# *Engine/Vehicle Systems Simulation as a Platform for Aftertreatment Modeling*

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Gamma Technologies

**Fourth and Fifth DOE Crosscut Workshop on Lean Emissions Reduction Simulation**

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# *Three Test Cases Using Traditional User Models*

- Modeling HCCI Combustion

  Luca Montorsi, University of Modena

- Modeling DPF-SCR for Heavy Duty Disel Engine

  John Kasab, Scania

- Aftertreatment Modeling Using Bistro™/GT-Power

  Robert Weber, TIAX/ADL

# MODELING HCCI COMBUSTION

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# 1-D CFD code – kinetic code interface

**1-D fluid-dynamics code:**

**GT-Power**

- In-Cylinder Processes (except Combustion)
- Injection system
- Turbocharger
- Waste-gate valve
- Intercooler
- EGR system

Control strategies

**Detailed kinetic code:**

**Combustion Code**

**(Lund Institute of Technology)**

- Chemical reactions occurring during combustion
- Ignition delay
- Combustion heat release
- Engine emissions

# 1-D CFD code – kinetic code interface

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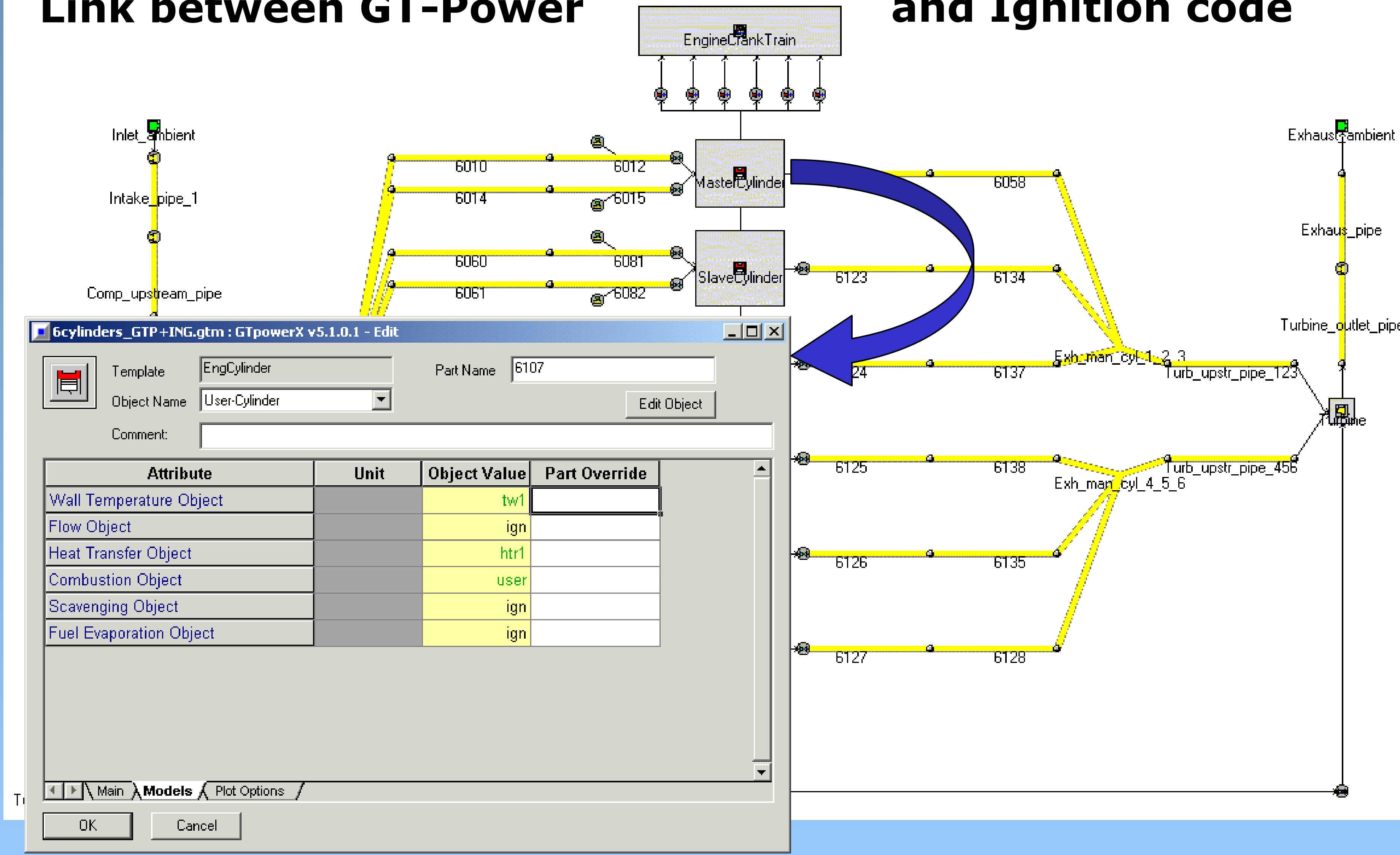
## Link between GT-Power and Ignition code



# 1-D CFD code – kinetic code interface

- **Cylinder's number, cycle's number**
- **Current crank angle degree, time step size**
- **Current in cylinder pressure and temperature values**
- **Air and fuel mass trapped into the cylinder**
- **User parameters**

**GT-Power**

***At every GT-Power time step***

**Combustion Model**

- **Ignition crank angle degree**
- **Burned fuel mass during the current time step**
- **Combustion end crank angle degree**
-

**The mass fractions of the in cylinder mixture components are stored in an external file**

**At every Ignition Code time step**

# Combustion Model

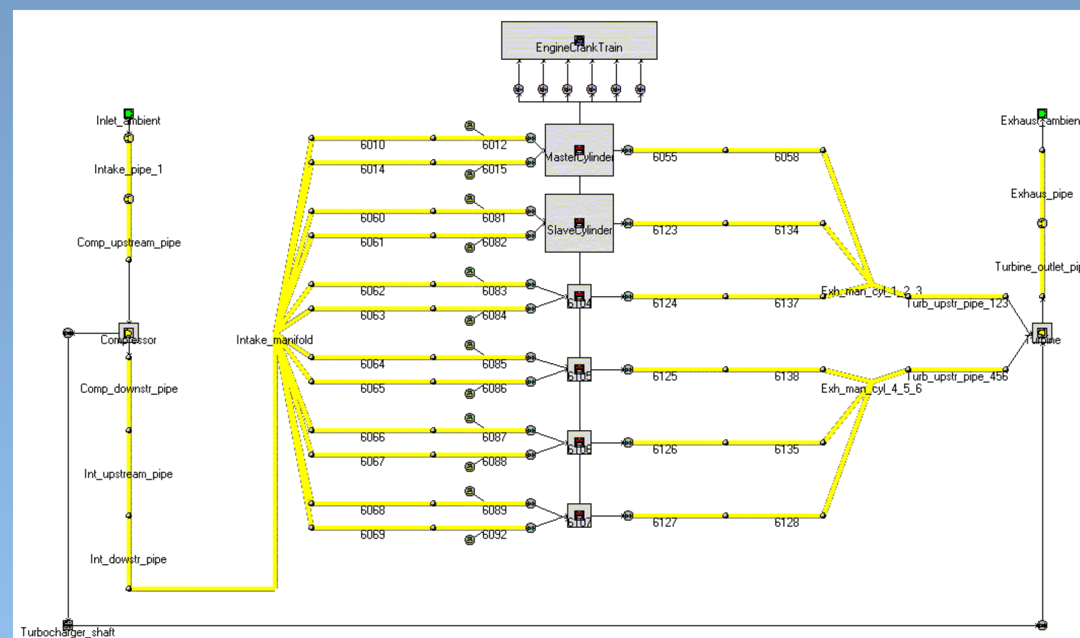
- **Combustion Model Contained 141 Species and 1405 Reactions (Yetter et al.)**
- **Formaldehyde Chemistry is based on work of Amneus et al.**
- **C2-C5 Chemistry Mostly Originated From the Work Of Warnatz and Baulch et al.**
- **C6-C8 Chemistry Developed According to Curran et al.**
- **A Simplied Scheme is used for low-temperature Chemistry (ASME 2002-ICE-457)**

# Test case

## SCANIA DSC12

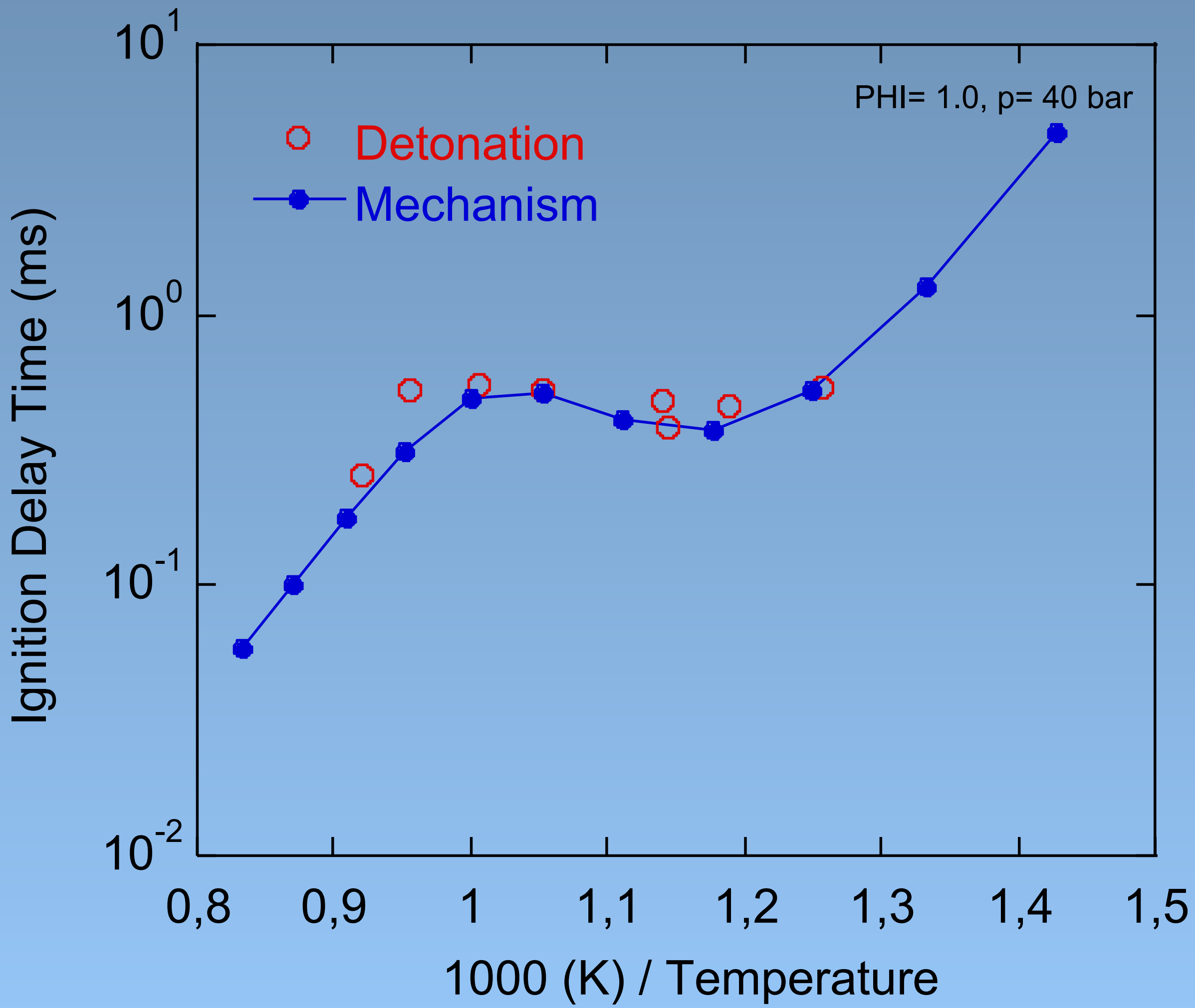
## (DI turbocharged Diesel engine)

