On Modeling of Emissions Aftertreatment Systems

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Wish list of Kinetics Modelers

- Accurate Transient Boundary Conditions

  - Major and Minor Compositions: Accurate In-Cylinder Chemistry

  - State

  - Flow rates

- Flow and Thermal Field Solved by the System Model
- Kinetics can be Easily Implemented

Modularization of the Problem

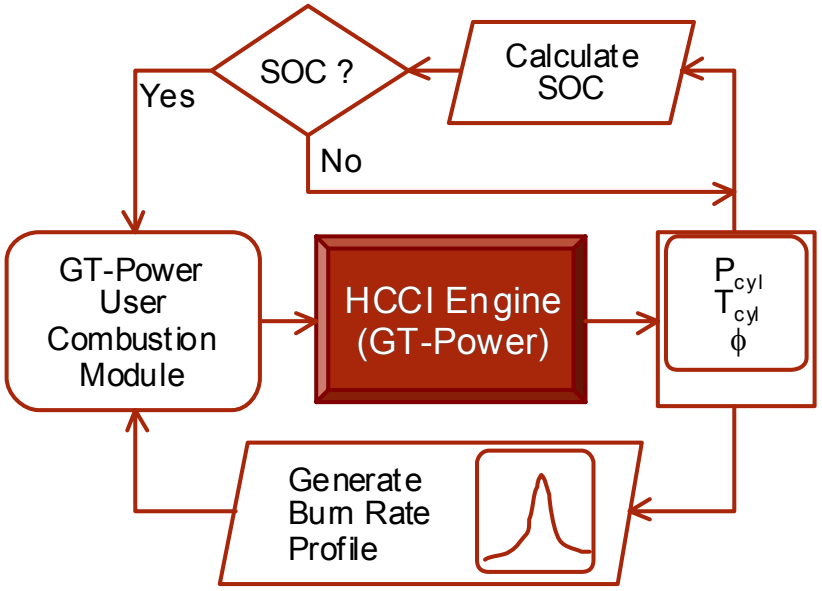
- Air and Fuel Systems (intake, exhaust, injection,cylinders, turbochargres)
- Thermal System
- Control System
- Aftertreatment System
  - Base Models
  - Infrastructure for implementation of proprietary models: user model facility
  - Link with 3-party Tools (Bistro™, Chemkin™, Simulink, CFD etc.)

User Developed Models

- Modeling With Built-in Tool
  - With Analysis and Control Tools
- Modeling with 3-Party Code
- Conventional User Models
  - Incorporation of User Written Code

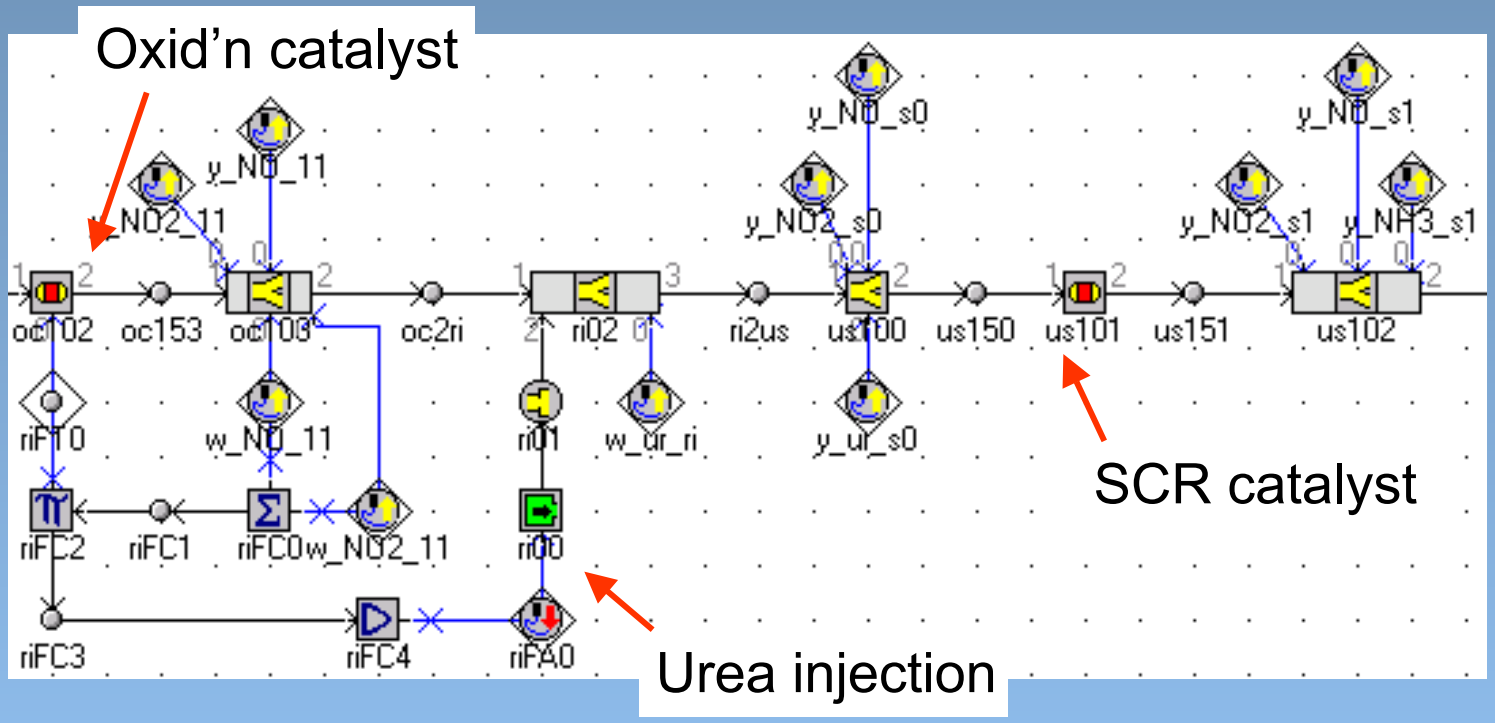
Sub-models for start of combustion (SOC), and rate of heat release (ROHR) were implemented in SIMULINK.

