EXHAUST AFTERTREATMENT IN THE FRAMEWORK OF SYSTEM ENGINEERING SIMULATION

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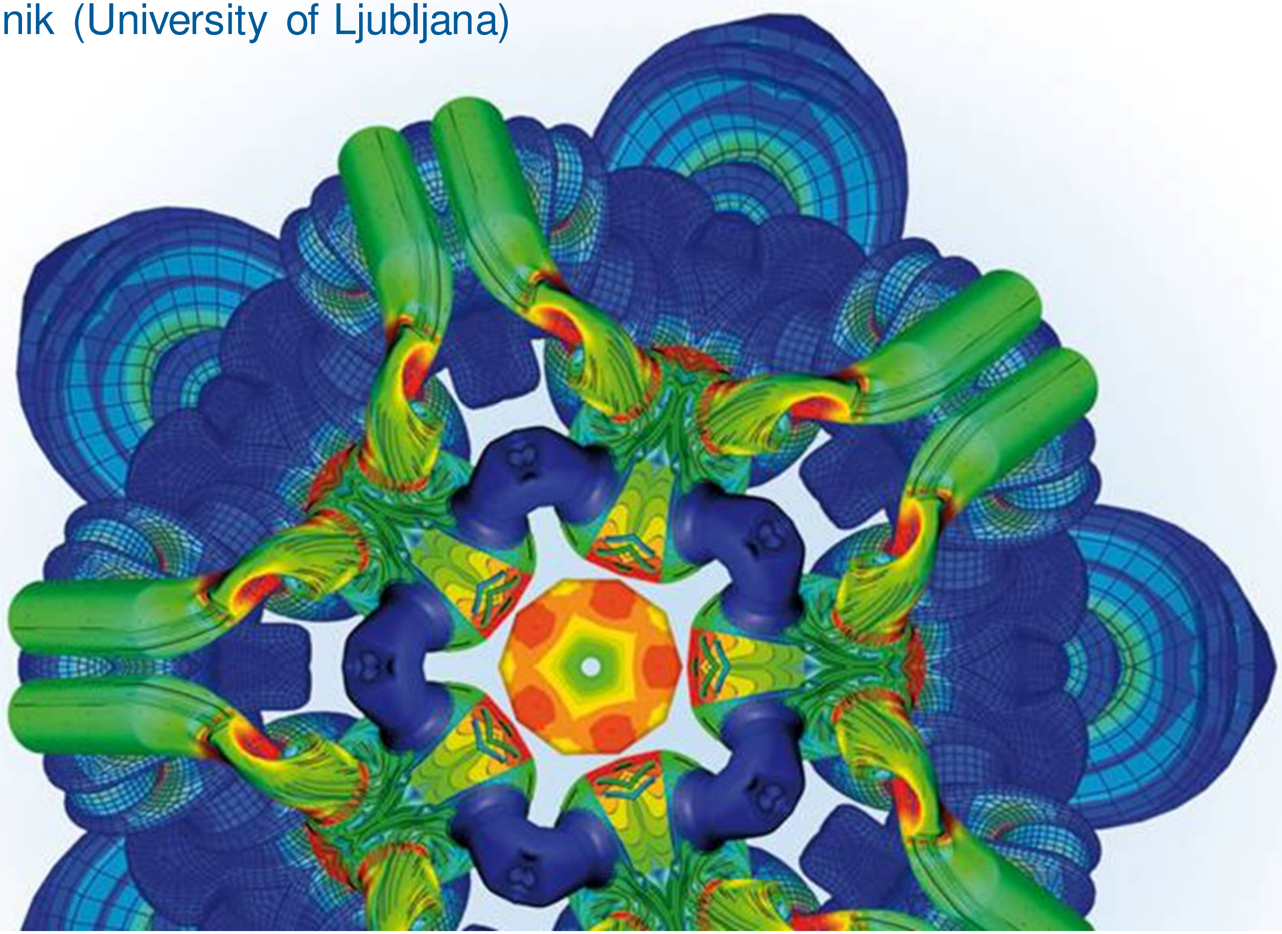
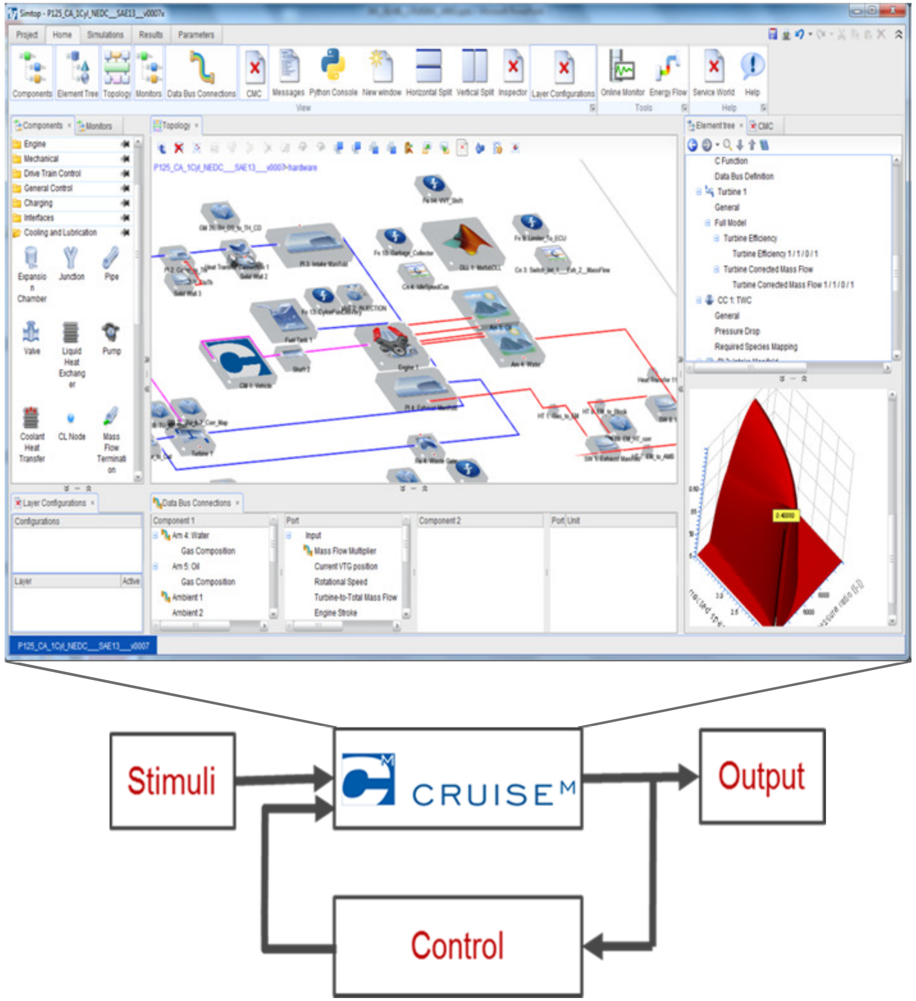


OVERVIEW

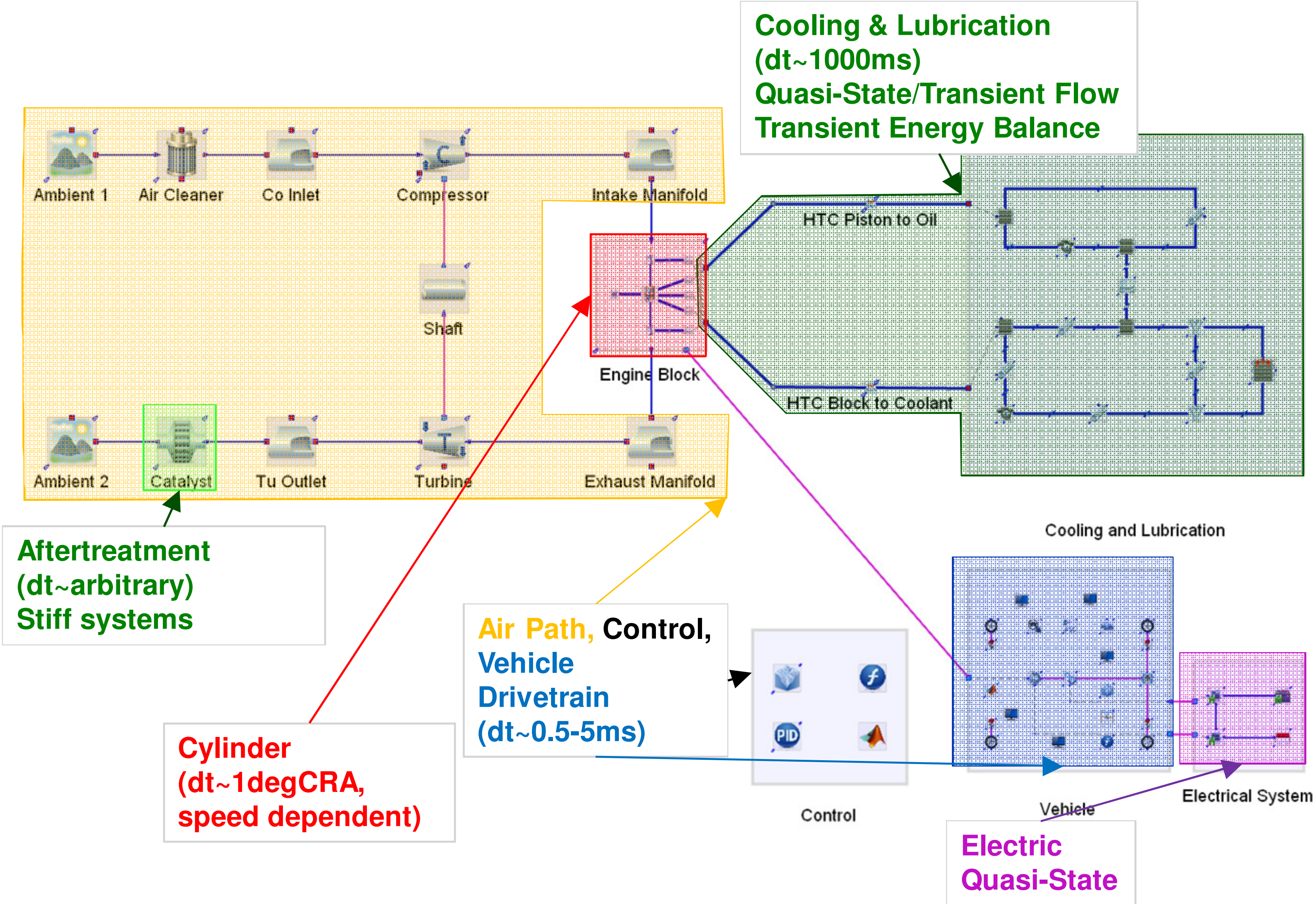
- System Engineering Simulation
  - Requirements
  - Functionalities
- Simulation Examples
  - TGDI Engine in Hybrid Passenger Car
  - HSDI Diesel Engine in Conventional Passenger Car
- Summary/Conclusions

