Machine Learning in Process Systems Engineering:
Opportunities and Challenges

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AI and ML in PSE

- AI & ML in PSE is a 35-year old idea with many success stories
- What is new and exciting is the availability of
  - Lots of data
  - New algorithms
  - New languages
  - Cheap & powerful computational/communication resources
- Barriers of entry lower now
  - My students used to program in Lisp to do AI & ML
- What took us months to accomplish can be done in days or hours now
- We have entered the "Watson" Era in PSE
- New Opportunities & Challenges

AI and ML in a "Big Data" Era: Importance of Hybrid Models

- Machine learning provides tools for learning Input-Output correlations
- But it's not the mere correlations that we want
  - Target vs ExxonMobil
  - Consumer behavior vs Catalyst design
  - Diaper-Beer vs Yield-Selectivity
- What are the fundamental physics/chemistry/biology principles and mechanisms?
- Desire in-depth knowledge of the phenomena
  - Mechanistic, first-principles based, understanding
  - Makes hybrid models very important: Mechanistic + Data Science
- To have confidence and explanatory power when we make decisions about design, control, optimization, and safety
- How do we go from Big Data to Deep Models and Insights quickly?

*V. Venkatasubramanian, "Drowning in Data: Informatics and Modelling Challenges in a Data-Rich Networked World", Perspective Article, AIChE J., **2009.***

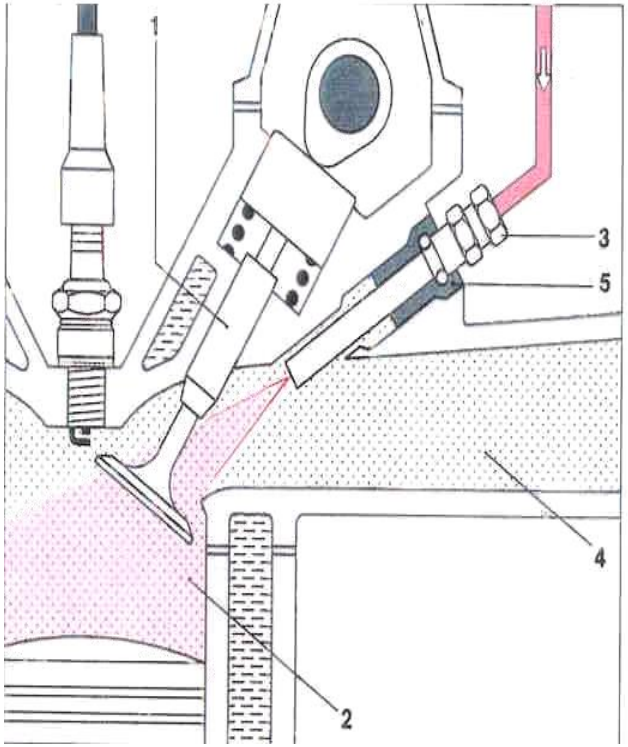
What is Watson?

- Question answering (QA) AI system built by IBM
- Advanced Natural Language Processing, Information Retrieval, Knowledge Representation and Reasoning, and Machine Learning technologies
- ~100 different techniques used to analyze natural language, generate hypotheses, score evidence, and merge and rank hypotheses

"Watson" for PSE?

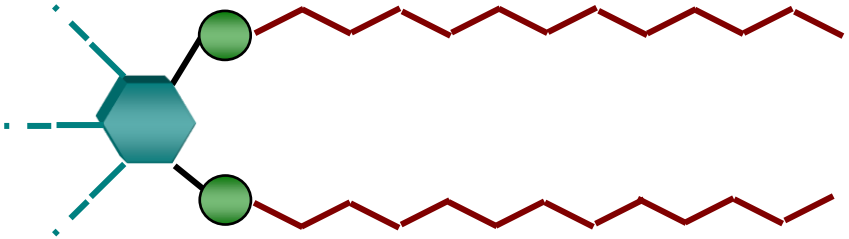
- What will it take to develop "Watson" for PSE?
- Can we develop "Watson" for fault diagnosis, risk analysis, materials design, etc.?
- More challenging than Watson for Jeopardy
  - Not just qualitative facts
  - Quantitative
  - Math Models
  - Charts, Tables, Spectra
  - Heuristic Knowledge

LUBRIZOL: AI for Fuel Additive Design (1995-99)



Mixture formation
1 Intake valve
2 Combustion chamber
3 Fuel-injection valve
4 Intake manifold (tube)
5 Heat-isolating mount

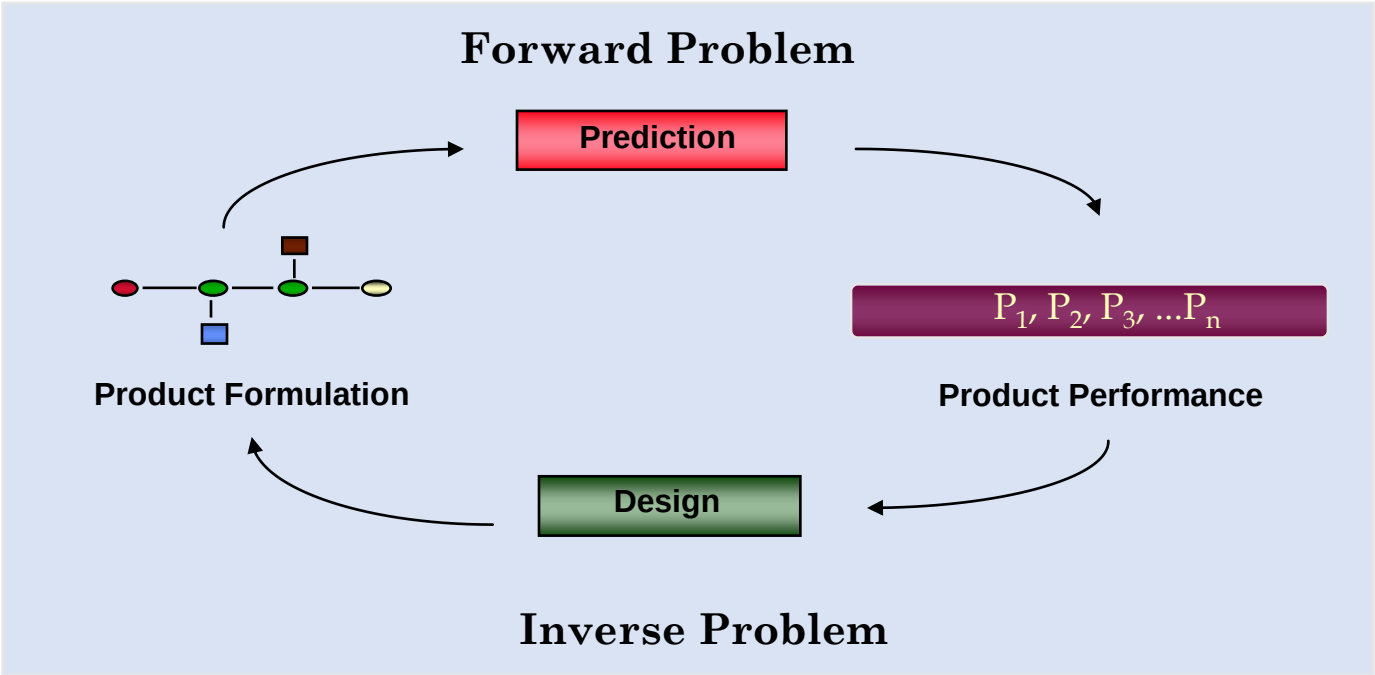
Intake Valve and Manifold



- **EPA Performance Measure**
  - BMW Test for Intake Valve Deposit
  - Stipulated to be less than 100 mg over a 10,000 mile road test
- Fuel-additives are added to gasoline to minimize IVD
- **Expensive testing**
  - Around $10K for a single datum
- **Molecular Product Design Problem:** ***Design fuel-additives that meet desired IVD performance levels***