| | |
|---|---|
| Total displacement | 11 705 $cm^3$ |
| Compression ratio | 18:1 |
| Bore | 127 mm |
| Stroke | 154 mm |
| Connecting Rod | 255 mm |
| IVO | 54° BTCD |
| IVC | 78° ABCD |
| EVO | 96° BBCD |
| EVC | 54° ATCD |




**FUEL ADOPTED FOR HCCI OPERATING CONDITIONS** ⇨ { **ISOOCTANE** / **N-HEPTANE** }

# Test case




*n - Heptane*

# Test case

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LUNDS TEKNISKA HÖGSKOLA

## *Model validation:*

### Operating conditions:

| | |
|---|---|
| $\lambda$ | **3.07** |
| **rpm** | **1500** |
| **ON** | **100** |
| **Eng. Inlet Temp. [K]** | **424** |
| **Internal EGR** | |

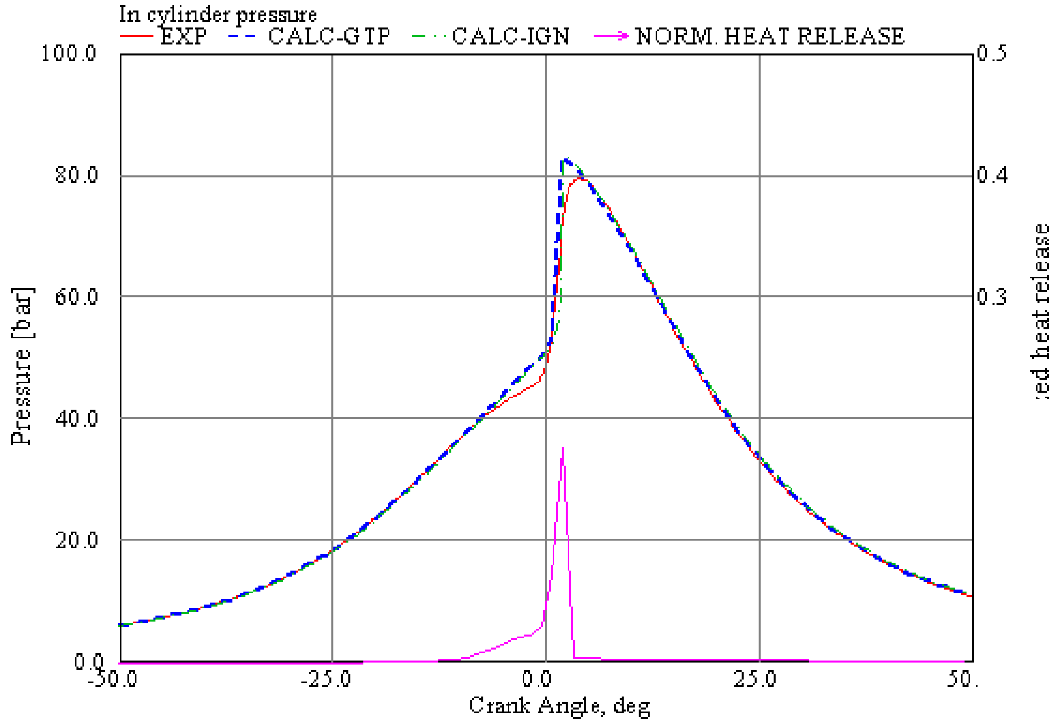
**Input data**

### Engine performaces:

| | EXP. | CALC. |
|---|---|---|
| Comp. Out. Press. [bar] | 0.98 | 1.00 |
| Turb. Inlet Temp [K] | 565 | 564 |
| Turb. Inlet Press. [bar] | 0.97 | 1.06 |
| IMEP [bar] | 3.92 | 3.91 |

# Test case

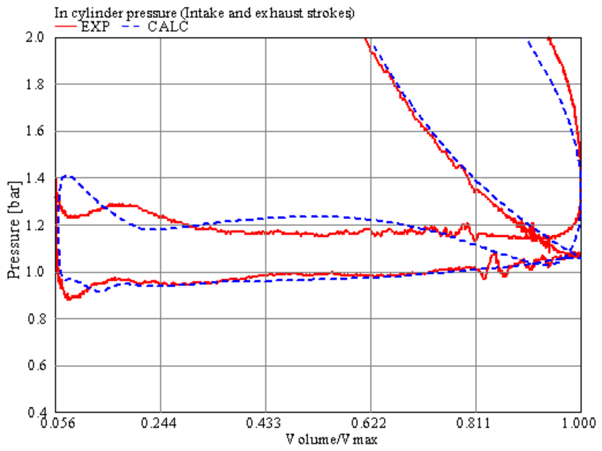
## *Model validation:*




**In cylinder pressure**

**In cylinder pressure during gas exchange**

**Cumulative Burned Fuel Rate Percent**




**Computational time:**

**Only GT-Power** 5 s/cycle
**Coupled run** 40 s/cycle

**Pentium IV 2 GHz**

# Test case

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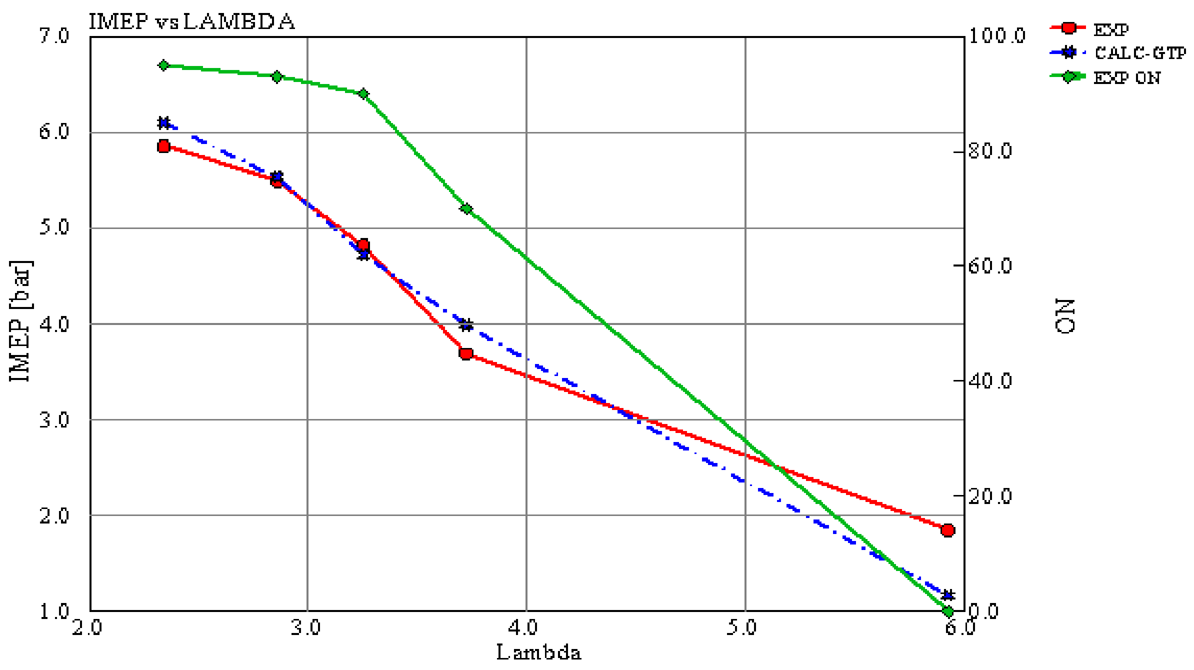
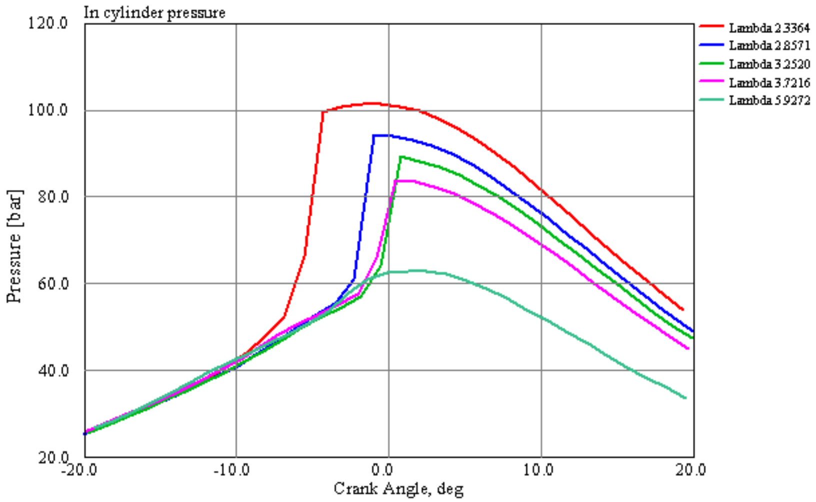
**<u>IMEP variation versus different LAMBDA values</u>**

