EXHAUST AFTERTREATMENT
IN THE FRAMEWORK OF SYSTEM ENGINEERING SIMULATION

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OVERVIEW

- System Engineering Simulation
  - Requirements
  - Functionalities
- Simulation Examples
  - TGDI Engine in Hybrid Passenger Car
  - HSDI Diesel Engine in Conventional Passenger Car
- Summary/Conclusions
REQUIREMENTS ON SYSTEM ENGINEERING SIMULATION SUPPORTING AND CONCEPT DESIGN AND CALIBRATION

- **Multi-physical system simulation**
  - Dedicated models and solvers for all vehicle domains (engine, cooling, drivetrain, e-system)

- **Consistent plant modelling**
  - Links development teams from concept to calibration phase

- **Scalable physical modelling depth**
  - Right balance of predictability and CPU speed

- **Flexible model customization**
  - Best combination of standard and custom models

- **Open interface in office and HiL**
  - Office co-simulation platform and model export on all relevant HiL systems

- **From engineering to commercial tools**
  - Experience of powertrain engineering as input for tool development
MULTI-PHYSICS SYSTEM SIMULATION ENGINE, COOLING, VEHICLE AND CONTROL

- Cooling & Lubrication (dt~1000ms) Quasi-State/Transient Flow Transient Energy Balance
- Air Path, Control, Vehicle Drivetrain (dt~0.5-5ms)
- Aftertreatment (dt~arbitrary) Stiff systems
- Cylinder (dt~1degCRA, speed dependent)
CONSISTANT PLANT MODELING
SCALABLE PHYSICAL MODELING DEPTH

Modeling Approaches

- Map Based:
  (e.g. conv=f(Temp., [educt])
- Surrogate modeling:
  (multidimensional input space)
- Physical, transient 1D/3D two-phase model
- Physical, transient 1D/3D two-phase model including 1D reaction diffusion modeling in arbitrary washcoat layers

Figures taken from SAE _2012-01-1296
AVL User Coding Interface

- GUI Supported Custom Kinetics
  - Arbitrary Species
  - Arbitrary Reactions (conversion, surface storage, …)
- Automatic generation of c-code and compilation of reaction dll
- Encapsulated reaction modelling
- Combination of multiple user-dll with pre-defined reaction models
- Simplified Workflow (Application of one single reaction dll in BOOST, FIRE and CRUISE™)
FLEXIBLE MODEL CUSTOMIZATION EXAMPLE: UREA DECOMPOSITION APPROACH

Model 12 reactions

(R1) urea → NH4+ + NCO-
(R2) NH4+ → NH3(g) + H+
(R3) NCO- + H+ → HNCO(g)
F (R4) urea + NCO- + H+ → biuret
D (R5) biuret → urea + NCO- + H+
F (R6) biuret + NCO- + H+ → cyanuric acid + NH3(g)
D (R7) cyanuric acid → 3 NCO- + 3 H+
F (R8) cyanuric acid + NCO- + H+ → ammelide + CO2(g)
D (R9) ammelide → 2 NCO- + 2 H+ + HCN(g) + NH(g)
(R10) urea(aq) → NH4+ + NCO-
(R11) NCO- + H+ + H2O(aq) → NH3(g) + CO2(g)
F (R12) urea(aq) + NCO- + H+ → biuret

F: formation reaction
D: decomposition reaction

\[
\dot{r}' = A \cdot e^{\left( -\frac{T_A}{T_s} \right)} \cdot \prod_j \left( Z_j^N \cdot v_j \right) \cdot \Gamma / 1000 \cdot \left( \sum_k Z_k^{init} \cdot \sigma_k \right)^\nu \left( 1 - \sum_j \nu_j \right)
\]

OPEN INTERFACE IN OFFICE APPLICATION

- **Flowmaster, Kuli**
- **AVL PUMA**
- **MATLAB/Simulink**
- **Car/TruckMaker**
- **LMS AMESim**
- **AVL VSM/Drive**
- **ETAS ASCET**
- **Car/TruckSim**
- **AST ACCI**
- **CUSTOM C-CODE**
- **FMI (Dymola, SimX...)**

**CRUISE™:**
Multi-Physics, Multi-Rate-Time-Integration
OPEN INTERFACE IN HIL APPLICATION
Mission compilation out of various sources

- Random-cycle generator: Compile random driving profile out from 20000 short trips
- In-Use data import: Load GPS (e.g. measured via M.O.V.E., NAVTEC)
- Legislation cycles: Selection of driving profile from built-in library
- Combine individual task to dedicated mission
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2 Front wheel driven passenger cars:

1. Conventional 5 speed gear box
2. Parallel Hybrid of Toyota Prius 2004 (schematic)

Common configurations for
- Vehicle chassis, tires
- Driver…
- TGDI and ECU
ENGINE, AIR PATH AND CYLINDER MODEL

Engine
- 4-Cylinder GDI
- Waste-gate TC
- TWC

Controller
- Fuelling
- Boost pressure: Waste-gate and throttle controlled in open and closed loop
Model Characteristics:

- Air path (IM, EM, Walls, TC, Air Cleaner, Intercooler, Fuel Tank, Catalysts etc.) elements are described in **time domain** by
  1. Mean Value approach (this study)
  2. Filling/Emptying approach
- Cylinder, ports, wall heat transfer, injector, etc. are described in **crank angle domain**
  - Single zone during gas exchange
  - Two zone during high pressure phase
- Combustion is modeled by GCA derived maps for Vibe parameters
- Pollutant Formation is modeled by surrogates taking advantage of the crank resolved cylinder (in particular in-cylinder A/F ratio)
- Port and Cylinder heat losses following Zapf and Wimmer

Mass / Species Conservation

\[
\frac{dm}{d\xi} = \frac{dt}{d\xi} \left( \sum m_{\text{j},\text{air}} + \sum m_{\text{k},\text{ads}} + m_{\text{inj}} \right) \quad \frac{dm_i}{d\xi} = \frac{1}{m} \frac{dt}{d\xi} \left( \sum m_{\text{j},\text{air}} \cdot w_{n,i-1} \right) + \sum m_{\text{j},\text{inj}} \cdot w_{n,i} + \frac{dw_C}{d\xi},
\]

Energy Conservation

\[
\frac{dT}{d\xi} = \frac{B}{m} \left[ (Q + \dot{H}) \cdot \frac{dt}{d\xi} + \left( K \cdot m - 1 \right) \cdot p \cdot \frac{dV}{d\xi} - (u + K \cdot T \cdot R \cdot m) \cdot \frac{dm}{d\xi} - m \cdot \left( K \cdot m \cdot T \cdot \frac{\partial R}{\partial w_n} + \frac{\partial u}{\partial w_n} \right) \cdot \frac{dw_n}{d\xi} \right]
\]
**NO FORMATION**

### Model Characteristics:

- **Crank-Angle resolved (physical) NO formation**
  - Based on two zone model
  - Equilibrium approach for 12 species according to De Jaeger
  - Kinetic approach for NO formation according to Zeldovich
  - Initial NO level defined by system species balances (considering NO in EGR)

- **Surrogate (data driven) NO formation**
  - Applies maps, Support Vector Machines, NNs, ... populated based on experimental data or high-fidelity simulations
  - Embedded in crank-angle resolved or surrogate engine model
PASSIVE SCALAR TRANSPORT

Model Characteristics:

- Transport of arbitrary species throughout the entire air path without influencing the flow/energy field calculation
- Addition to classic and general species transport (enable a minimum of transport equations for pollutant formation and aftertreatment)
- Arbitrary link of passive species with in-cylinder pollutant formation models and catalyst conversion models
- Arbitrary link with user-defined pollutant formation models

\[
\begin{align*}
B \cdot \frac{d\Phi}{dt} &= + \sum \dot{F}_k \\
\Phi &= \begin{bmatrix} m \\ T \\ w_A \\ w_P \end{bmatrix} \\
\dot{F} &= \begin{bmatrix} \dot{m} \\ \dot{H} \\ \dot{W}_A \\ \dot{W}_P \end{bmatrix}
\end{align*}
\]
• Non-linear Reaction-Diffusion Problem:

\[ 0 = a_{\text{trans}} \cdot \beta_k \cdot (c_k^L - c_k^B) - \sum_i v_{i,k} \cdot \dot{r}_i(c_k^L, T_s) \]

• Transient Surface Storage Balance:

\[ a_{\text{trans}} \cdot \Theta \cdot \partial_i Z_{S,j} = \sum_i v_{i,j} \cdot \dot{r}_i(Z_{S,j}, c_k^L, T) \]