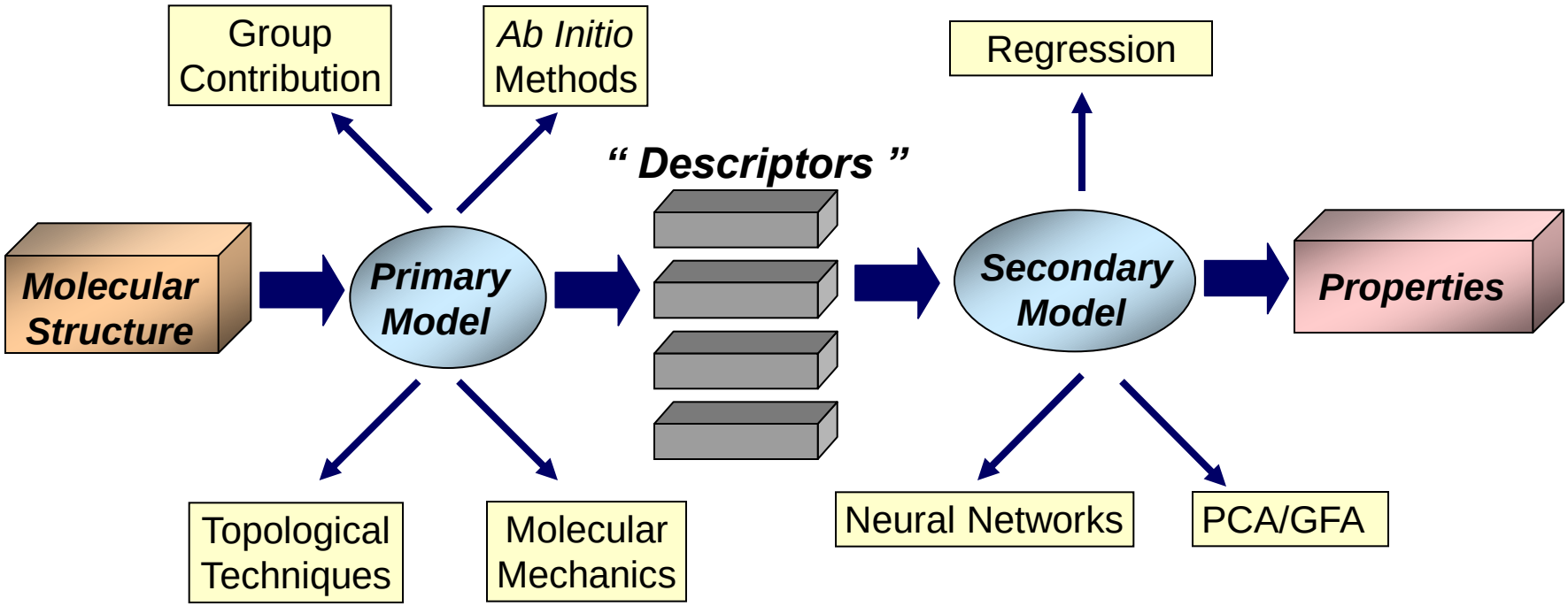
Sundaram, A., Ghosh, P., Caruthers, J.M. and Venkatasubramanian, V., "Design of Fuel Additives Using Neural Networks and Evolutionary Algorithms", *AICHE J.*, 47 (6), pp. 1387 – 1406, **2001.**

Product Formulation and Design

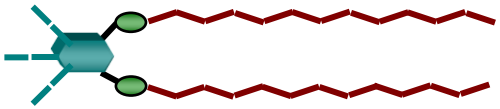


- Forward Problem: Prediction
  - Estimate Product Performance from Formulation
- Inverse Problem: Design
  - Determine a set of products that satisfy desired performance criteria

Hybrid Model: First-principles + Data Science

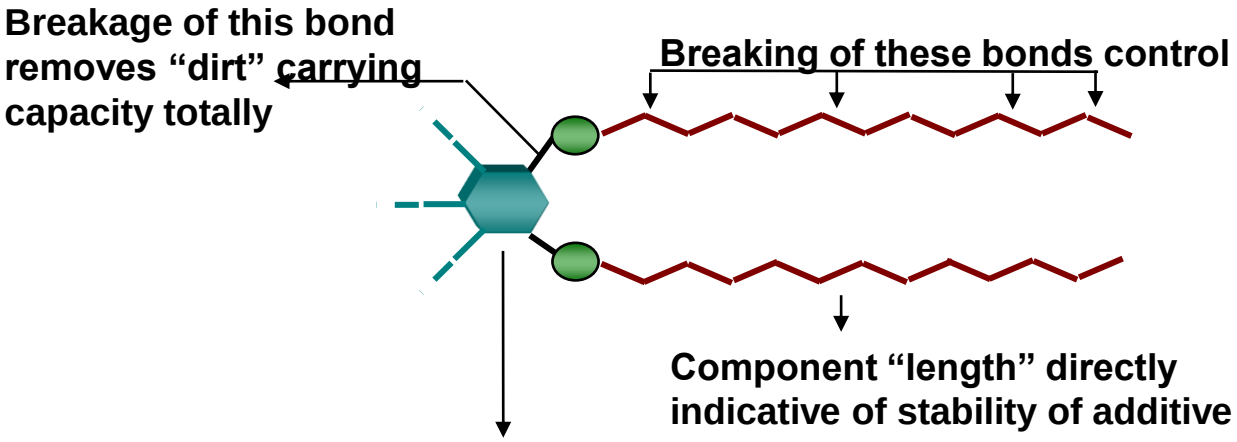


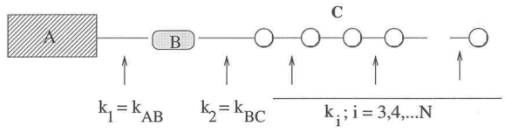
First-principles Model:
Polymer link breakage dynamics



Data Science Model

First-Principles Model for Additive Degradation: Population Balance Equations





- First-principles model
- Tracks the structural distribution of fuel-additive with time due to reactive degradation

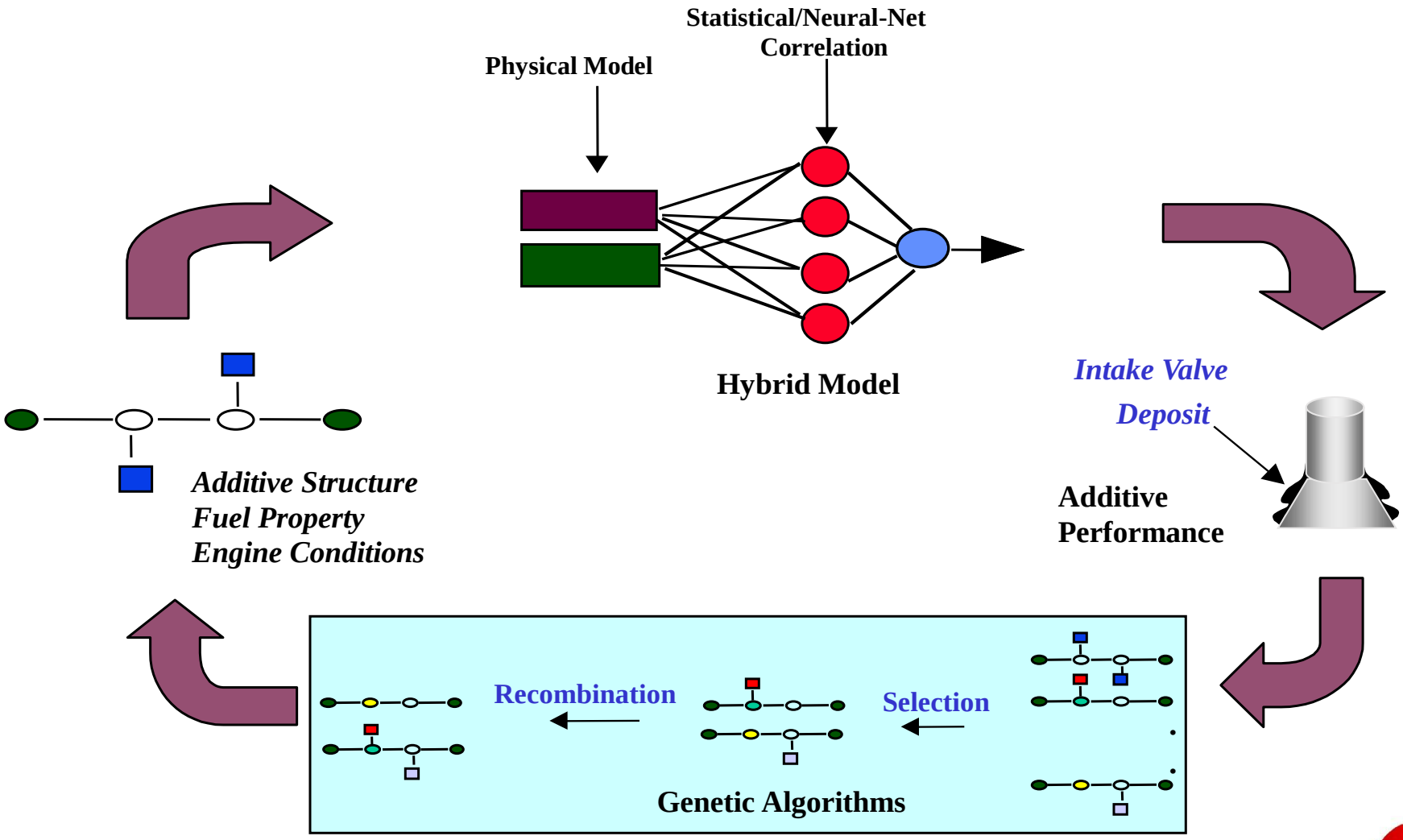
$$\frac{d\mathbf{X}}{d\tau} = A \bullet \mathbf{X};\ \mathbf{A} = \begin{bmatrix} -k_1 & k_2 & k_3 & \cdots & k_N \\ 0 & -k_1-k_2 & k_2 & \cdots & k_N \\ \cdot & 0 & -k_1-k_2-k_3 & k_3 & \cdots & k_N \\ \cdot & \cdot & 0 & \cdots & k_N \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdot & -\sum_{i\le j} k_i & k_{i+1} & \cdots & k_N \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ 0 & 0 & 0 & 0\ 0 & 0 & \cdots & -\sum_{i=1}^{N} k_i \end{bmatrix};\ \mathbf{X} = \begin{bmatrix} X_1 \\ X_2 \\ X_3 \\ \cdot \\ X_j \\ \cdot \\ X_N \end{bmatrix}$$

$$X_0 = \sum_{i=1}^{N} k_i * X_i$$

$$\mathbf{X}(\tau = 0) = \mathbf{P}(\mu, \sigma)$$

Population Balance Eqns

Discovery Analytics for Fuel-Additives Design



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CRIS.lab

Objective: Determine a structure with IVD < 10 mg

Rank/Identifier	Fitness	Predicted IVD	Structural Description
III-1	1.000	8.9 mg	**Novel Structure New Chemistry**
I-2	0.996	11.5 mg	**Novel Structure New Chemistry**
I-6	0.993	12.0 mg	Found by the traditional approach also