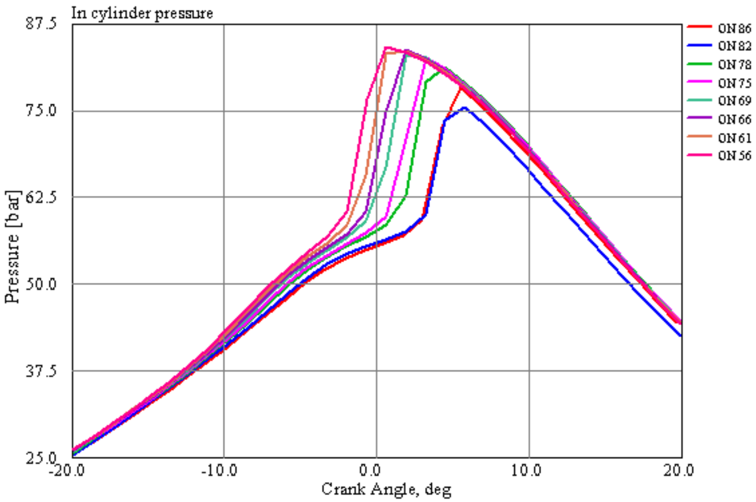


# Test case

**IN CYLINDER PRESSURES**




**IMEP versus LAMBDA**




**IGNITION CAD versus ON**

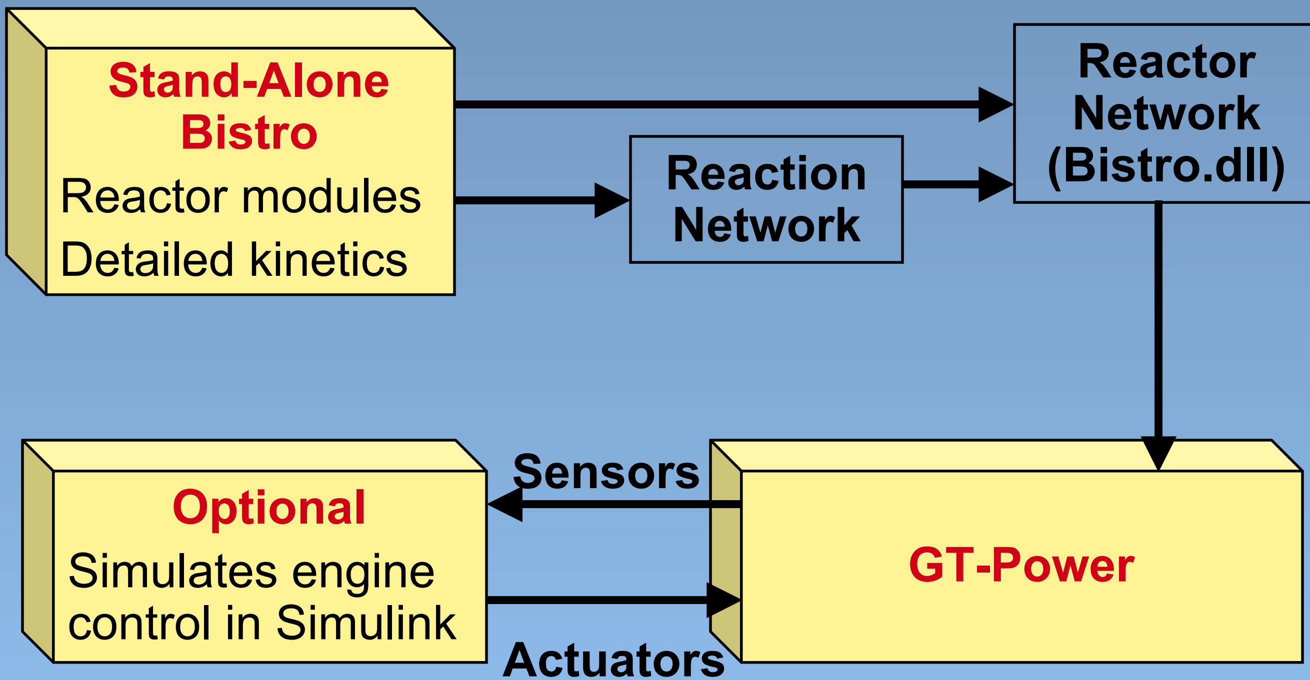
- Aftertreatment Modeling Using Bistro™/GT-Power

TIAX/ADL

**The combination of GT-Power/C-Power and Bistro provides an efficient framework for the creation of engine/catalyst/control system models.**

- Catalyst models are created in Bistro and “plugged-in” to GT-Power/Simulink models via the UserModel option.
- The Bistro concentration results are written to output files for post-processing.
- Through GT-Power, the user can adjust many of the physical parameters of the catalyst such as length, cell density, and initial temperature.
- Each component provides flexibility in its own domain.

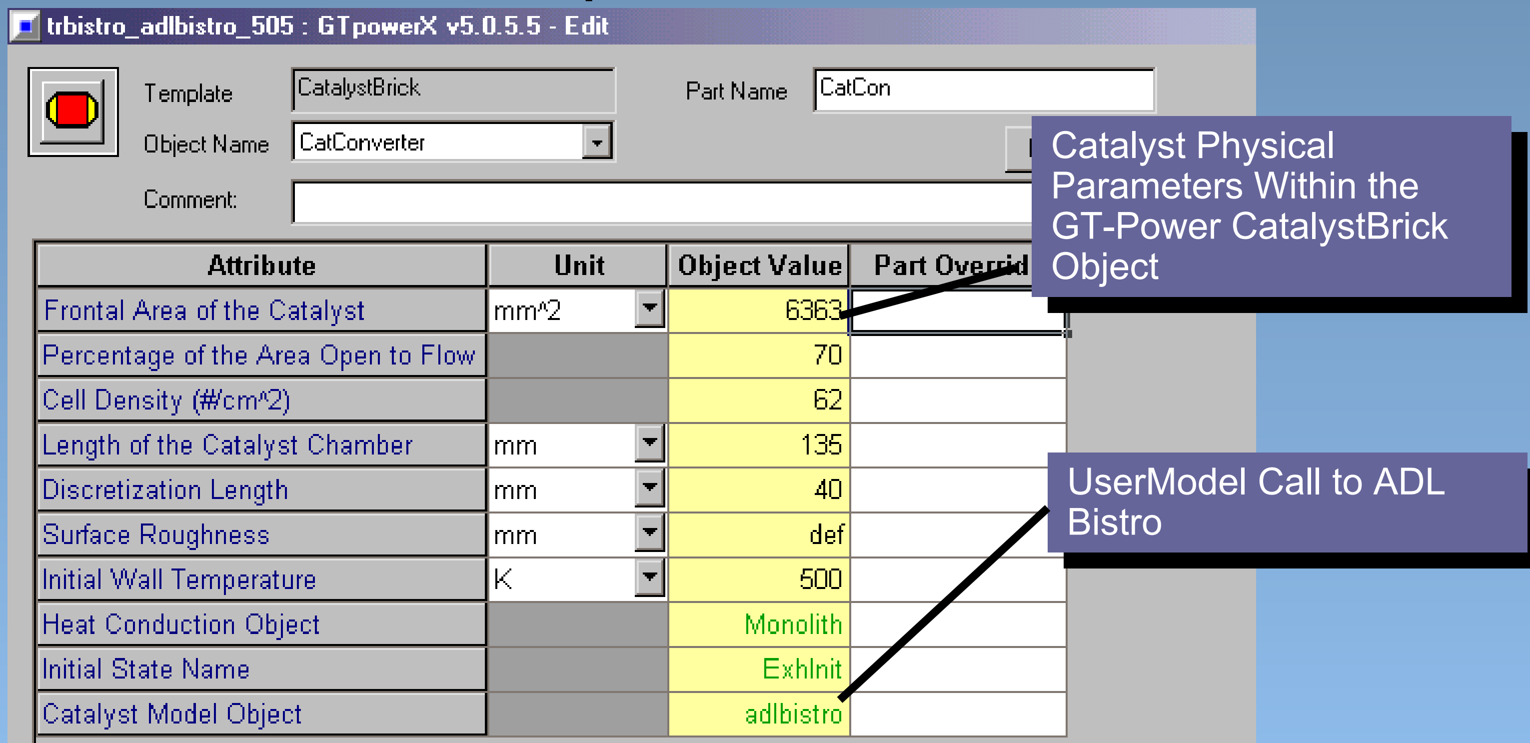
**Catalyst models are created with Bistro and "plugged-in" to GT-Power/C-Power models via the UserModel option.**




**Construction of the reactor network, the reaction network, and the engine controller is done outside of the GT-Power environment, which allows each researcher to contribute specialized information).**

The GT-Power/Bistro Framework

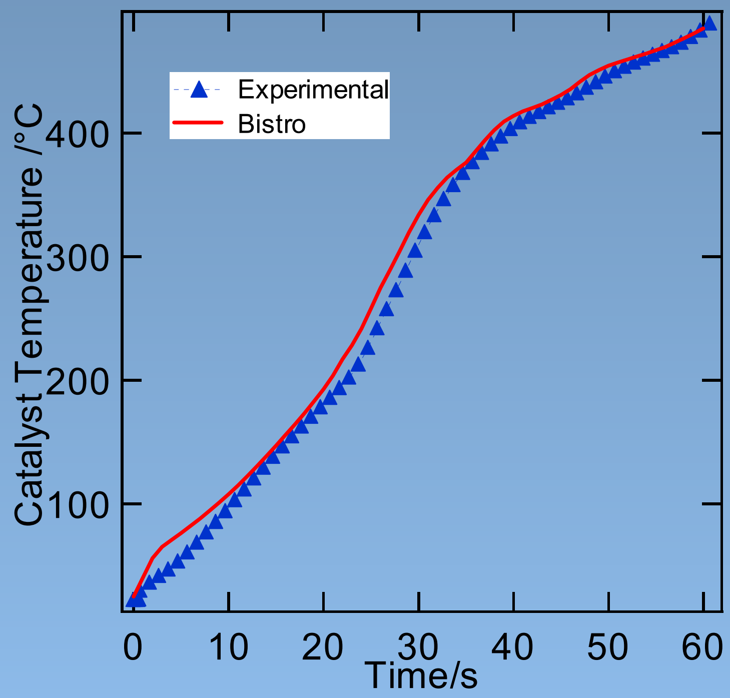
## Through GT-Power, the user can adjust many of the physical parameters of the catalyst such as length, cell density, initial substrate temperature...