The sub-models, which are based on published data, are detailed enough to capture the correct system behavior and response to variations in input parameters, yet they are simple enough to allow for cost-effective evaluation of many different system configurations.



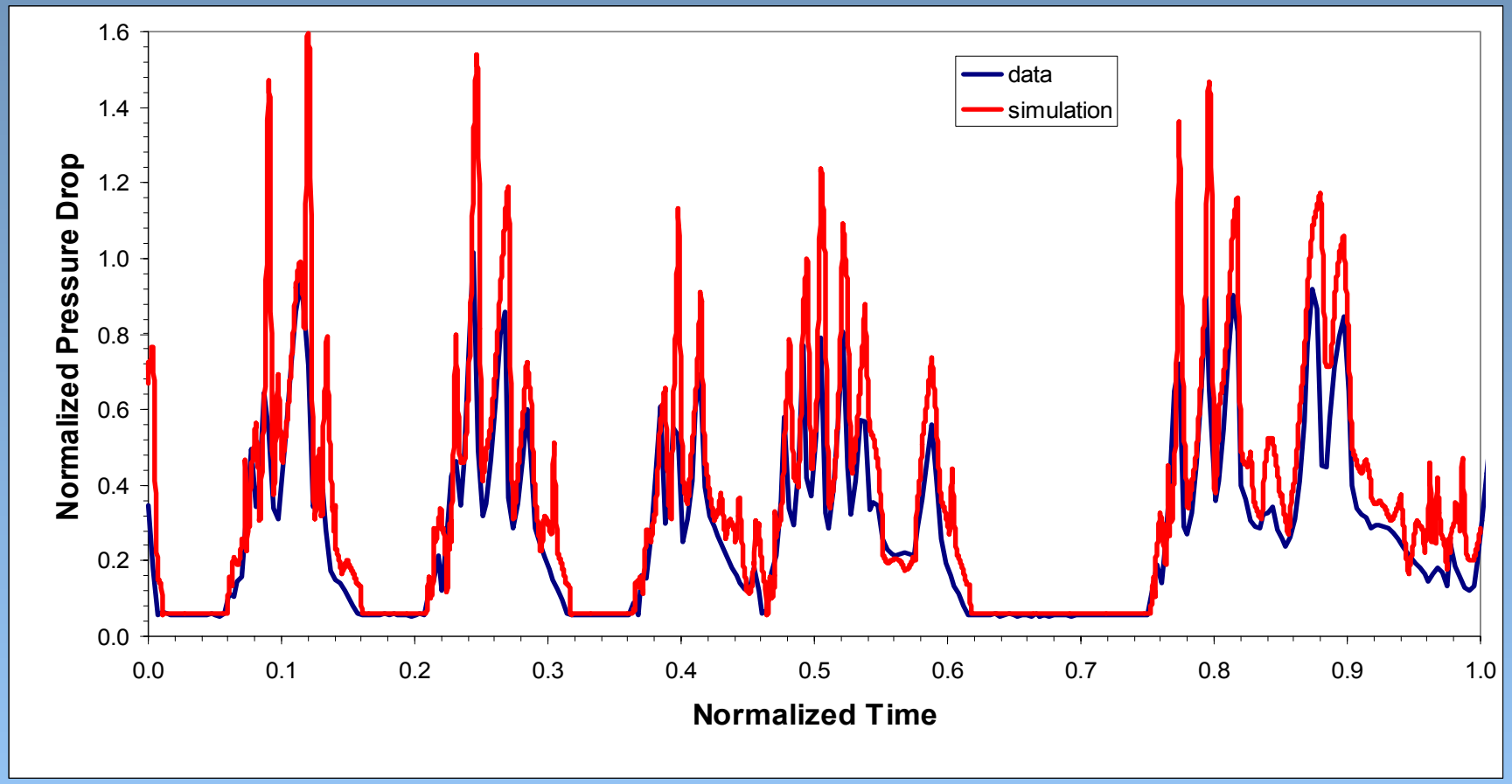
Start of Combustion (SOC)	Rate of Heat Release (ROHR)
Description	
• Calculates start of combustion. • Based on "*Ryan and Callahan", SAE 961160*, modified to match data for natural gas supercharged experimental data by "*Christiensen et. al.", SAE 980787*.	• Specifies rate of heat release. • Burn rate profiles adopted from "*Christiensen et. al.", SAE 980787*.