Found new candidates in minutes

Opened up new possibilities: New Insights

Think "Out of the Box"

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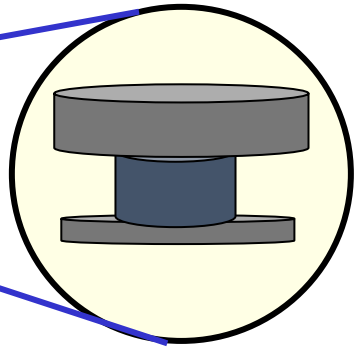
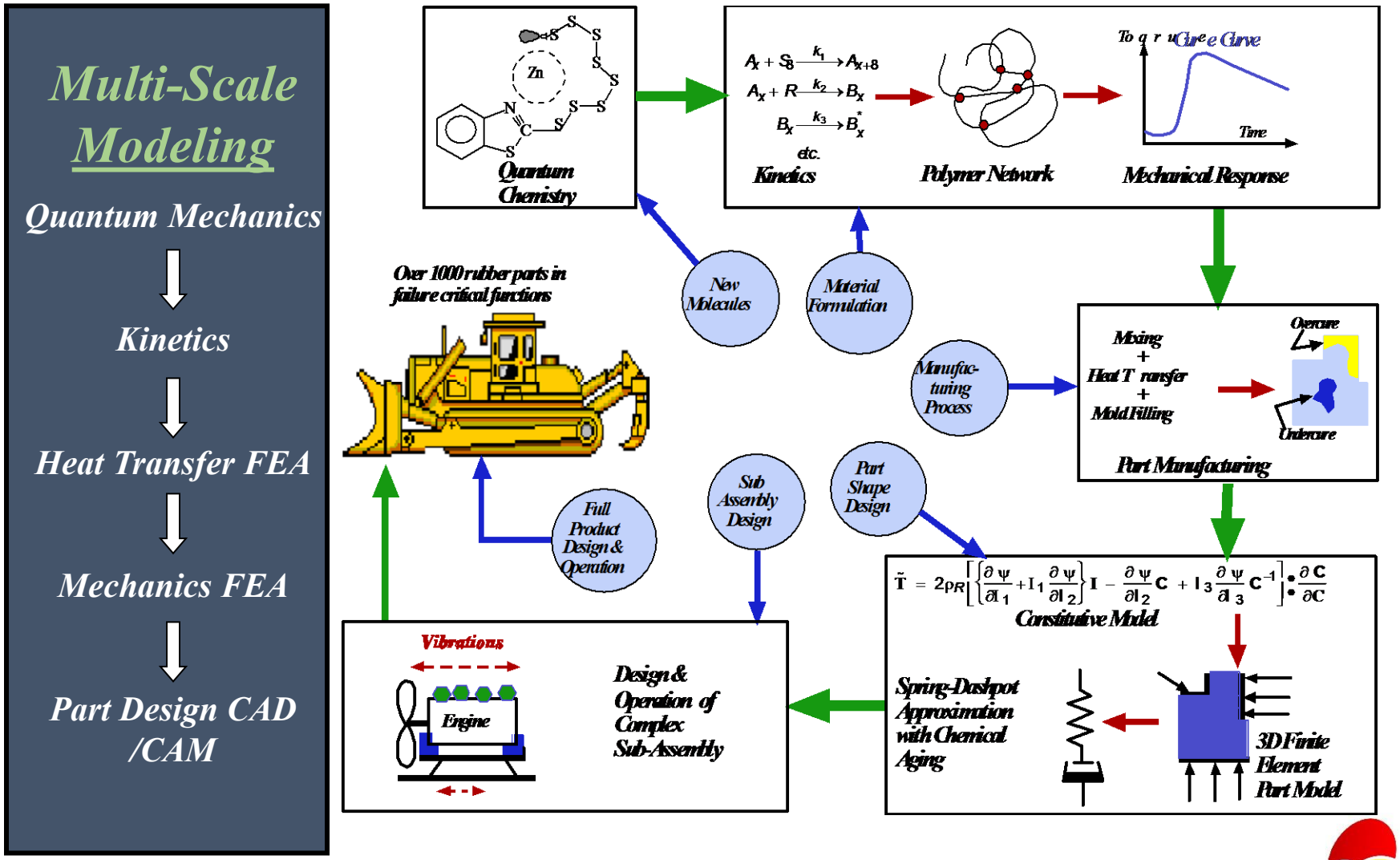
CATERPILLAR (1998-2001)

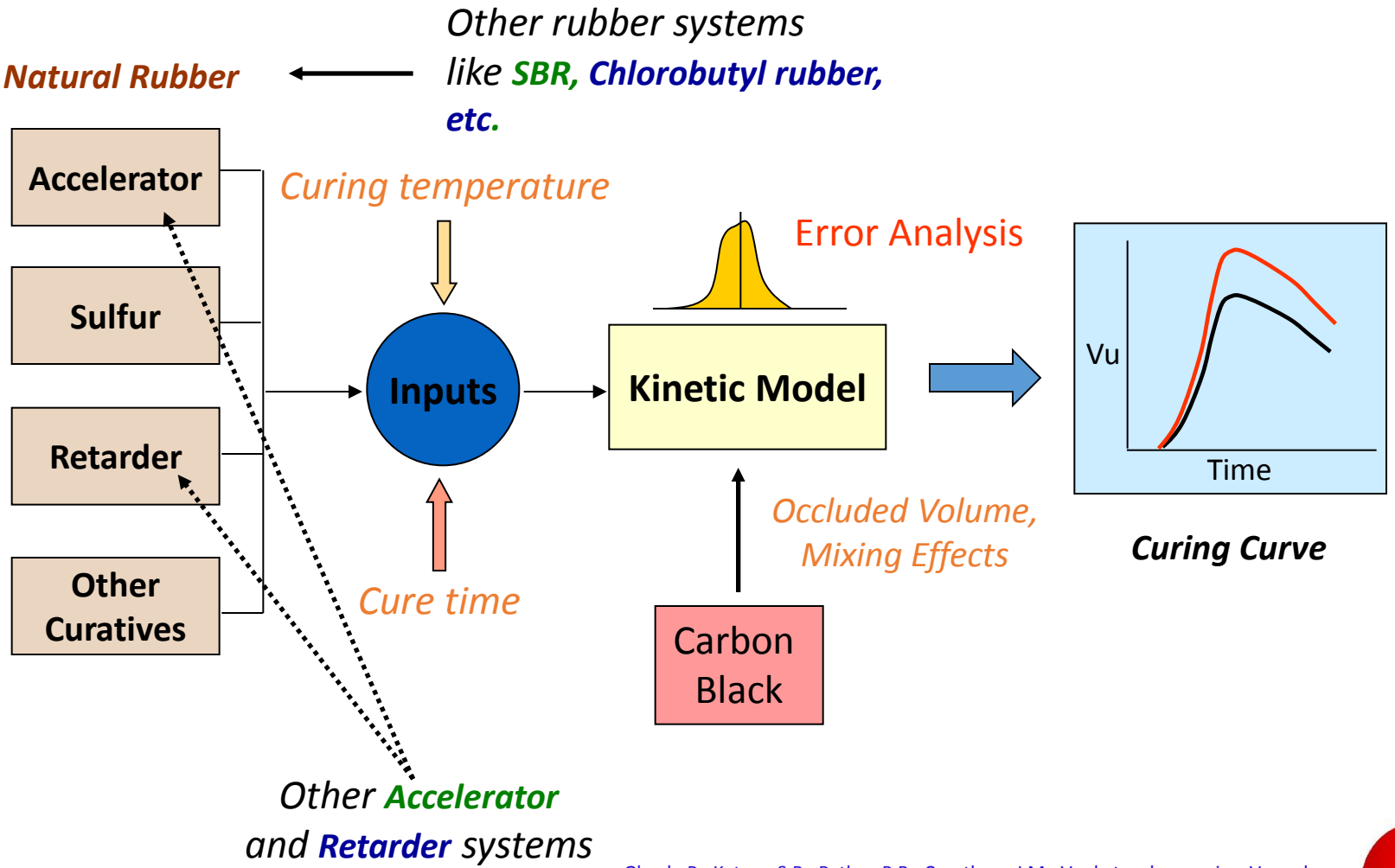


- About 1000 Rubber Parts in Failure Critical Functions
- Tires, Treads, Hoses, Shock Absorbers, O-rings, Gaskets, Mounts …
- Reliability and Warranty Problems