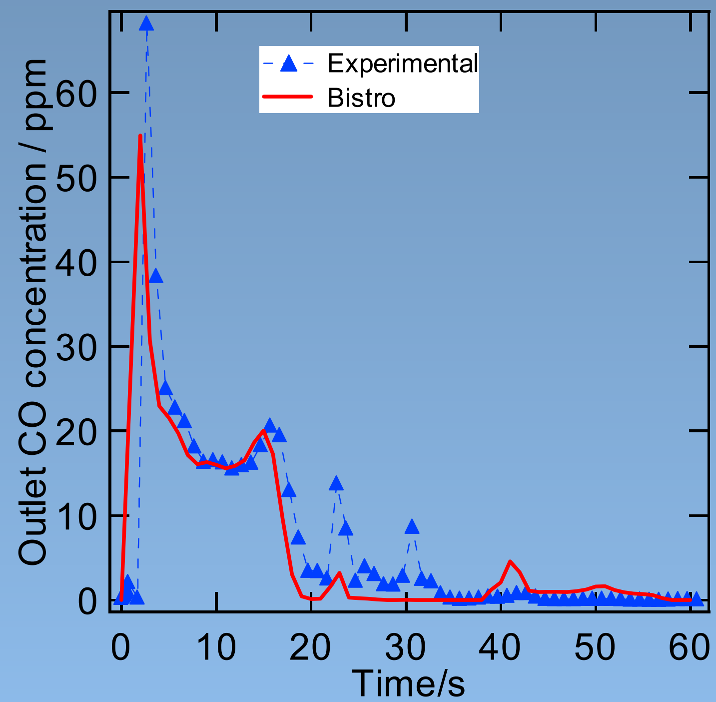



as well as the engine parameters and conditions that affect the catalyst inlet conditions….

**Putting it all together** Comparisons with data from a 3-way converter

## With only 1 adjustable parameter, we predict well the experimentally observed trends in the performance of a typical catalytic converter.



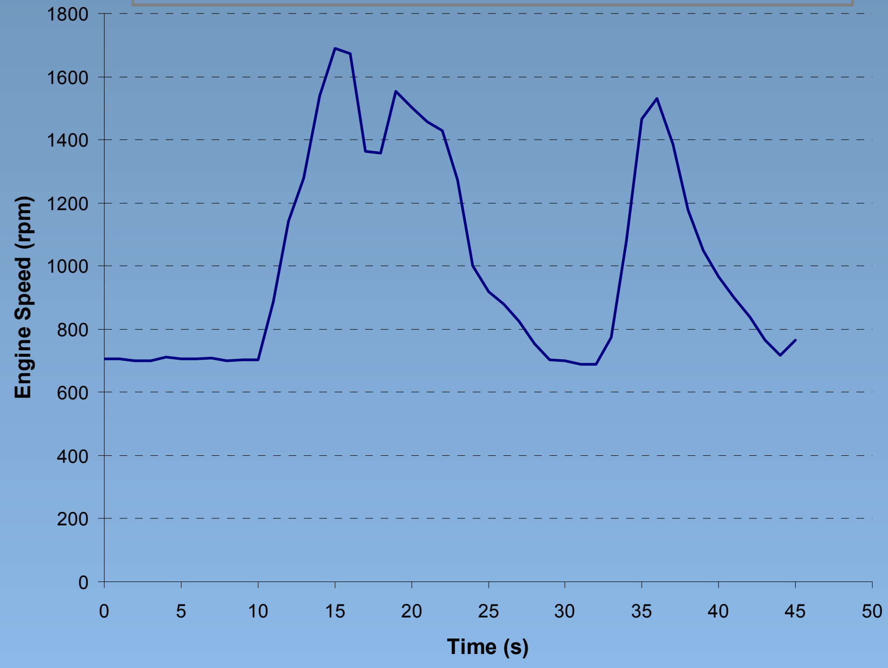

- Measurements were from an engine-dyno attached to a 3-way catalytic converter. The experiment corresponded to cold-start in a US FTP cycle.
- We used typical literature values for the catalyst surface area, and for the thermo-physical properties of the monolith. Only the reactor size was adjusted.

The GT-Power/Bistro Framework

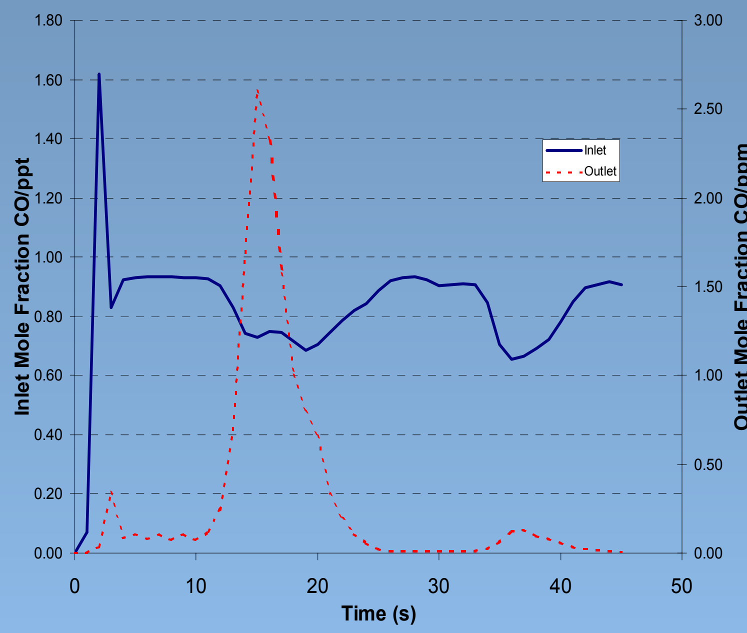
D

….and study the subsequent effect on catalyst performance.

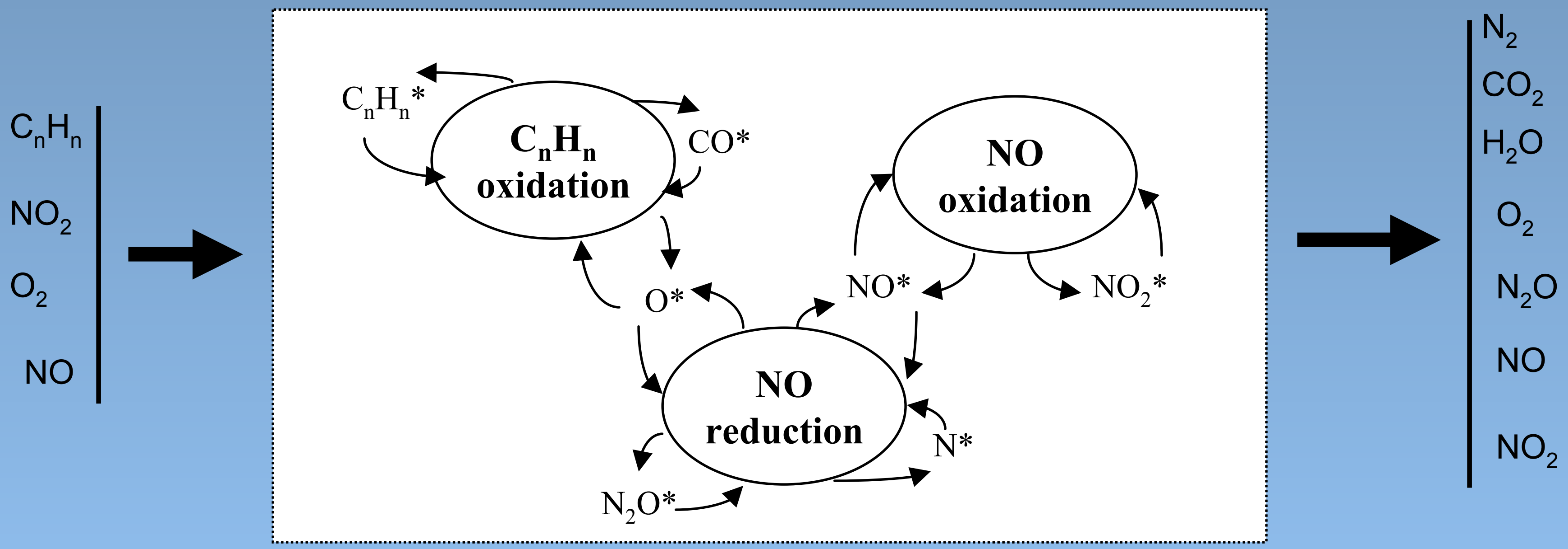
Simulated Engine Speed




Simulated CO inlet and outlet concentrations



# ADL has developed an SCR network that includes NO oxidation and reduction of $NO_x$ by hydrocarbons catalyzed by platinum group metals.



$NO_x$ reaction modeling

# Kinetic parameters in this network were drawn from both the literature and predictions of computational chemistry for three major pathways.

