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System Simulation of Modern Powertrain Concepts

- From an Industrial Perspective

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Outline

Introduction

- Emission Standards – Motivation - Challenges

Modeling Challenges

- Exhaust Gas Aftertreatment Simulation
 - BlueTEC Technology for Passenger Cars
- Engine emission modeling
- Full Vehicle Simulation
- Summary Conclusion



Motivation: NOx- and PM-Emissions

The major challenge is to fulfill the worldwide emission standards



DAIMLER Political Surroundings





It is expected that fuel consumption and emission targets will tighten even further in the future!



Challenges Related To Emission Legislation



To meet future standards, fuels with closely restricted specifications and extensive improvements in combustion and exhaust gas after treatment systems are obligatory



Innovative powertrain systems towards sustainable mobility for the future





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Motivation

AGN-Simulation as sub-component of systemsimulation for the development of lowemission vehicles with combustion engines including alternative propulsion (e-Drive)



→ high complexity of aftert-treatment and propulsion systems and fundamental role of simulation
 → Without simulation it`s impossible to adapt a system to all the different vehicle and engine variants offered on the markets around the world



Introduction Modeling EGA



Exhaust Aftertreatment Component Toolbox (ExACT)

History

- <u>1996</u>: Technology-Monitoring: Tools EGA-Sim commercially not available
- 1997: Start FVV-Project, Lead Daimler (PhD: Daniel Chatterjee)
- <u>2000</u>: Start Modeling in R&D Projects: TWC, DOC, NO-Oxidation Cooperation with Universities Prague, Milano, Thessaloniki (Models or SCR, TWC, NSC, DOC, DPF)

\rightarrow Tool *ExACT*





ExACT toolbox consists of 1D models for SCR, DOC, DPF, LNT, TWC and ASC. Simulation of combined aftertreatment systems. Model generation by drag & drop. **Focus:** Testcycle simulation, system design, operating strategies, DCU development



Modeling of most relevant physical and chemical processes required for predictive simulations. Variation of geom. parameters (cell density etc.) in the simulation makes separation of transport effects and chemistry kinetics necessary.



• Real axiale distribution

• Temperature distribution



DAIMLER EGA 1D M



Modeling of NSC and SCR: NOx Conversion and NH3 Yield (Simulation versus Experiment)



NSC: NH₃ selectivity during regeneration favoured around 350 °C. SCR: Conversion efficiency is influenced by the NO₂/NO_x feed ratio. Model correlates well with measured product selectivity and NO_x conversion.



Reaction Mechanism: How important is the detailed chemistry?



Eley-Rideal unable to explain the inhibition of N2-formation by NH3.

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2. Modified Redox kinetics (MR)



With a modified mechanism MR excellent compliance between Sim and Experiment

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Kinetic Parameter Calibration Dr. V. Schmeißer, Dr. B. Ganz

Kinetic Parameter Calibration



Model calibration

global kinetics

• change of washcoat or ageing condition requires calibration

• only kinetic parameters calibration – geometry not affected reactions and rates - example:

$$CO + \frac{1}{2}O_{2} \longrightarrow CO_{2}$$

$$R_{NSRC1} = k_{NSRC1}y_{CO}y_{O_{2}}\frac{1}{G_{1b}}$$

$$K_{inh,l} = K_{infl}O_{l} \cdot \exp\left(\frac{E_{l}}{T^{s}}\right)$$

$$K_{inh,l} = K_{inh,l} \cdot \exp\left(\frac{E_{l}}{T^{s}}\right)$$

• numerous

• to be determined according to measurements



- new catalysts/PGM-loadings/aging require kinetic calibration
- effective techniques necessary:
 - using conventional parameter estimation tools (e.g. simplex)
 - using automated calibration





Advanced calibration methods

Demand:

availability of kinetic parameters for new technologies/conditions within a short time!



New Calibration Methodology could be used for all tested cases fast calibration process due to parallelization on computer cluster **D**

* Souther & Workedienten basierth, NSGAM (Noon-sorting agenetic algorithm) BFGS (Broyden-Fletcher-Goldfarb-Shanno)



1D EGA simulation: Heavy Duty EGA-System Dr. F. Hofmann, Dr. J. Koop

EGA 1D Model Application



example:

ATS-Box

Euro6 Swenox

Heavy Duty EGA-System

Motivation

- high complexity of EAT systems and increased requirements
- support by simulation required

Technical and Functional Approach

- > EAT model development using Matlab/Simulink (ExACT) and StarCD
- ➢ pipes, DOC, (c)DPF, SCR, ASC, TWC, NSC, AdBlue[®] dosing and processing

Current Status

- status of in-house developed models: high quality
- model application in various projects (Euro6, Tier4, Helo)
- further development according to future technologies (e.g. hybrids)



exhaust gas

from enaine

particulate filte

AdBlue

njection

SCF

ASC

EAT modeling and simulation for:

- > development of operation strategies
- > prediction of conversion behaviour

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NO2-ratio[%]

temperatures[°C]

efficiency around 10-20% by improving the NH₃-uniformity.