SCR System

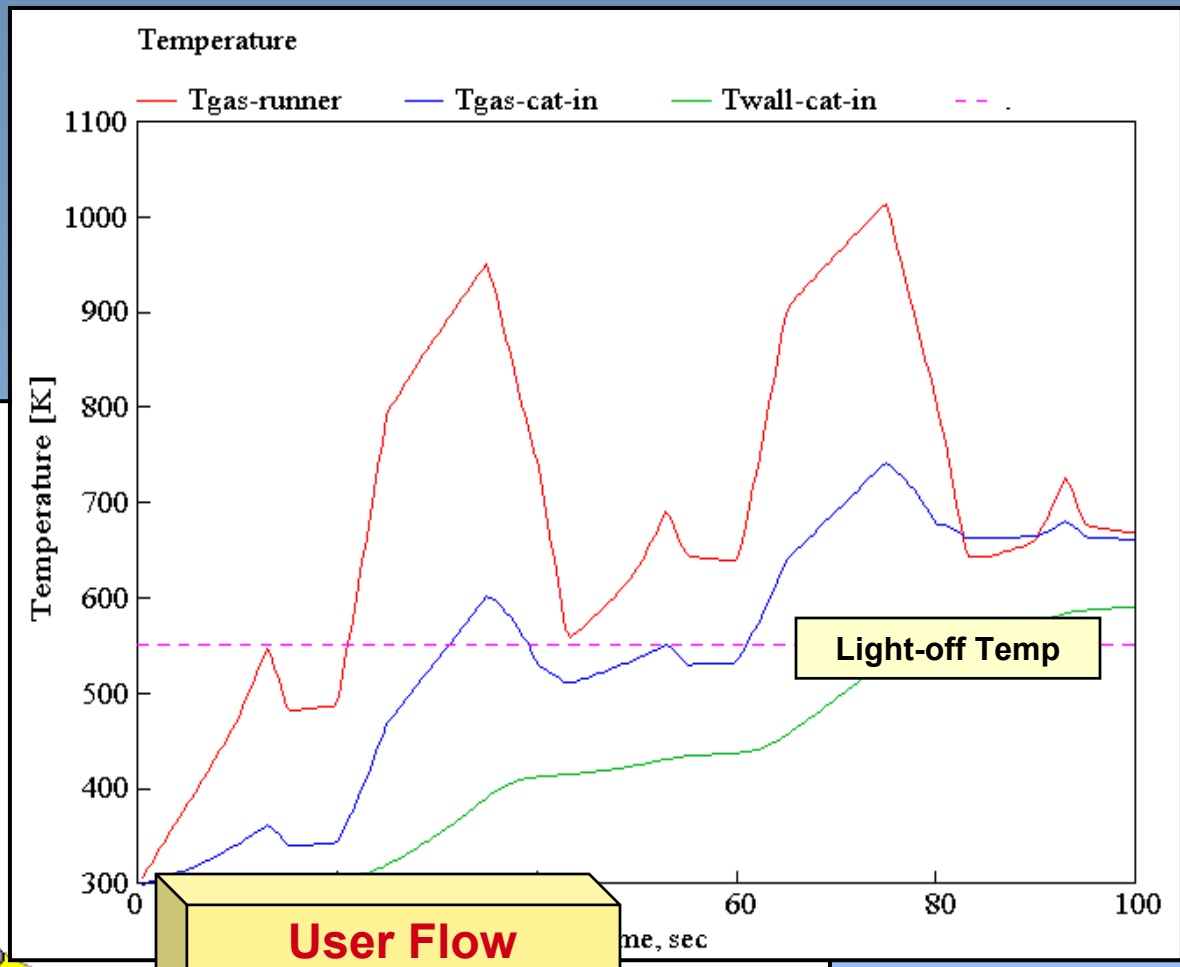


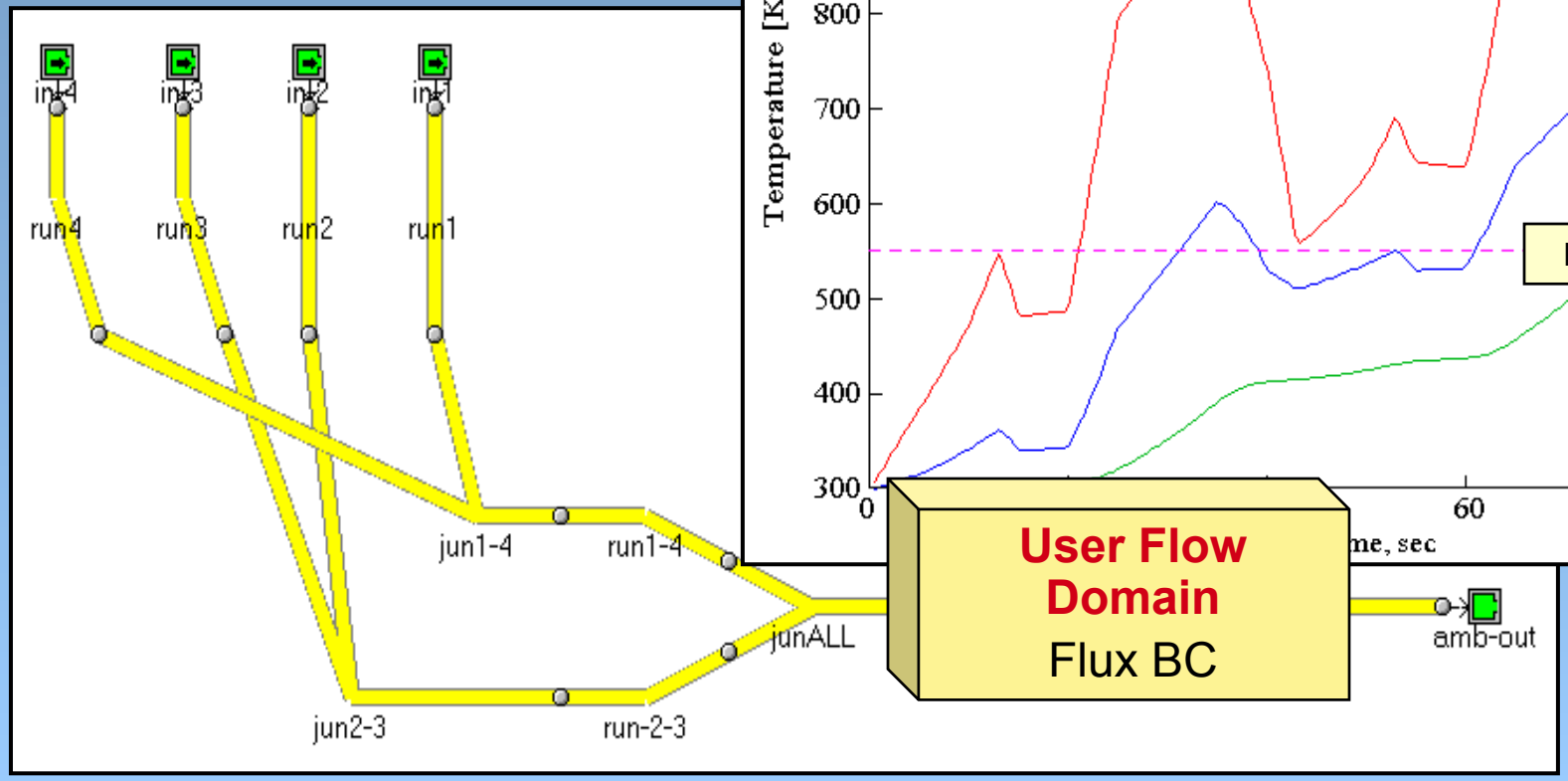
Courtesy of SCANIA

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