## NO oxidation/$NO_2$ reduction

| | | |
|---|---|---|
| $NO_2$ + * | ⇔ | $NO_2$* |
| NO + * | ⇔ | NO* |
| $NO_2$* + * | ⇔ | *$NO_2$* |
| *$NO_2$* | ⇔ | NO* + O* |
| CO* + $NO_2$* | ⇔ | $CO_2$* + NO* |

## NO oxidation/NO reduction

*high-temperature pathway*

| | | |
|---|---|---|
| NO* + * | ⇔ | N* + O* |
| 2N* | ⇔ | $N_2$* + * |
| $N_2$* | ⇔ | $N_2$ + * |

*low-temperature pathway*

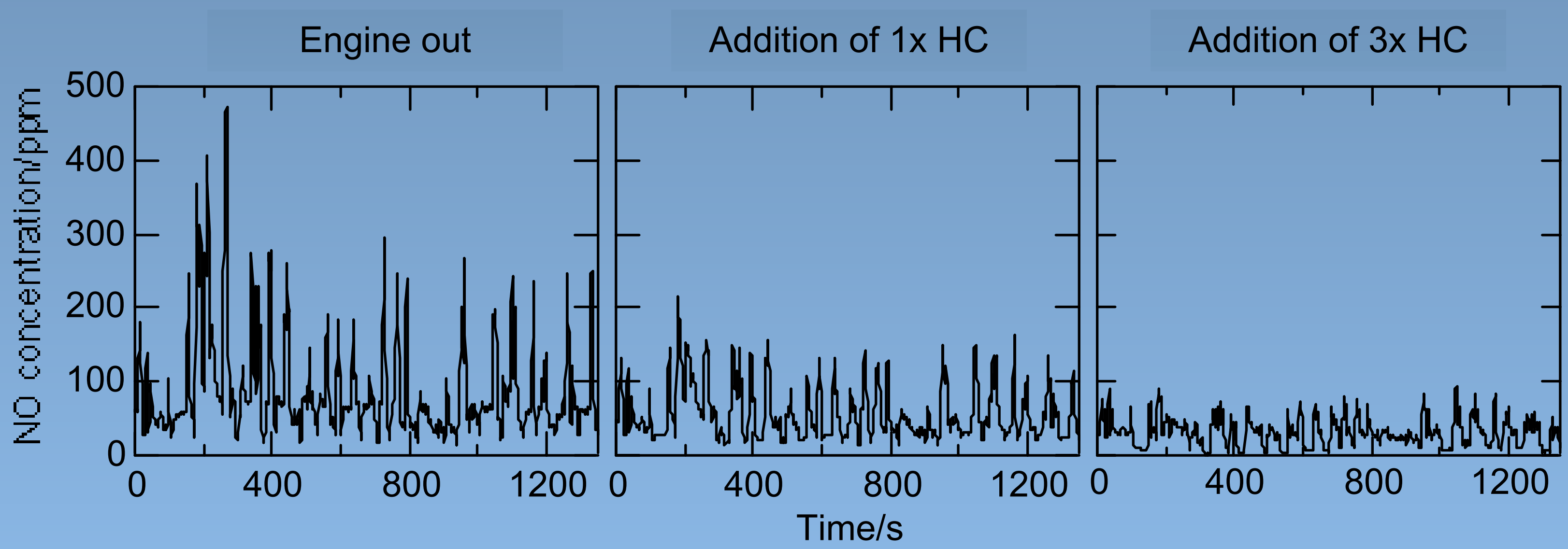
| | | |
|---|---|---|
| NO* + N* | ⇔ | $N_2O$* + * |
| $N_2O$* | ⇔ | $N_2O$ + * |
| $N_2O$* + * | ⇔ | $N_2$* + O* |

## $C_nH_n$ ($C_3H_6$) oxidation

| | | |
|---|---|---|
| $C_3H_6$ + * | ⇔ | $C_3H_6$ |
| $O_2$ + * | ⇔ | $O_2$* |
| $O_2$* + * | ⇔ | 2O* |
| $C_3H_6$ + O* | ⇔ | $C_3H_5$* + OH* |
| $C_3H_5$* + H* | ⇔ | $C_3H_6$* + * |
| $C_3H_5$* + O* | ⇔ | $C_3H_4$* + OH* |
| $C_3H_4$* + H* | ⇔ | $C_3H_5$* + * |
| $C_3H_4$* + O* | ⇔ | $C_3H_3$* + OH* |
| $C_3H_3$* + H* | ⇔ | $C_3H_4$* + * |
| $C_3H_3$* + O* | ⇔ | $C_2H_3$* + CO* |
| $C_2H_3$* + O* | ⇔ | $C_2H_2$* + OH* |
| $C_2H_2$* + H* | ⇔ | $C_2H_3$* + * |
| $C_2H_2$* + O* | ⇔ | $C_2H$* + OH* |
| $C_2H$* + H* | ⇔ | $C_2H_2$* + * |
| $C_2H$* + O* | ⇔ | $C_2$* + OH* |
| $C_2$* + H* | ⇔ | $C_2H$* + * |
| $C_2$* + O* | ⇔ | C* + CO* |
| C* + O* | ⇔ | CO* + * |
| CO* | ⇔ | CO + * |
| CO* + O* | ⇔ | $CO_2$* + * |
| $CO_2$* | ⇔ | $CO_2$ + * |
| H* + OH* | ⇔ | $H_2O$* + * |
| $H_2O$* | ⇔ | $H_2O$ + * |

**X* indicates that species X is bound to a surface site ***

ADL has used the model to estimate the effect of hydrocarbon addition on the efficiency of NOx aftertreatment for Diesel exhaust




3x Stoichiometric addition corresponds to a fuel penalty of about 2%.

Courtesy of ADL

# Modeling DPF-SCR for Heavy Duty Diesel Engine

SCANIA

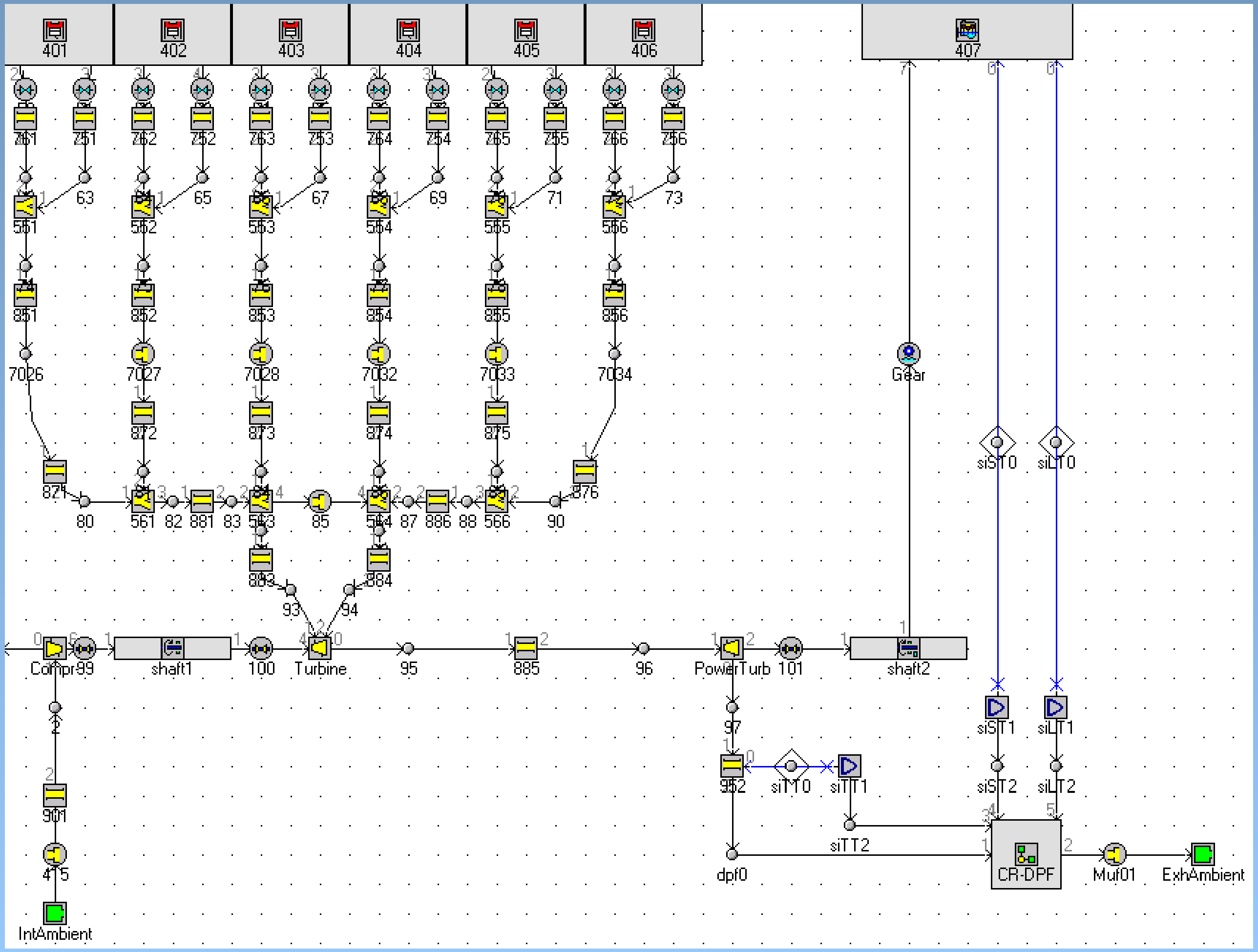
# Catalyst Package

- NO Oxidation Catalyst
- Soot oxidation Catalyst
  - $2\ NO_2 + C = 2\ NO + CO_2$
  - Continuous regeneration
- NH3-SCR Catalyst
  - Urea hydrolysis
  - Ammonia Reduction