NOx-conversion-deviation-map (sim *-exp.) [%]

Analyis of Urea Processing on SCR-Performance



OM460 with ATS-Katbox EURO6 (17L DOC; 27L cDPF; 39,7L SCR), mexh 300 kg/h

Simulation reveals a potential of improvement of the low temperature SCR



NO2-ratio[%] * 1D ExACT Simulation



NOx-conversion map experiment [%]

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Heavy Duty EGA-System:





1D EGA simulation: NSC + SCR-combination (BlueTEC I) Dr. Weibel et. al.

EGA 1D Model Application



Exhaust gas after treatment with Bluetec I / Bluetec II



Target: Diesel engines as clean as gasoline engines thanks to BLUETEC - on the way to the most stringent emission standards EU5 and EU6

EGA 1D Model Application



ExACT-simulation: NSC + SCR-combination

BlueTEC I: on-board generation of NH₃



BlueTEC 1 as complex aftertreatment system with influence and interaction between catalyst modules including a lean / rich strategy by the engine

1D EGA Simulation



ExACT-simulation: NSC + SCR-combination

lean/rich-cycles (steady state), SV = 35.000 1/h, lean: 180s, rich: 7s



EGA 1D Model Application



BlueTec I (NSC Technology) Detailed analysis of the cycle



•NOx absorption starts after 150 sec

•Practically all NOx emitted between 150 sec and 800 are completely absorbed

•conversion in SCR after 800 sec due to low temperatures

- \Rightarrow NOx conversion in NSC 62%
- NOx conversion in SCR 8%
- BlueTec I has the potential to meet Euro 6 targets



Coupling engine emission data with 1D EGA simulation

T. Rappe



EGA-Simulation DI-Gasoline: Study of





Numerical NEDC-Simulation of axial NO_{χ} and NH₃ profile with **3s** rich spikes



With 3s rich time NSC NO_X regeneration insufficient however for overall NO_X performance sufficient NH3 in SCR catalyst.

Results: Coupling engine data with EXACT DAIMLER Numerical simulation of lean gasoline vehicle to achieve EU6 regulations. SCR **SCR** TWC TWC **NSC** 00 Urea 3000 3000 Lambda [-] -NOx upstream 0.8 0.8 -NOx downstream TWC 2500 2500 NOx downstream SCR -NOx_upstream -NOx downstream NSC -TWC 0.6 0.6 -NOx downstream SCR 0.0 [Lux]/b] -SCR 2000 -NSC 2000 0.4 [may/6] ×ON EU6 N SCR [wad] 1500 XON [udd] 1500 XON Lambda 0.2 Ŏ EU6 0 0 1000 1000 500 500



Simulation is useful to compare different EGA-systems and operation strategies. Pre-optimizations of operation strategies can simplify test bench application.



Summary

- *ExACT*: in-house developed and well-established1D-simulation tool for EGA components
- description of complex exhaust aftertreatment systems possible
- simulation tasks for:
 - improved system configuration
 - improved component design and layout (catalyst size, position)
 - sensitivity analysis
 - potential estimation

Conclusion

Modeling and **simulation** will be the **key factor** for different applications of engine-vehicle combinations on markets around the world.



ExACT "virtual testbench": DCU-methodology for TP/PME

Dr. F. Hofmann



DCU-Methodology

Model based DCU*-development for EURO6 and DCU-calibration with ExACT *DCU: Dosing Control Unit



• ExACT "virtual testbench": combined DCU and EGA simulation
 • DCU control algorithm testing & precalibration of a-maps
 → precalibration saves approx. 1-2 months in development time



*DCU: Dosing Control Unit

DCU-Methodology

Further Development of Urea-Dosing Strategy for Cu-SCR based on ExACT

Motivation:

SCR NO_x conversion depends on <u>NH₃ storage</u> (θ_{NH3}) (*Cu-SCR* !) **approach**:

- 1.) control of NH_3 loading
- 2.) accelerated NH_3 loading by overdosing at cold-start
- → development of loading control and testing: with ExACT

Simulation Results:

- θ_{NH3} control
 → increased NO_x-conversion
- for both: Fe- or Cu-SCR
- generation of NH₃ storage map based on ExACT

Next Step:





• Validation on engine test bench

higher NO_x-conversion due to improved dosing control

 \rightarrow enables higher NO_x raw emissions & reduced fuel consumption:

[U NOx] max NH3 slip min

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3D-CFD-Modeling & 1D-3D coupling

Dr. Schöffel, H. Echtle







3D Simulation AdBlue Processing Example: mixer optimization



• reduced mixer length \rightarrow investigating reason for less uniform distribution (350°C, 200kg/s)

• reason: wall film formation due to decreased overlap of blades \rightarrow poor evaporation

→ 3D-Simulation applied for diagnostics and optimization

1D-3D coupling



Cooperation with CD-adapco Monolith with fine representative channel subdivision

Example: water condensation on DOC





M. Weaver, CD-adapco, CLEERS-Workshop 2010

- integration of DOC 1D-reactions validated \rightarrow model compatibility 1D 3D
- pilot application for test bench simulation in progress
- next steps: integration DPF and SCR reactions



Control-oriented SCR-Model (COM) Methodology (HiL, SiL, ..)

