Object-oriented modelling, dynamic simulation and optimization of heat-integrated exhaust purification systems with ProMoT and DIANA
Outline

1. Introduction

2. Modelling and Simulation
   with ProMoT and Diana

3. Simulation Results - Examples

4. Summary and Outlook
1. Automotive exhaust purification – state of the art

**state of the art → multi-component exhaust lines**

![Diagram showing exhaust purification process](image)

- **EGR-Valve**
- **Diesel-oxidation** $T > 250°C$
- **NO$_x$-storage-reduction catalyst** $T = 250 - 450°C$
  - (sulphur removal: $T ≈ 750°C$)
- **Diesel soot filter** (regeneration at $T ≈ 450 - 750°C$)

Exhaust temperature: $150 – 800°C$

Commercial tools for simulation available
1. Exhaust purification – heat-integrated approach

Exhaust treatment separated from engine control
in one compact, autonomous exhaust treatment unit

- Full flexibility of equation based modelling
  necessary (programming languages)

- Convenience of “block oriented” tool preferred

→ Lack of commercial tools
1. Heat integrated concepts – modeling approaches

Modular approach: Models reusable for different constellations, complex system to solve

Fully integrated approach: new models and extensive numerical studies necessary

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1. Heat integrated concepts – modeling approaches

Requirements:

• easy set-up of model constellations and simulation scenarios

• user-friendly “block-oriented” modelling

• flexibility of equation based modelling

• efficient solvers for complex coupled DAE problems

• full access to the source code

• efficient tools for parameter estimation, optimization and numerical analysis

→ our choice: ProMoT and DIANA
2. ProMoT and DIANA
(Max Planck Institute Dynamics of Complex Technical Systems, Magdeburg)

Modelling tool ProMoT
(Process Modelling Tool)

- Equation-based modelling
  - DAE (index 1)
- Object-oriented concept
  - Multiple inheritance
  - Aggregation
- Model implementation
  - Graphical modelling with GUI
2. ProMoT and DIANA
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- Model implementation
- Graphical modelling with GUI
- Text-based in language MDL
- Equation analysis and optimization
- Symbolic differentiation in ProMoT

```plaintext
# define-module
:class "bilansen-dpf"
:super-classess (["kinetik-dpf"])
:documentation "subsystem"
:variables
df
:indices ("a" :lower "0" :upper "n")
:system-theoretic "real-parameter"
:value "0.0000"
"q_h2"
:indices ("a" :lower "1" :upper "n")
:system-theoretic "real-parameter"
:value "1.00-10"
"q_h2c"
:indices ("a" :lower "1" :upper "n")
:system-theoretic "real-parameter"
:value "1.00-10"
"q_o2"
:indices ("a" :lower "1" :upper "n")
:system-theoretic "real-parameter"
:value "1.00-10"
|equations |
|"coupling1" |
|"coupling2" |
|"coupling3" |
|"coupling4" |
|"coupling5" |
|"coupling6" |
|"coupling7" |
|"coupling8" |
|"coupling9" |
```
### Modelling tool ProMoT

- Equation-based modelling
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### Simulation tool DIANA

- Equation based models
- Object-oriented architecture
- Modular and extensible
- Efficient numerical kernel
  - (solvers based on free code)
- Control via scripts
- Contains methods for dynamic simulation and numerical analysis

- free for academic groups under GNU General Public License
- full access to source, good support (MPI) and extensibility
3. Simulation Results – Heat-integrated system

Favorable mode of operation:

1) Fast start-up of the unit
2) Keep unit in ignited mode

Two showcases how to use DIANA concerning heat-integrated exhaust purification systems

Dynamic simulation of heat-up under drive-cycle conditions to show behaviour of the system

Steady-state continuation to show theoretical limits of ignited states
3. Simulation Results – Example 1

Heat-up under drive cycle conditions (no cold-start application!)

Comparison of three system set-ups (Diesel):

DOC (stand alone)

a) DOC with cold start burner

b) HEX with DOC and cold start burner → heat-integrated system

Set point: \( T_{\text{DOC}}^{\text{IN}} = 350°C \) \( T_{\text{DOC}}^{\text{IN}} = 400°C \)

Source: CaPoC8 Brussels; J. Bernnat et. al. - Heat integrated concepts for automotive exhaust purification
3. Dynamic Simulation –
Heat-up under drive cycle conditions

Fast heat-up due to efficient use of the burner

Concerning DIANA:
Easy and fast set-up of simulation scenario
Efficient simulation of different coupled systems under drive-cycle conditions
Second Example: Steady-state continuation: stability of operation states

Simple model of integrated system for exhaust after treatment of CNG-engine

Counter-current heat exchanger with partially catalytically coated walls

*www.ingas-eu.org
3. Steady-state continuation – principle

Parameter continuation vs. dynamic simulation

Condition for steady-state points of an autonomous system $x \in \mathbb{R}^n, \nu \in \mathbb{R}^p$ is:

$$\dot{x} = f(x, \nu) = 0$$

Stability is determined by eigenvalues of a linearized system at the steady-state point $x_s, \nu_s$:

$$V \Lambda = \frac{\partial f}{\partial x} V$$

Source: Mykhaylo Krasnyk, DIANA — An object-oriented tool for nonlinear analysis of chemical processes, Max Planck Institute for Dynamics of Complex Technical Systems
3. Steady-state continuation in one parameter

Variable: Inflow Temperature

Constant: 2000 ppm Methane, 100 kg/h

Conversion [-]

Inflow temperature [°C]

Limit points correspond to stability bounds

extinction

ignition
3. Steady-state continuation in one parameter

Steady state profiles of the wall temperature

→ extinction

- Conversion [-] vs. Inflow temperature [°C]
  - Conversion: 0 → 1
  - Inflow temperature: 100 → 600

- Wall temperature vs. length [cm]
  - Wall temperature: 0 → 600
  - Length: 0 → 25

- Inflow temperature: 186°C and 187°C
  - Extinction points

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3. Steady-state continuation in two parameters

Variable: Temperature, Methane Concentration

Constant: 100 kg/h

Conversion vs. inflow temperature

Conversion [\%]

- upper stable branch
- unstable branch
- lower stable branch

Inflow temperature [°C]

- Ignition line
- Extinction line

Cusp gives the limits of ignition and extinction

Inflow temperature [°C]

Methane concentration [ppm]

- 2000 ppm
3. Steady-state continuation in two parameters

Variable: Temperature, Methane Concentration
Constant: 100 kg/h

Cusp gives the limits of ignition and extinction

850 ppm

2000 ppm
3. Steady-state continuation – CNG

From the limit points we can extract more useful information! e.g.
4. Summary and outlook

Summary:

• Object-oriented, equation-based modelling
• Flexible and fast set-up of model configurations
• Easy set-up of simulation scenarios
• ProMoT\(^1\) and DIANA\(^1\)
• Advanced numerical packages for system design
• Simulation results

Outlook:

• Extension of model library
• Analysis and optimization of after treatment systems
• Development of control strategies

\(^1\) Max Planck Institute for Dynamics of Complex Technical Systems
Acknowledgement:

*Support of the*
- Deutsche Forschungsgemeinschaft (DFG),
- European Community (EU)
- MPI Magdeburg

*is gratefully acknowledged.*

*Thank you for your kind attention!*

*Questions?*