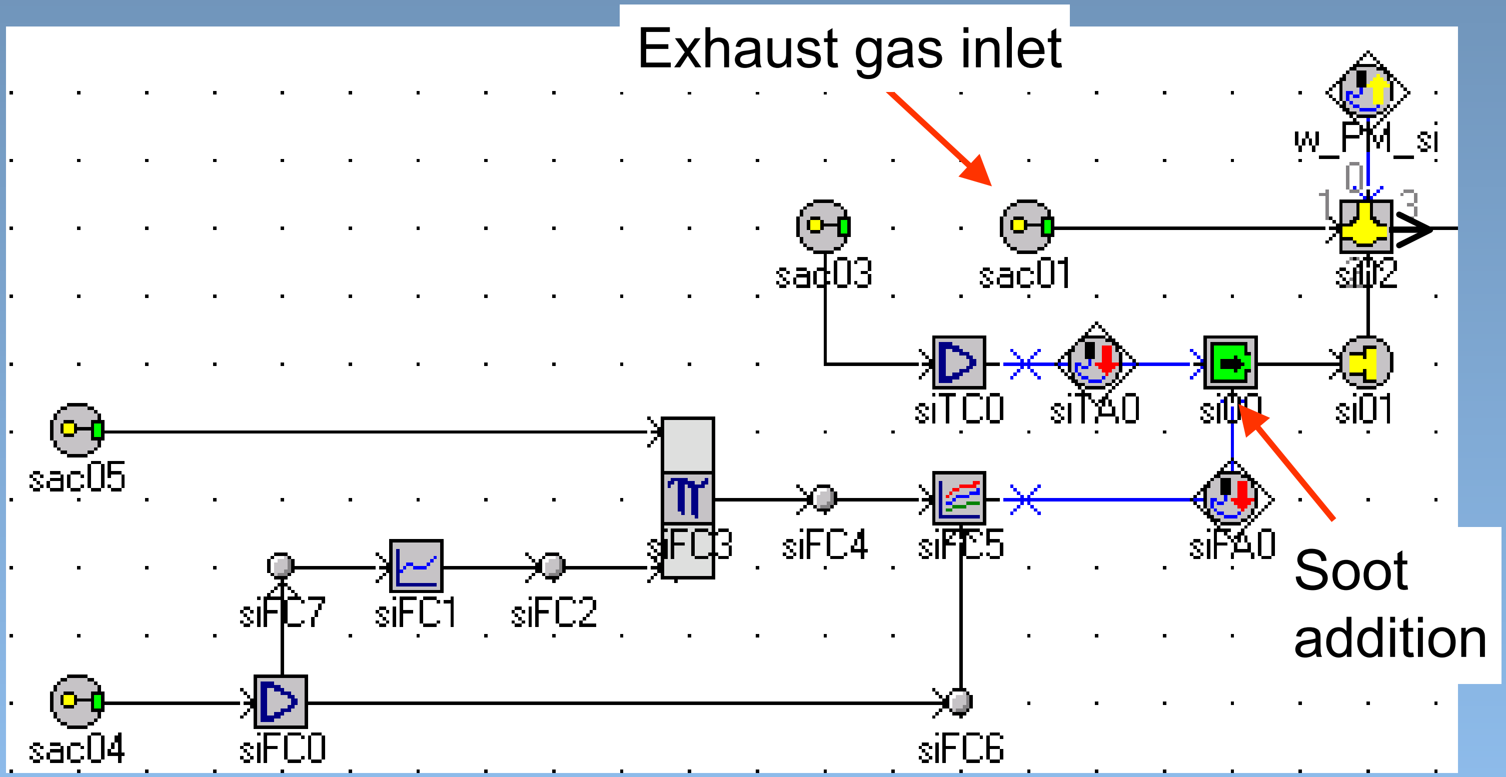
# Implementation in GT-Power

- Catalyst Package and Exhaust System are Placed in the Subassembly Section of the Model
- Subassembly was Attached to the Main Engine Model
- Catalyst Brick Object are Used to Access User Developed Kinetics Model
- Measured Value of Soot is Introduced Down Stream of the Exhaust Manifold
- Control Object are Used to Model Pressure Drop Across the DPF (Masoudi et al. SAE 2000-01-0184)

# CR-DPF Subassembly



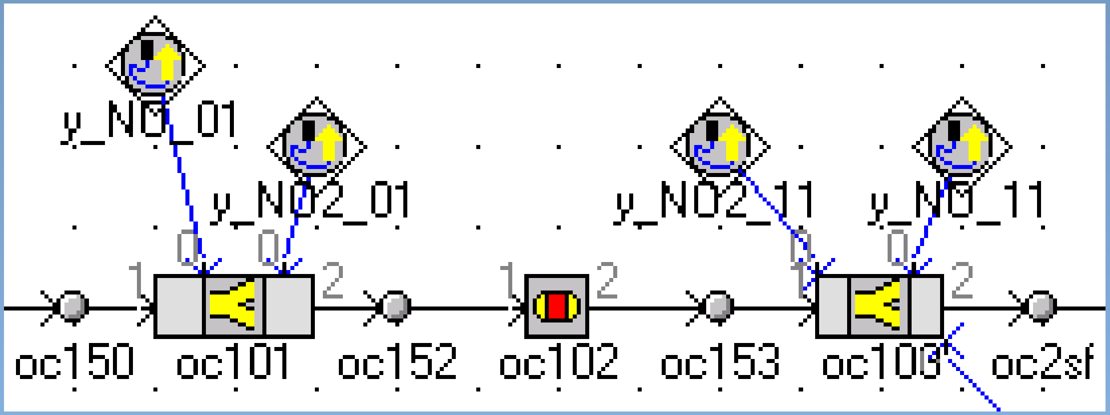
# Exhaust Gas Manipulation



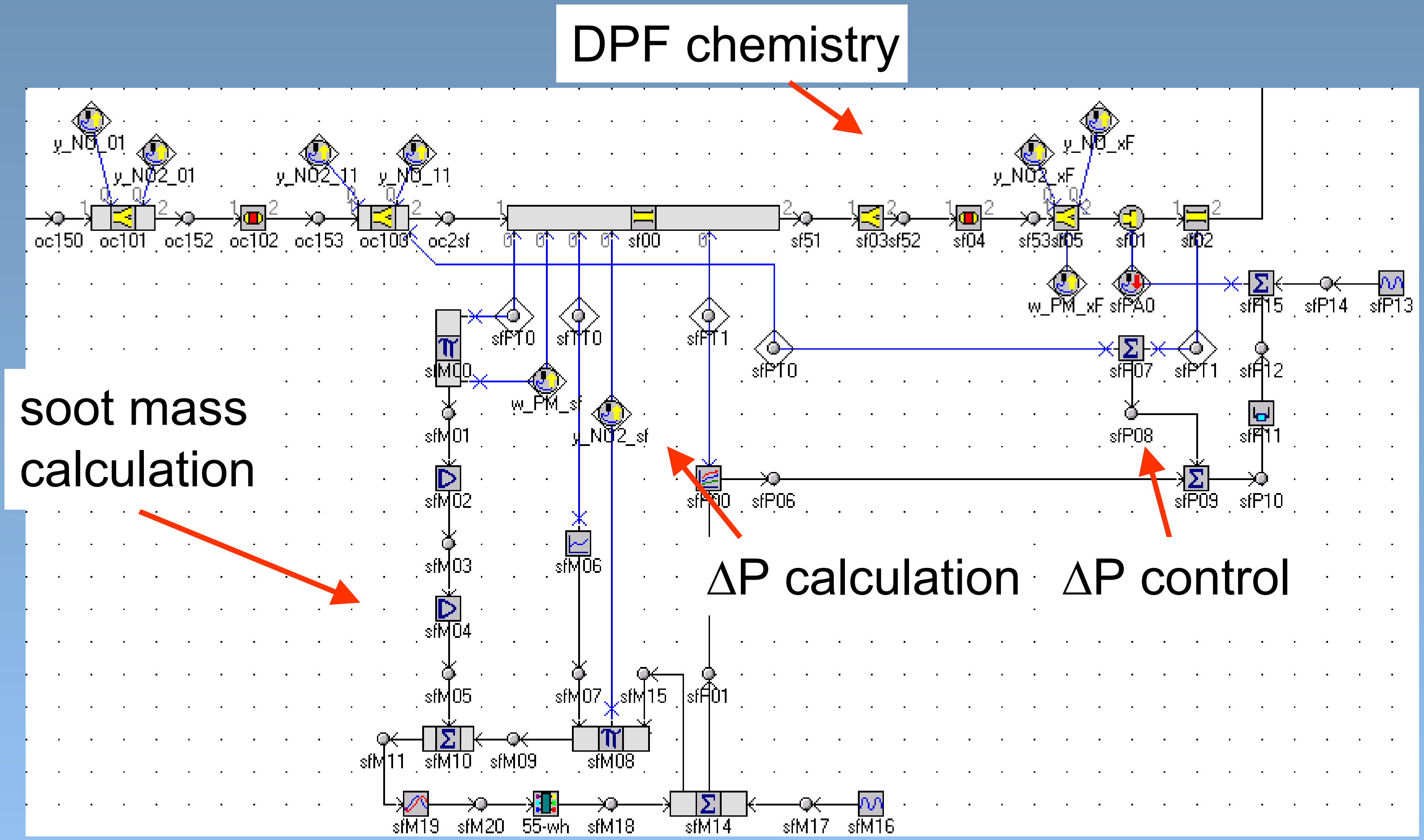
# Oxidation Catalyst System

- Use CatalystBrick object in GT-Power
- Chemistry in user-defined module
  - CO, HC oxidation
  - 2 NO + $O_2$ = 2 $NO_2$, reversible
  - Thermodynamic or kinetic limitations
  - Reaction equations taken from literature

