Diesel Aftertreatment System Analyses with DOC and SCR Models

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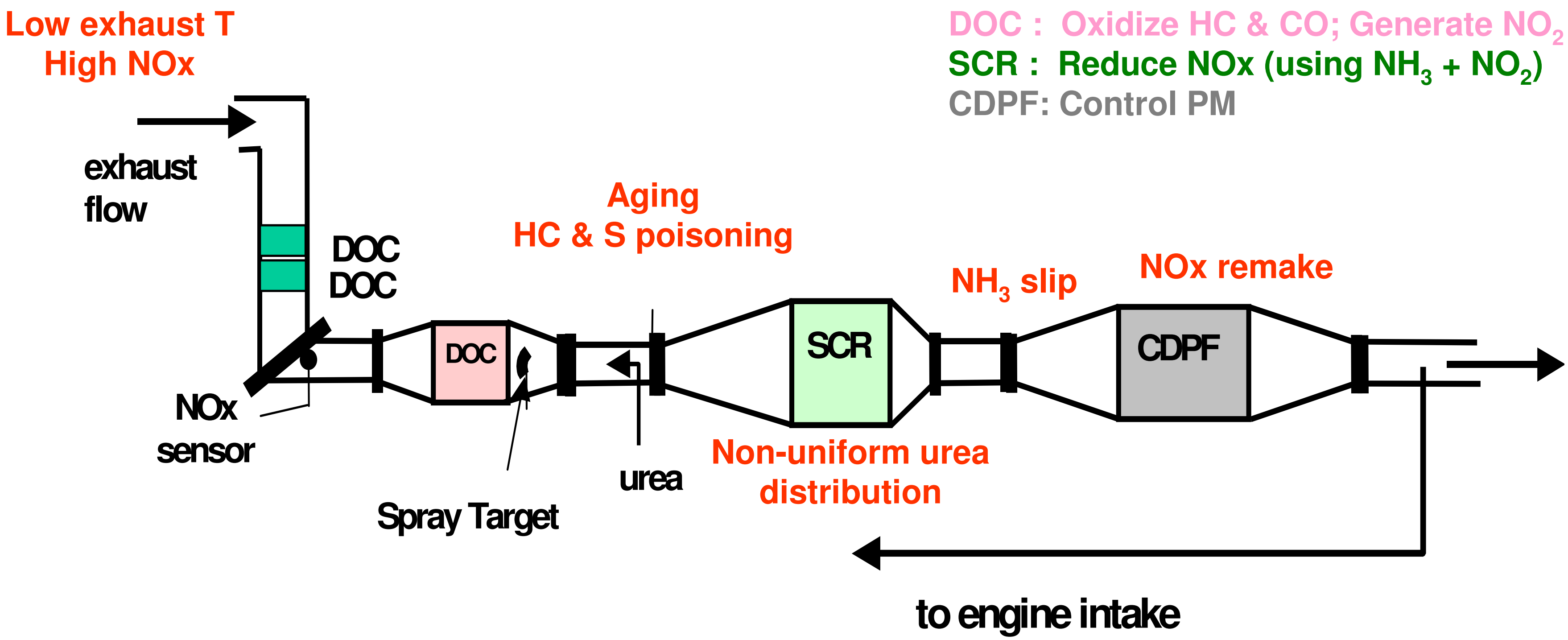
Recent progress & key challenges

C. Lambert *et al.*, DOE funded project, 2001 – 2005

DOC : Oxidize HC & CO; Generate NO_2

SCR : Reduce NOx (using NH_3 + NO_2)

CDPF: Control PM



- Typical AT system for lean NOx control: DOC + SCR + CDPF
- Several challenges but good progress
- Models facilitated progress
- Current modeling efforts to support vehicle programs

CDPF: Catalyzed Diesel Particulate Filter

Diesel Oxidation Catalyst (DOC) model

- Model calibration
- Prediction of post-DOC NO_2 on a vehicle

Selective Catalytic Reduction (SCR) model

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- Prediction of tailpipe NOx and NH_3 slip in a vehicle

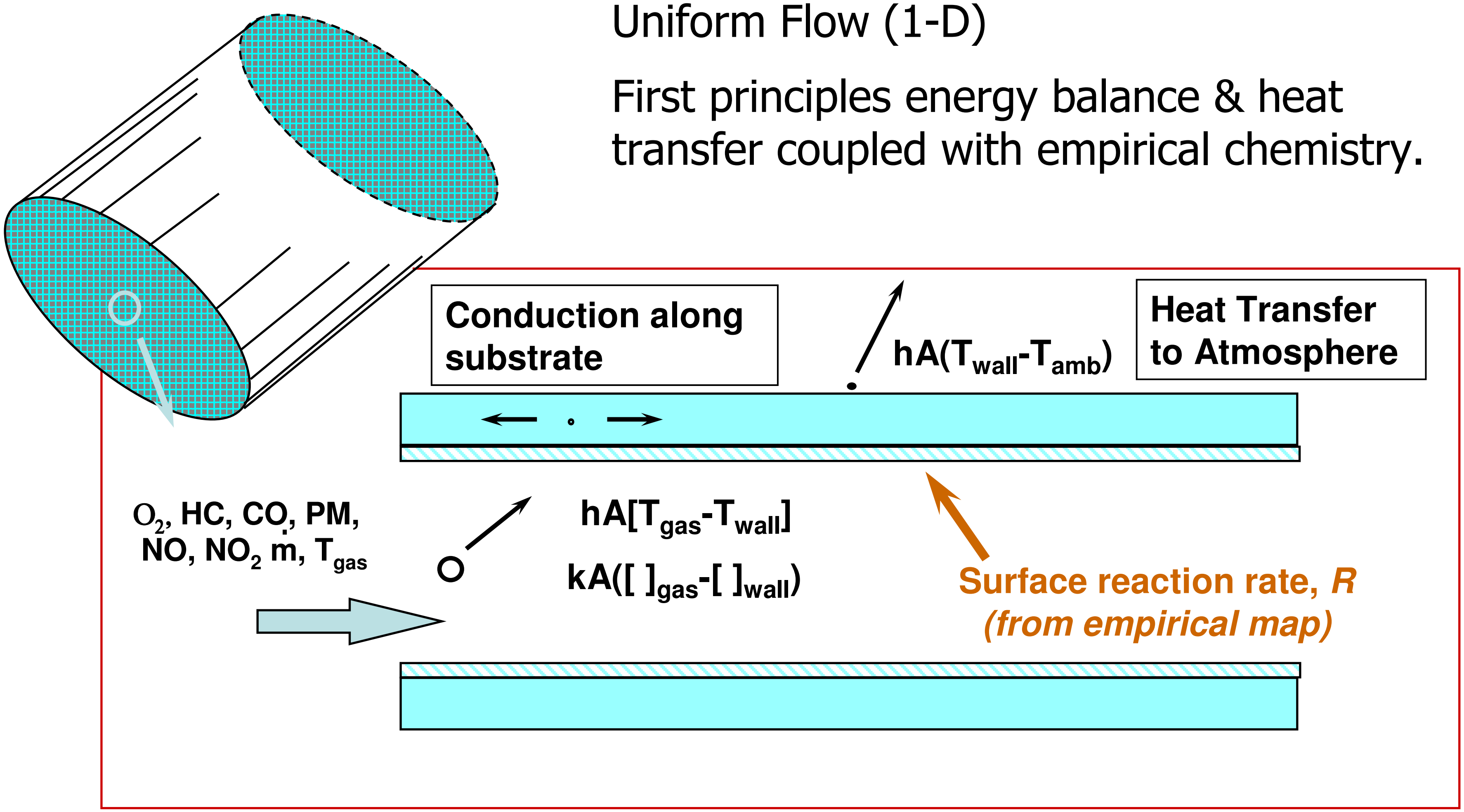
DOC+SCR system applications

- Importance of post-DOC NO_2 on SCR performance
- Optimization of urea injection strategy