Caterpillar's Multi-Scale Modeling Challenge: Design of Formulated Rubber Parts



Forward Model: First-principles



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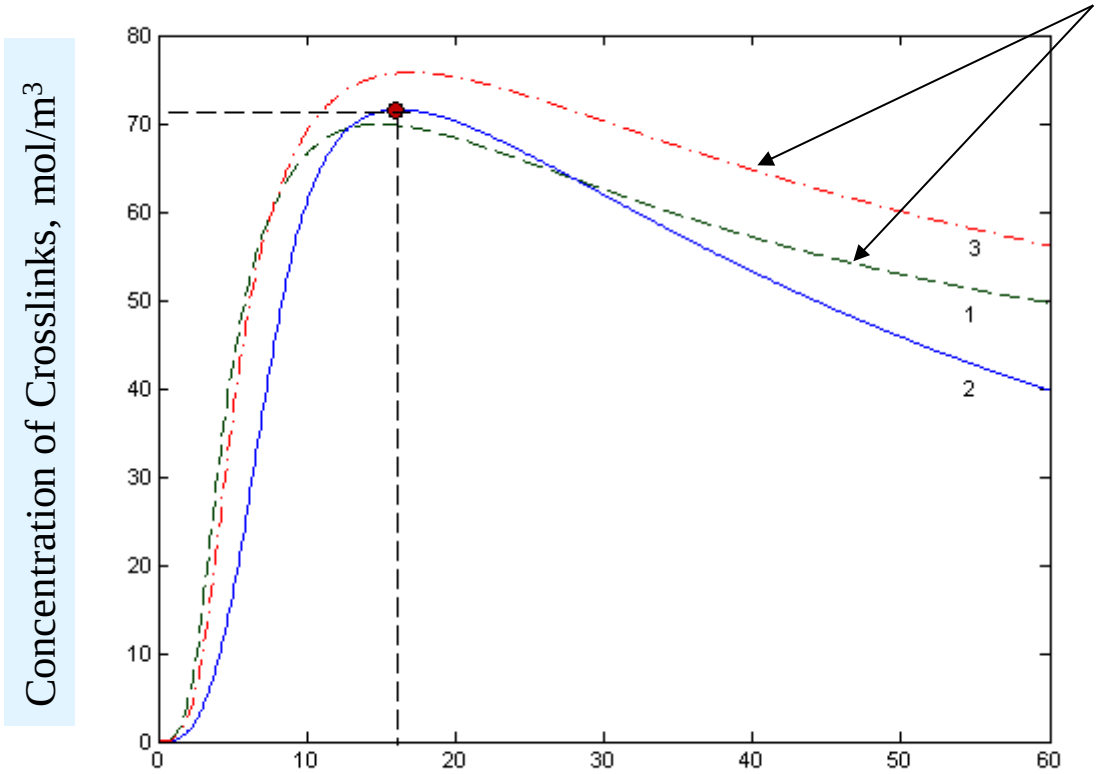
Inverse Problem Solution

Formulation	Fitness	T_{max}	Vu_{max}	σ_{100}	σ_{200}
[1.75 1.25 0.05 0 315]	0.9999	15	69.92	0.91	1.63
[0.50 4.00 0.10 0 310]	0.9999	16	71.57	0.92	1.65
[1.75 1.50 0.05 0 310]	0.9996	17	75.75	0.97	1.75
[0.75 2.75 0.10 0 315]	0.9994	13	67.88	0.88	1.58



New Formulations

Better Formulations

Designed in hours instead of about 2 weeks taken by human experts

Used daily at Caterpillar

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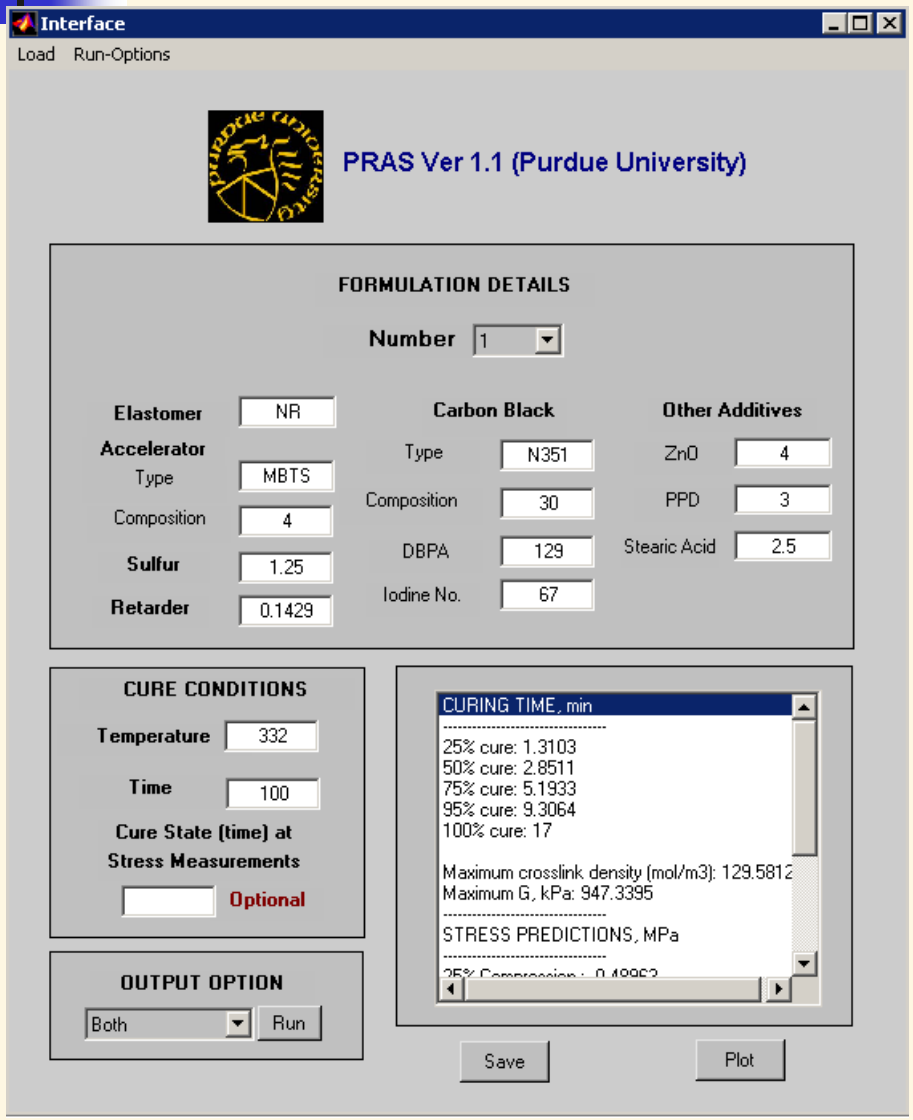
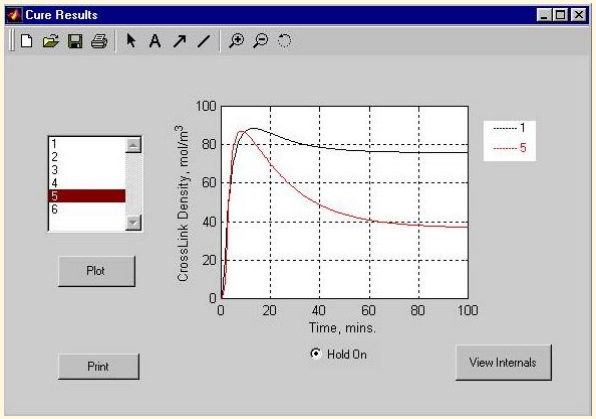
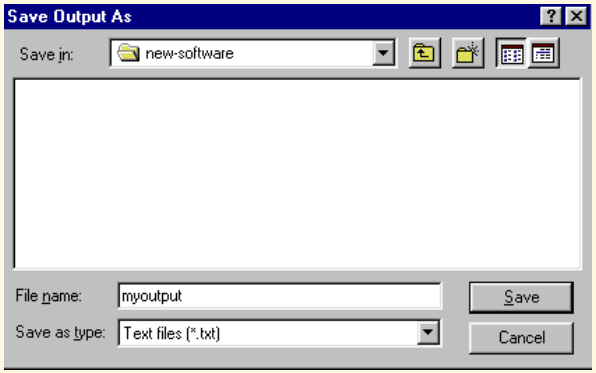
CRIS.lab

