Catalyst Modeling Using the GT-Power/Bistro Interface

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The GT-Power-Bistro interface is a powerful and flexible tool with the potential to significantly reduce current powertrain development cycles.

- "In-house" models of aftertreatment systems are typically inadequate for the range of conditions and designs of interest in vehicular applications.
- ADL's Bistro™ is a novel approach to modeling exhaust aftertreatment systems that addresses the deficiencies of conventional models.
- The combination of GT-Power/C-Power and Bistro provides a unique framework for the creation of engine/catalyst/control system models.
- Future versions of GT-Power/Bistro will optimize simulation speed, user-friendliness, and accuracy.

1 Current Situation

2 The Bistro Approach

3 The GT-Power/Bistro Framework

4 Next Steps

“In-house” models of aftertreatment systems are typically inadequate for the range of conditions and designs of interest in vehicular applications.

- Conventional, ad hoc catalyst models can only represent the data over limited ranges and afford no cross-system learning.

- Advanced microkinetics models provide insight into catalyst performance, including degradation, that bears directly on cost, reliability and control.

Conventional, ad hoc catalyst models can only represent the data over limited ranges and afford no cross-system learning.

- In conventional models the parameters in the empirical rate expressions are just fitting coefficients and have no physical meaning.
- Moreover, the form of conventional models is not well adapted to describe transient performance—neither startup nor acceleration.
- Therefore conventional models cannot be tied to the properties or formulation of the catalysts and must be retuned from scratch for each new system.

Example of a conventional expression used to describe the rate of a reaction catalyzed by a catalytic converter

Functional form forces numerical correlation between parameters, making it difficult to determine accurate values

Based only on observable species, ignores available information about surface species

$$r = \frac{k \cdot K \cdot P_{CO} P_{O_2}}{1 + K \cdot P_{CO}}$$

Assumes that adsorption is equilibrated and that surface species are in steady state, precluding accurate description of fast transients

Advanced microkinetics models provide insight into catalyst performance, including degradation, that bears directly on cost, reliability and control.

- Microkinetics models are sets of coupled differential equations built from a fundamental understanding of the chemical steps that occur on the surface of the catalyst.
- The models can be accurate over a wide range of conditions and are intrinsically capable of representing very sharp transients.
- The generality and extensibility of microkinetics models allow simulations that can lead to new catalysts which are cheaper and more robust (different metals, lower loading, use protocols).
- Extending a microkinetics model to include other sorts of reactions, notably catalyst degradation, is straightforward.
- Since the models represent many levels of performance, they can be interrogated to devise model-based control.

Microkinetics network for oxidation of propene

$C_3H_6 + Rh = C_3H_6Rh$
$C_3H_6Rh + Rh = C_3H_5Rh + HRh$
$Rh + C_3H_5Rh = C_2H_4Rh + CHRh$
$C_2H_4Rh + Rh = 2\ CH_2Rh$
$CH_2Rh + Rh = CHRh + HRh$
$CHRh + ORh = CORh + HRh$
$CO + Rh = CORh$
$CORh + ORh = CO_2 + 2\ Rh$
$O_2 + 2\ Rh = O_2Rh_2$
$O_2Rh_2 = 2\ ORh$
$H_2 + Rh = H_2Rh$
$H_2Rh + Rh = 2\ HRh$
$HRh + ORh = OHRh + Rh$
$H_2O + Rh = H_2ORh$
$H_2ORh + ORh = 2\ OHRh$
$HRh + OHRh = H_2ORh + Rh$
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•
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Reactions are not assumed to be equilibrated or irreversible

Reaction rates are expressed in Arrhenius form, $r = A\ \exp(-E_a/RT)$, with parameters derived from transition state theory or fundamental measurements

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ADL's Bistro™ is a novel approach to modeling exhaust aftertreatment systems that addresses the deficiencies of conventional models.

- Reaction equation parameters are easily added, adjusted, and stored through an intuitive, windows-based relational database.
- Overall reaction networks are built from microkinetic subnetworks that are easily extensible to include additional reactions.
- As the overall network is built, it is checked for thermodynamic consistency and physical reasonableness.