SIMTWC – Heat transfer equations + catalyst conversion data

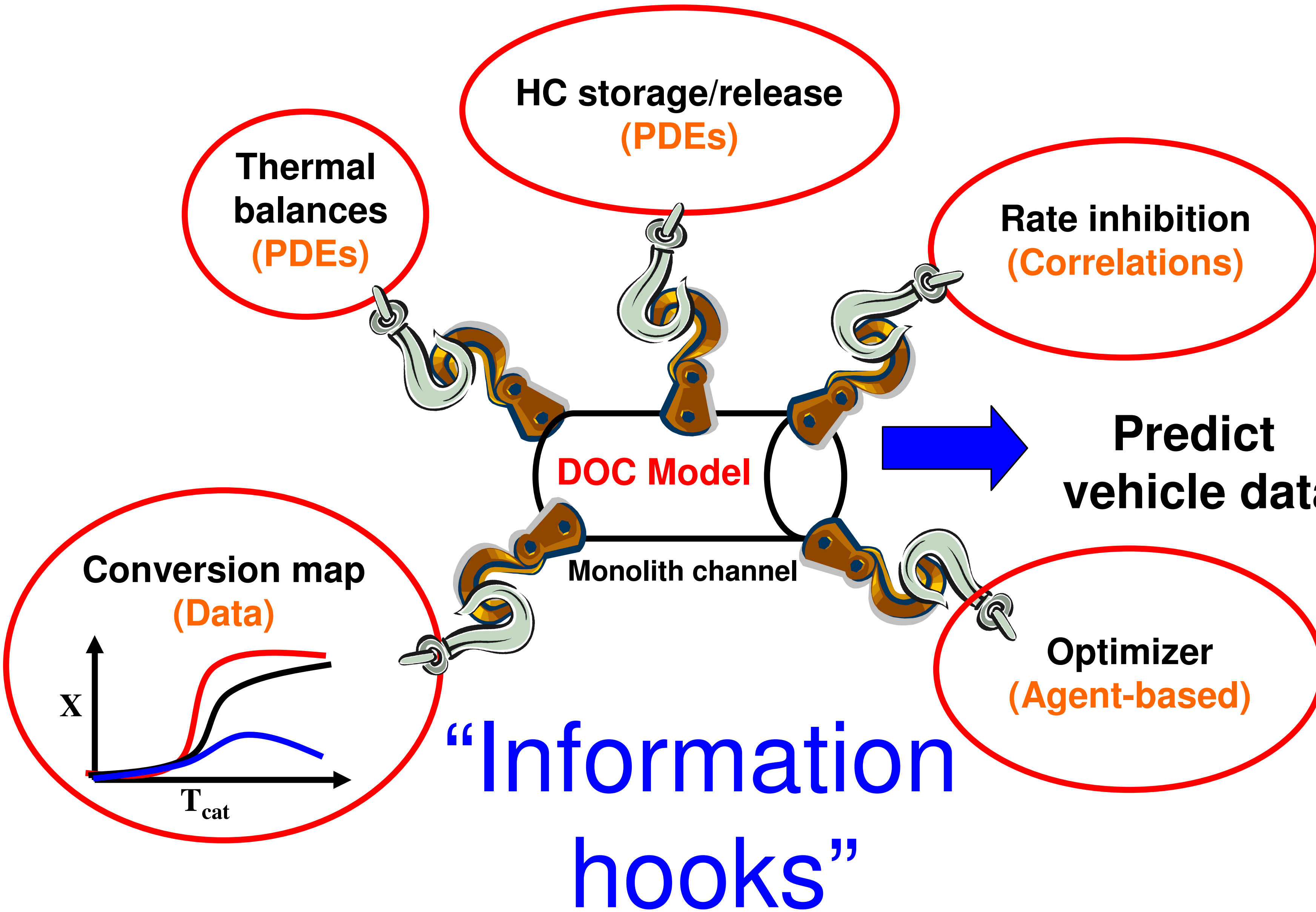
Uniform Flow (1-D)

First principles energy balance & heat transfer coupled with empirical chemistry.

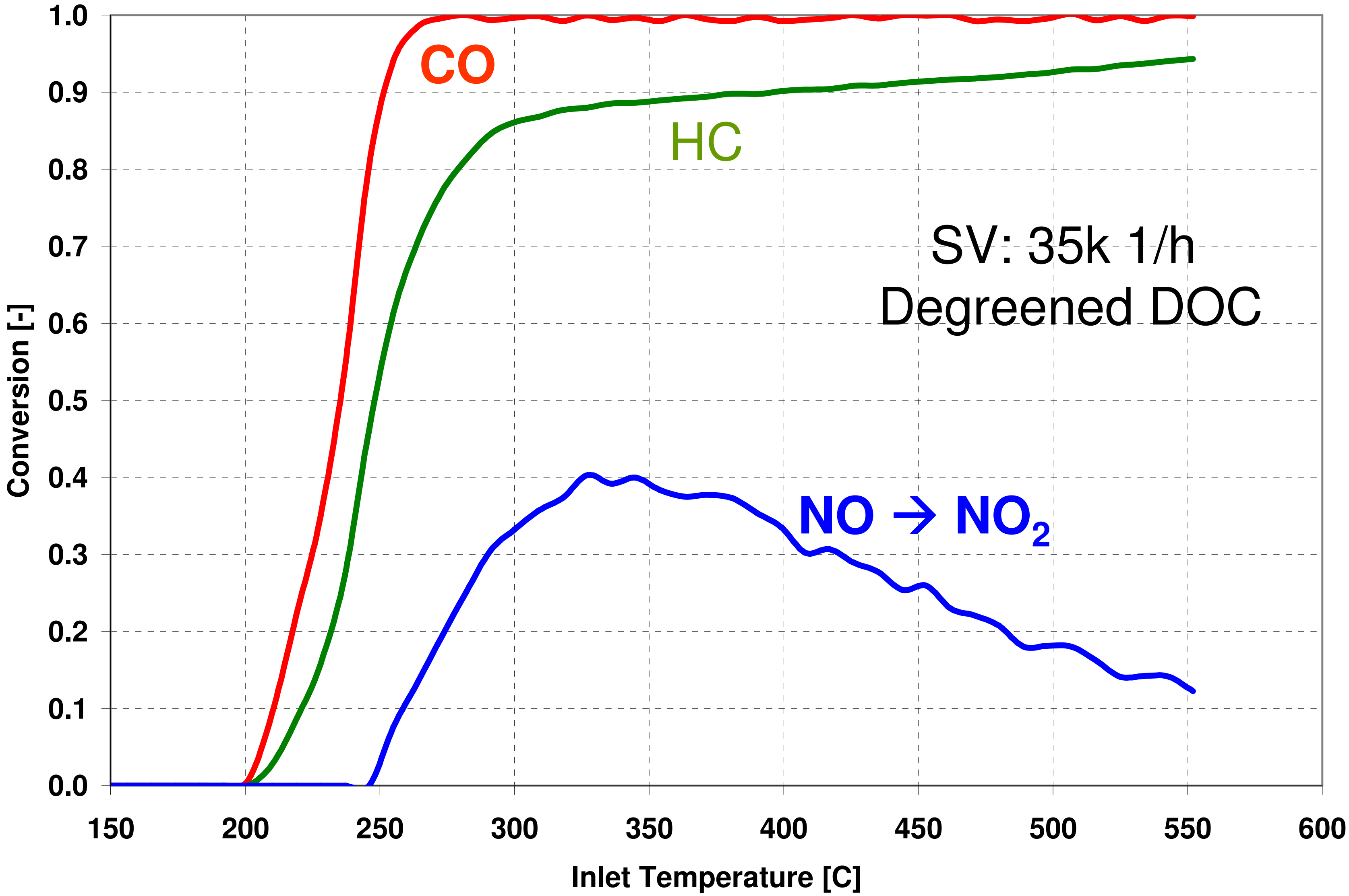


Computationally non-intensive semi-empirical modeling approach

DOC model – Hybrid approach to leverage data



Typical pulsator map



Key input to the DOC model

At the bulk-solid interface

$$\frac{dC_s}{dt} = k_c S\left(C_f - C_s\right) - k_a\left(1-\theta\right)C_s N + \boxed{k_d \theta N} = 0$$