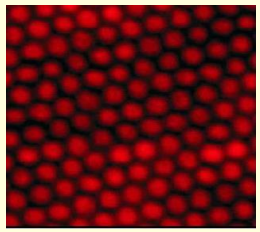
AI System Used at Caterpillar on a Daily Basis



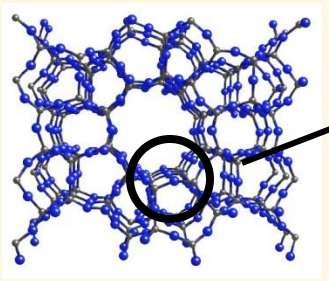


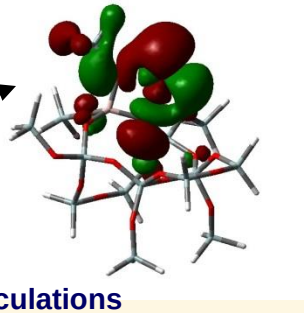


ExxonMobil's Grand Challenge: Catalyst Design via Combinatorial Chemistry



Catalyst Structures





Quantum calculations

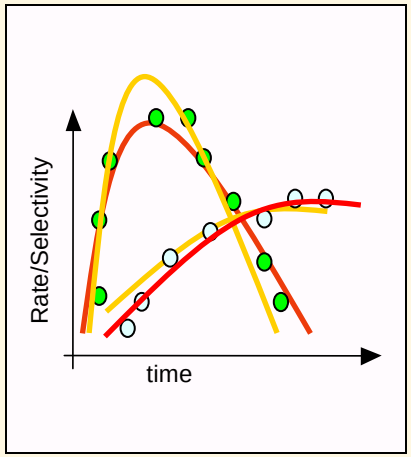
d band center
Electronegativity
⋮
Electronic/Structural descriptors

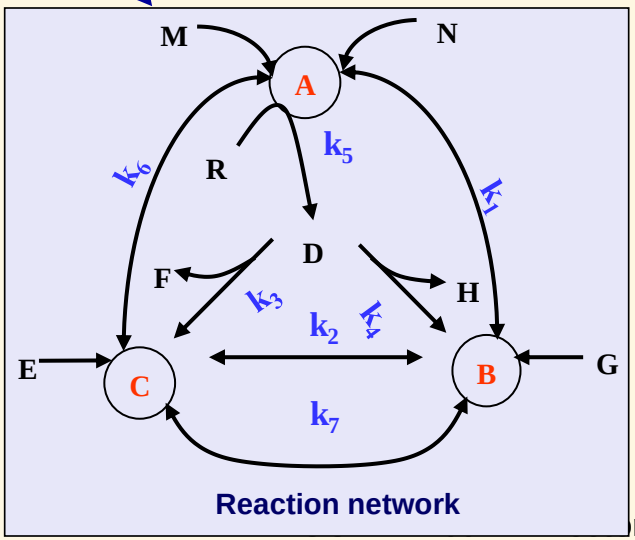
Fundamental Chemistry

Reaction kinetics

Performance measures

Synthesis Characterization





Reaction network

Paraffin Aromatization

- Identify a catalyst formulation for light paraffin aromatization that is superior to Ga/H-ZSM-5 in terms of:
  - Higher Benzene, Toluene, Xylene (B/T/X) selectivity
  - Higher Hydrogen selectivity

- Microkinetic model development for the kinetic description of the system

Caruthers, J.M., Lauterbach, J.A., Thomson, K.T., Venkatasubramanian, V., Snively, C.M., Bhan, A., Katare, S. and Oskarsdottir, G., "Catalyst Design: Knowledge Extraction from High Throughput Experimentation", *Journal of Catalysis*, vol. 216/1-2, pp. 98 – 109, **2003**.

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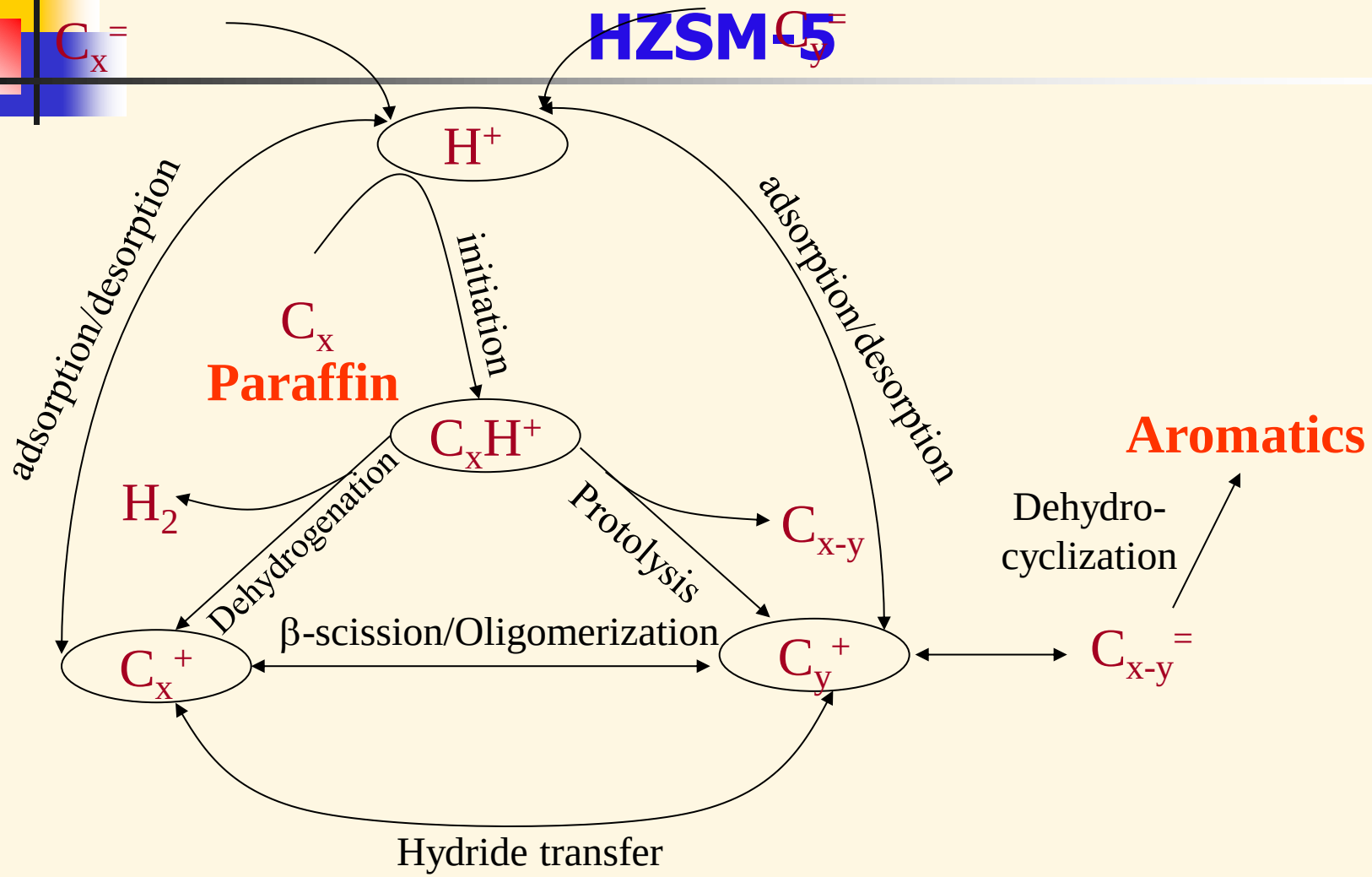
Reaction Network – Propane Aromatization on HZSM-5