• Transient Substrate Enthalpy Balance:

\[ \rho_s \cdot c_p \cdot \partial_i T_s = \partial_z (\lambda_s \cdot \partial_z T_s) - a_{\text{trans}} \cdot \alpha_h \cdot (T_s - T_g) + \sum_i \Delta h_i \cdot \dot{r}_i(c_k^L, T) + \dot{Q}_{\text{ext}} \]
ENGINE PERFORMANCE CALIBRATION
ENGINE LOAD POINT VARIATION AT 3 ISO-SPEED LINES

Comparison of simulation and experiment at selected speeds

Figures taken from SAE _2012-01-0359

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Light-Off Comparison:

- Model calibrations represent well given measurements at 3 AF-ratios

Figures taken from SAE _2012-01-0359
Result Discussion:

- Engine in HEV only runs in acceleration phases except first non-zero speed period
- HEV engine runs at higher BMEP → Higher efficiency and lower overall fuel consumption
- ICEV engine runs at low BMEP during steady-state cruising and consequently at low engine efficiencies
- HEV engine features higher effective work (integrated “positive” power) due to
  - Higher vehicle mass (~10%)
  - Efficiencies of energy transformation from mechanical to electrical and back
  - Regenerative breaking does not compensate the above energy losses
Result Discussion:

- Hybrid features significant fluctuations in exhaust mass flow and temperature
- Not fired engine pumps “cold” air and cools the catalyst (perfect control was not attempted)
- Both engines run in approximately the same lambda controlled excess air ratio window at slightly rich conditions
- Lean/rich fluctuations are buffered in the TWC by Cerium oxide
UDC SIMULATION: CONVENTIONAL VEHICLE VS. HEV ACCUMULATED ENGINE / TAILPIPE EMISSIONS

Result Discussion:

- Hybrid produces significant emission steps (due to higher load points and emission mass flows)
- Conventional vehicle features “continuous engine out emissions
- Hybrid shows shorter light-off time due to higher mass flows at the between 12s and 50s
- Conventional vehicle shows CO and HC tail pipe emissions between 150s and 200s caused by missing oxygen
- Overall conversion performance of both vehicle configurations shows no significant differences

Figures taken from SAE _2012-01-0359
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ENGINE AND VEHICLE MODEL

System engineering model assembled out library elements

**Engine**
- 4-Cylinder HSDI Diesel
- Intercooler
- Cooled EGR
- VTG turbocharger
- DOC DPF SCR

**Controller**
- Boost pressure (VTG)
- EGR
- Fuelling and smoke limitation
- idle speed
- Urea dosing

**Vehicle**
- Front Wheel Passenger Car
- Manual 6 Speed Gear Box
- ASC
- Driver
CATALYST MODEL CALIBRATION

Catalyst Model Calibration:

- Comparison with experimental data
  - Rates approaches are reasonable
- Comparison with reference model
  - Allows modeling workflow of rate approaches

- **DOC:**
  - CO, HC. Voltz approach
  - NO: reversible power-law

- **SCR:**
  - NH3 ad/desorption
  - Standard/Fast/Slow SCR reaction
  - NH3 oxidation

Figures taken from EAEC 2011_A32 | Valencia

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NEDC COLD START SIMULATION BASE LINE MODEL

NEDC with Engine Base Calibration:

- NO emissions are calculated according to Zeldovich, NO2 is estimated
- CO2, H2O, O2 N2 are calculated based on equilibrium assumption
- DPF is assumed to be non-catalytic and therefore a pure thermal inertia
- Urea-dosing control is set to provide NH3/NO ratio of 1.05

- Model matches measured data with reasonable accuracy

Figures taken from EAEC 2011_A32 | Valencia
NEDC with Modified Engine Calibration:

- EGR variation shows increasing NO emissions with decreased EGR due to higher combustion temperatures and higher O2 concentrations
- Lower EGR (0.9) shows stronger tailpipe emission deviation from base case than higher EGR (1.1)
- SOC variation show increasing NO emissions with earlier SOC due to higher combustion temperatures
- Earlier SOC (-10degCRA) shows more pronounced deviation in NO emissions that late SOC (+10degCRA)
- Earlier SOC and therefore lower engine out temperatures do additionally deteriorate the DeNOx performance in the exhaust line
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SUMMARY AND CONCLUSIONS

- A system engineering simulation model is presented covering the areas vehicle (1), engine (2) and cooling (3) and control (4)
- Dedicated numerical techniques are applied to ensure fast (RT) running models
- The models are configured out of standard and custom components
- System engineering simulation is a promising approach to address current and future challenges in the area of
  - In-use emission compliance
  - HiL based function calibration