REQUIREMENTS ON SYSTEM ENGINEERING SIMULATION SUPPORTING AND CONCEPT DESIGN AND CALIBRATION

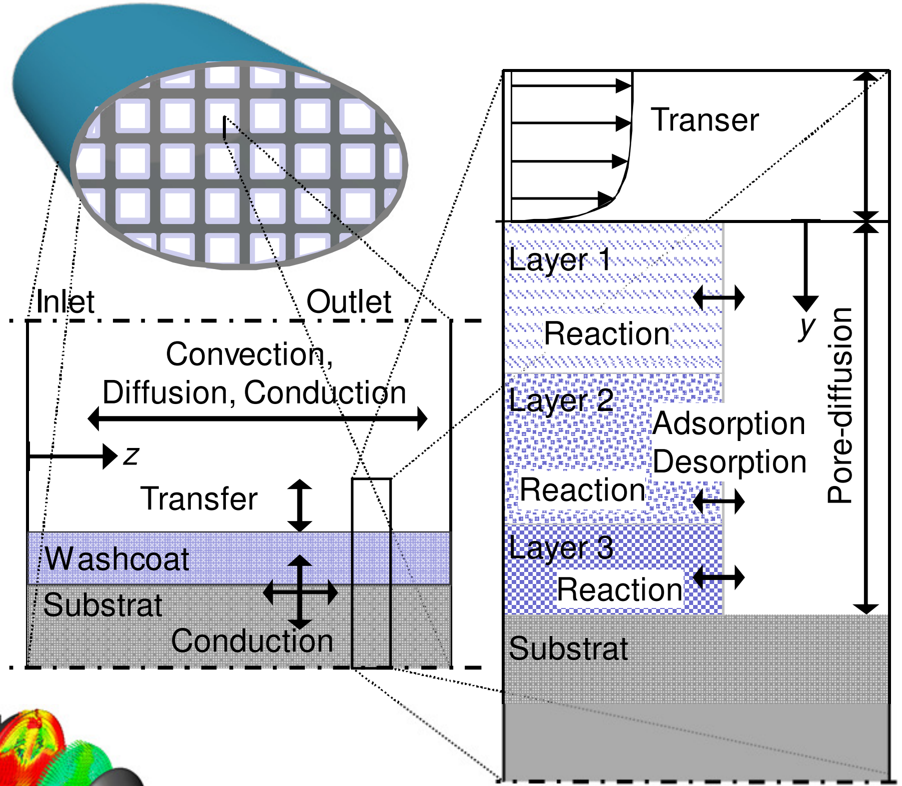


- **Multi-physical system simulation**
  → Dedicated models and solvers for all vehicle domains (engine, cooling, drivetrain, e-system)
- **Consistent plant modelling**
  → Links development teams from concept to calibration phase
- **Scalable physical modelling depth**
  → Right balance of predictability 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



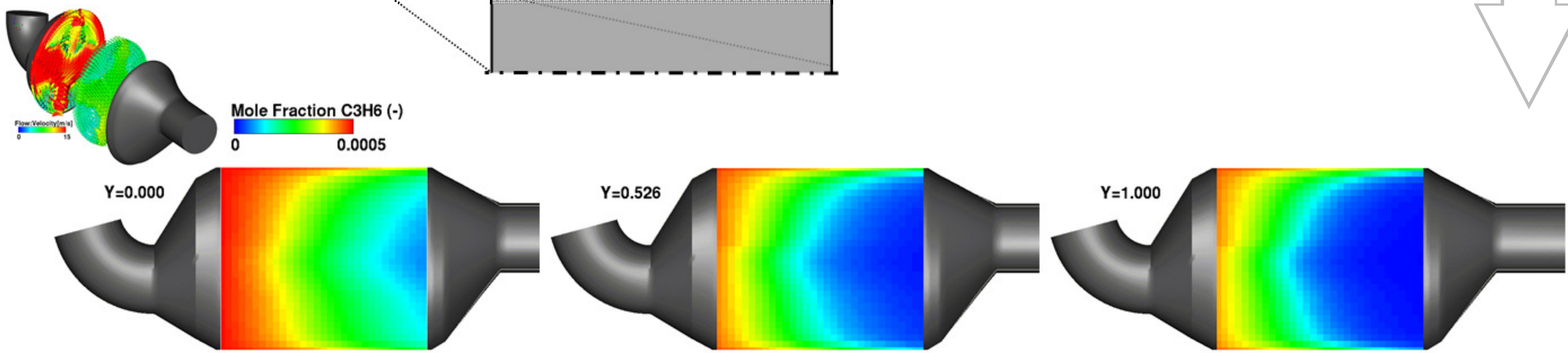
CONSISTANT PLANT MODELING
SCALABLE PHYSICAL MODELING DEPTH



Modeling Approaches

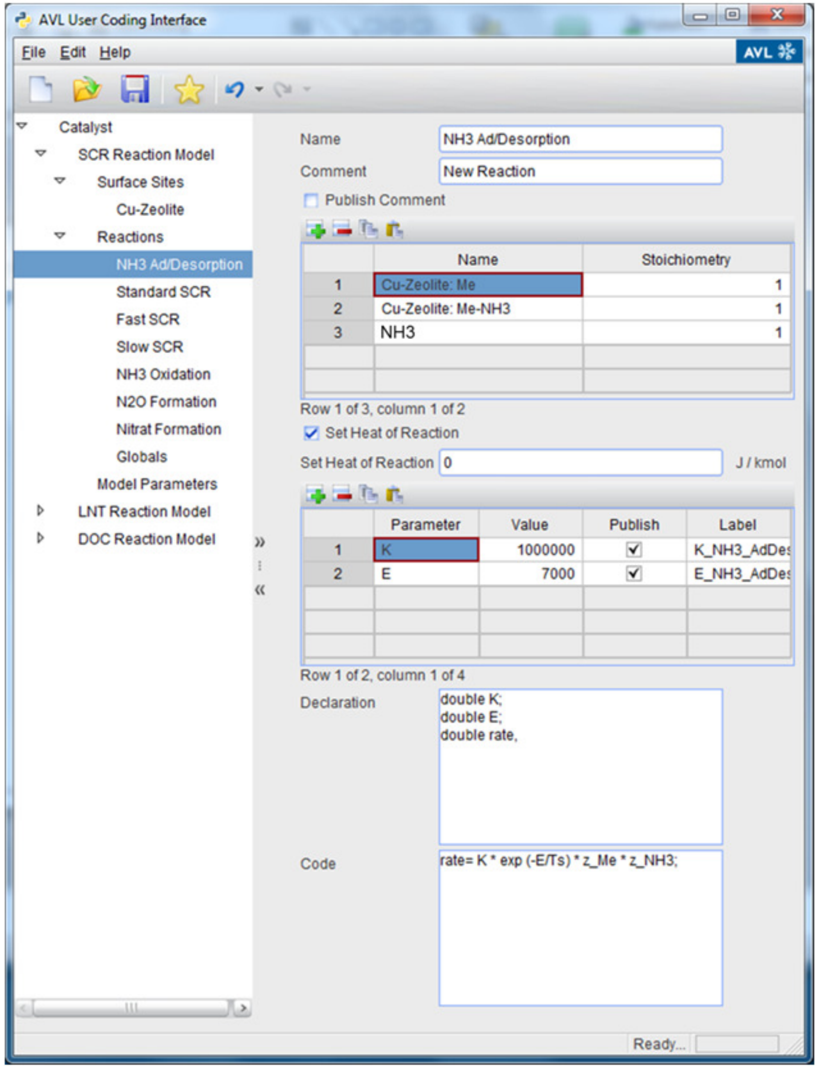
- Map Based:
  (e.g. conv=f(Temp., [educt])
- Surrogate modeling:
  (multidimensional input space)
- Physical, transient 1D/3D two-phase model
- Physical, transient 1D/3D two-phase model including 1D reaction diffusion modeling in arbitrary washcoat layers

Modeling Depth



Figures taken from SAE _2012-01-1296

FLEXIBLE MODEL CUSTOMIZATION
GRAPHICALLY SUPPORTED REACTION DESIGN



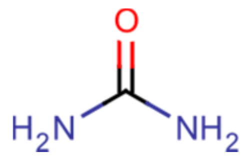
AVL User Coding Interface

- 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[M])

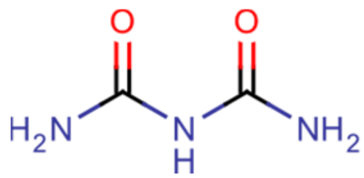
FLEXIBLE MODEL CUSTOMIZATION
EXAMPLE: UREA DECOMPOSITION APPROACH