Exhaust Catalyst Warm-up with FE/Thermal Network

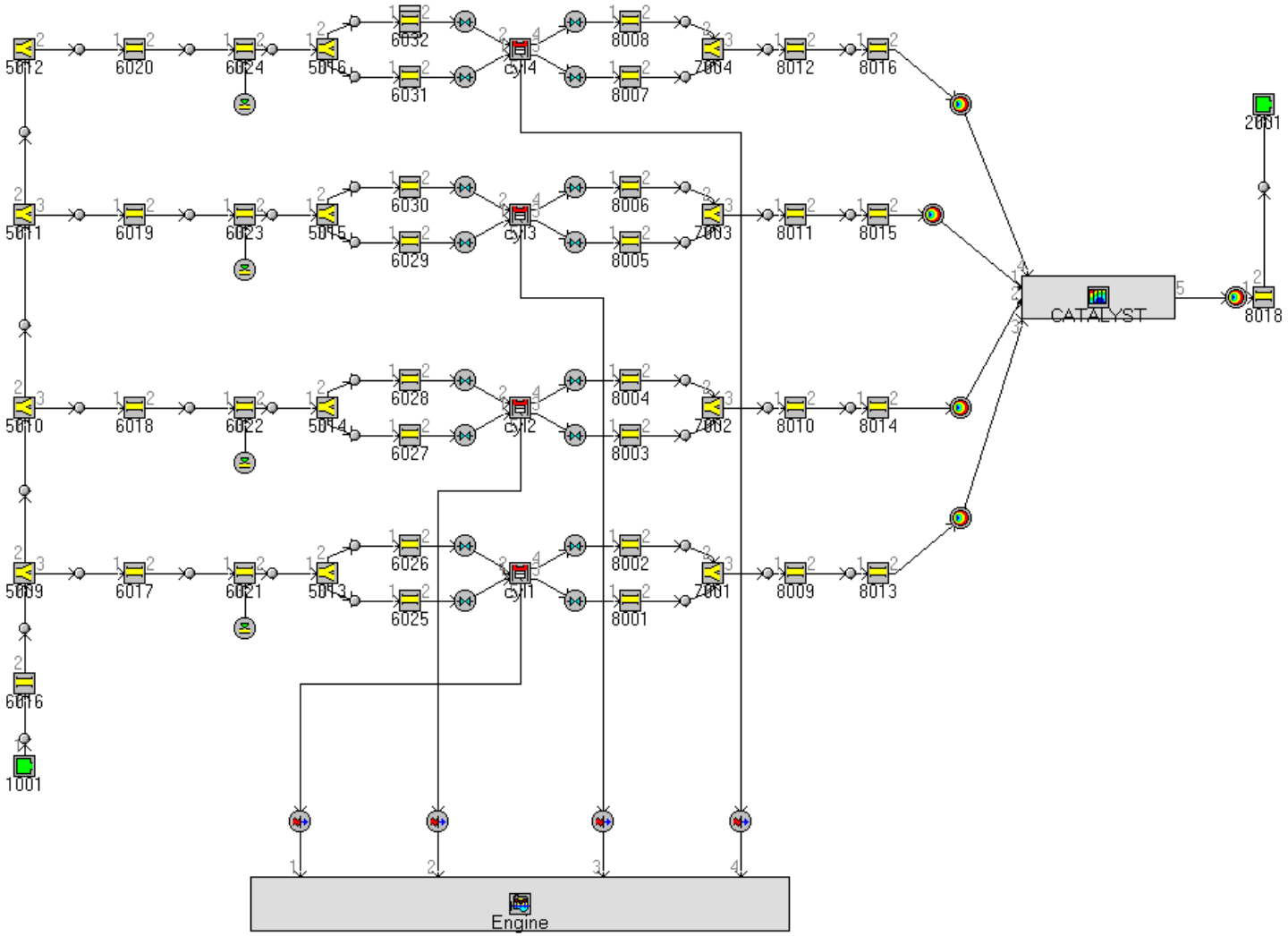




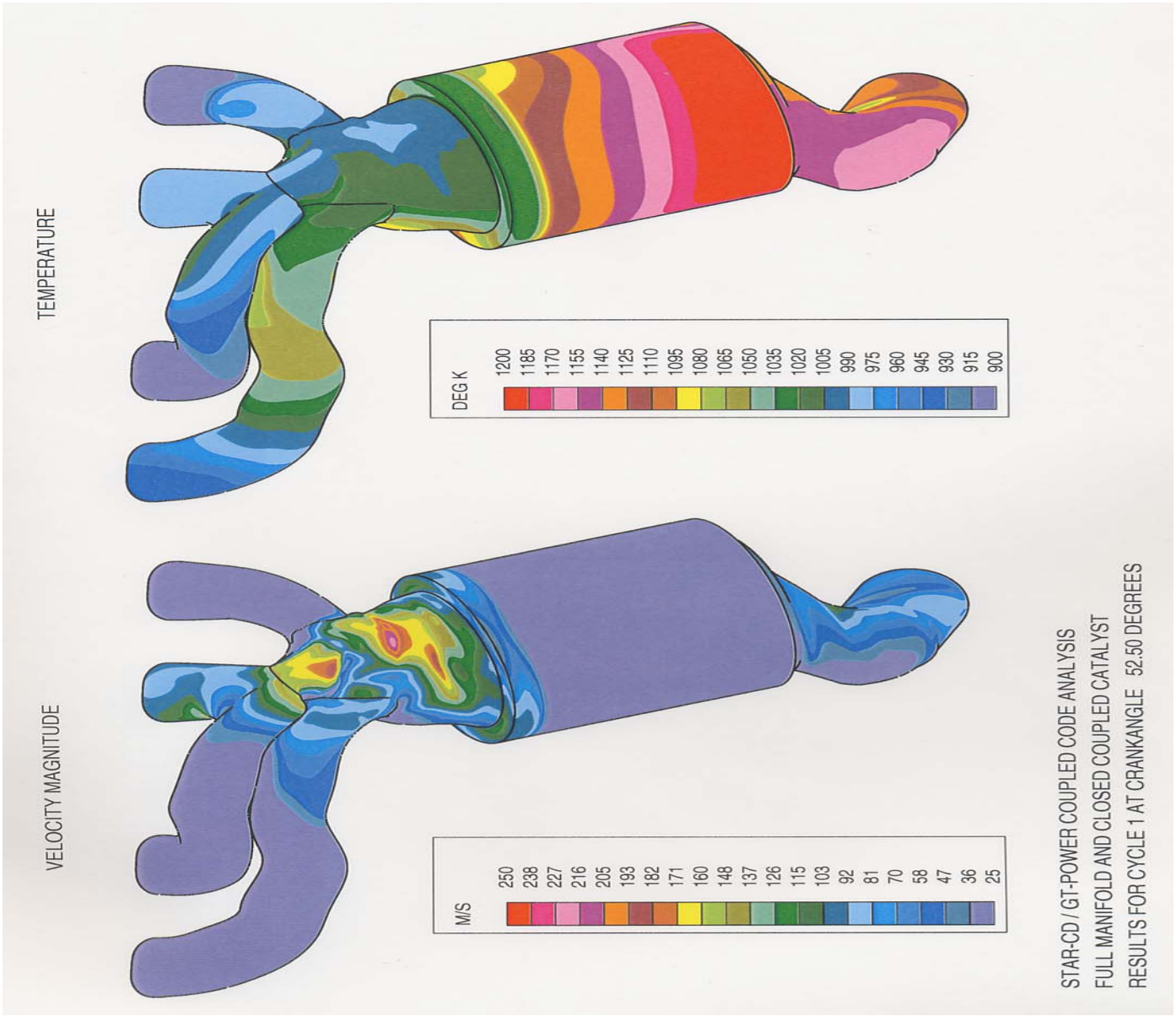
User Flow Domain

Flux BC

Coupled 1-D/3-D Simulation of A Catalyst