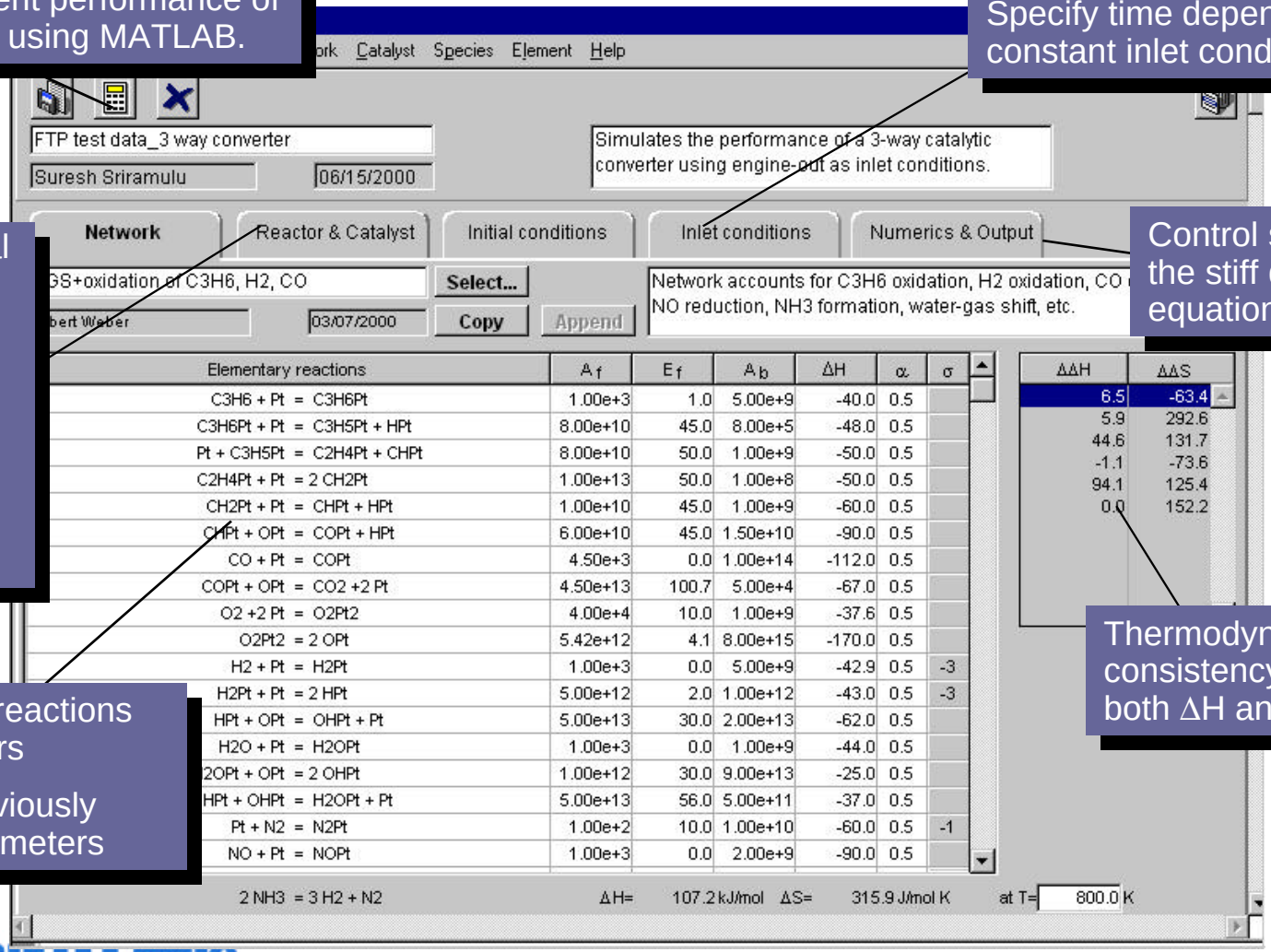
Reaction equation parameters are easily added, adjusted, and stored through an intuitive, windows-based relational database.

Calculate transient performance of chemical reactor using MATLAB.