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



urea
CH_4N_2O



biuret
$C_2H_5N_3O_2$

cyanuric acid
$C_3H_3N_3O_3$

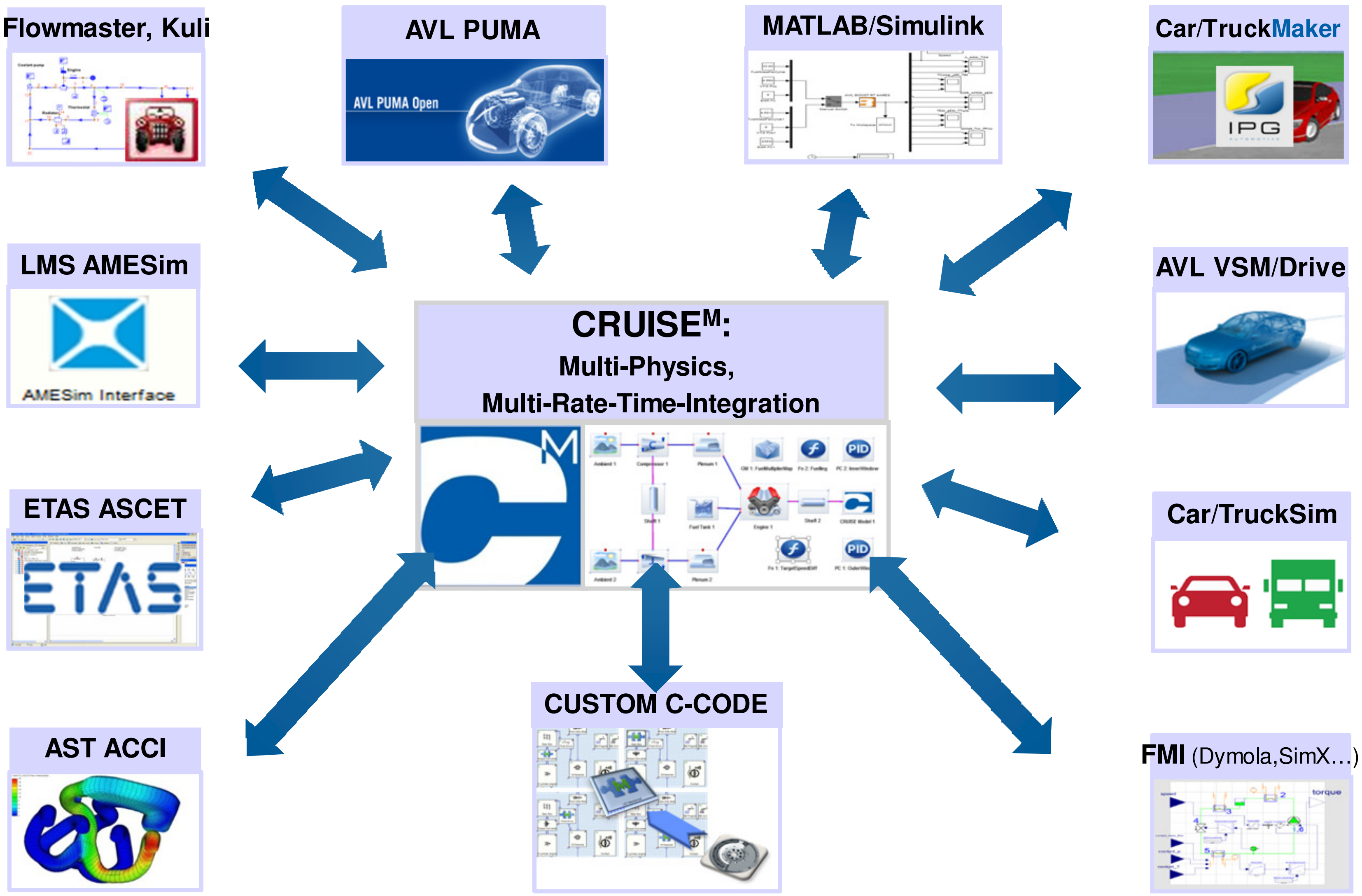
ammelide
$C_3H_4N_4O_2$

F: formation reaction
D: decomposition reaction

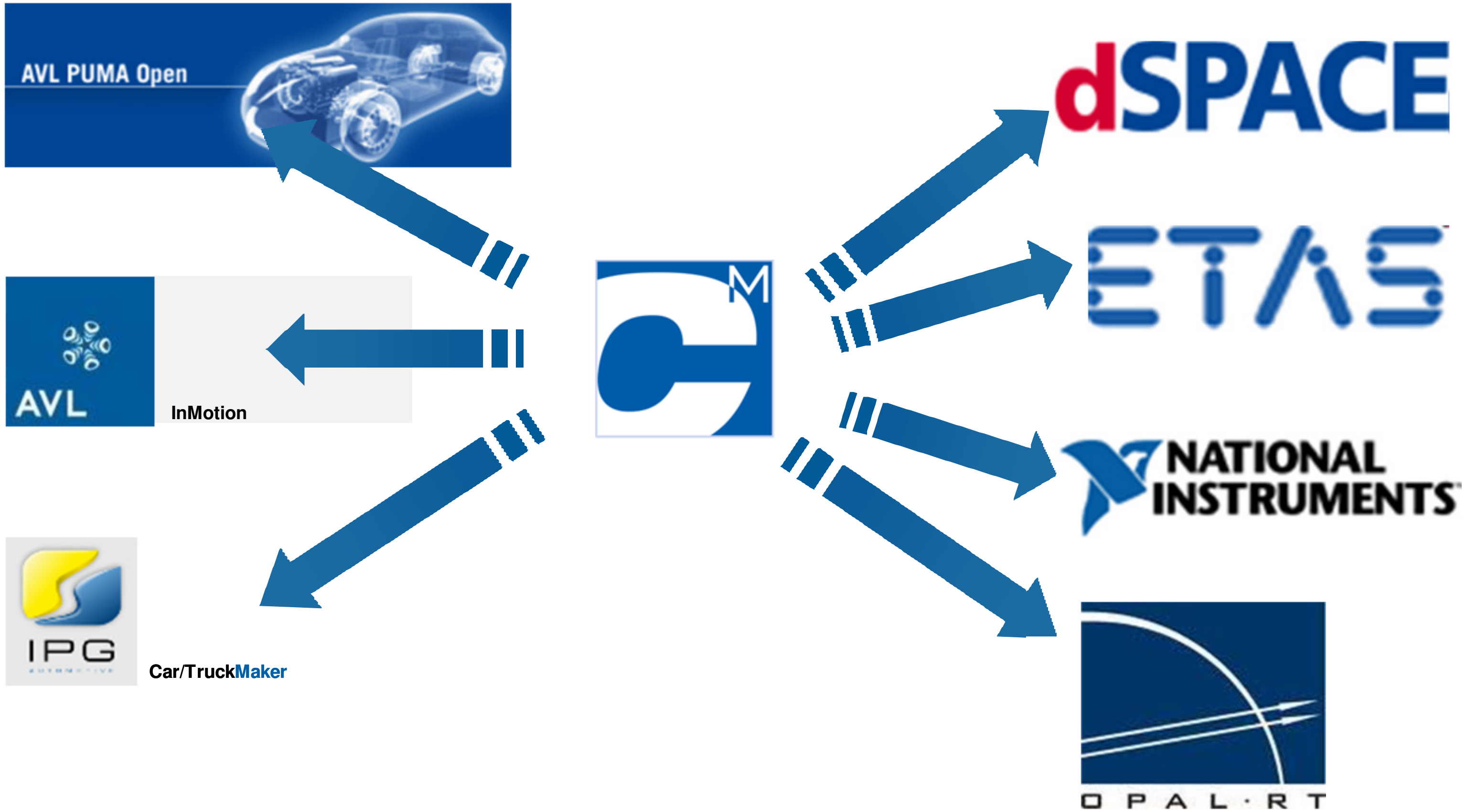
$$\dot{r}' = A\cdot e^{\wedge}\left(-\frac{T_A}{T_s}\right)\cdot\prod_j\left(Z_j{}^{\wedge}v_j\right)\cdot\Gamma/1000\cdot\left(\sum_k Z_k^{init}\cdot\sigma_k\right)^{\wedge}\left(1-\sum_j v_j\right)$$

Ebrahimian, V.: “Development of multi-component evaporation models and 3D modeling of NOx-SCR reduction system”, PhD thesis, L‘Universitè de Toulouse, 2011