In the zeolite phase

$$\frac{d\theta}{dt} = k_a(1-\theta)C_s - \boxed{k_d \theta}$$

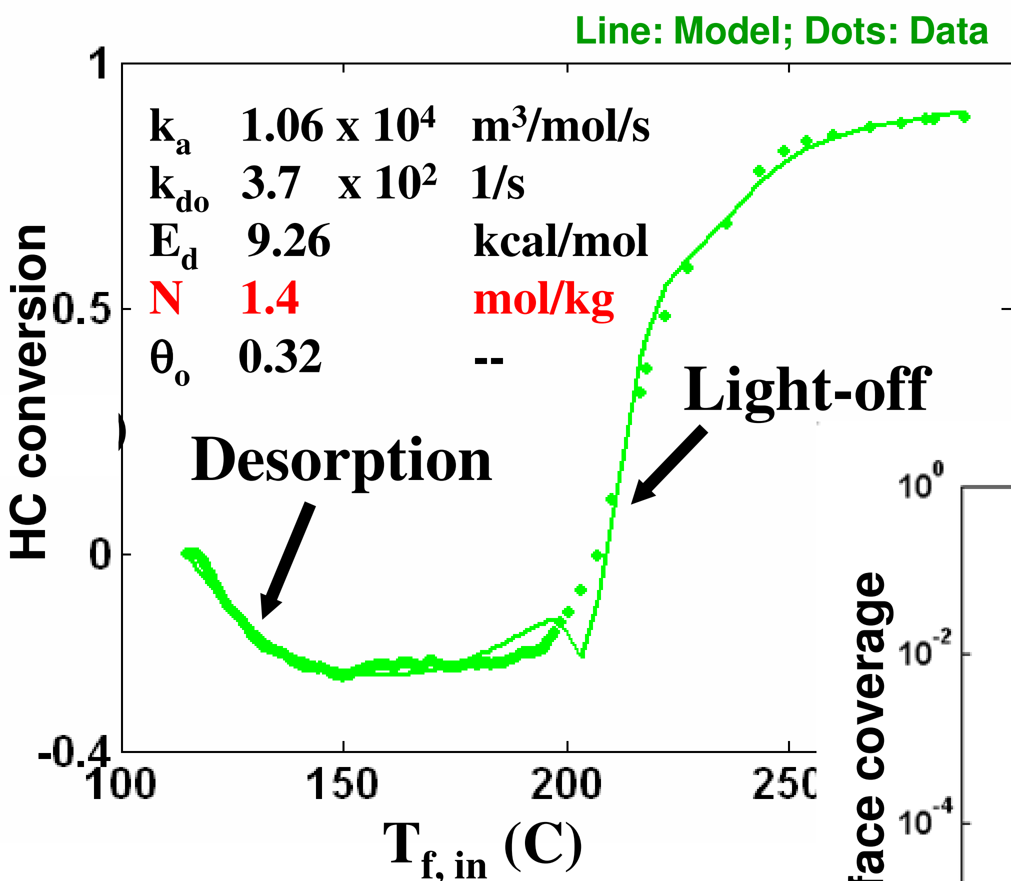
Adsorption

Desorption

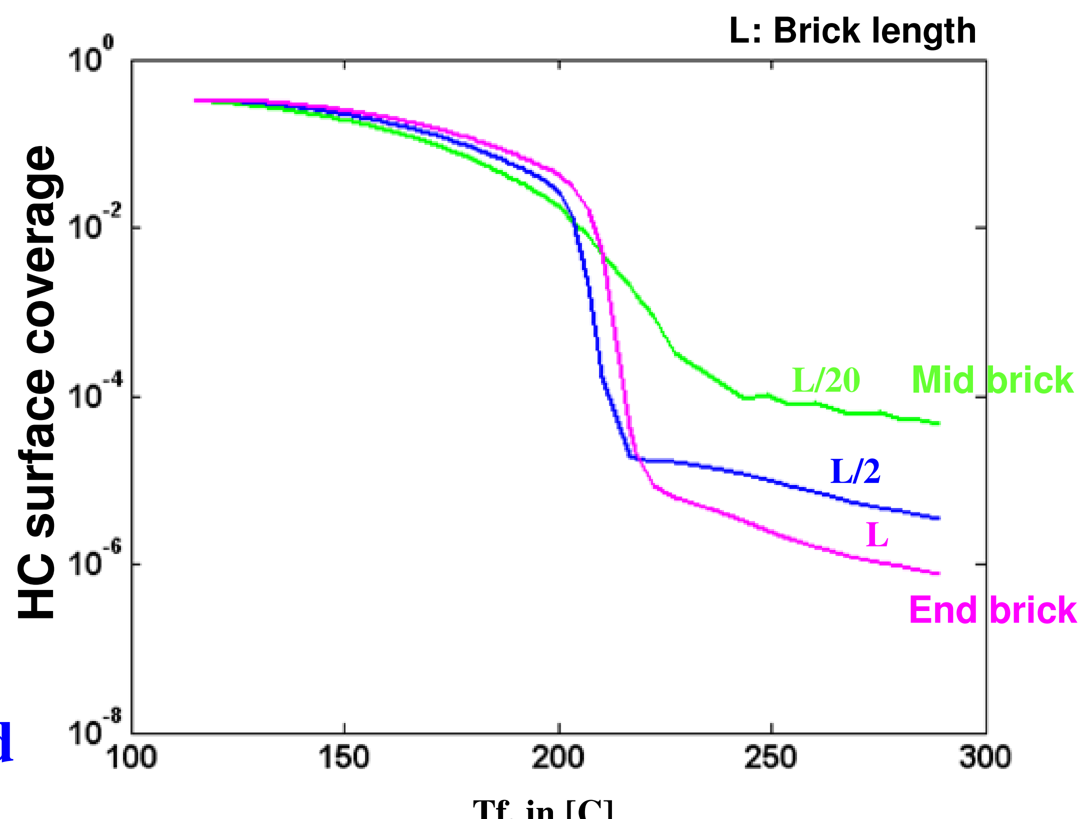
$$\boxed{\begin{array}{l} k_d = k_{do}\exp(-E_d / RT) \\ k_a, N, \theta_o \end{array}}$$