Dr. Frank Hofmann





Example: Comparison COM vs. ExACT in NEDC with Cu-SCR-catalyst





Summary

- For the **overall system simulation** of future powertrain concepts there is no alternative to EGA-simulation (conventionel & e-Drive)
- **ExACT** is physical/chemical based and effective for **predictive simulation**
- **ExACT** + 3D-Simulation urea process in exhaust is used intensively for application work in the **product development**
- The use for **model-based control** and ECU capable models is of increasing importance
- And will be **further developed** together with our academic and industrial partners

 $|\triangleright$



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| DAI | MLER |
|-----|------|
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Virtual Powertrain – engine emission modeling

Dr. R. Steiner et. al. in cooperation with ETH Zürich



Engine Emission Modeling General Modeling Requirements:

Overall system simulation (and sub-models!) needs to be

fast for offline predictions: results for driving cycles are in focus!

real-time for HiL applications (for total system: time steps <10 ms, <100 HZ)</p>

> very fast when using an engine air-path model: time steps <1ms, <1000HZ)

Compromise between computational efficiency and accuracy: As accurate as needed, as simple and fast as possible!!!

Accounting for most relevant physics-based process variables!

Most challenging part in sub-model development, prediction of → transient behaviour of heat release and raw emission formation

^{*1} :Depending on computer platform







Control-oriented Modeling: State-of-the-art Mean value model for control-oriented applications (ODEs) Gas path: \rightarrow good compromise between computational efficiency and accuracy Combustion: Quasi-static modeling approach \rightarrow based on static engine maps **Raw Emissions** 3D CFD models (Kiva...) Usually crank-angle based. CPU costs too high! Phenomenological models (Hiroyasu. Empirical Models (Barba...) Large-number of measurements needed; reduced portability; very poor extrapolation capability! 400 800 QSS Engine torque [Nm] Measurement 300 PM [FSN] NO [ppm] 200 400 100 0 0 0 0 0 2 6 8 2 6 0 8 Time [s] Time [s] Time [s] Comparison between measurement data (black) and quasi-stationary simulations (red) during a load step at constant engine speed.

Quasi-stationary modeling approach is adequate for computing torque generation (and fuel consumption) but inappropriate for predicting emissions!

DAIMLER Control-Oriented Models: Analysis



Transient boundary conditions of combustion process

Differences to static engine operation



The **turbocharger inertia** causes the most relevant dynamic effects for a modern Diesel!

The relevant boundary conditions for combustion and emission formation are:

> cylinder charge at IVC (mass, gas composition, and gas temperature)

boost pressure, exhaust gas recirculation rate and the temperature after intercooler

- injection (mass, pressure, timing)
- operating point (injected fuel, engine speed)



DAIMLER Transient control-oriented engine models





With the approach "Transient control-oriented engine models" Well Prediction of heat release and raw emissions

DAIMLER Transient control-oriented engine models



Comparison between measurement and simulation Soot:



Influence of transient transitions on soot-emissions are predicted well!

UDC= urban-driving-cycle EUDC=Extra-urban-driving-cycle

DAIMLER Transient Simulation Results: NEDC



Comparison between measurement and simulation NOx:



Influence of transient transitions on NOx-emissions are predicted well!

UDC= urban-driving-cycle EUDC=Extra-urban-driving-cycle



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DAIMLERFull Vehicle Simulation @ Daimler



Example: Support within the Blue-Zero Project





Reduction of development time by strong link between soft- and hardware (Plug 'n Play)

Validation





Ready to use for "offline" optimization (Model-, ECU-, Powertrain-in-the Loop)!

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Source: P. Macri-Lassus

Validation





Validation based on arbitrary driving cycle shows good results! Ready to use for "offline" optimization (Model-, ECU-, Powertrain-in-the Loop)!

Source: P. Macri-Lassus



Summary

The mobility of the future is dependent on a lot of boundary conditions that become more and more stringent! CO2 and emissions are in focus!

Future mobility is also shaped by the electrification of the powertrain! Portfolio of powertrain concepts and its complexity is dramatically increasing! Increase of levers for optimization. Operation strategies make the difference! Overall system optimization is the key to success!

Without advanced simulation tools it will be impossible to meet these challenges. This includes sub-system and overall system models.

"Best components with best operation strategies!"

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Thank you for your attention !