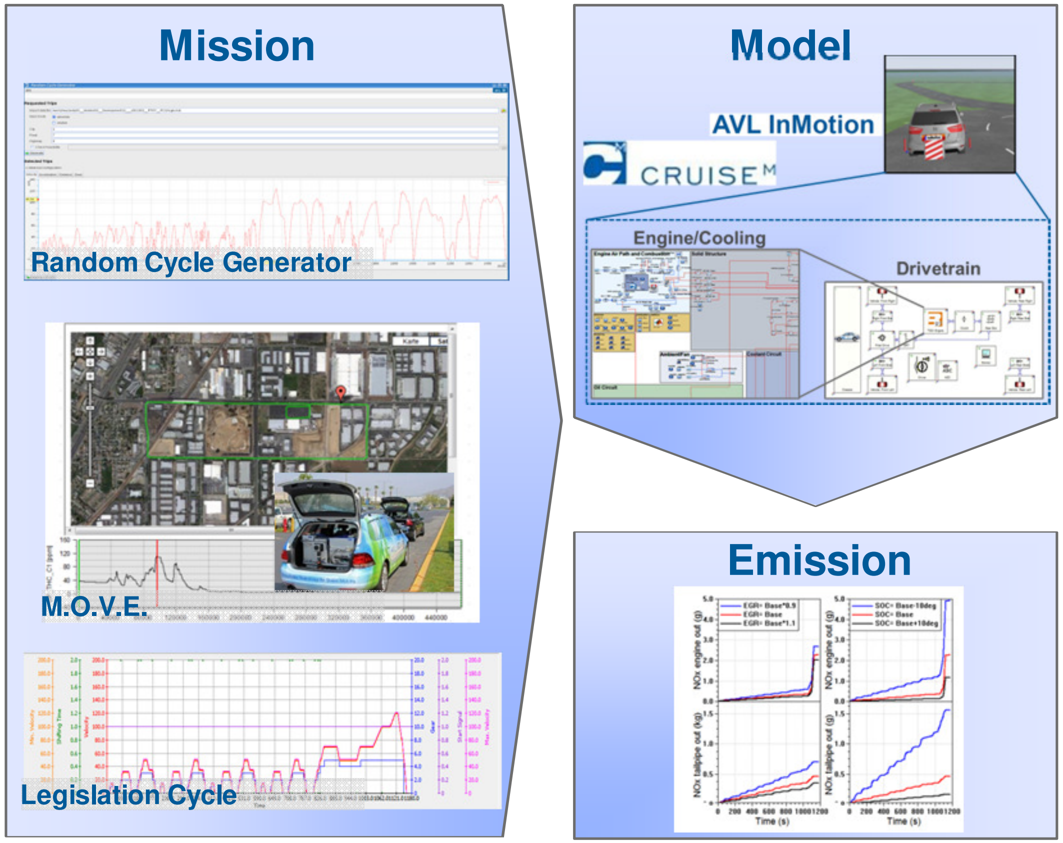
OPEN INTERFACE IN OFFICE APPLICATION



OPEN INTERFACE IN HIL APPLICATION



REAL-LIFE EMISSIONS IN OFFICE SIMULATION



Mission compilation out of various sources

- Radom-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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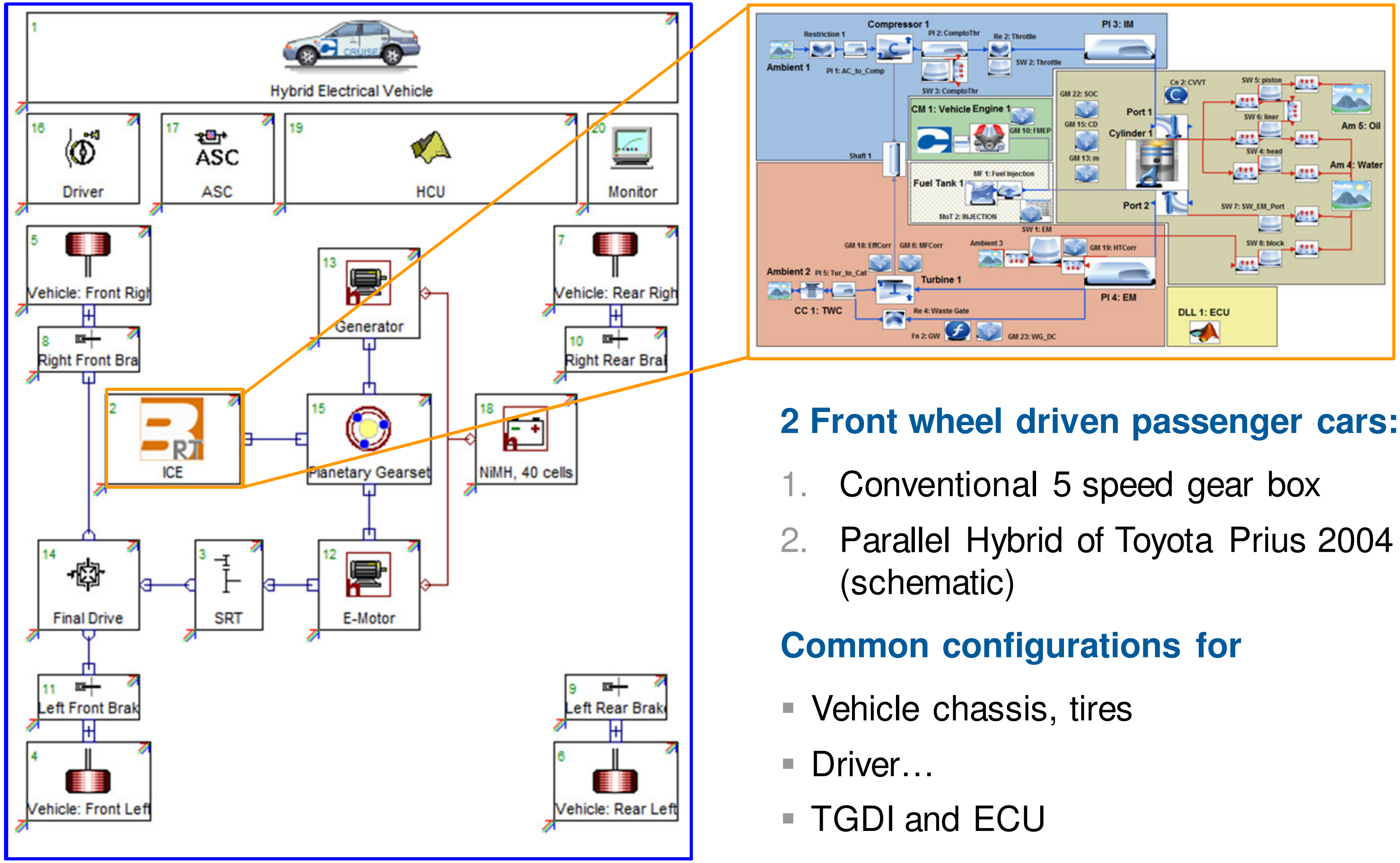
VEHICLE, ENGINE AND CONTROL



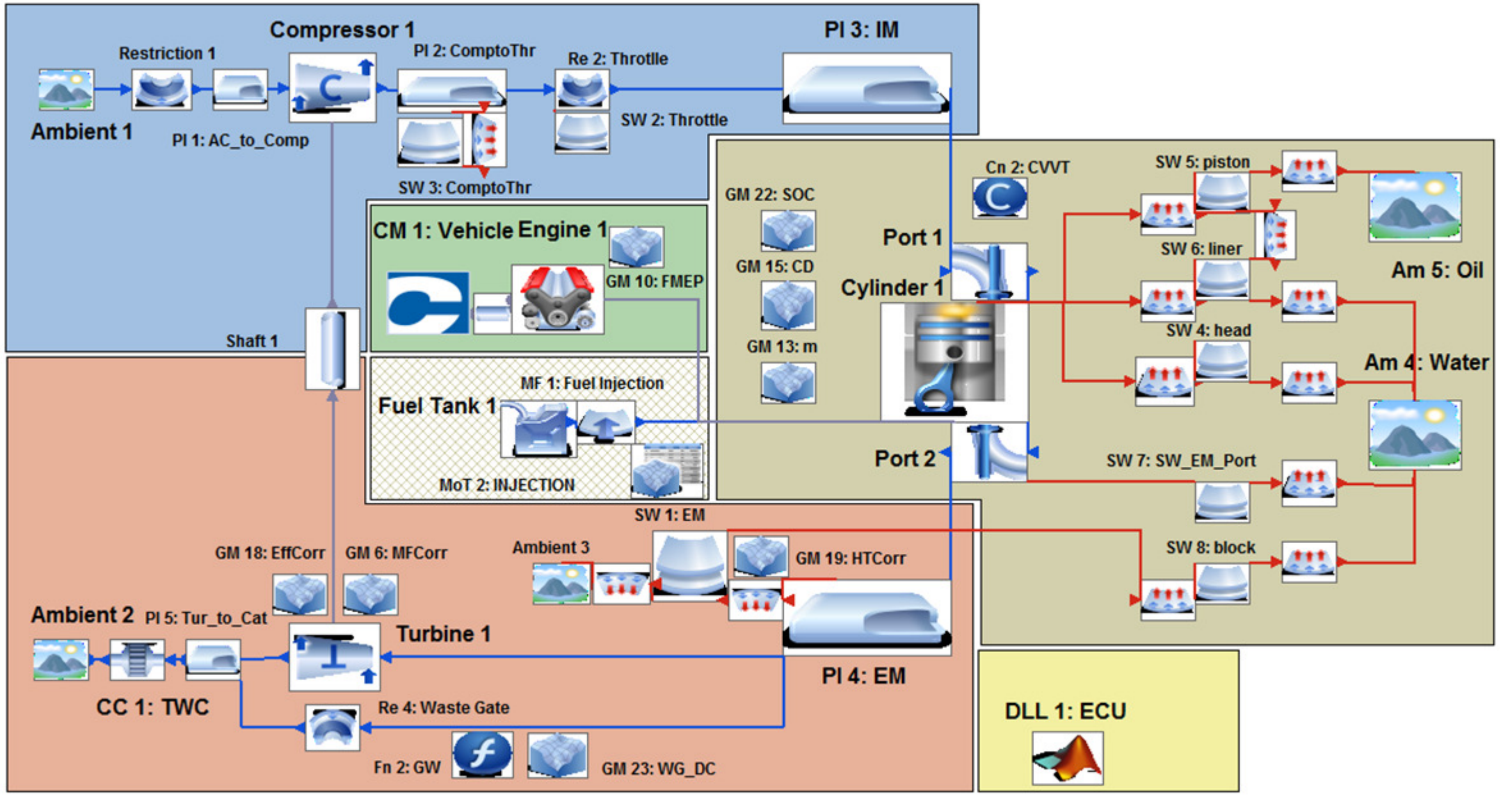
2 Front wheel driven passenger cars:

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



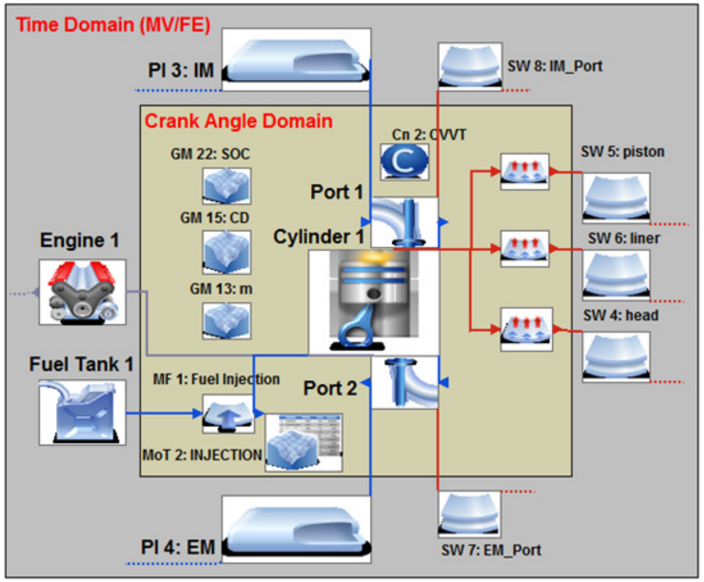
Engine

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

Controller

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

CYLINDER, COMBUSTION AND POLLUTANT FORMATION



Mass / Species Conservation

$$\frac{dm}{d\xi} = \frac{dt}{d\xi}\cdot\left(\sum \dot{m}_{j,us} + \sum \dot{m}_{k,ds} + \dot{m}_{inj}\right)$$

$$\frac{dw_n}{d\xi} = \frac{1}{m}\cdot\frac{dt}{d\xi}\cdot\left(\sum \dot{m}_{j,us}\cdot w_{n,i-1} + \sum \dot{m}_{j,us}\cdot w_{n,i}\right) + \dot{m}_{inj}\cdot w_{inj}, + \frac{dw_C}{d\xi},$$