2 nonlinear equations & 5 parameters

Model can predict HC adsorption, desorption and light-off

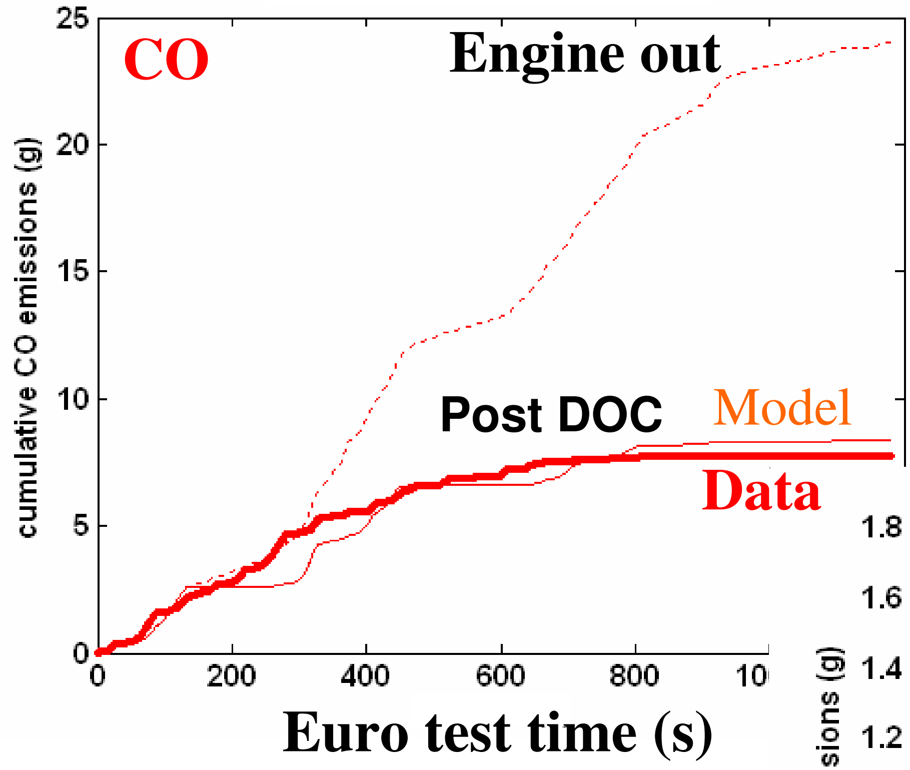


Parameter estimation using in-house "stochastic optimizer" *

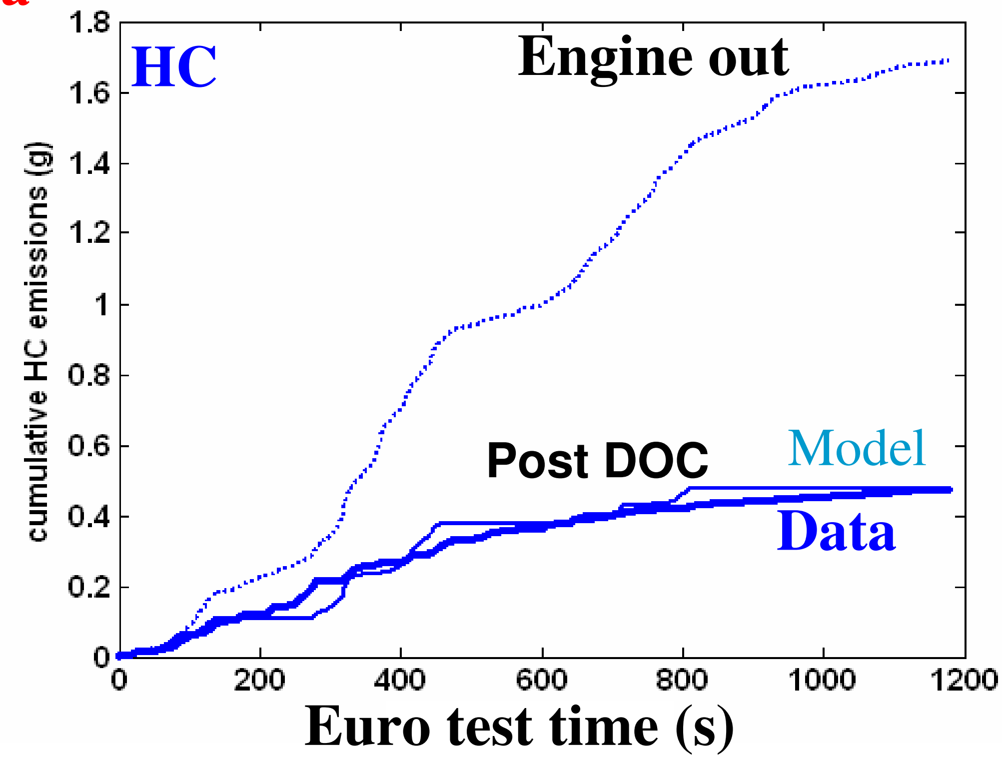


Total amount of the trap material (N) could be optimized

* Katare & West, *Complexity*, 11, 4, 2006

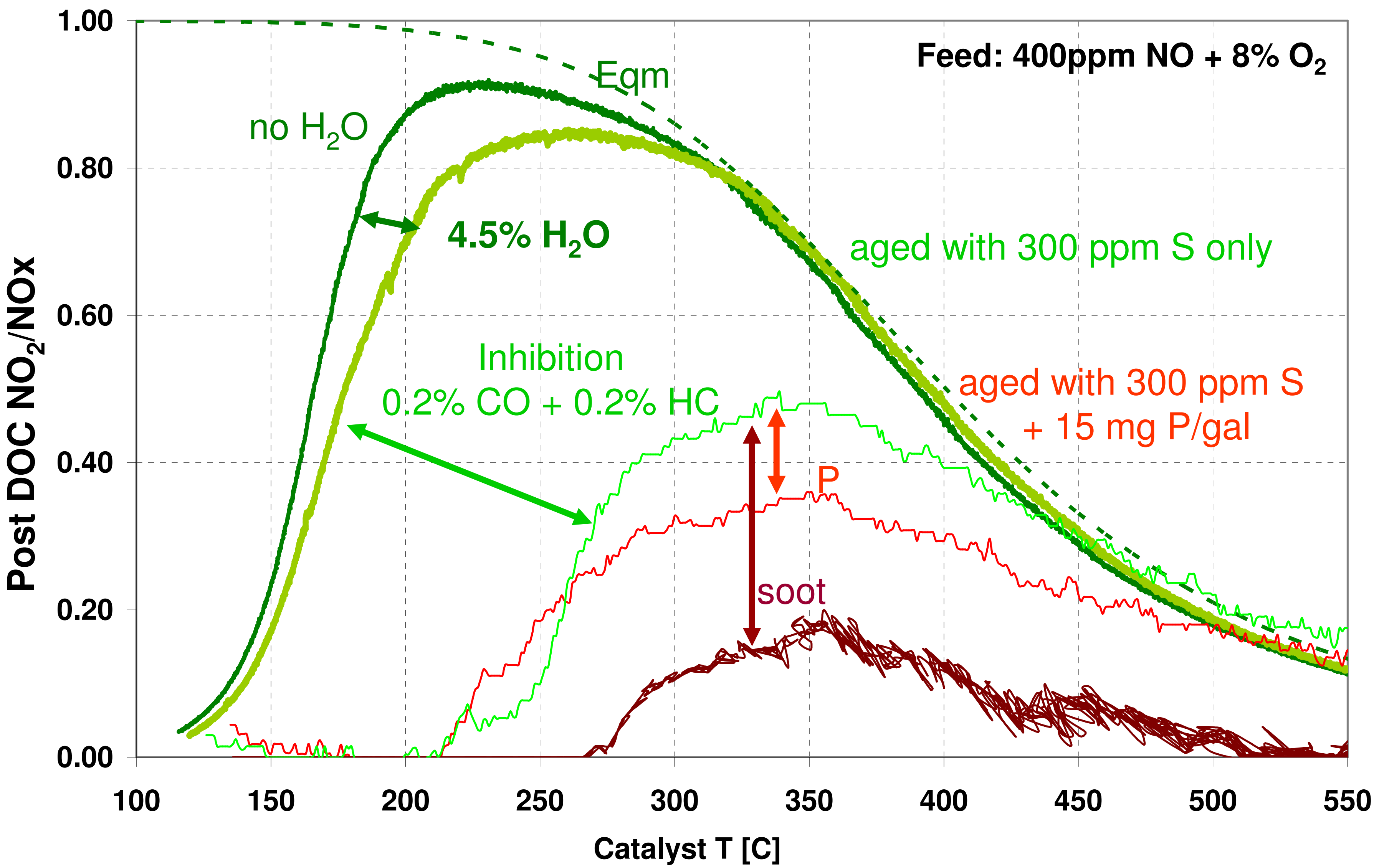


2.2 L Puma engine



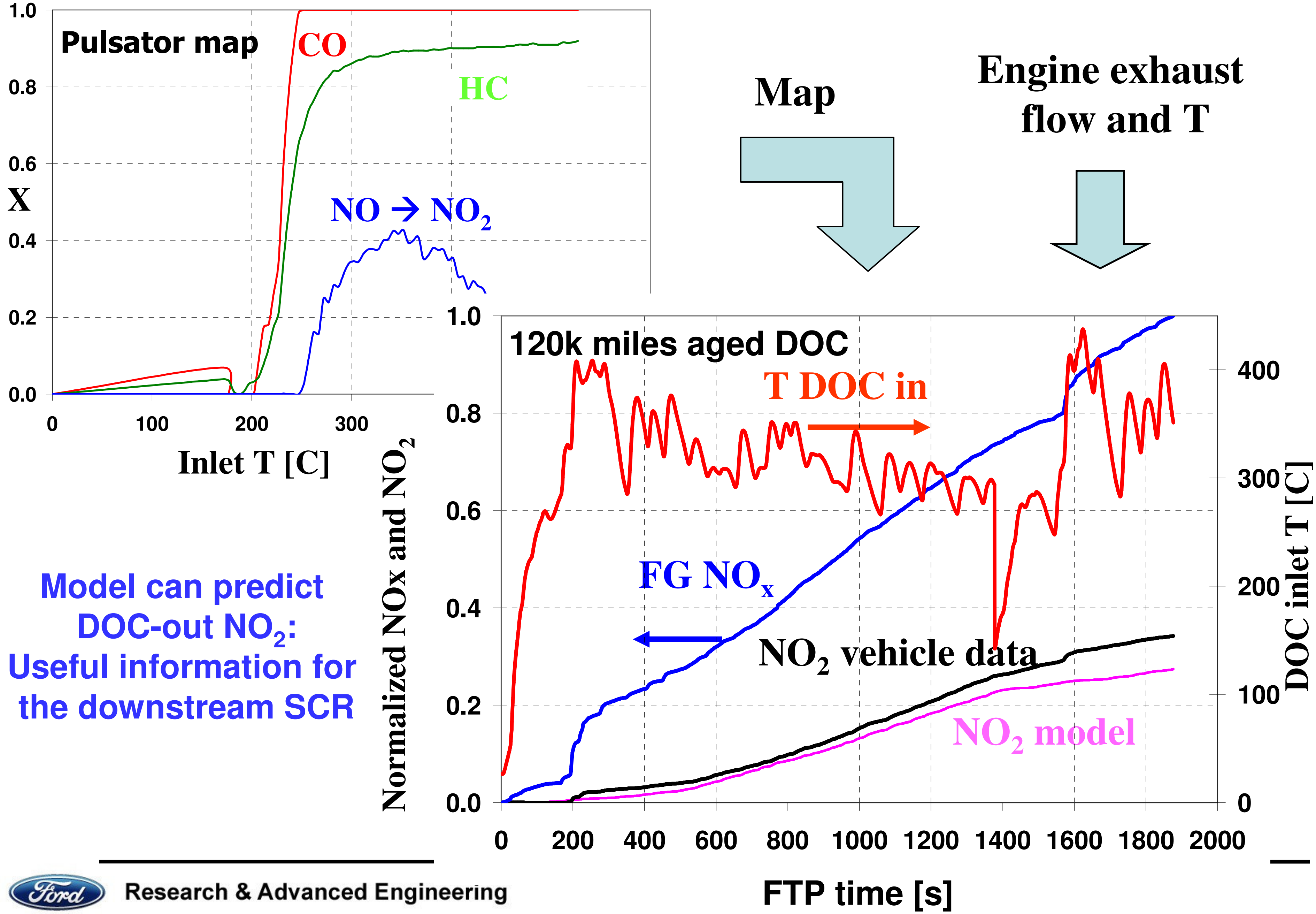
Model predictions reasonable

DOC oxidizes NO to NO_2 – critical for SCR operation



NO oxidation chemistry is complex

Predicting post DOC NO_2 on a Ford developmental vehicle



Model can predict DOC-out NO_2: Useful information for the downstream SCR

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DOC+SCR system applications

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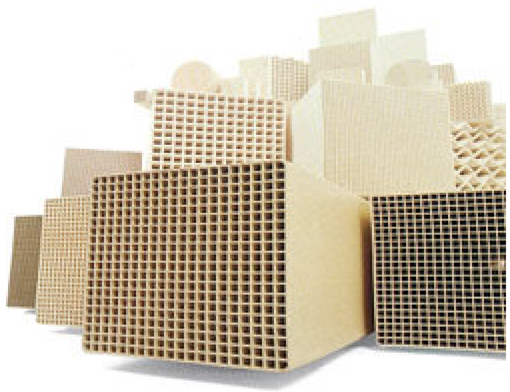
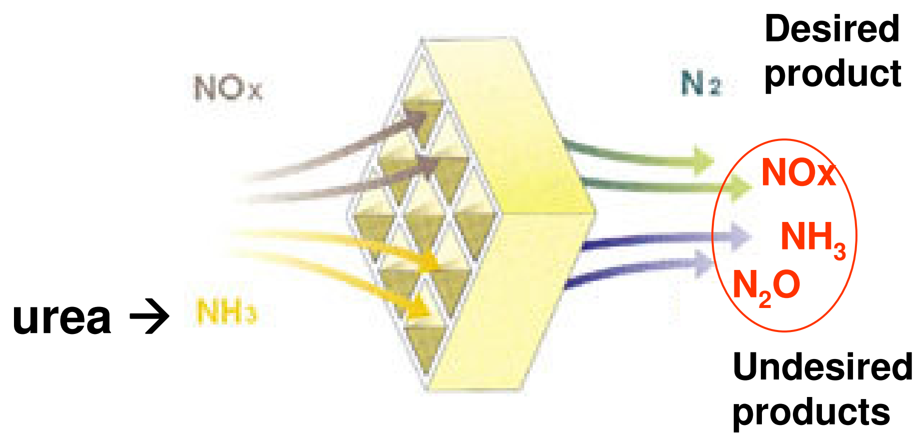
Introduction to Selective Catalytic Reduction (SCR)