Specify time dependent or constant inlet conditions

- Thermo-physical properties
- Adiabatic
  - CSTR, PFR, Film PFR
- TPD and TPR
  - CSTR, PFR
  - Sensitivity analysis

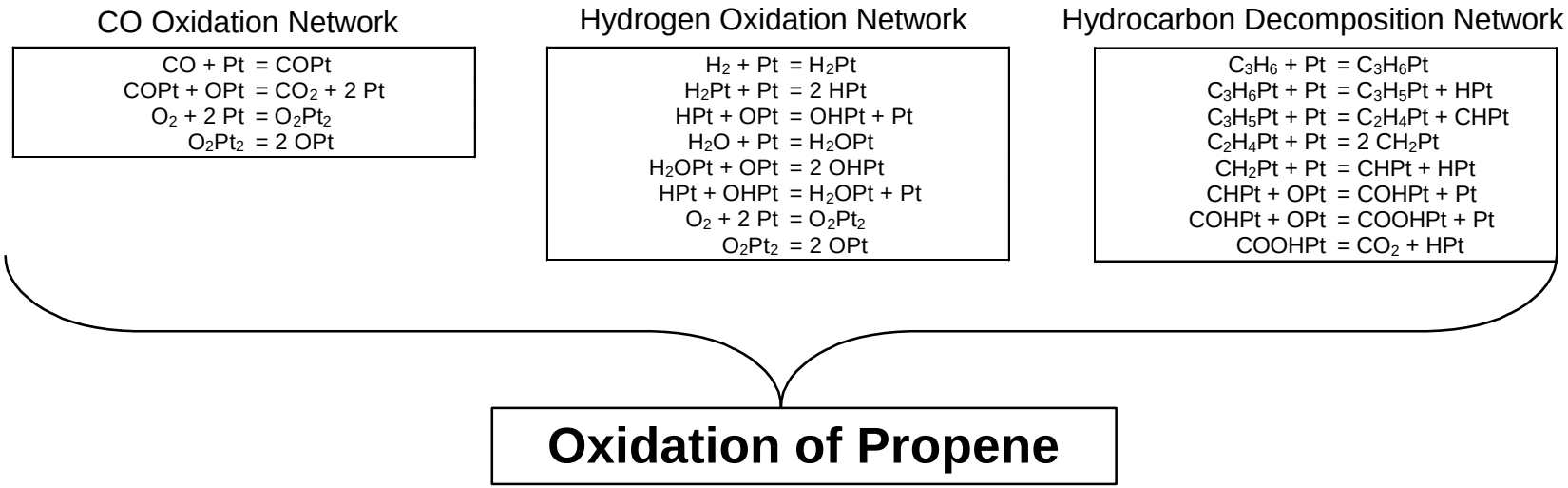
Control solution of the stiff differential equations.



- Easy entry of reactions and parameters
- Re-use of previously validated parameters