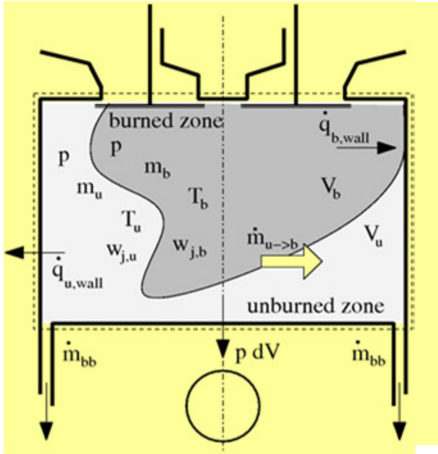
Energy Conservation

$$\frac{dT}{d\xi} = \frac{B}{m}\cdot\left[\left(\dot{Q}+\dot{H}\right)\cdot\frac{dt}{d\xi} + (K\cdot m - 1)\cdot p\cdot\frac{dV}{d\xi} - (u + K\cdot T\cdot R\cdot m)\cdot\frac{dm}{d\xi} - m\cdot\left(K\cdot m\cdot T\cdot\frac{\partial R}{\partial w_n} + \frac{\partial u}{\partial w_n}\right)\cdot\frac{dw_n}{d\xi}\right]$$

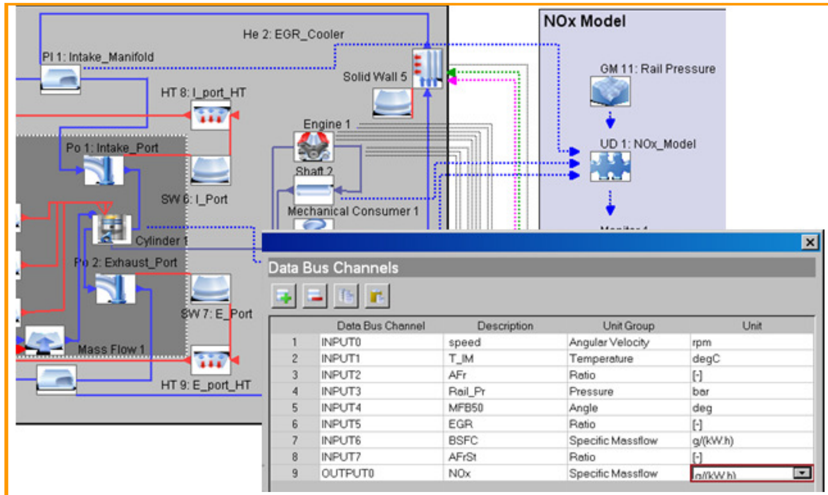
Model Characteristics:

- Air path (IM, EM, Walls, TC, Air Cleaner, Intercooler, Fuel Tank, Catalysts etc.) elements are descripted 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

NO FORMATION



R1	$N2 + O = NO + N$
R2	$O2 + N = NO + O$
R3	$N + OH = NO + H$
R4	$N2O + O = NO + NO$
R5	$O2 + N2 = N2O + O$
R6	$OH + N2 = N2O + H$

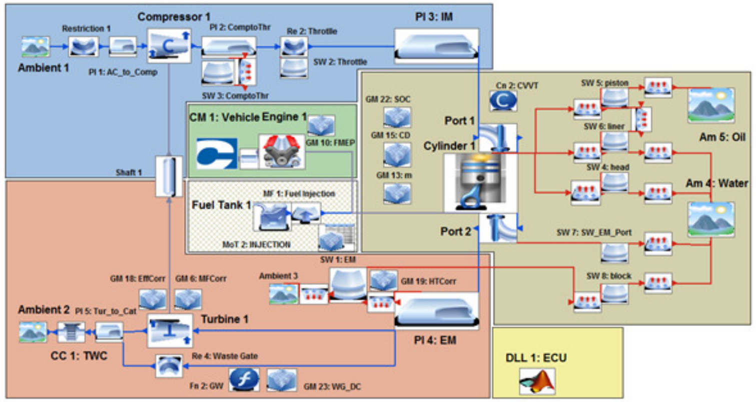


	Data Bus Channel	Description	Unit Group	Unit
1	INPUT0	speed	Angular Velocity	rpm
2	INPUT1	T_IM	Temperature	degC
3	INPUT2	AFr	Ratio	[-]
4	INPUT3	Rail_Pr	Pressure	bar
5	INPUT4	MFB50	Angle	deg
6	INPUT5	EGR	Ratio	[-]
7	INPUT6	BSFC	Specific Massflow	g/(kW.h)
8	INPUT7	AFrSt	Ratio	[-]
9	OUTPUT0	NOx	Specific Massflow	g/(kW.h)

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



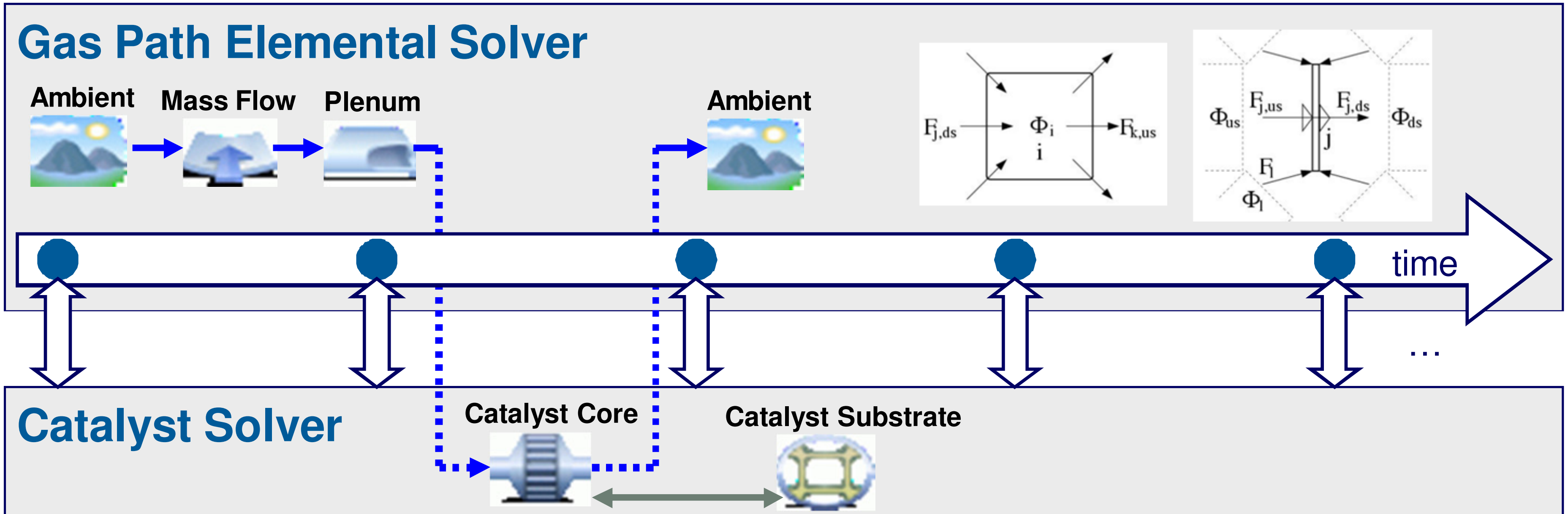
$$\mathbf{B}\cdot\frac{\mathrm{d}\boldsymbol{\Phi}}{\mathrm{d}t}=+\sum\dot{\mathbf{F}}_{\mathrm{k}}$$

$$\boldsymbol{\Phi}=\begin{bmatrix} m \\ T \\ \mathbf{w}_{\mathrm{A}} \\ \mathbf{w}_{\mathrm{P}} \end{bmatrix} \qquad \dot{\mathbf{F}}=\begin{bmatrix} \dot{m} \\ \dot{H} \\ \dot{\mathbf{W}}_{\mathrm{A}} \\ \dot{\mathbf{W}}_{\mathrm{P}} \end{bmatrix}$$