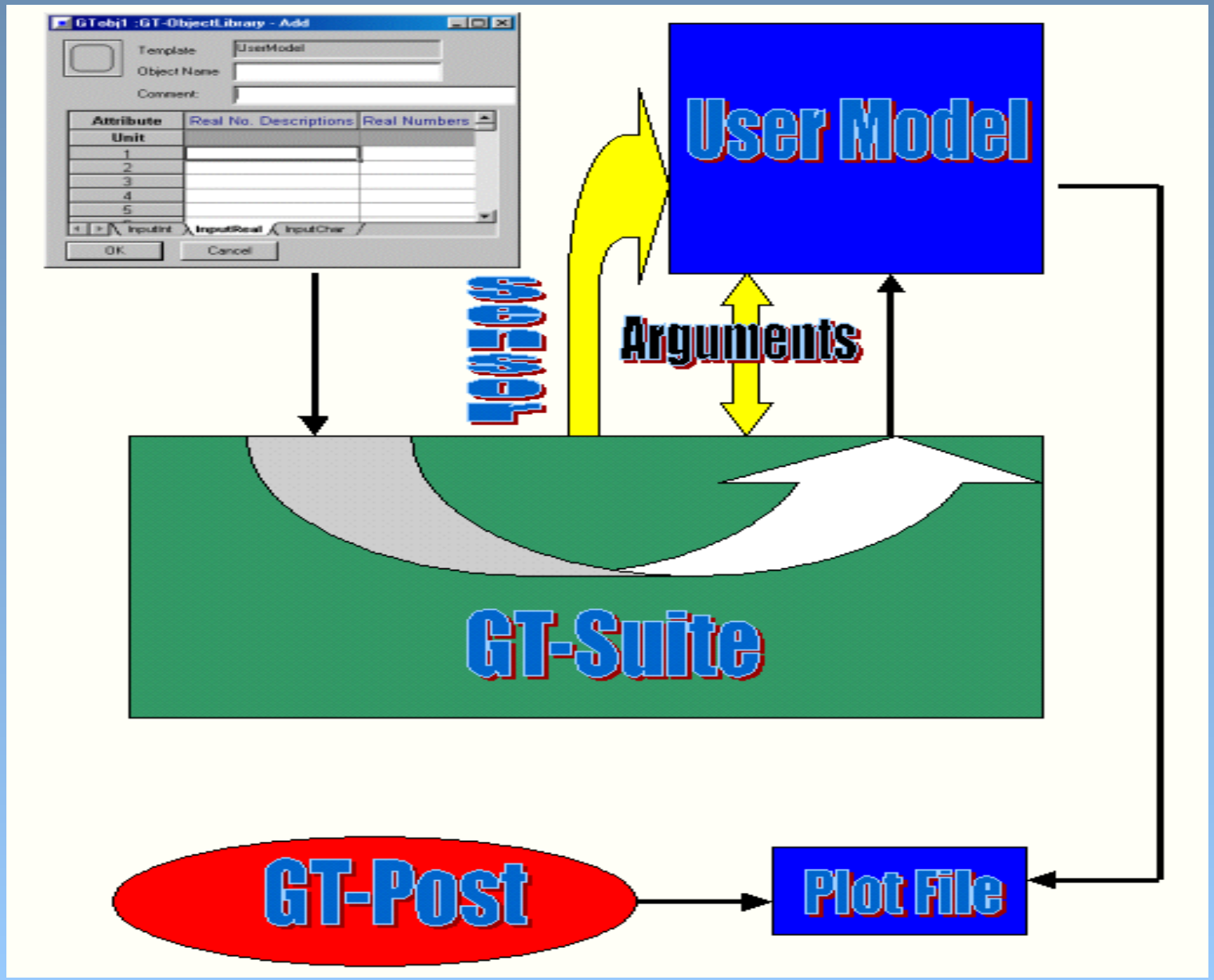
Velocity and Pressure Distribution in a Catalyst



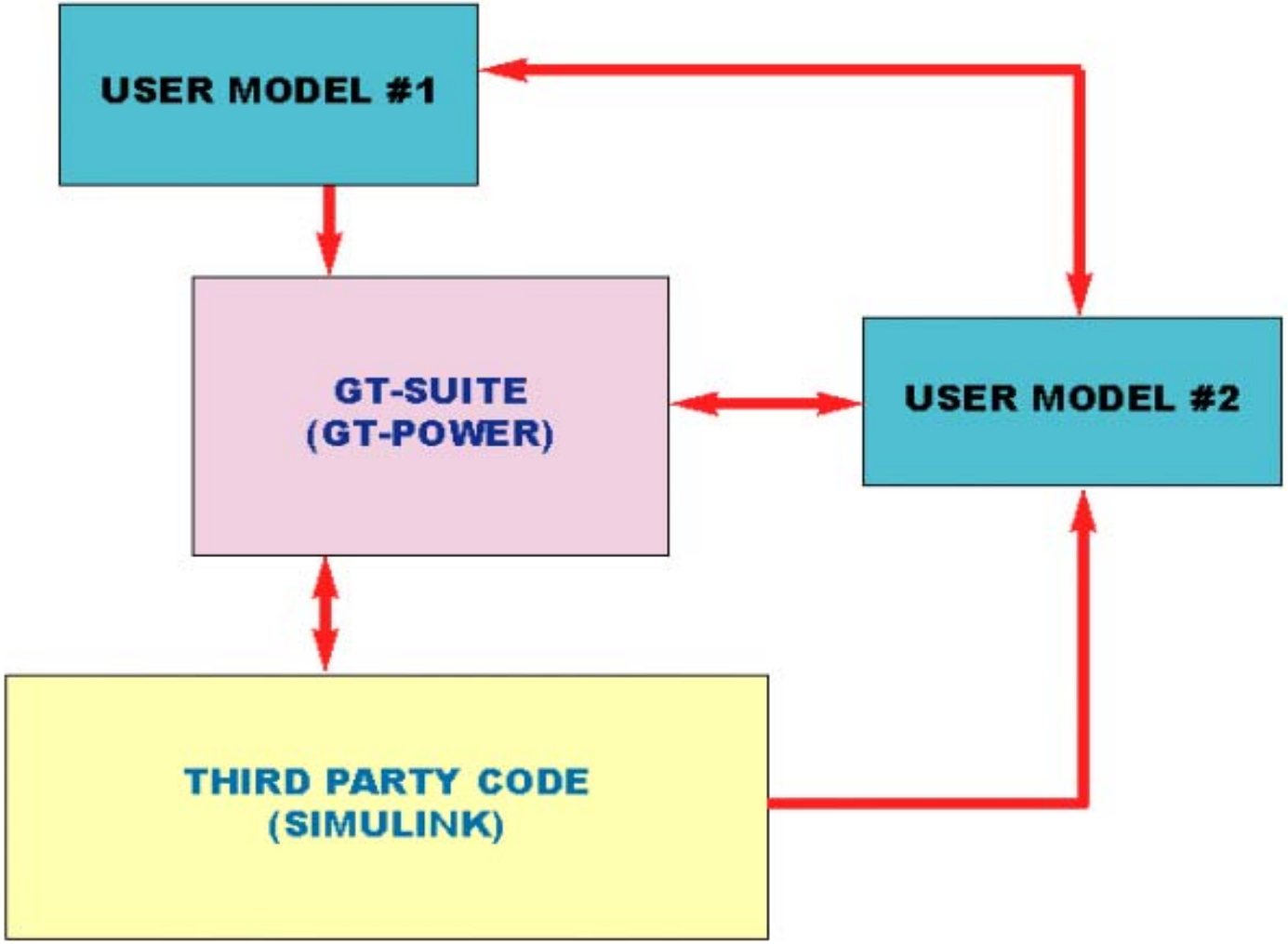
CONVENTIONAL USER MODELS

- Incorporate client-developed models into GT-Suite
- Serves as a bridge to third party software (e.g., Bistro™)
- Can interact with integrated codes (e.g., Simulink, MATRIXx)
- Exchange information through sensors and actuators