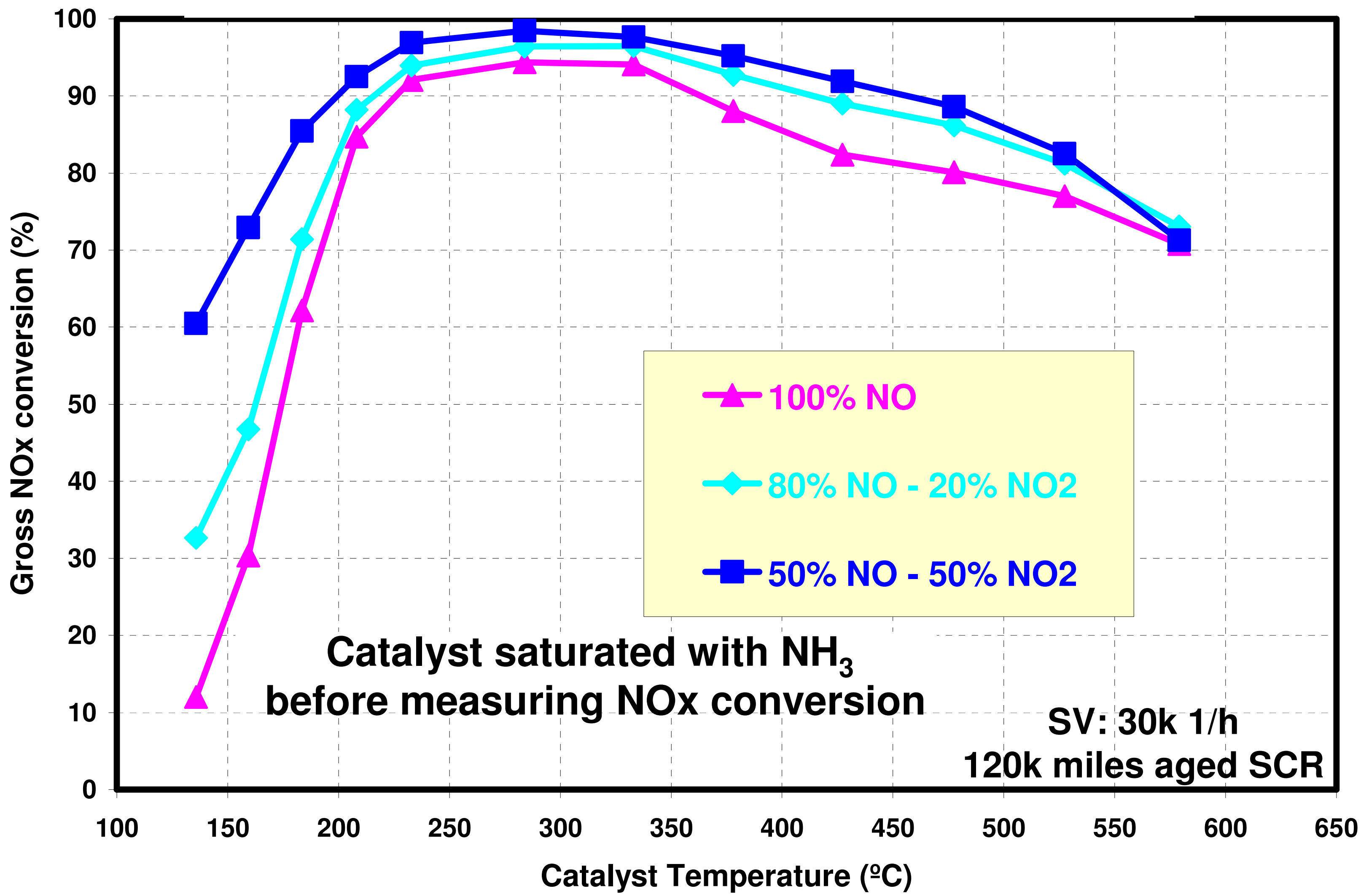
- **Base metals such as Cu and Fe on honeycombs**
- **Selectively reduce NOx to N_2**
- **Aqueous urea sprayed onto the catalyst**
- **Urea → thermal decomposition + hydrolysis to NH_3 on the catalyst**

$$4NH_3 + \boxed{4NO} + O_2 \rightarrow 4N_2 + 6H_2O$$ **Standard SCR**

$$4NH_3 + \boxed{2NO + 2NO_2} \rightarrow 4N_2 + 6H_2O$$ **Fast SCR**

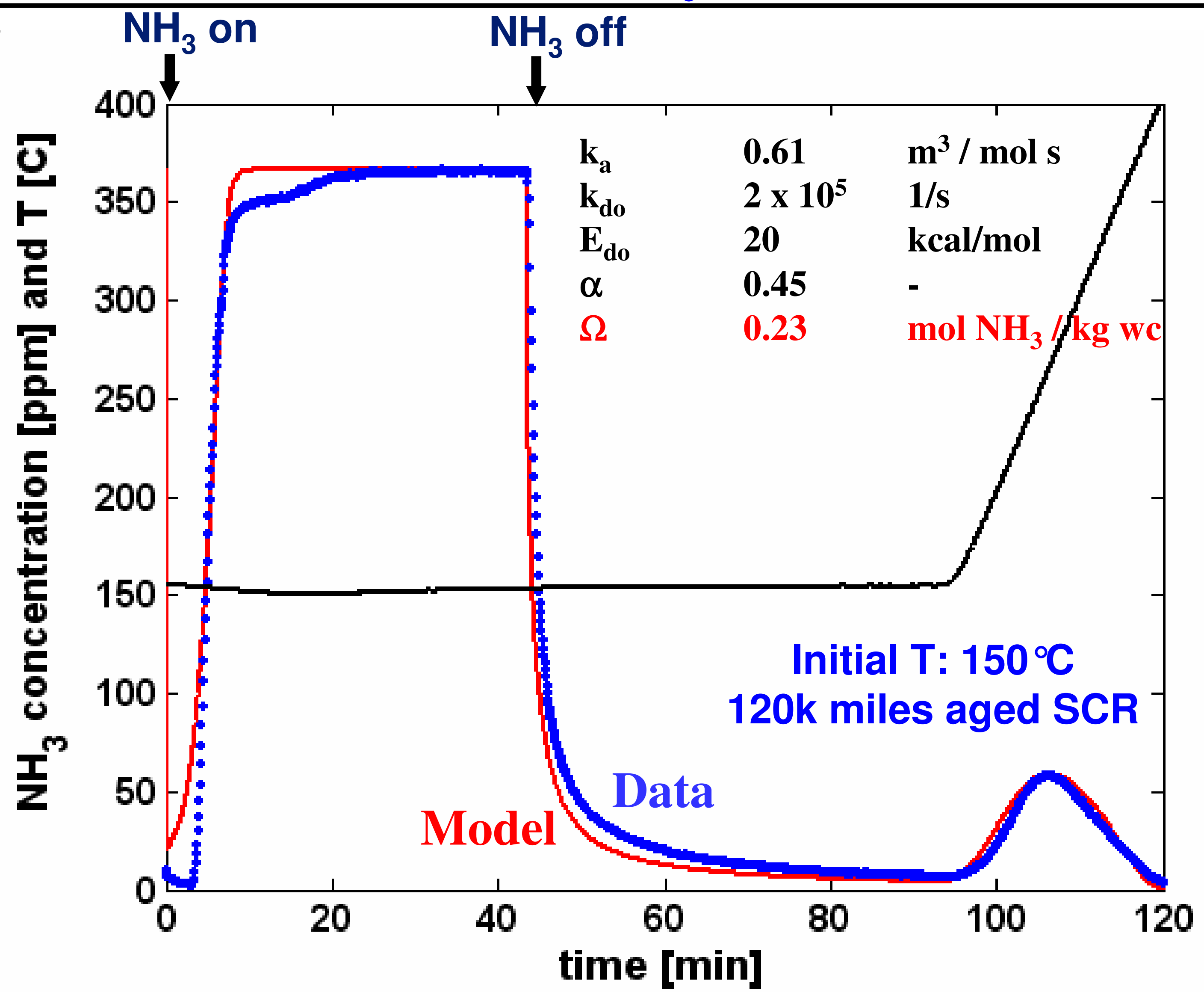
When feed NO = NO_2 SCR reaction is faster