# Oxidation Catalyst System

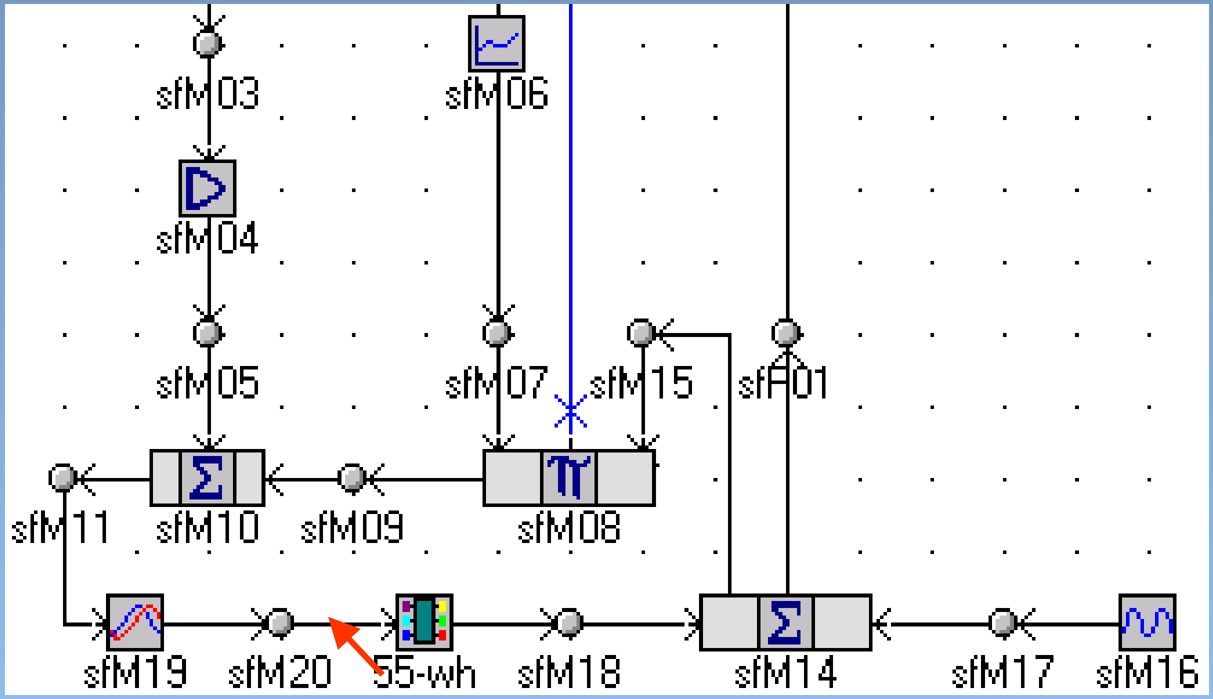


# CR-DPF System



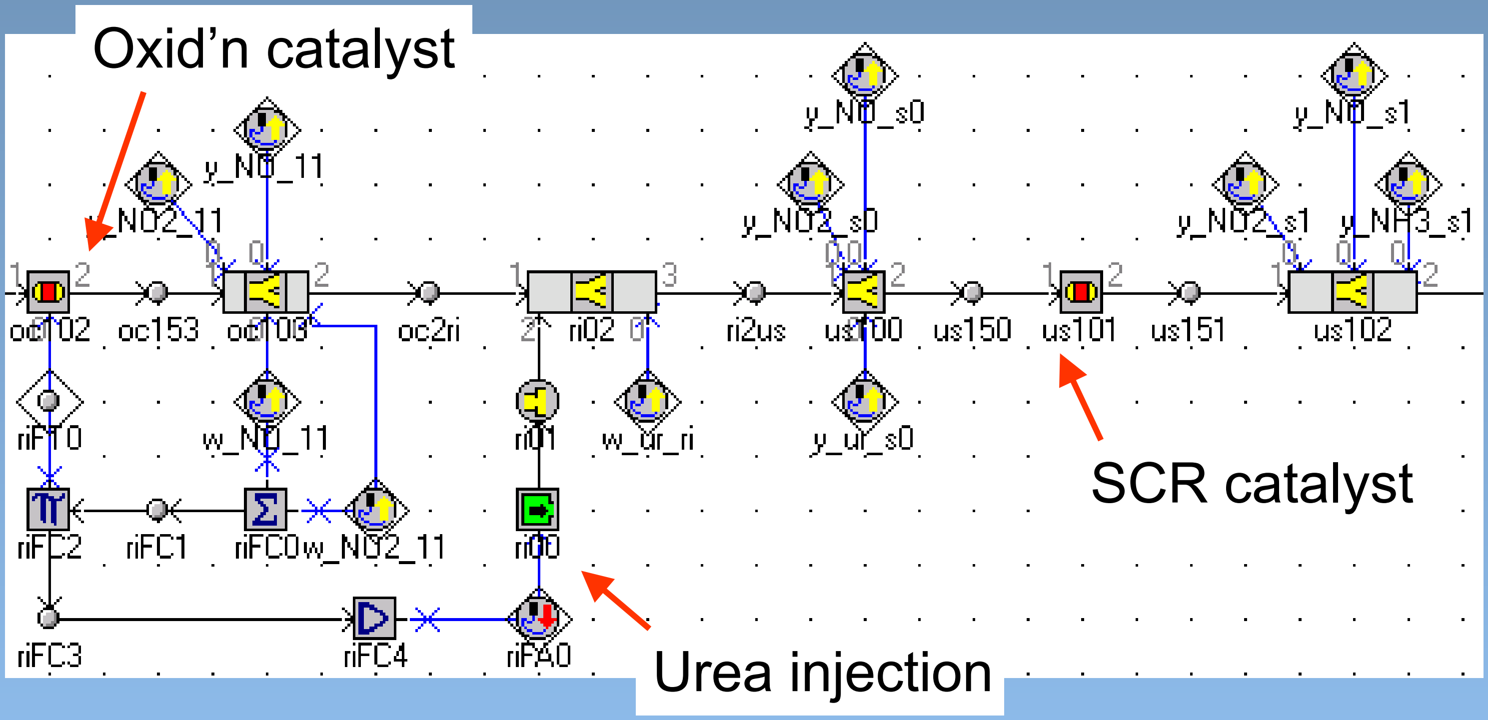
# CR-DPF System

Soot mass balance objects in detail




Soot integrator

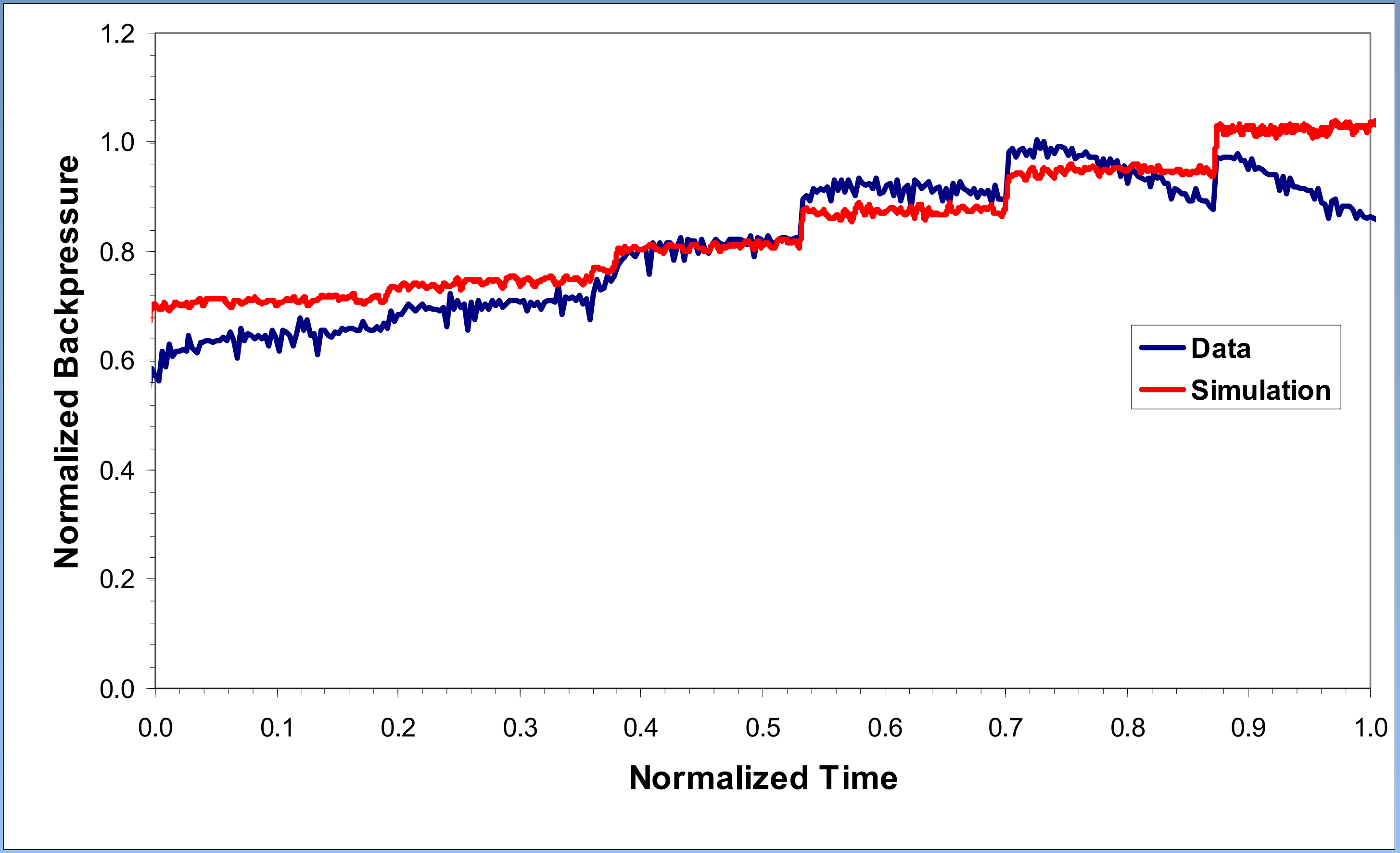
# SCR System


Oxid'n catalyst
SCR catalyst
Urea injection
y_NO_11
y_NO2_11
oc102
oc153
oc100
oc2ri
ri02
ri2us
us100
us150
us101
us151
us102
y_NO_s0
y_NO2_s0
y_NO_s1
y_NO2_s1
y_NH3_s1
riFT0
w_NO_11
ri01
w_ur_ri
y_ur_s0
riFC2
riFC1
riFC0
w_NO2_11
ri00
riFC3
riFC4
riFA0