Thermodynamic consistency check of both ΔH and ΔS

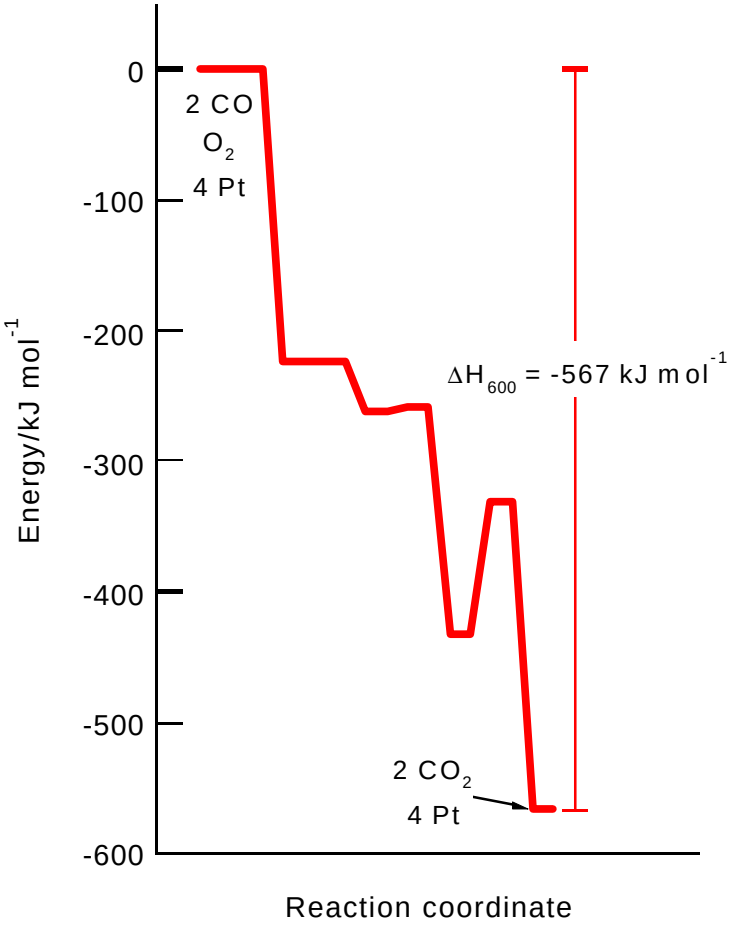
Overall reaction networks are built from microkinetic subnetworks that are easily extensible to include additional reactions.



- Subnetworks are comprised of a sequence of elementary steps, which are hypothesized to proceed molecularly as written.
- No assumptions concerning rate determining reactions, reactions in equilibrium, most abundant surface intermediates, irreversibility, etc.
- The parameters in a microkinetic model have chemical and physical meaning.

As the overall network is built, it is checked for thermodynamic consistency and physical reasonableness.