UserModel I/O



POSSIBLE INTERACTIONS

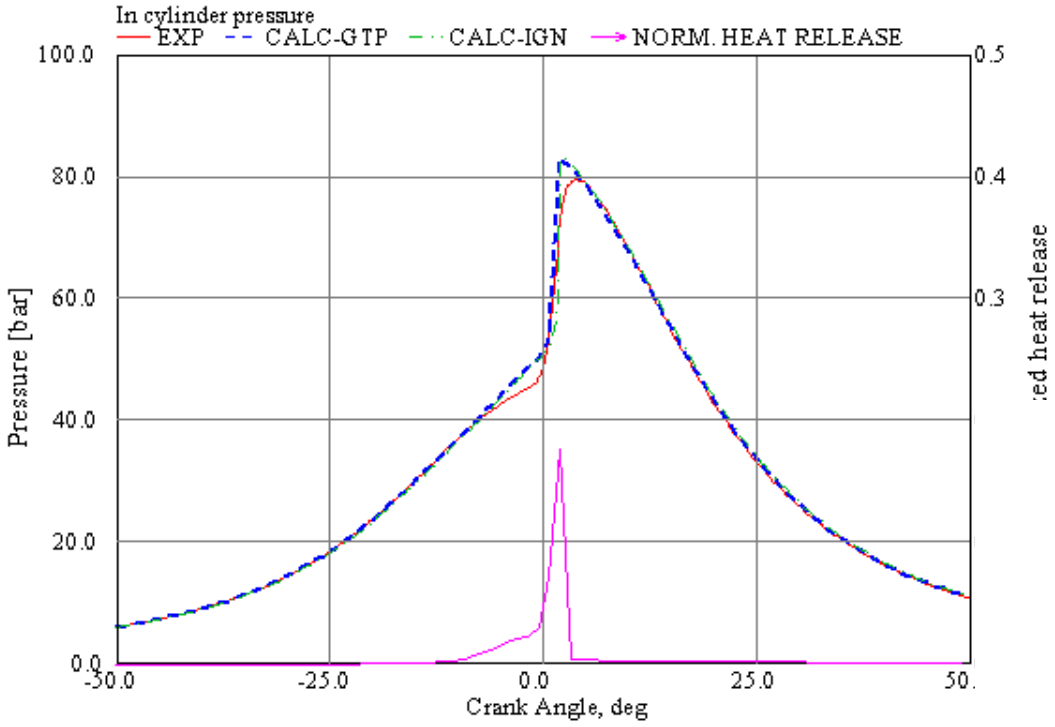


EXAMPLES OF USER MODELS

- Combustion
- Catalysts
- Heat Transfer
- Tumble
- Swirl
- Turbulence
- Scavenging
- Knock
- Turbine
- Compressors

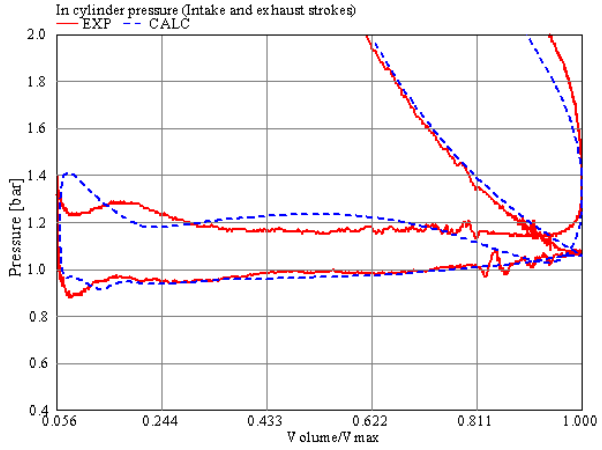
Test case

Model validation:



In cylinder pressure

In cylinder pressure during gas exchange

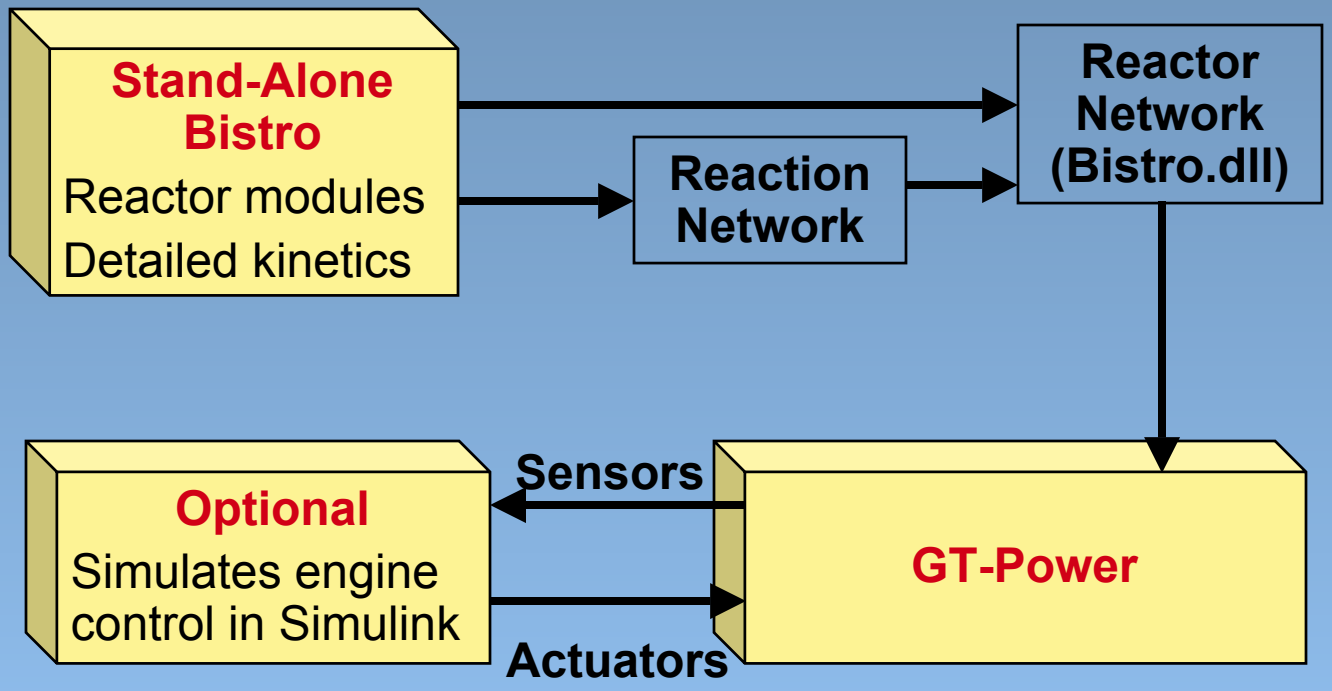


Computational time:

Only GT-Power	**5 s/cycle**	**Pentium IV 2 GHz**
Coupled run	**40 s/cycle**	

The GT-Power/Bistro Framework

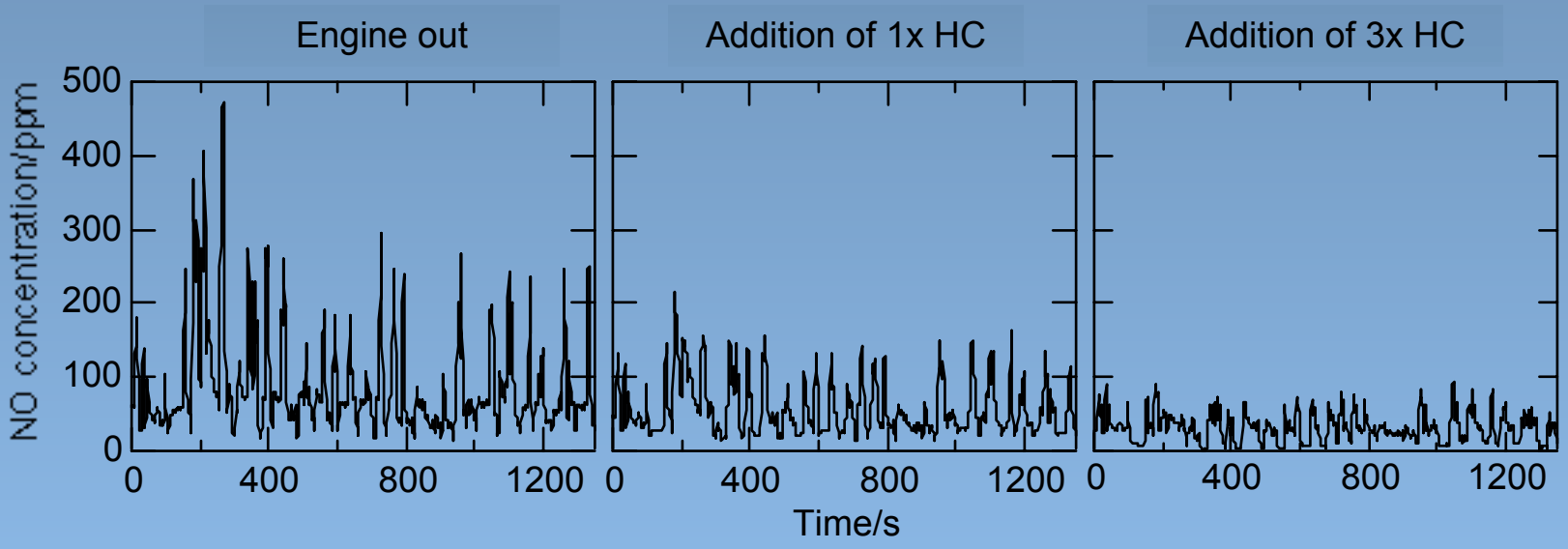
Catalyst models are created with Bistro and "plugged-in" to GT-Power/C-Power models via the UserModel option.



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).

Reactor modeling

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%.

Curtsy of ADL

Conclusions

- **Better in-cylinder models are needed.**
- **There is need for development of improved numerical methods, adaptive (automatically reduced) mechanisms.**

  - 141 species, 1405 reaction, single zone combustion calculation caused a eight to ten fold increase computational time

  - 3-way catalyst,namely 3.0h of calculation time for the first 60secs of an FTP cycle (GT-Power calculation alone took 2 .5h).

Conclusions

- Lack of validation data is a serious bottleneck
- There is no magic bullet solution: it is a field in itself
- 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