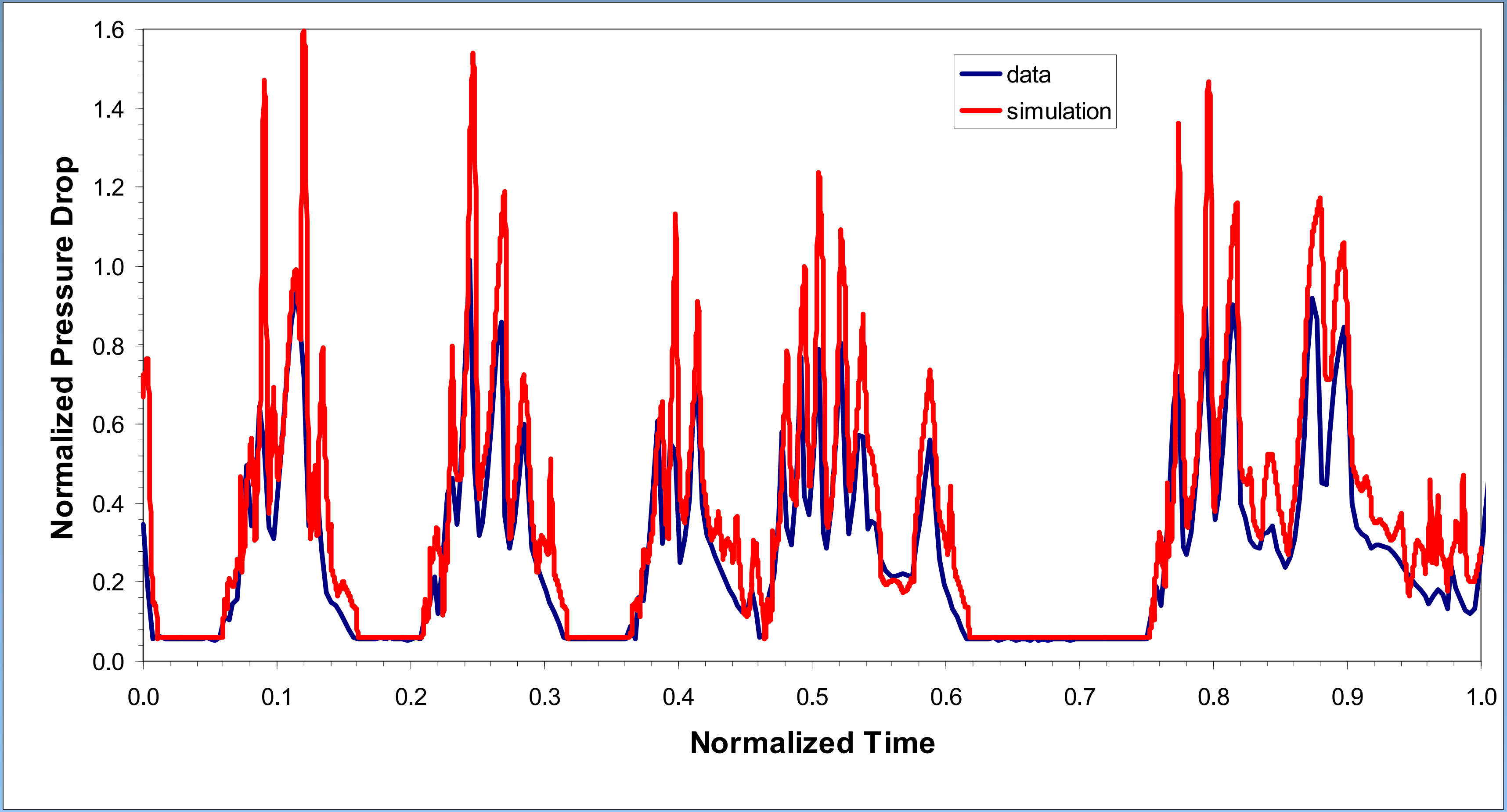
# Examples

- Soot balance-point test
- ETC results
- ESC results
- Dimension optimization

# Soot Balance-Point Test

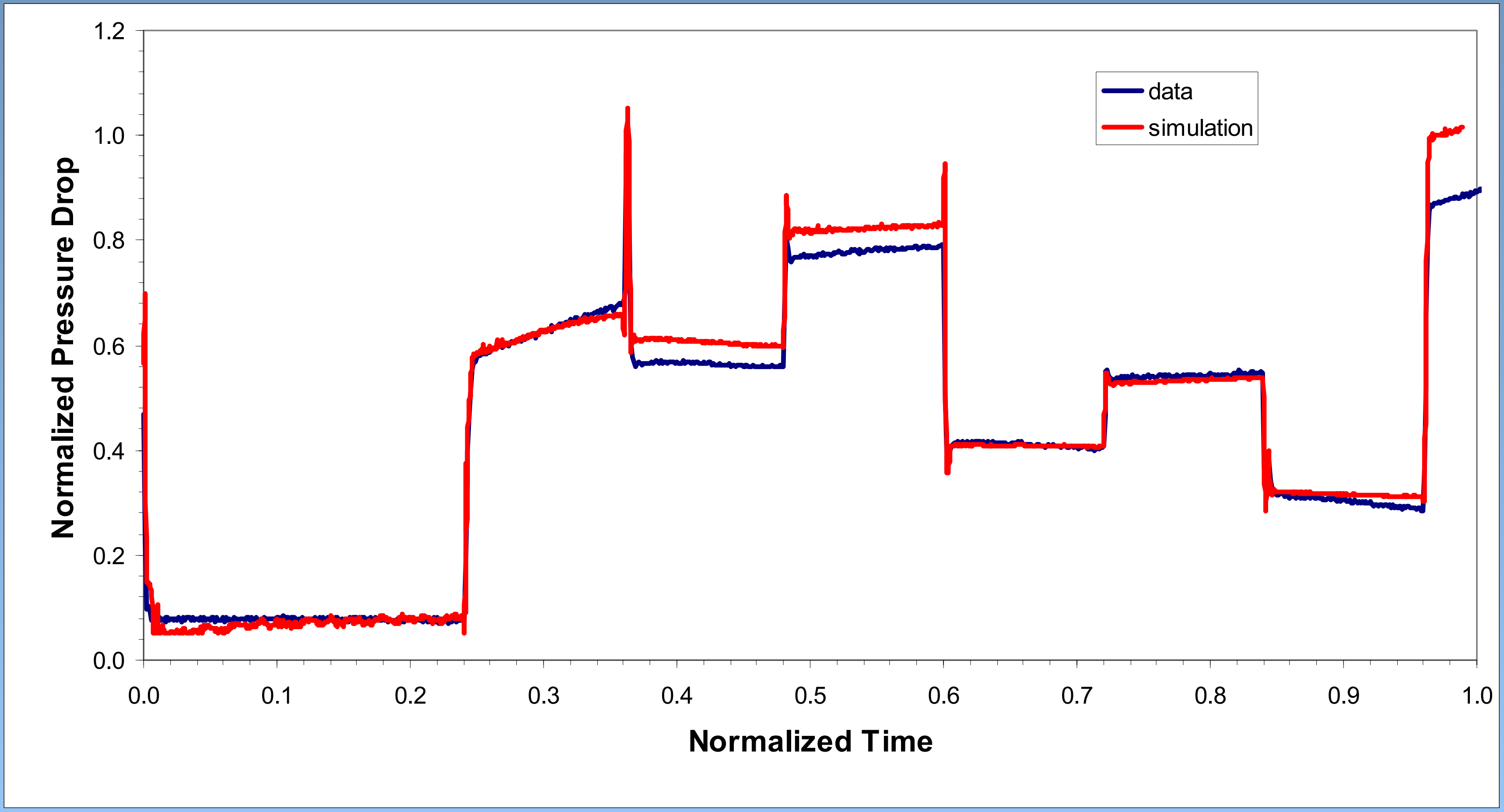


# ETC Test



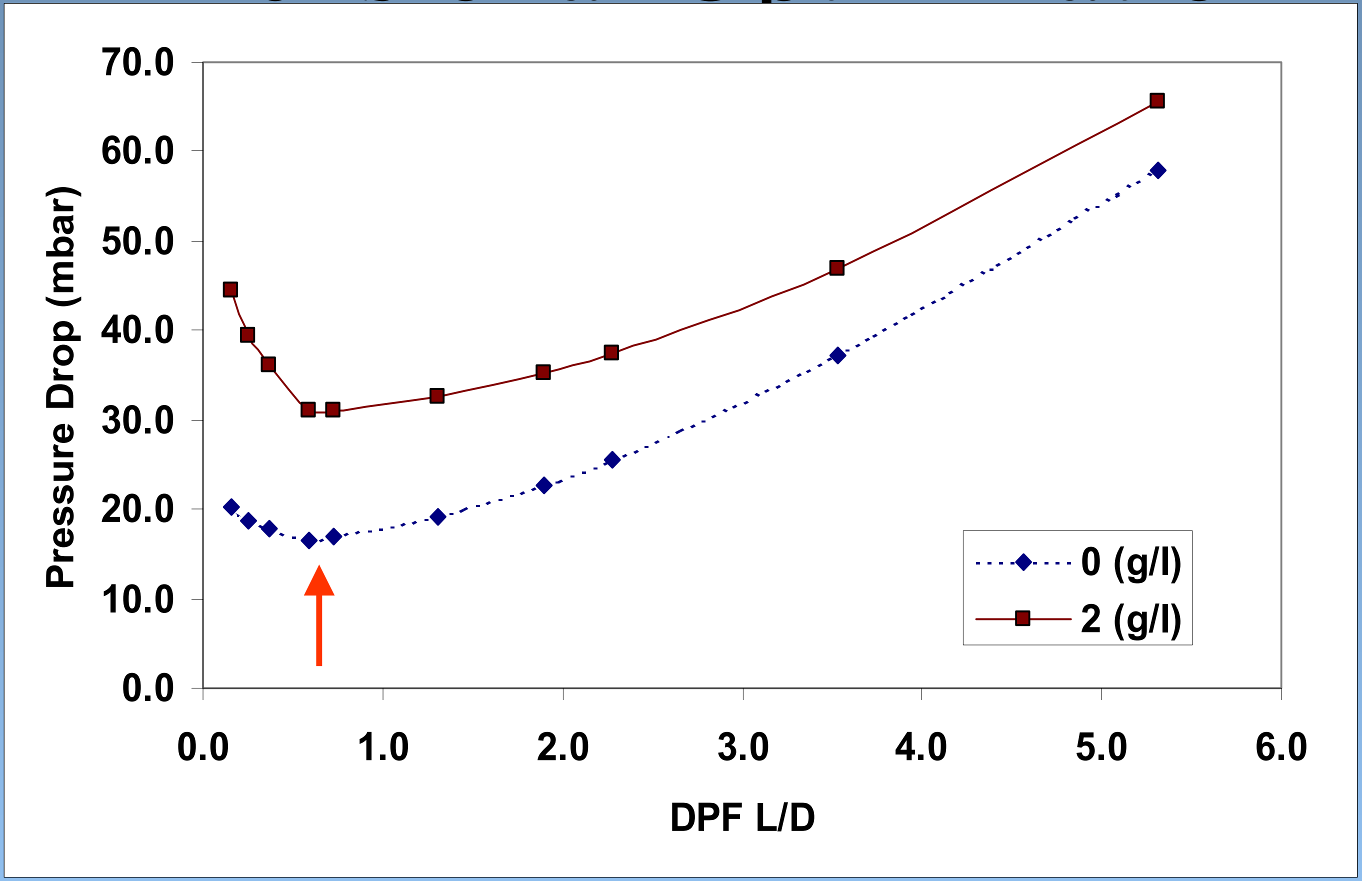
data
simulation
Normalized Pressure Drop
Normalized Time
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0

# ESC Test



data
simulation
Normalized Pressure Drop
Normalized Time
0.0
0.2
0.4
0.6
0.8
1.0
1.2
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0

# Dimensional Optimization



# SUMMARY

- User model facility offers aftertreatment modelers with the flexibility of use of external tools and/or proprietary model development
- IPR can be  effectively protected
- Separation of system level modeling and kinetics modeling can be efficiently used to take advantage of distributed expertise within an organization
- We must agree on a common interface (API) for calling third-party kinetics tools
- Kinetics calculations are the computation bottleneck. There is an urgent need for development of efficient numerical schemes (e.g. faster solvers and integrators, adaptive or automatically reduced mechanism).
- Better in-Cylinder models are needed to accurately predict species distribution