- Rate parameters for subnetworks are obtained from the literature, quantum chemical modeling, or estimated from transition state theory.
- Subnetworks are constructed, validated against available data, and assembled into larger networks.
- Parameters are deemed to be physically reasonable if they are within the limits expected from transition state theory.
- In the overall chemistry, the activation energies should be comparable to bond strengths.



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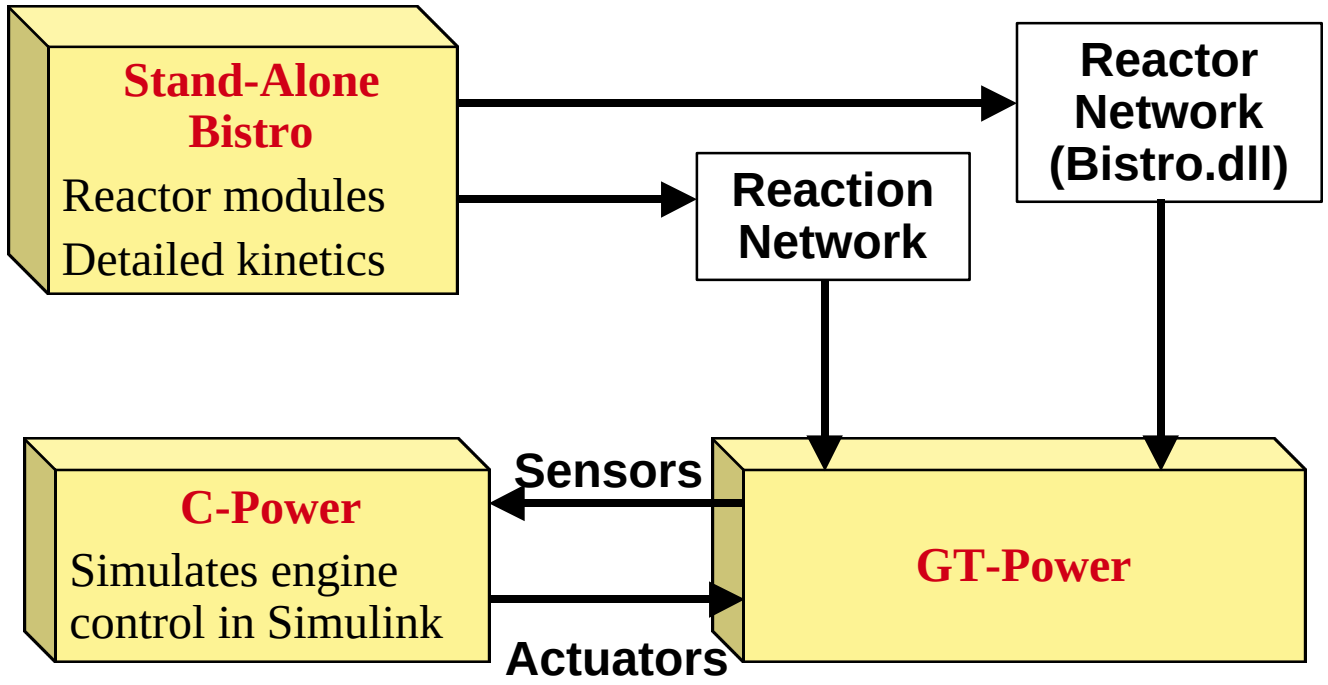
The combination of GT-Power/C-Power and Bistro provides an efficient framework for the creation of engine/catalyst/control system models.