SCR NOx performance increases with NO_2 in the feed



NO_2 information from DOC model is key for simulating SCR performance

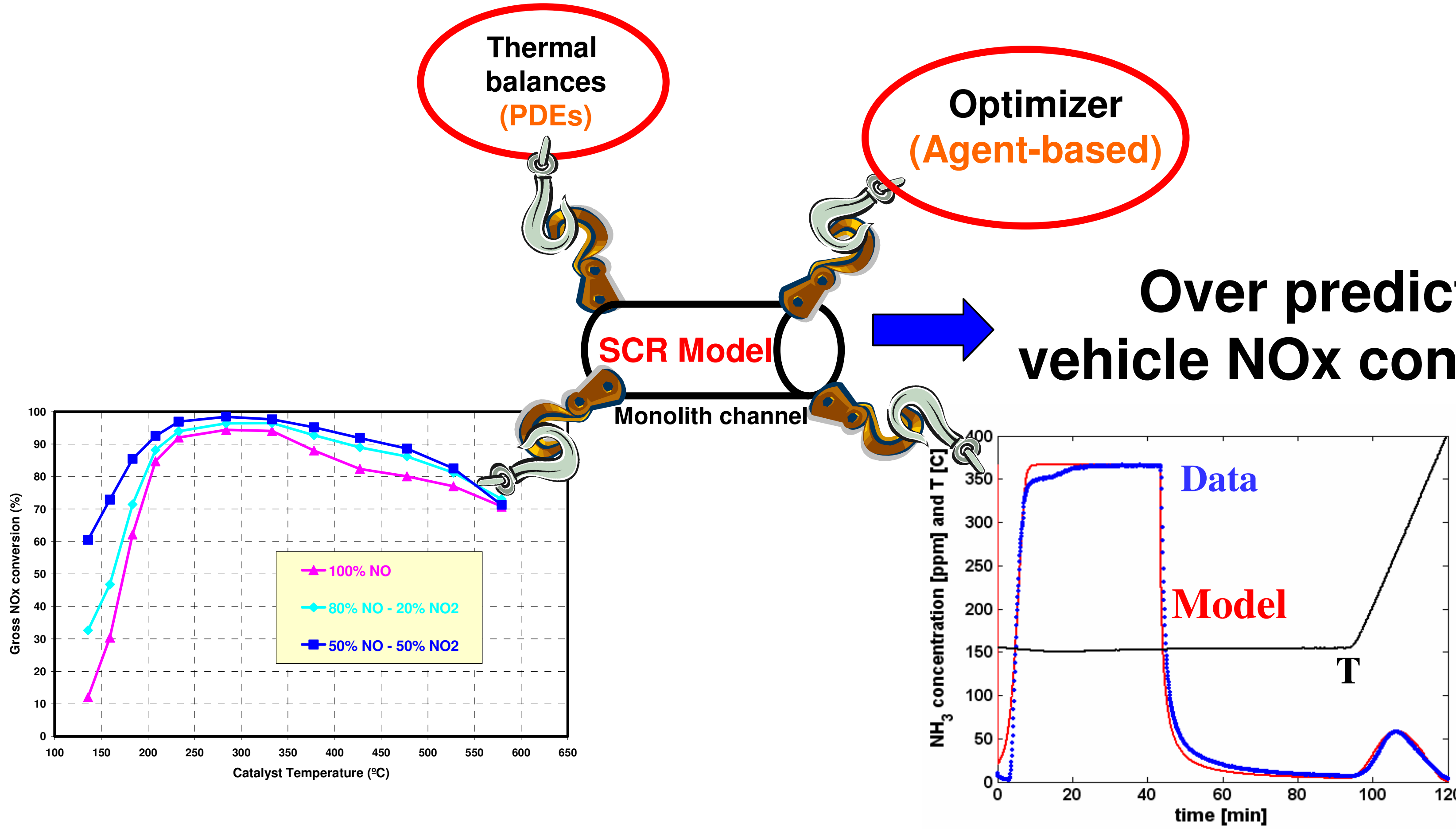
Temperature programmed desorption of NH_3



Temkin isotherm captures NH_3 ads/des data reasonably

Model calibrated at 150℃ and verified at other T and C_{NH3}

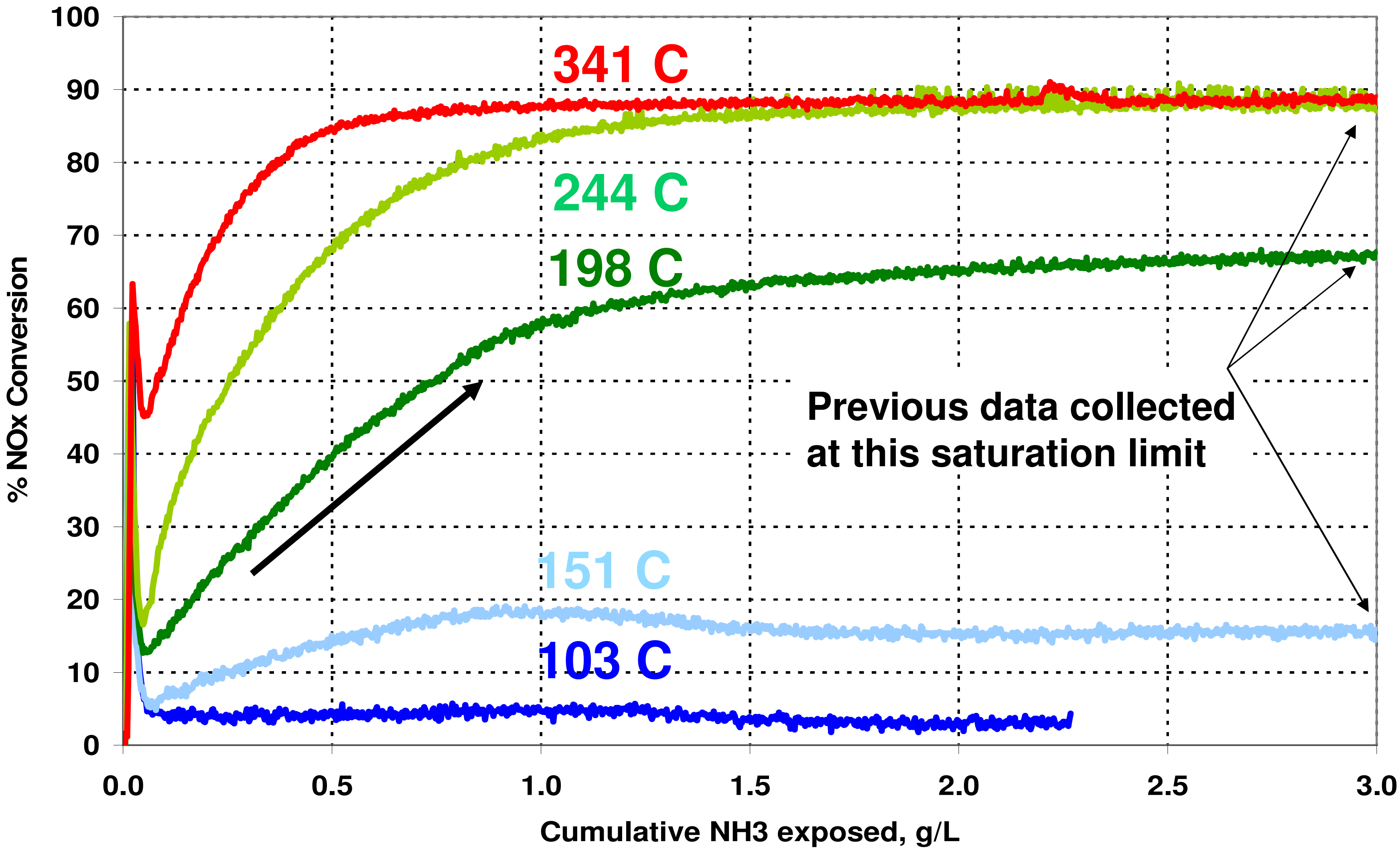
Calibrated model over predicted vehicle NOx conversion