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

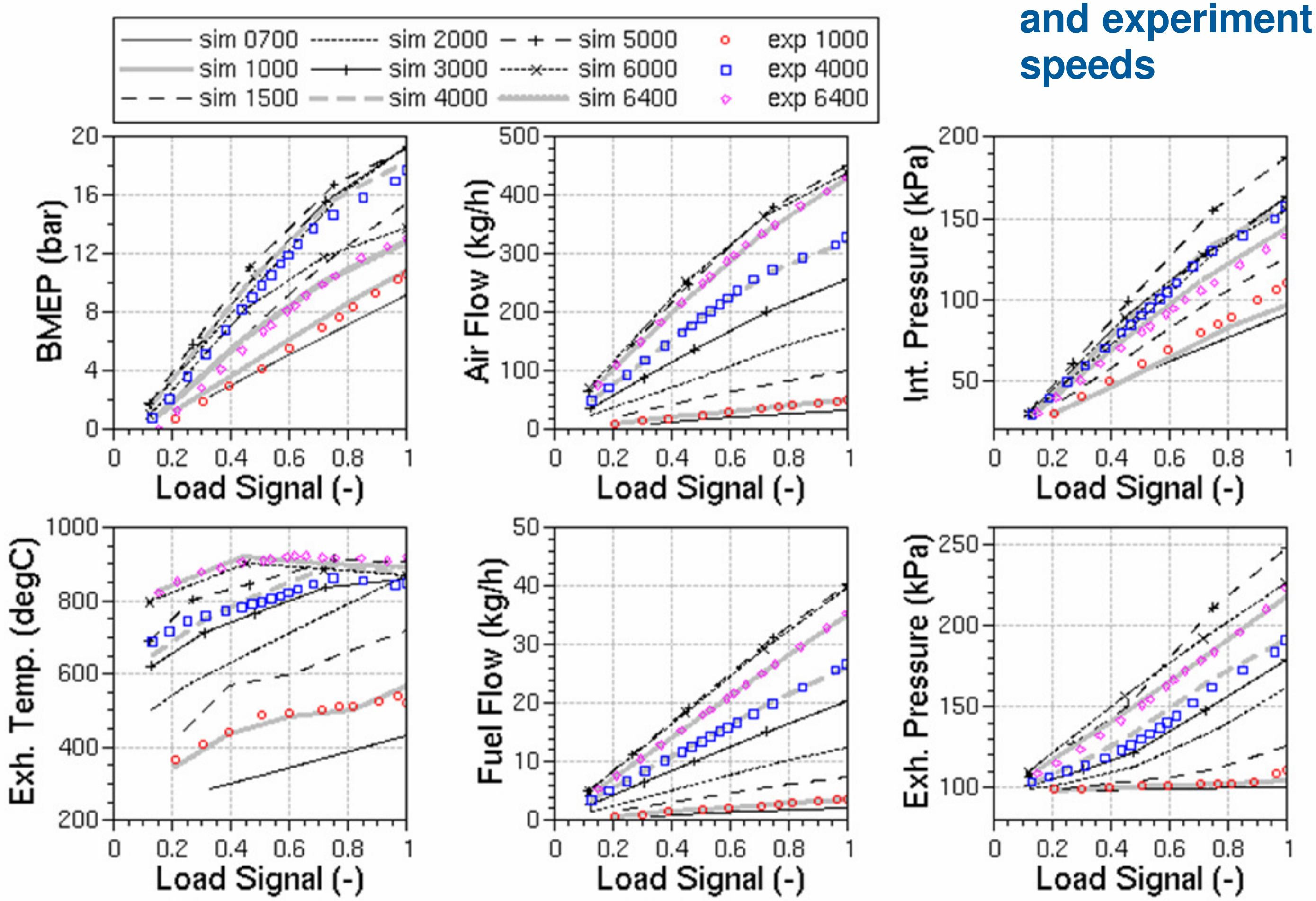
CATALYST AIR PATH BINDING



- Non-linear Reaction-Diffusion Problem: $0 = a_{trans}\cdot\beta_k\cdot\left(c_k^L - c_k^B\right) - \sum_i^I \nu_{i,k}\cdot\dot{r}_i\left(c_k^L, T_s\right)$
- Transient Surface Storage Balance: $a_{trans}\cdot\Theta\cdot\partial_t Z_{S,j} = \sum_i^I \nu_{i,j}\cdot\dot{r}_i\left(Z_{S,j}, c_k^L, T_s\right)$
- Transient Substrate Enthalpy Balance: $\rho_s\cdot c_{p,s}\cdot\partial_t T_s = \partial_z\left(\lambda_s\cdot\partial_z T_s\right) - a_{trans}\cdot\alpha_h\cdot\left(T_s - T_g\right) + \sum_i^I \Delta h_i\cdot\dot{r}_i\left(c_k^L, T_s\right) + \dot{Q}_{ext}$

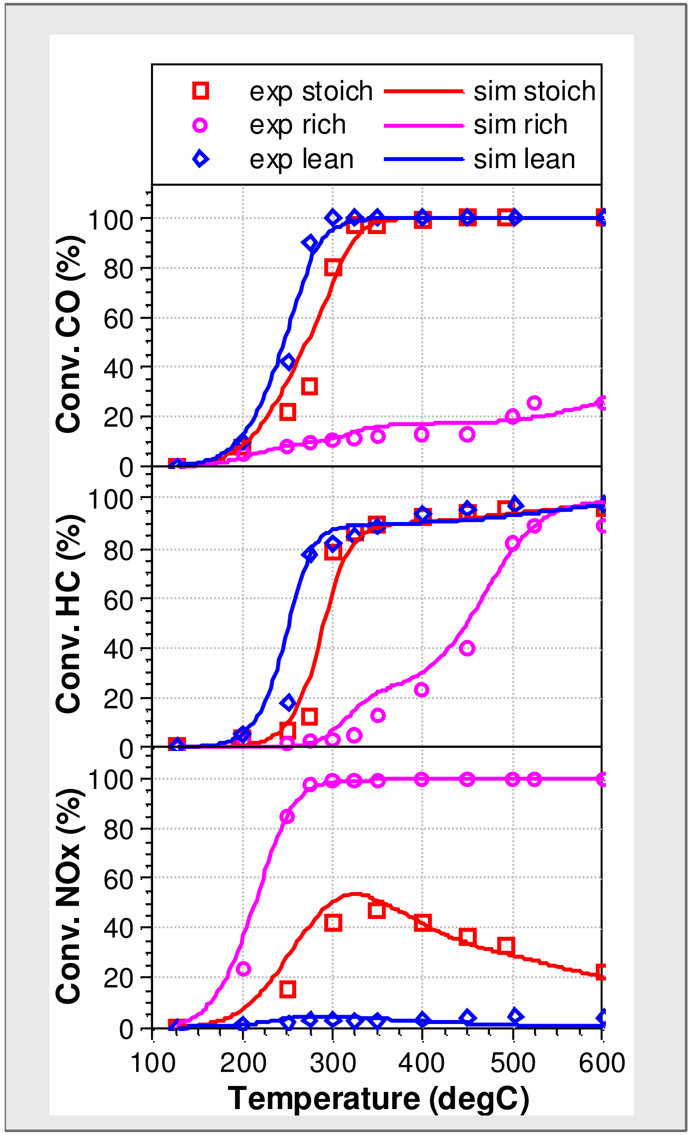
ENGINE PERFORMANCE CALIBRATION
ENGINE LOAD POINT VARIATION AT 3 ISO-SPEED LINES

Comparison of simulation and experiment at selected speeds



Figures taken from SAE _2012-01-0359

TWC CALIBRATION



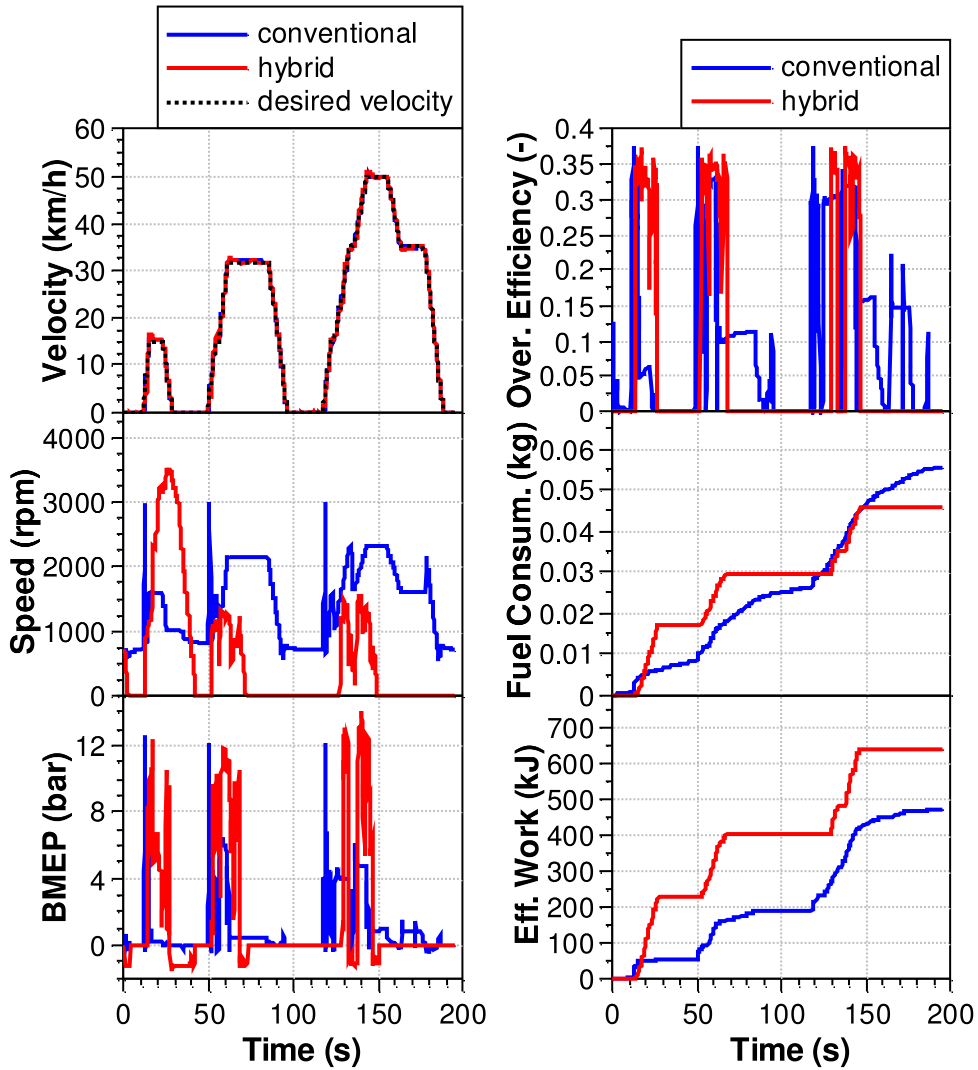
Figures taken from SAE _2012-01-0359

Light-Off Comparison:

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

- ☑ R1: $CO + {}^1\!/_2 O_2 \longrightarrow CO_2$
- ☑ R2: $C_3H_6 + {}^9\!/_2 O_2 \longrightarrow 3CO_2 + 3H_2O$
- ☑ R3: $2CO + 2NO \longrightarrow 2CO_2 + N_2$
- ☐ R4: $H_2 + {}^1\!/_2 O_2 \longrightarrow H_2O$
- ☑ R5: $2NO + O_2 \longleftrightarrow 2NO_2$
- ☑ R6: $CO + H_2O \longleftrightarrow CO_2 + H_2$
- ☑ R7: $C_3H_8 + 5O_2 \longrightarrow 3CO_2 + 4H_2O$
- ☑ R8: $C_3H_6 + 3H_2O \longleftrightarrow 3CO + 6H_2$
- ☑ R9: $C_3H_8 + 3H_2O \longleftrightarrow 3CO + 7H_2$
- ☑ R10: $Ce_2O_3 + {}^1\!/_2 O_2 \longrightarrow 2CeO_2$
- ☑ R11: $2CeO_2 + CO \longrightarrow Ce_2O_3 + CO_2$
- ☑ R12: $12CeO_2 + C_3H_6 \longrightarrow 6Ce_2O_3 + 3CO + 3H_2O$
- ☑ R13: $14CeO_2 + C_3H_8 \longrightarrow 7Ce_2O_3 + 3CO + 4H_2O$

UDC SIMULATION: CONVENTIONAL VEHICLE VS. HEV PERFORMANCE AND FUEL CONSUMPTION

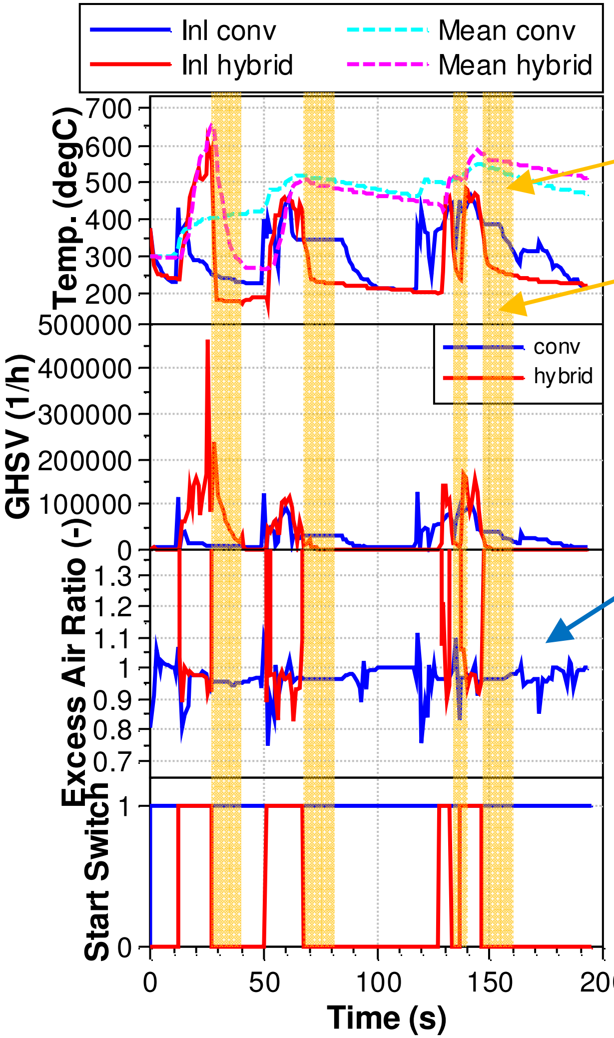


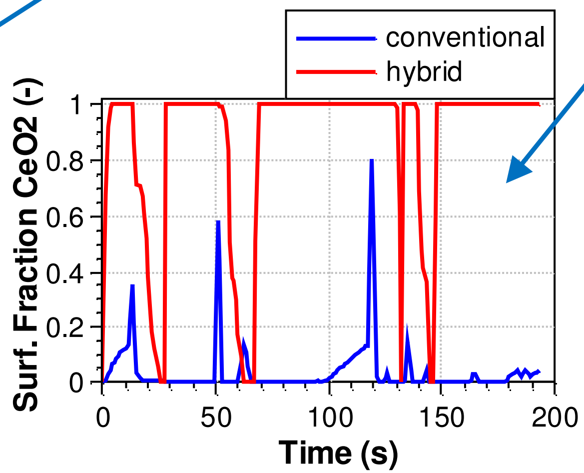
Figures taken from SAE _2012-01-0359

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

UDC SIMULATION: CONVENTIONAL VEHICLE VS. HEV ENGINE OUT / TWC INLET



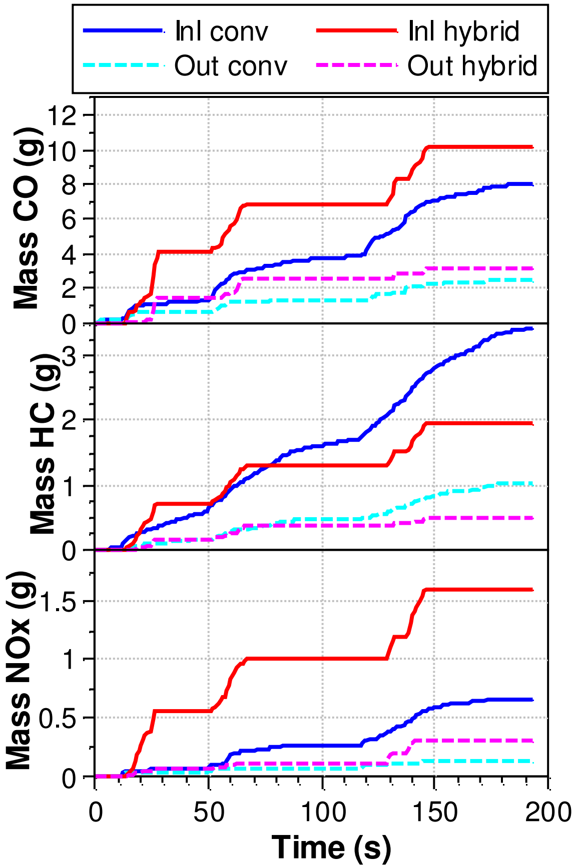


Result Discussion:

- 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

Figures taken from SAE _2012-01-0359

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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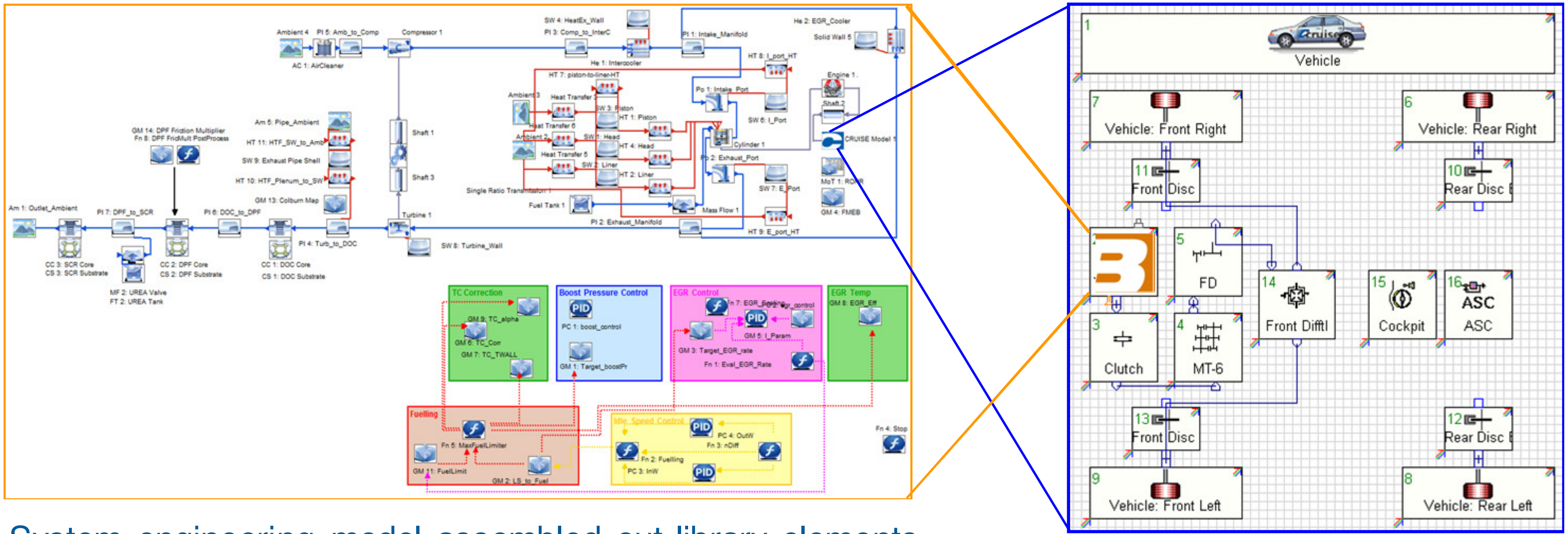
ENGINE AND VEHICLE MODEL