- Catalyst models are created in Bistro and “plugged-in” to GT-Power/C-Power 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 Bistro concentration results are written to output files for post-processing.

Simulation time

Temperature of discretized catalyst volumes

Mole fractions of species at the catalyst exit

el - results_outlet.txt

File Edit View Insert Format Tools Data

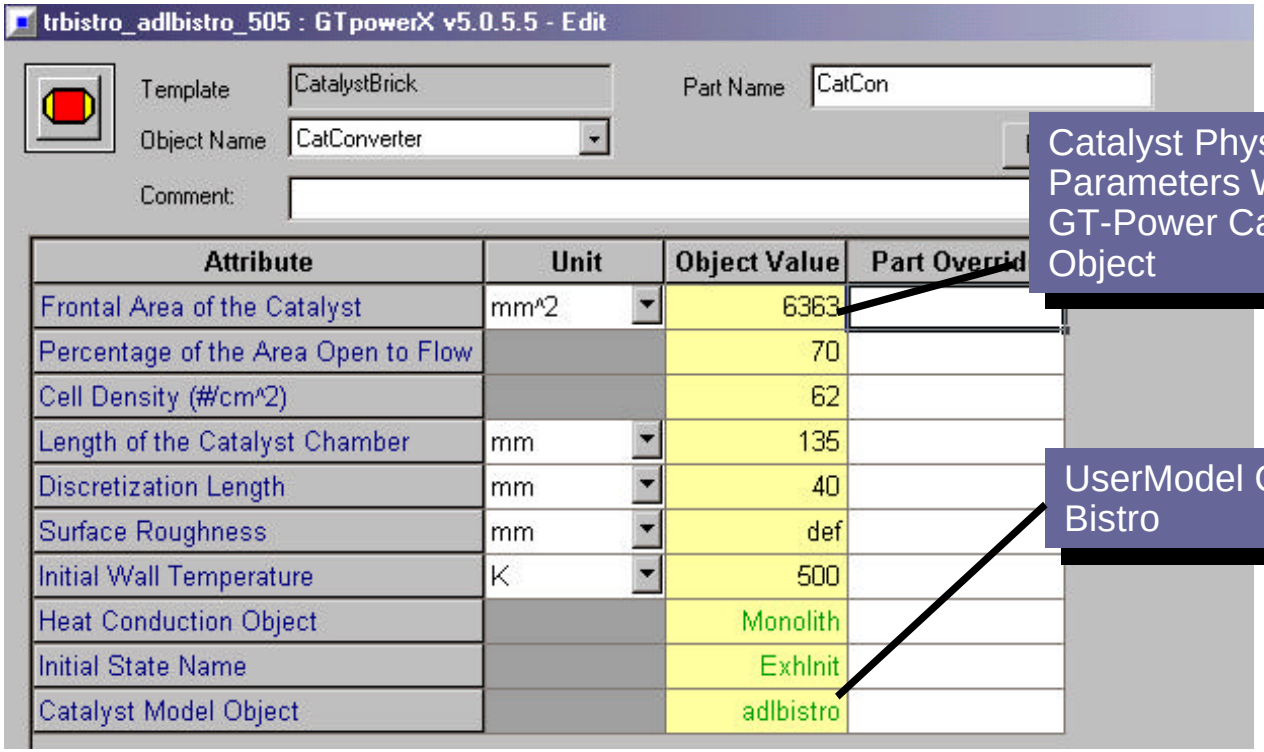
Arial 10 100%

A1 = Time

	A	B	C	D	E	F	G	H	I	J	K	L
1	Time	Temp_1	Temp_2	Temp_3	Temp_4	H2	H2O	O2	NO	N2	CO	CO2
2	seconds	Kelvin	Kelvin	Kelvin	Kelvin	Mole_Frac	Mole_Frac	Mole_Frac	Mole_Frac	Mole_Frac	Mole_Frac	Mole_Fr
3	0.00E+00	6.00E+02	6.00E+02	6.00E+02	6.00E+02	-1.30E-15	3.43E-12	5.53E-02	1.76E-02	9.28E-01	1.00E-21	7.05E-2
4	1.00E+00	6.00E+02	6.00E+02	6.00E+02	6.00E+02	2.14E-33	1.80E-18	5.54E-02	1.76E-02	9.28E-01	-1.74E-31	-7.28E-2
5	2.00E+00	6.00E+02	6.00E+02	6.00E+02	6.00E+02	7.16E-34	2.01E-18	4.42E-02	1.89E-02	9.38E-01	1.12E-32	-3.50E-2
6	3.00E+00	6.00E+02	6.00E+02	6.00E+02	6.00E+02	5.73E-34	2.14E-18	4.42E-02	1.89E-02	9.38E-01	-1.22E-33	-1.59E-2
7	4.00E+00	6.00E+02	6.00E+02	6.00E+02	6.00E+02	4.78E-34	2.22E-18	4.42E-02	1.89E-02	9.38E-01	8.27E-35	8.08E-3
8	5.00E+00	6.00E+02	6.00E+02	6.00E+02	6.00E+02	4.11E-34	2.28E-18	4.42E-02	1.89E-02	9.38E-01	-3.64E-34	1.41E-2
9	6.00E+00	6.00E+02	6.00E+02	6.00E+02	6.00E+02	3.60E-34	2.33E-18	4.42E-02	1.89E-02	9.38E-01	-1.31E-34	-1.73E-2
10	7.00E+00	6.00E+02	6.00E+02	6.00E+02	6.00E+02	3.20E-34	2.37E-18	4.42E-02	1.89E-02	9.38E-01	3.13E-34	-1.51E-2
11	8.00E+00	6.00E+02	6.00E+02	6.00E+02	6.00E+02	2.88E-34	2.40E-18	4.42E-02	1.89E-02	9.38E-01	4.92E-34	8.17E-2
12	9.00E+00	6.00E+02	6.00E+02	6.00E+02	6.00E+02	2.62E-34	2.42E-18	4.42E-02	1.89E-02	9.38E-01	4.01E-35	8.69E-2
13	1.00E+01	6.00E+02	6.00E+02	6.00E+02	6.00E+02	2.41E-34	2.44E-18	4.42E-02	1.89E-02	9.38E-01	-1.48E-34	-2.09E-2