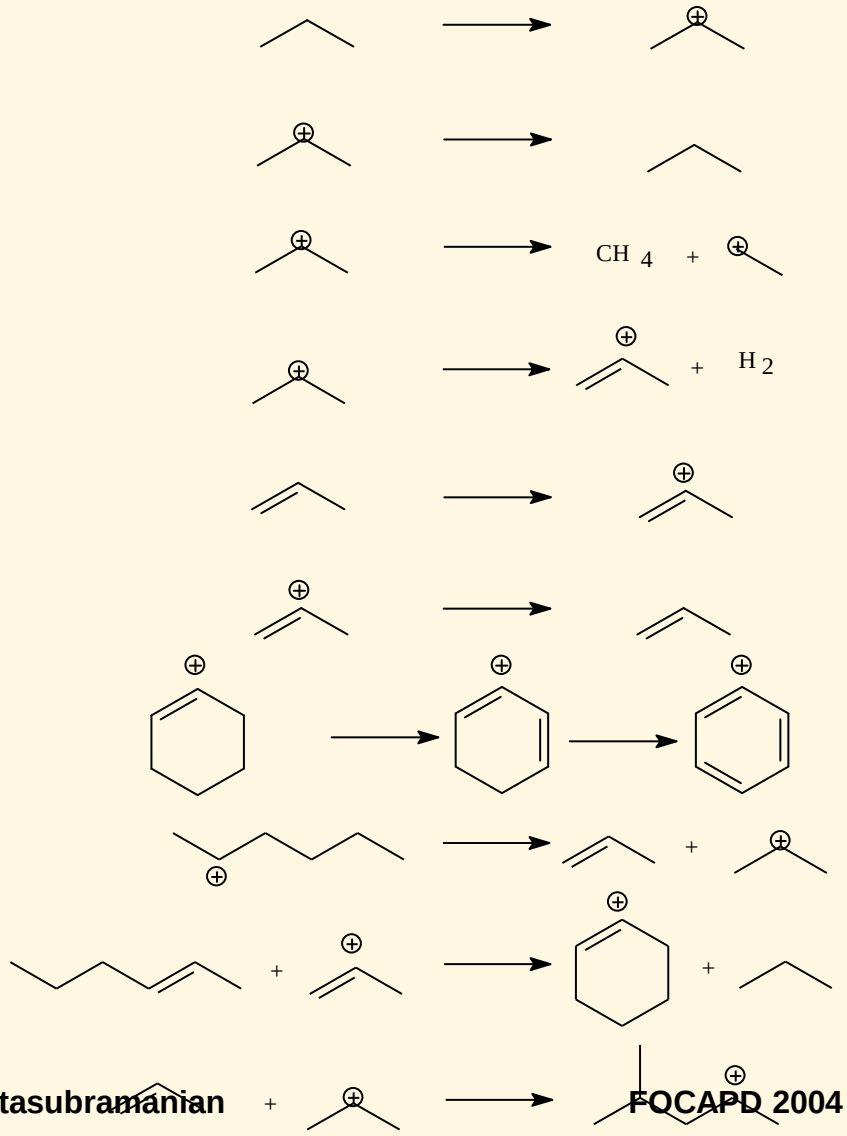
- 31 gas phase species + 29 surface species + 271 reaction steps
- Model with 31 ODEs, 29 algebraic equations
- 13 parameters with up to 10 orders of magnitude bounds on each

Chemistry Rules for Propane Aromatization on HZSM-5

Chemistry Rules

1. Alkane adsorption
2. Alkane desorption
3. Carbonium ion protolysis
4. Carbonium ion dehydrogenation
5. Olefin adsorption
6. Olefin desorption
7. Aromatization
8. Beta-Scission
9. Hydride Transfer
10. Oligomerization

Representative Chemical Reactions



Reaction Modeling Suite (RMS)

English Language Rules

Chemistry

8. Beta Scission
transforms a carbenium ion into a smaller carbenium ion and an olefin

Grouping

8. a. Formation of a secondary carbenium ion
is 20 times faster than a primary carbenium ion

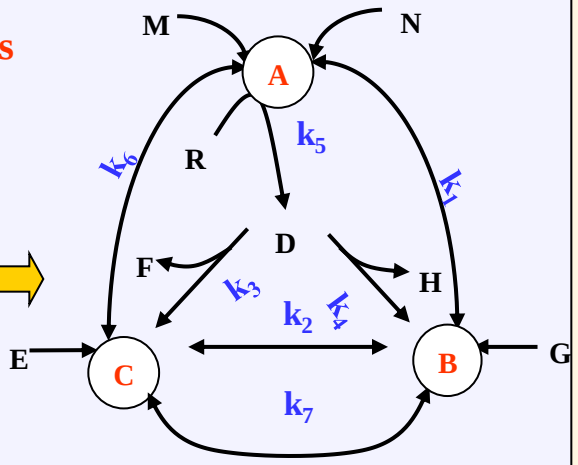
b. Formation of a tertiary carbenium ion
is 60 times faster than a primary carbenium ion

Reaction Description Language Plus

Beta Scission
Label-site c1+ (find positive carbon)
Label-site c2 (find neutral-carbon attached-to c1+)
Label-site c3 (find neutral-carbon attached-to c2)
Forbid (primary c3)
Forbid (less-than (size-of reactant) 9)
Disconnect c2 c3)
Increase-order-of (find bond connecting c1+ c2)
Add-charge c3
Subtract-charge c1+

Beta Scission
Label-site c1+ (find positive carbon)
Require (c1+ primary and product)
set-k k1
Label-site c2+ (find positive carbon)
Require (c2+ secondary and product)
set-k 20*k1
Label-site c3+ (find positive carbon)
Require (c2+ tertiary and product)
set-k 60*k1

Reaction Network



Model Generator

Mathematical Equations

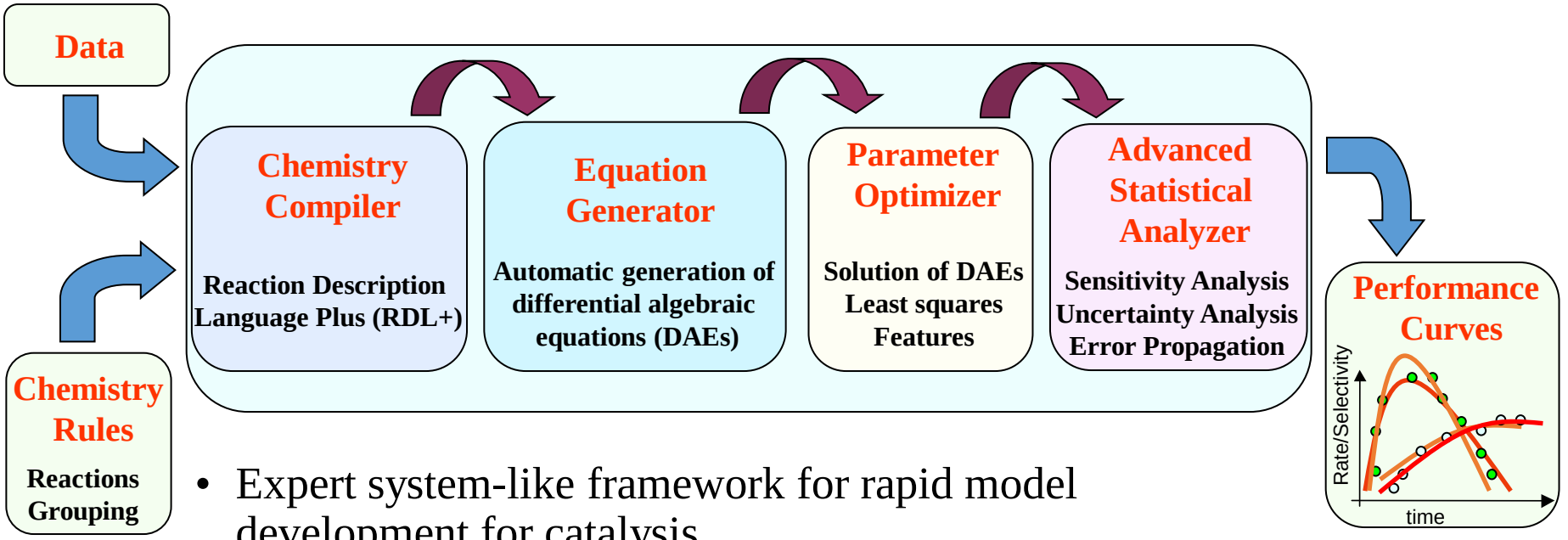
$$dC_A/dt = -k_1 C_A$$

$$dC_B/dt = k_1 C_A + k_4 D - k_5 B$$

$$\theta_A + \theta_B + \theta_C = 1$$

100's of DAE's

Discovery Analytics: AI-based Modeling Environment



- Expert system-like framework for rapid model development for catalysis
- Differential-Algebraic Equation (DAE) System
- Dozens of equations and parameters
- Real-time model development

