2.5% in average and extrapolation is possible.
- Combination of these properties is unique and allows for numerical optimal control.

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ABSTRACT

To date, models for the nitrogen-oxide emissions of Diesel engines are either of empirical or phenomenological nature. The former are fast and quantitatively accurate in the identified region, but lack the generality and extrapolation capability of the latter. The model presented in this work combines the advantages of both model types and thus complies with typical requirements of computationally intensive fields such as dynamic optimisation and model-based control. This unique aggregation of features is achieved by extracting the most relevant physical phenomena and extending them by physically motivated empirical elements. Exploiting the assumptions made and using a setpoint-relative formulation leads to a simple model structure, comprising one map and 10 scalar parameters only. Execution speed is roughly 500 times faster than real-time and throughout the entire engine operating-range, also during transient operation, relative errors are below 10% even for the largest allowable, simultaneous variation of all inputs. Apart from engine speed and injected fuel-mass, the model requires the cylinder-charge, its composition, and the start of combustion with the corresponding pressure and temperature as inputs. The latter can either be obtained from measured in-cylinder pressure signals, or may be calculated from quantities provided by a model for the air path of the engine.

1. Introduction

Optimal control of Diesel engines becomes increasingly important. More stringent emission regulations require the exploitation of the remaining potential of reducing emissions, not only in stationary operation but especially during transients. Simultaneously, fuel consumption has to be minimised for economical and environmental reasons. Current and near-future pollutant limits [1,2] guide the attention towards transient operation [3,4]. The classical approach to generate reference trajectories for control, which extends stationary engine-map calibration by empiric corrections during transients, lacks consideration of the engine dynamics. Dynamics may be incorporated either online by using model-predictive control [5] or offline by optimising the control trajectories globally w.r.t. time. The resulting control trajectories with corresponding fuel consumption and pollutant emissions can be used as a benchmark to disclose scenarios in which the performance of actual control systems is suboptimal. An analysis of these cases provides insight in how to improve control structure, feedforward control and reference-trajectory generation. The generally high dimensionality and complexity of Diesel-engine models, including non-analytical sub-models, exclude dynamic programming and indirect methods from application to dynamic optimisation. Direct numerical approaches for optimal control [6,7] are thus most prominently applied.

Emission models apt for optimal control are subject to a multitude of requirements as described in the following. Since emission limits typically appear as inequality constraints, quantitative accuracy is key. The optimisation process itself is allowed to explore the full input space in all possible directions, subject to mechanical constraints only. Therefore, the model has to reliably provide qualitative trends of the input–output relations on the entire input space. This capability of physically plausible extrapolation improves the

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Nomenclature

$\dot{x} := \frac{dx}{dt}$	derivative w.r.t. time
$[X]$	concentration of species X (mol/m^3)
$\tilde{x}$	setpoint-relative quantity

Uppercase letters

$\mathscr{F}$	generic model function (–)
H	heating value, formation enthalpy (J/kg), (J/mol)
M	molar weight (kg/mol)
N	rotational speed (1/min)
Q	molar or mass-specific heat (J/mol), (J/kg)
R	specific gas constant (J/kg K)
T	torque (Nm)
S	number of species in mixture (–)
V	volume (m^3)

Lowercase letters

a	coefficients of linearised enthalpies (–)
c	mass-specific or molar heat capacity (J/kg K), (J/mol K)
f	factor (relative change), reference quantity (–)
h	mass-specific or molar enthalpy (J/kg), (J/mol)
k	reaction constant, fitting parameter (–), (misc.)
m	mass (kg)
n	(molar) amount (mol)
p	pressure (Pa)
r	reaction rate, ratio (mol/m^3 s), (–)
u	control input (–)
x	fraction $\in[0,1]$ (–)
y	generic model output (–)

Greek symbols

α,β	average composition of fuel ($C_\alpha H_\beta$) (–)
γ	polytropic exponent (–)
ζ	molar fraction (and volume fraction for ideal gases) (–)
ϑ	temperature (K)
κ	isentropic exponent (–)
ξ	mass fraction (–)
ν	stoichiometric coefficient (–)
φ (°)	crank angle $\in[0,720]$, ignition top dead-center at 360

Abbreviations and indices

A	activation (temperature)
AFM	air-flow meter (measurement device)
af	adiabatic flame
AFT	adiabatic flame-temperature
bC, aC	before, after combustion
bw, fw	backward, forward
CA	crank angle
cyl	cylinder
EGR	exhaust-gas recirculation
eng	engine
ETC	European Transient Cycle
EVO	crank angle/time at exhaust-valve opening
f	fuel, formation
fb	forward-to-backward (ratio)
hl	heat losses
ID	ignition delay
IM, EM	intake manifold, exhaust manifold
is	isentropic
IVC	crank angle/time at intake-valve closure
l	lower (in contrast to higher)
ms	measured
M	molar
offs	offset
p	w.r.t. pressure, products (in contrast to reactants)
r	reactants (in contrast to products)
reac	reaction
rg	residual gas
rpm	revolutions per minute
s	sensible (enthalpy; in contrast to formation)
SOC, SOI	start of combustion, injection
SP	setpoint, value in setpoint
surr	surroundings
thr	threshold
ub	unburned
v	w.r.t. volume
VGT	variable-geometry turbine

convergence properties of the optimisation by eliminating the need for factitious constraints and providing inherent stability to the problem. The smooth nature of physically motivated relations contributes to the robustness of the optimisation problem and in turn reduces the number of measurements required for model identification by allowing coarser sampling. Obviously, the reduced measurement burden helps in lowering costs of both stationary and transient engine calibration. Finally, models for optimal control have to be computationally efficient, given the vast amount of model evaluations performed during numerical optimisation. Compared to a mean-value model for the air-path, running at least 100 times faster than real-time during forward simulation, the emission models should require less operations in order not to significantly increase the execution time. A simple structure and the avoidance of involved calculations such as the solution of differential equations are the basic means to achieve sufficient performance.

1.1. Survey on modelling of NO_x emissions

Models for the nitrogen-oxide (NO_x) emissions of Diesel engines may be split into two main groups, namely phenomenological and empirical models. Notice that the class of spatially resolved models [8,9] used to investigate turbulent-flame phenomena and to perform pre-experimental studies is excluded from this review due to prohibitively high computational costs.

The term phenomenological already indicates the inherent difficulty of describing the emission formation using physical first principles only. In fact, the complex nature of Diesel combustion and pollutant formation described in [10–13] requires macroscopic phenomena to be modelled directly. First promising attempts date back to the early 1970s [14,15]. Together with later contributions [16–20], they provided a generally accepted framework comprising the following key components: Subdivision of the injection spray into individual fuel packages, calculation of spray breakup, ignition and combustion, and superposition of the NO-formation kinetics using the well-known (extended) Zeldovich mechanism. The tracking of multiple packages through these phases motivated the term quasidimensional to designate this type of model. More recent research has focused on two main aspects: On one hand, the required detail of the formation mechanism is examined. More complex [21–25] as well as simple single-equation approaches have been investigated [26–30]. On the other hand, the main phenomena defining the evolution of temperature and composition of the packages over crank angle are elaborated. The initial temperature is commonly assumed to be the adiabatic flame-temperature (AFT). Its calculation is sometimes simplified by considering the main influence of oxygen availability only [31–33] or by treating dissociation effects as additional fitting parameters of the model [28,29,34]. Polytropic compression and expansion is certainly the most influential factor defining the further course of temperature.