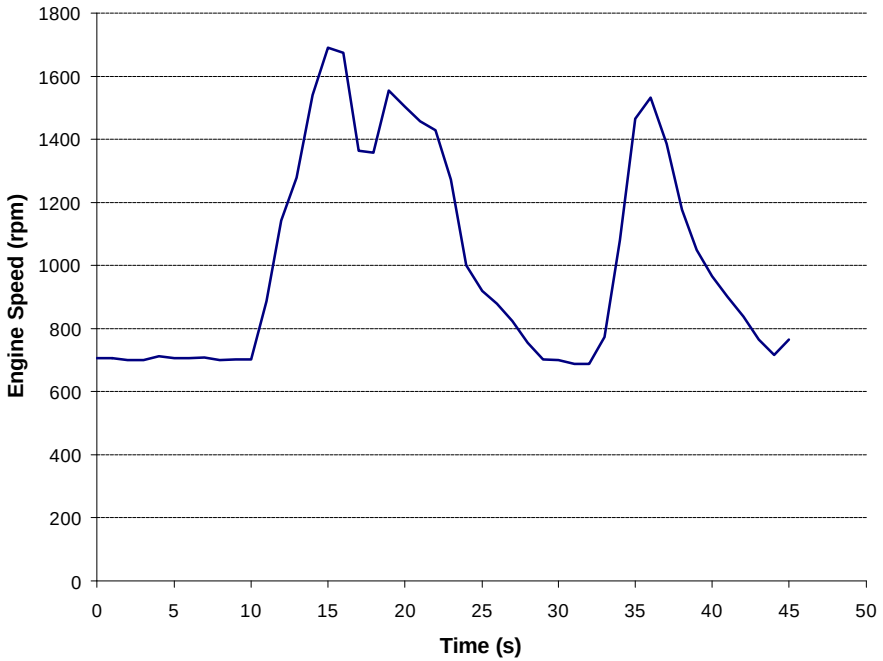
Future enhancements will include post-processing of Bistro results from within GT-Power.

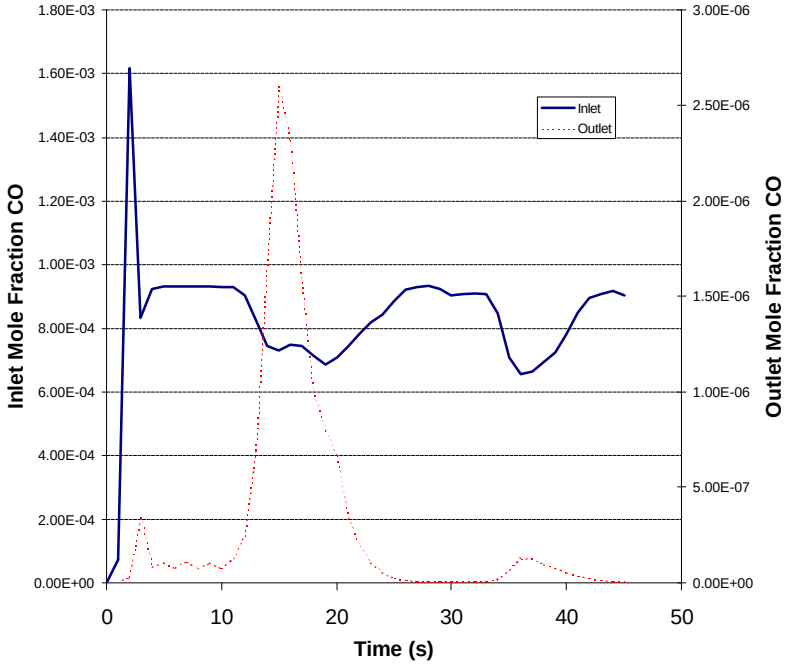
Through GT-Power, the user can adjust many of the physical parameters of the catalyst such as length, cell density, initial substrate temperature...



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

….and study the subsequent effect on catalyst performance.





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Future versions of GT-Power/Bistro will optimize simulation speed, user-friendliness, and accuracy.

- Currently, there is a trade-off between the temporal resolution of the catalyst model and computation time, which can be optimized in the future.
  –
- In future embodiments, the interface will be more closely incorporated into the GT-Power GUI.
  – Reference module instead of a user module
  – Graphical output interface
- A truly accurate representation of the catalyst can be achieved only if we succeed in modeling all of the complications of the exhaust system.
  – Speciated hydrocarbons in exhaust stream
  – NOx speciation
  – Higher dimensionality flow models

The GT-Power-Bistro interface is a powerful and flexible tool with the potential to significantly reduce current powertrain development cycles.

- ADL's Bistro offers several advantages over typical ad hoc models and extends the modeling capability of GT-Power.
- The modularity of GT-Power/Bistro/and C-Power can be used to appropriately leverage expertise within an enterprise.
- A demonstration version of a Bistro reactor and reaction network will be distributed with GT-Power.
- Arthur D. Little is ready to help organizations create customized catalyst models for their own specific applications.