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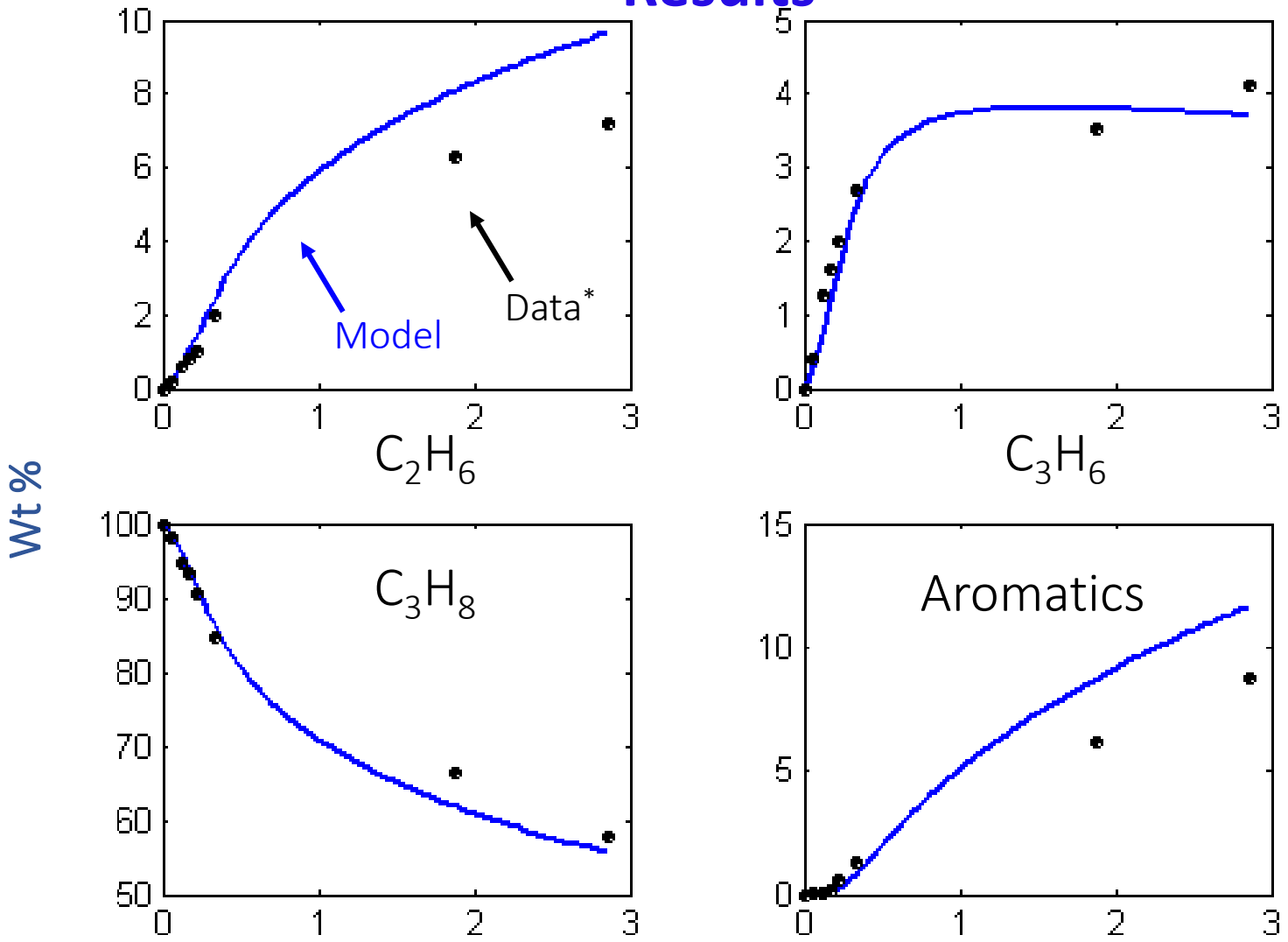
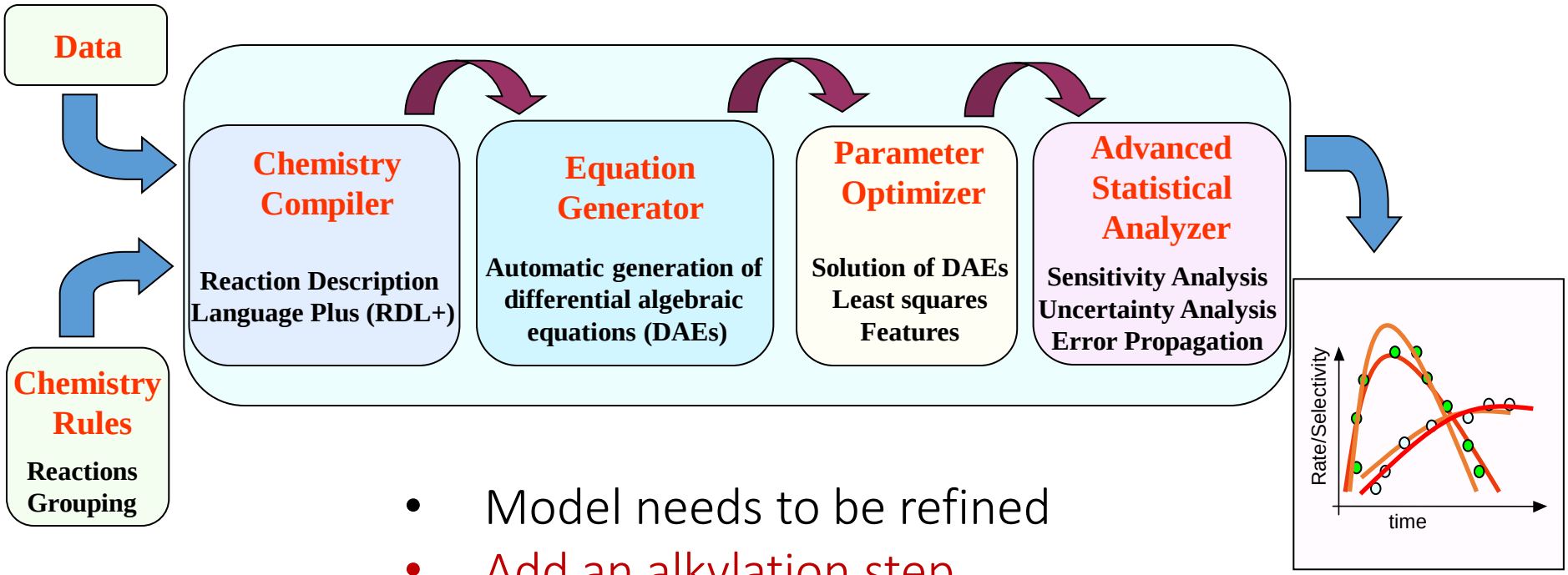
Results



Over prediction of C_2s and under prediction of C_3s

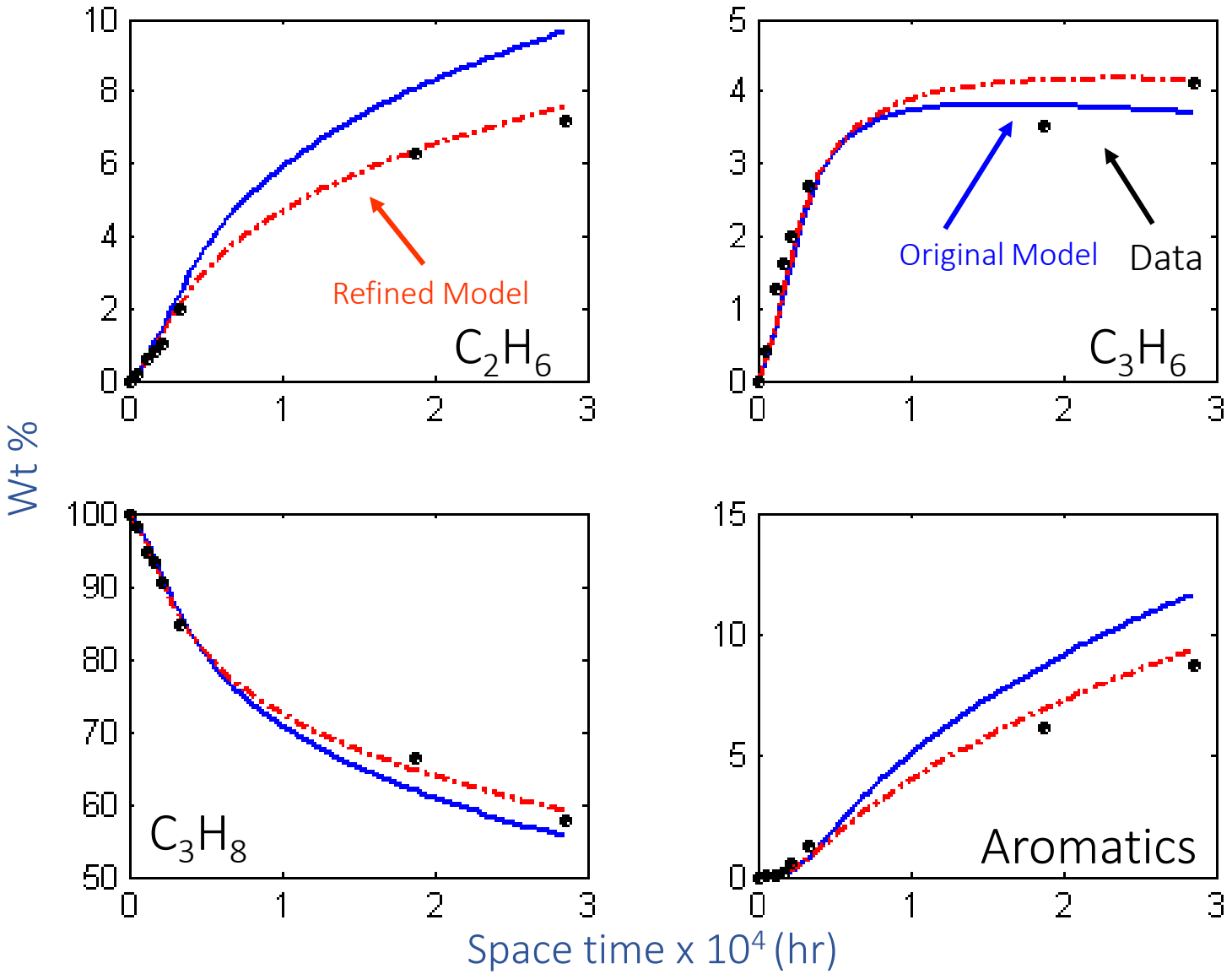
* Lukyanov et. al., Ind. Eng. Chem. Res. , 34, 516-523, 1995