Over predicted vehicle NOx conversion

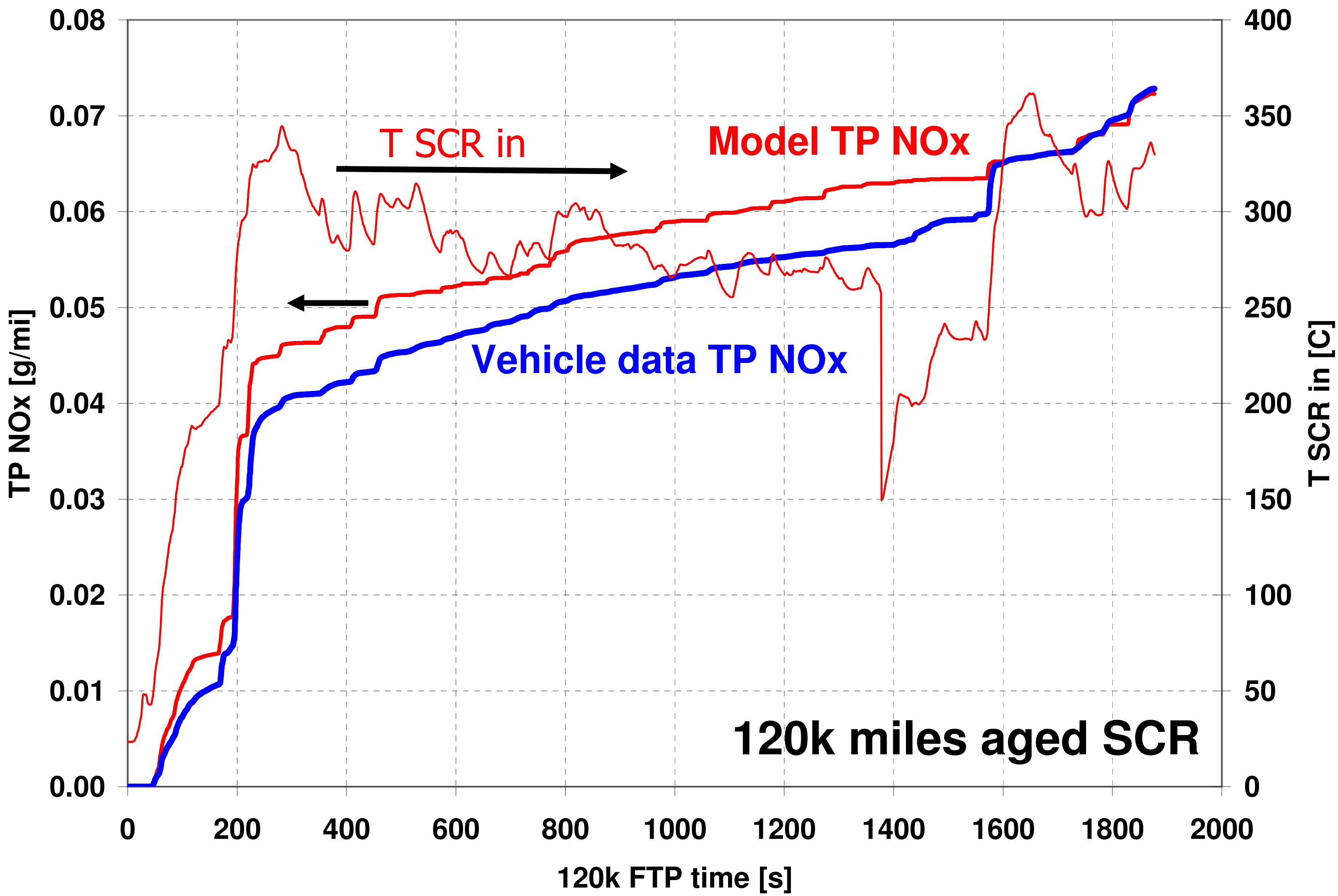
Model showed the right trends but had to assume
(1) low urea to NH_3 conversion or
(2) very high HC deactivation to explain vehicle data