System engineering model assembled out library elements

Engine

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

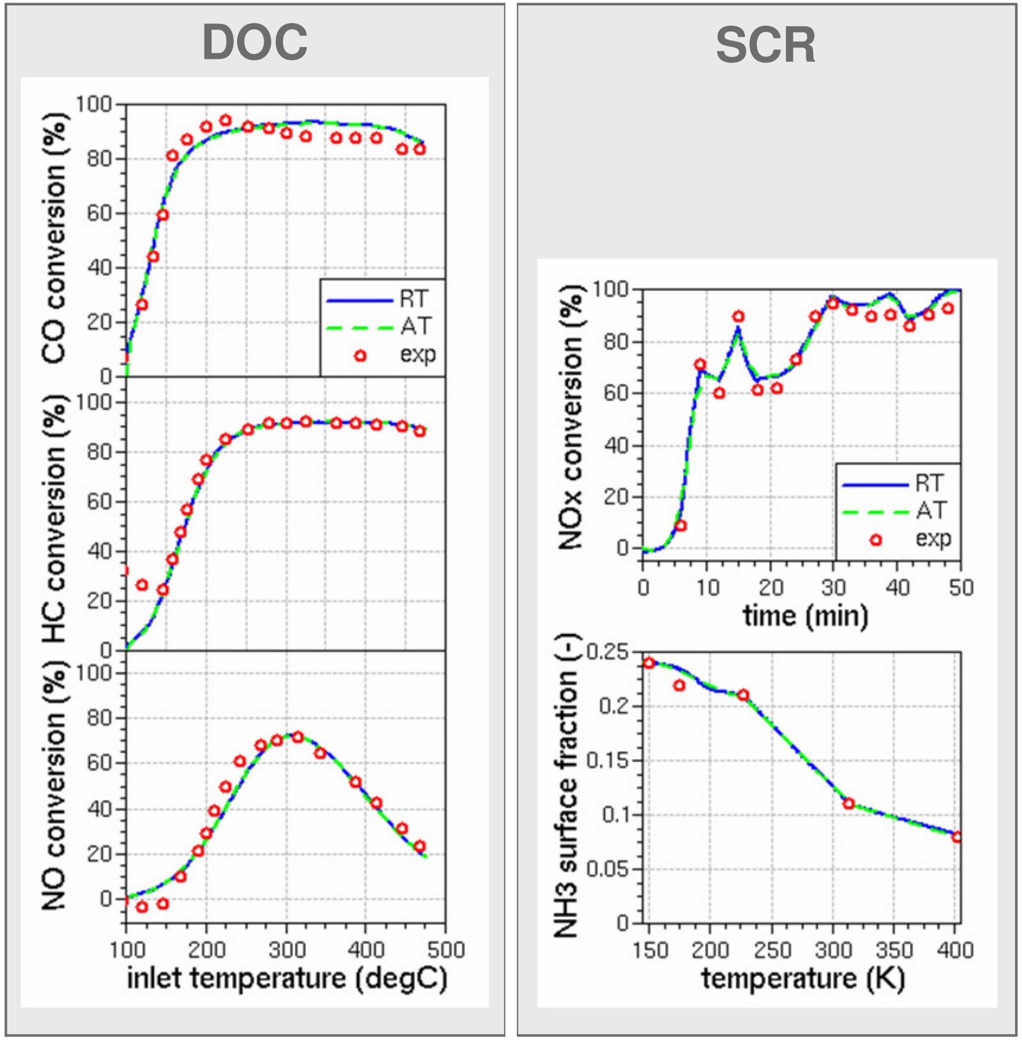
Controller

- 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

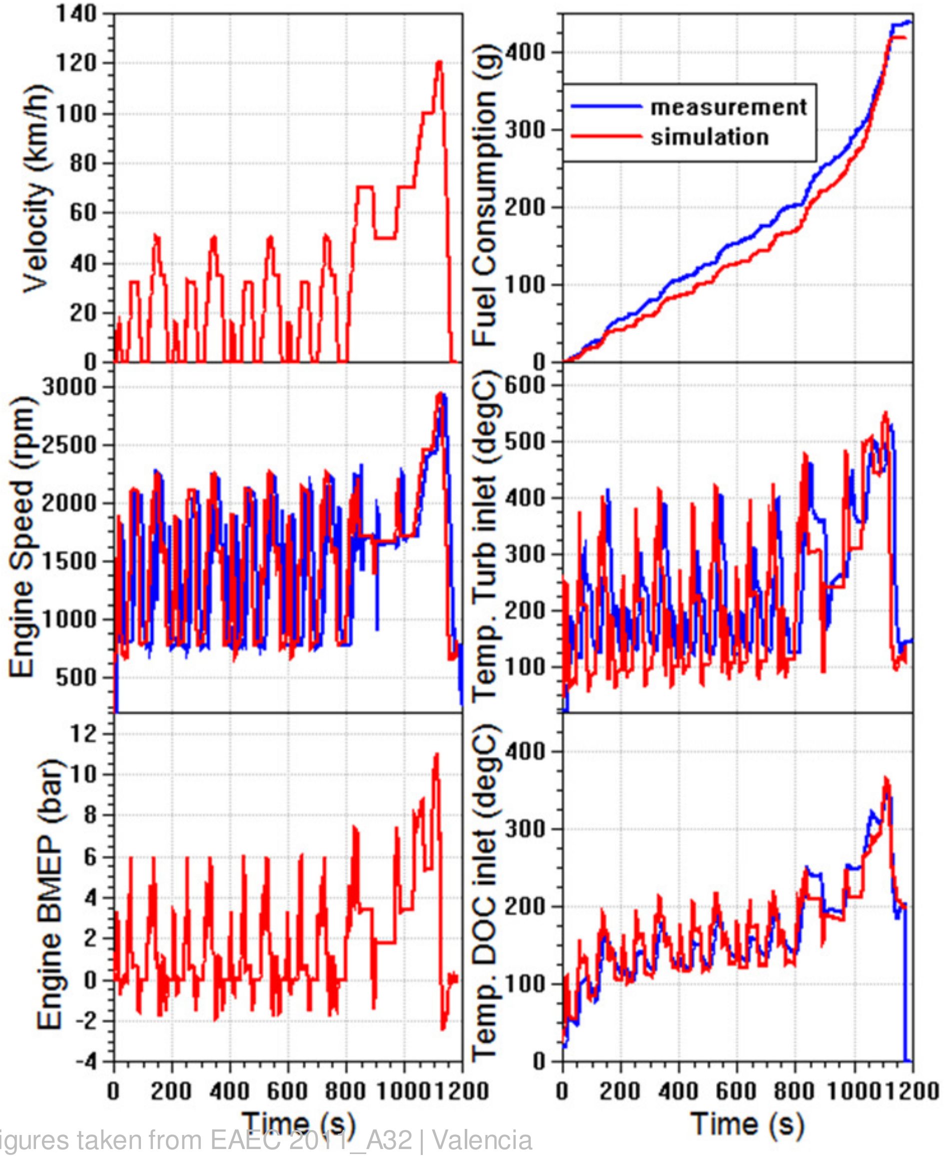


Catalyst Model Calibration:

- 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

NEDC COLD START SIMULATION BASE LINE MODEL

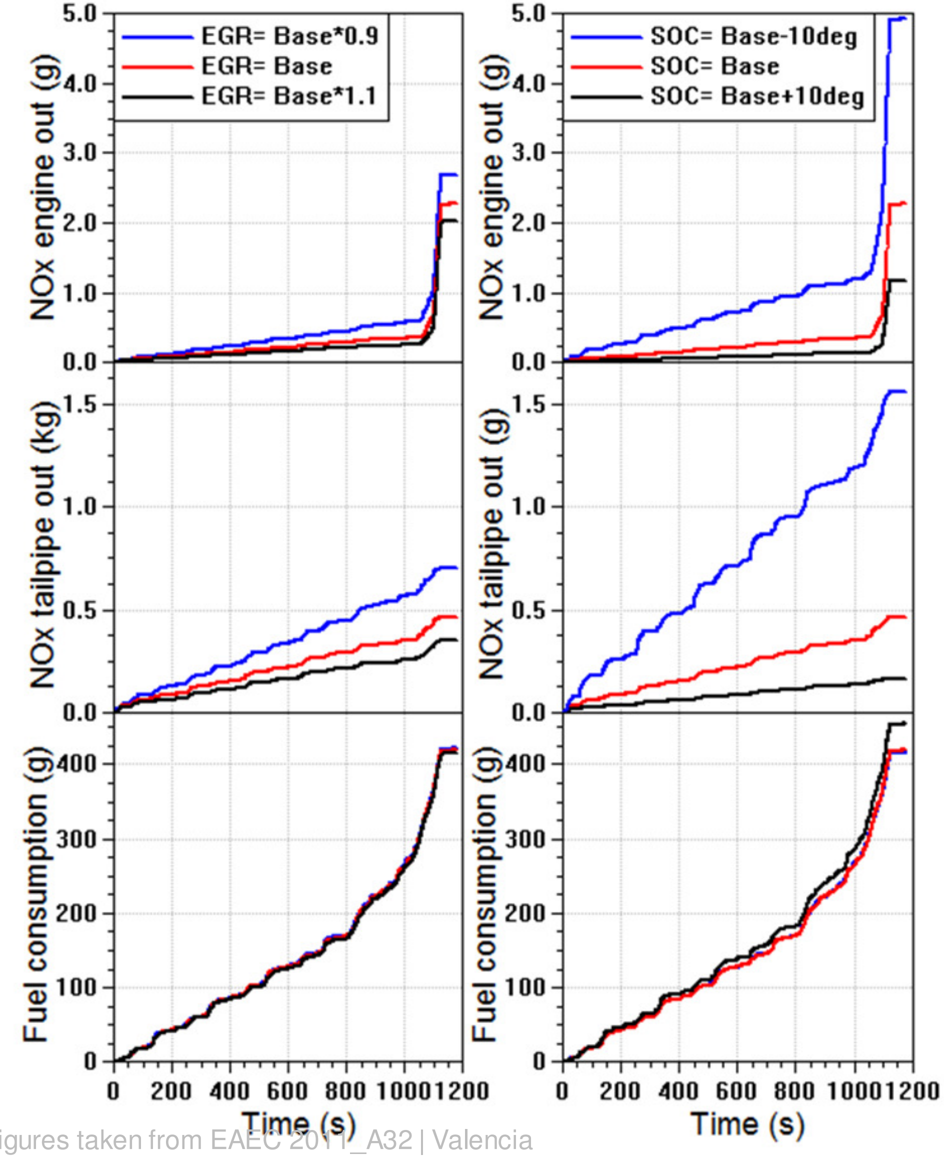


Figures taken from EAEC 2011_A32 | Valencia

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

NEDC COLD START SIMULATION ENGINE CONTROL VARIATIONS



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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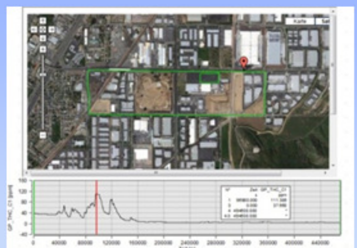
SUMMARY AND CONCLUSIONS



- 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