Ontological Informatics Cyberinfrastructure: Reaction Modeling Suite (RMS++)



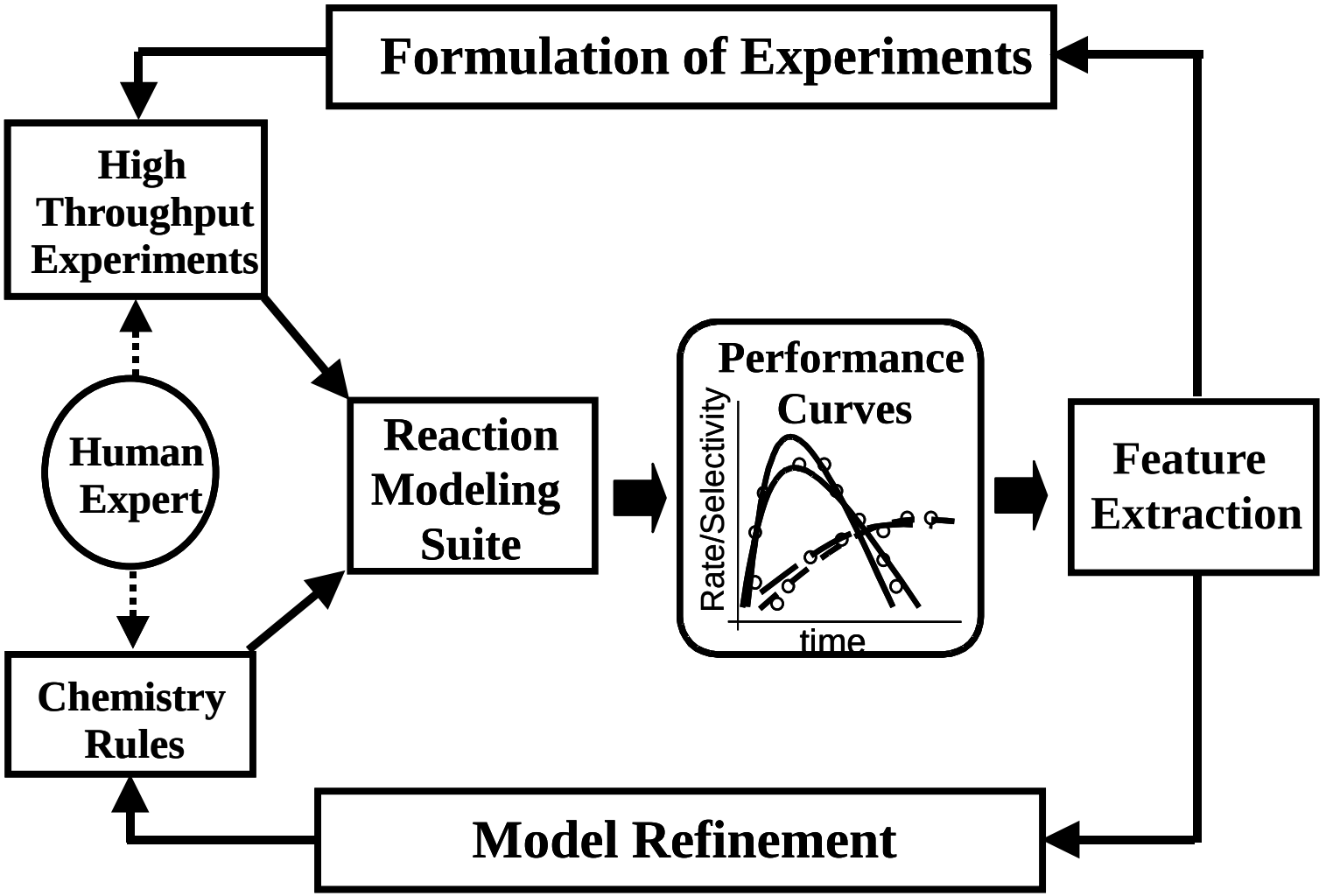
- Model needs to be refined
- Add an alkylation step
- To convert lighter alkanes to higher ones

Results – Model Refinement



Refined model adds alkylation step to convert lighter alkanes to higher ones

Materials Discovery Analytics Cycle: Active Learning



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Summary

- Vision: "Watson" for PSE
  - AI & ML in PSE is a 35-year old idea with many past success stories
  - What is new is the availability of great amounts of data, new algorithms, new languages, and cheap & powerful computational/communication resources
  - What took us months to accomplish can be done in days or hours now
- Most scientific & engineering applications likely require hybrid models: First-principles + Data Science
- Need to develop modeling environments to build hybrid models quickly
- Require progress in building domain-specific components
  - Ontologies, Compilers, Molecular Structure and Semantic Search Engines
  - Chemical entities extraction systems, Languages for modeling chemical reaction pathways, etc.
  - These are the next generation Aspen+ and gPROMS

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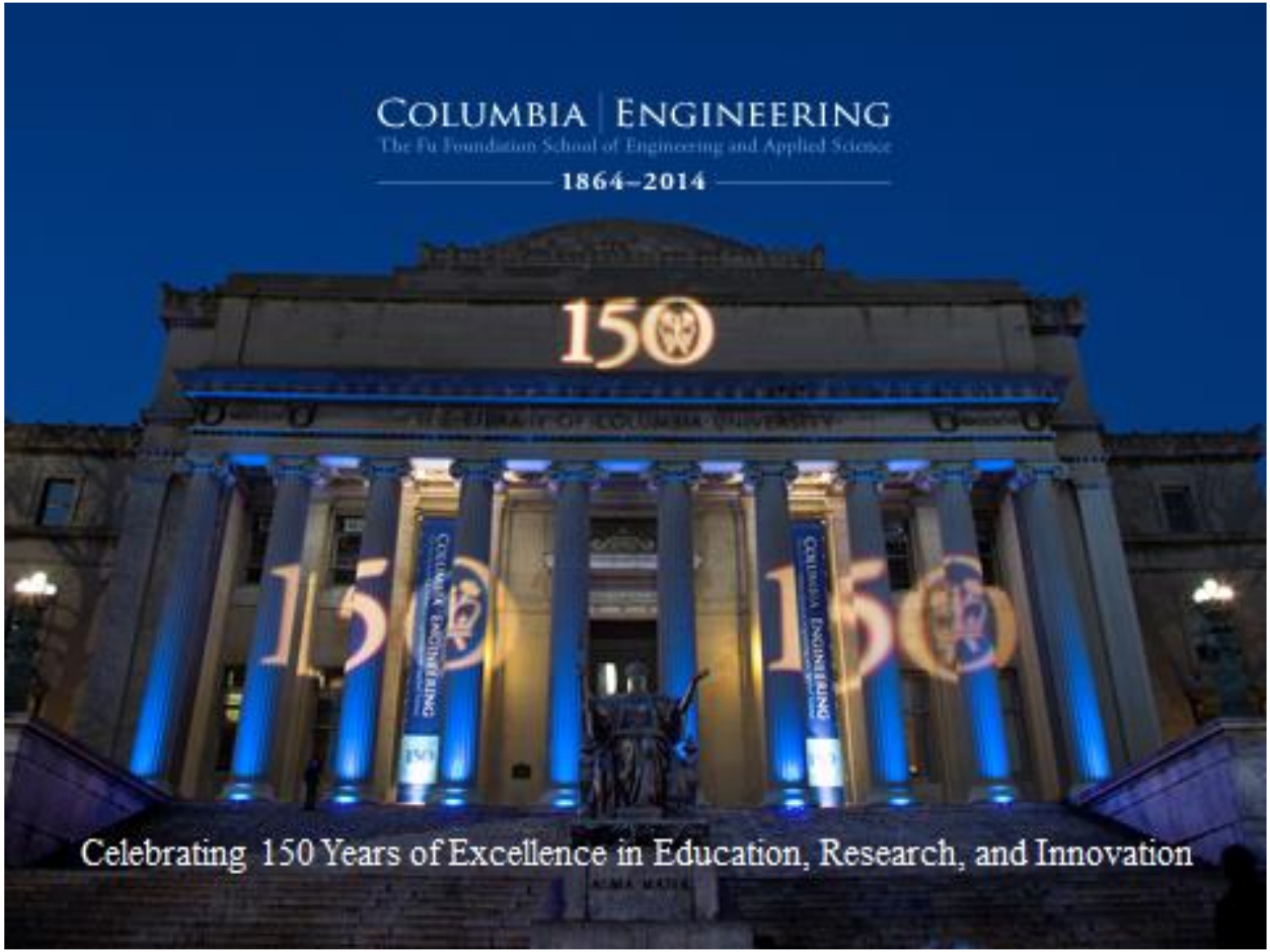
Thank You for Your Attention!



Questions?