NOx performance increases with increasing NH_3 storage

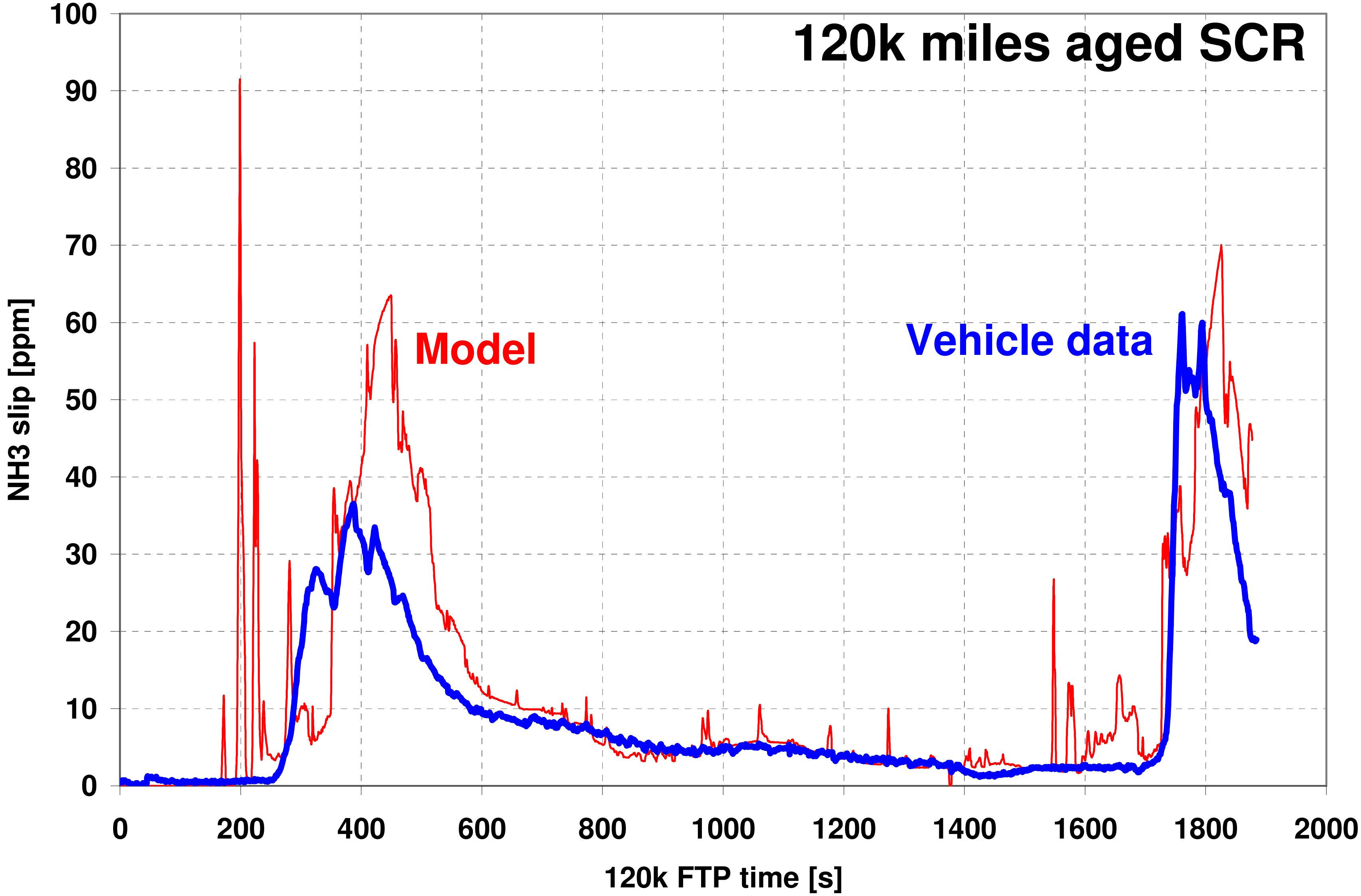


Currently a standard protocol for screening catalysts

Model predicts vehicle Tail Pipe (TP) NOx



NH_3 slip prediction



Model – experiment closure: Model → Experiment → Data → More accurate model

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DOC+SCR system applications

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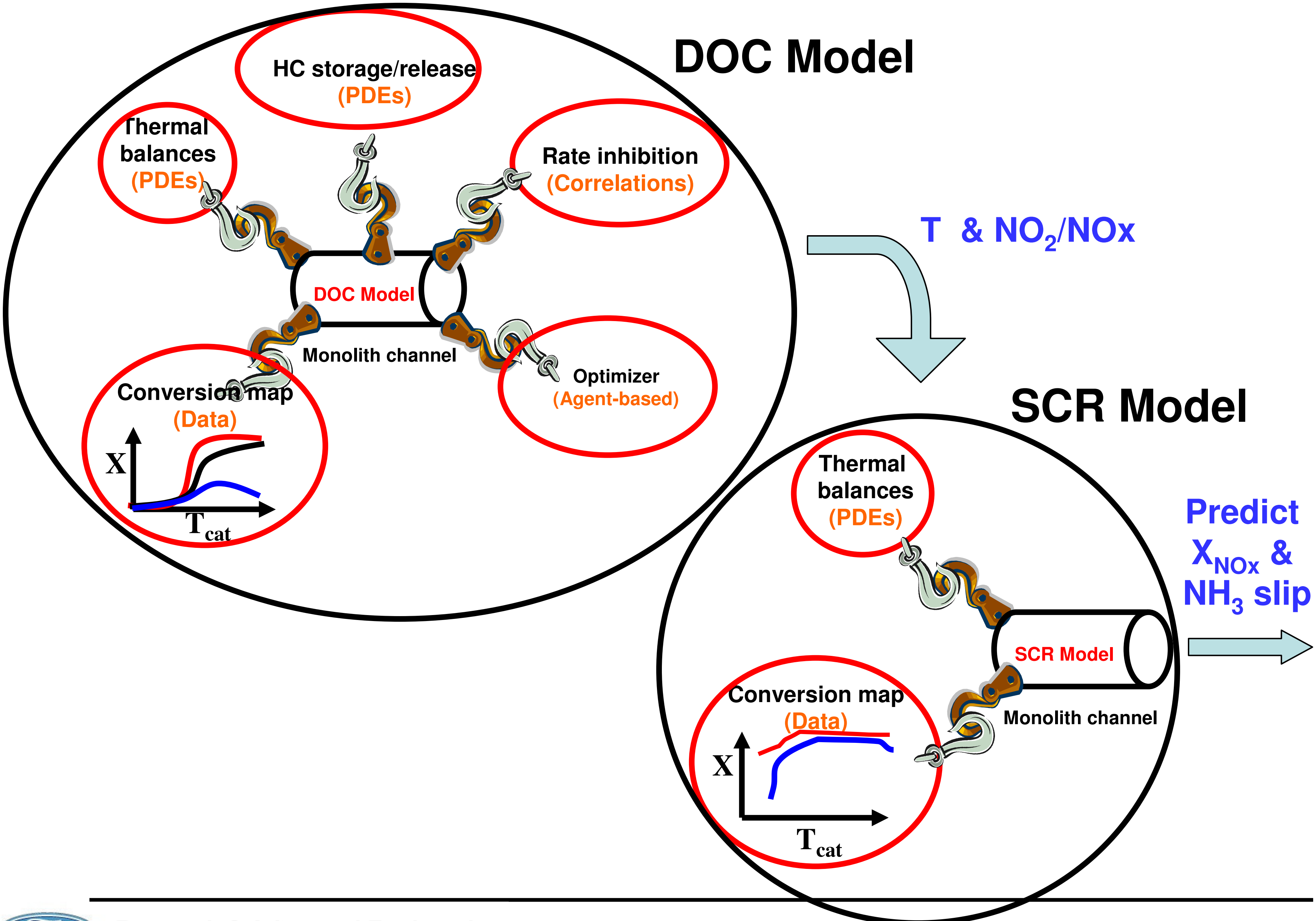
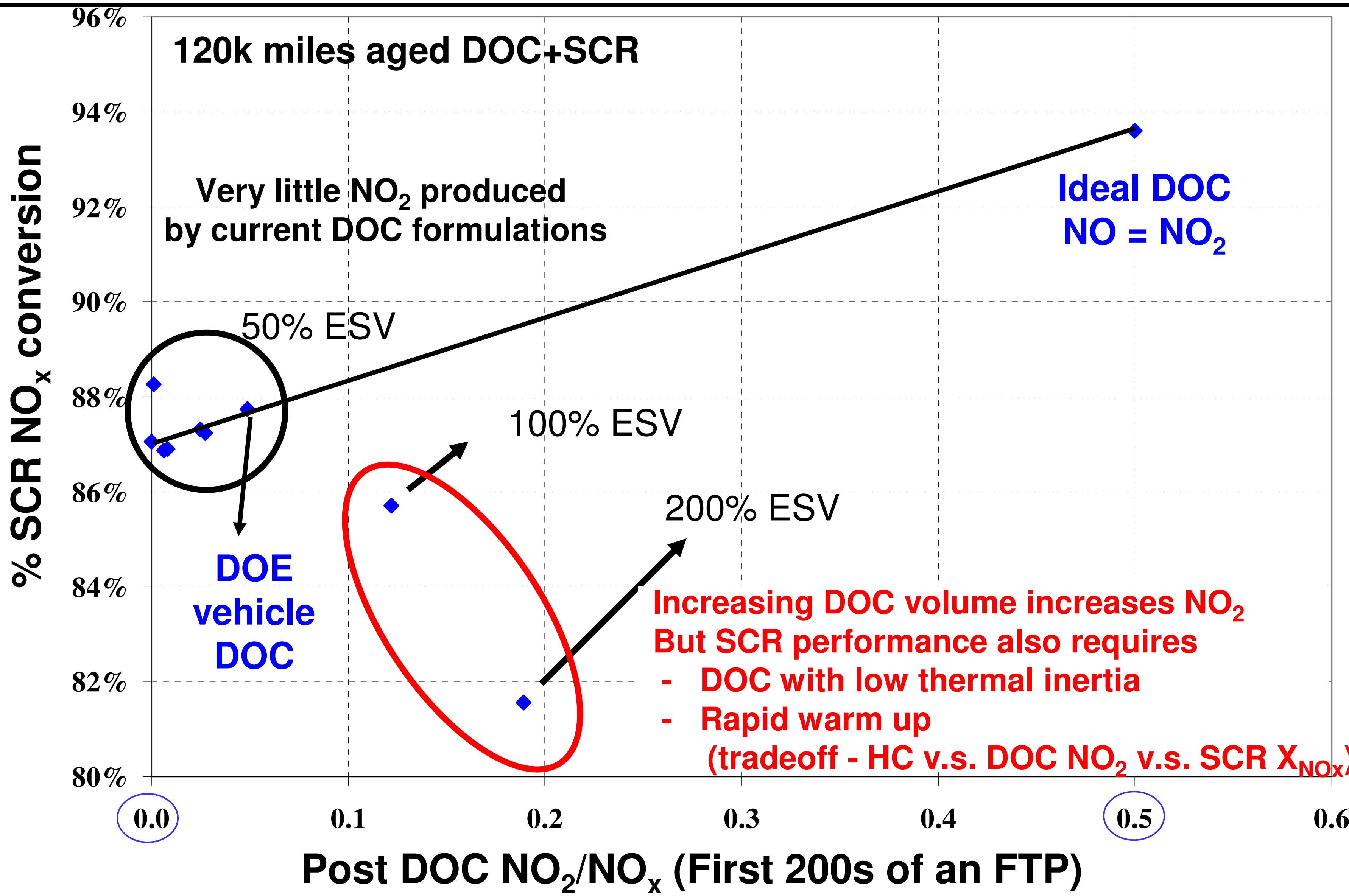
System: DOC + SCR Models



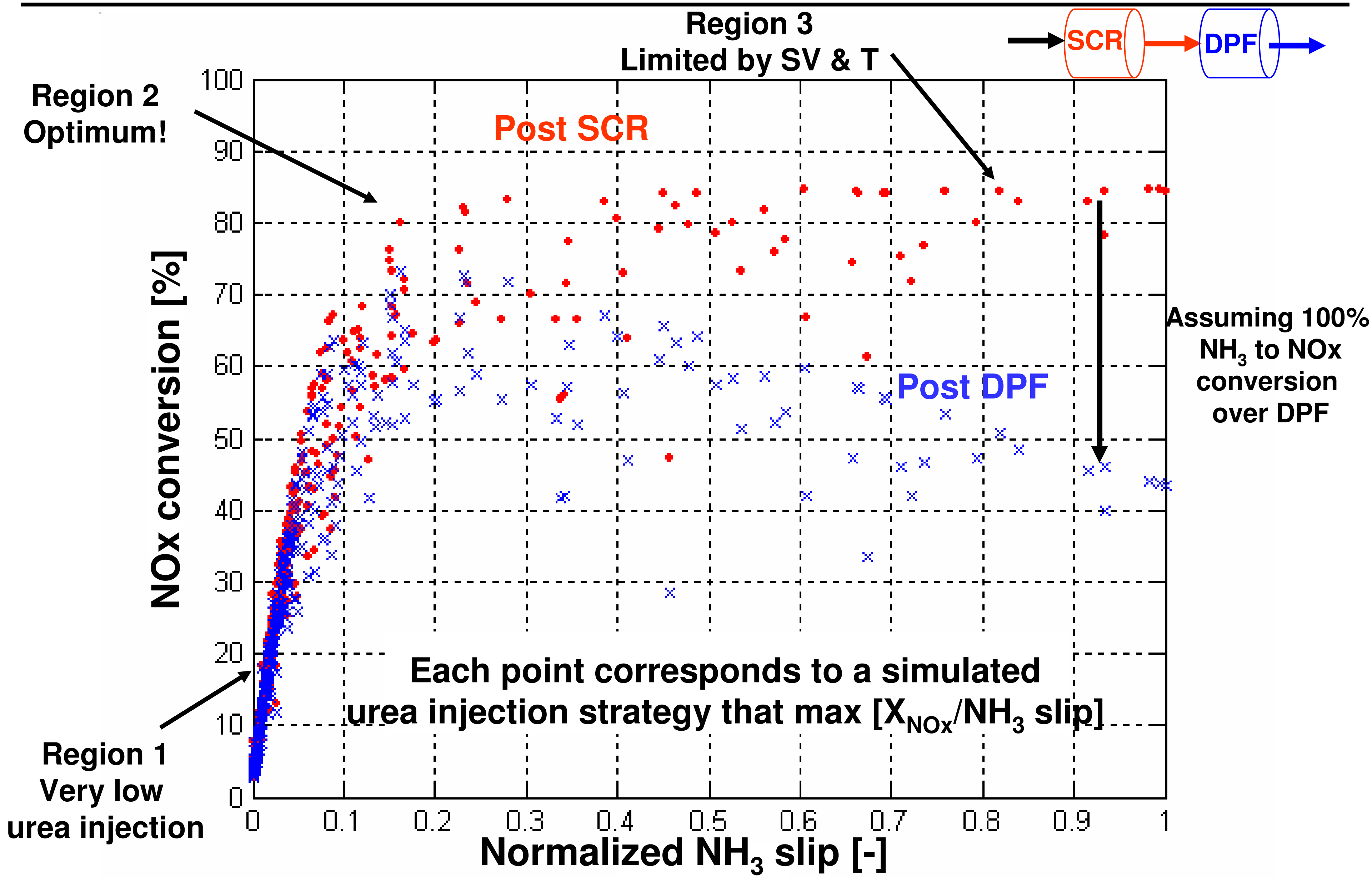
Optimum DOC for an efficient SCR ?



Model provided insight into system design issues

Katare *et al.*, *Ind. Eng. Chem. Res.*, 46, 2007, 2445

Urea injection strategy as a function of vehicle speed over an FTP test



Possible to use models to come up with effective urea injection strategies

Summary

Math models enable effective analysis and afford insight into diesel AT systems

Models leverage laboratory data to predict vehicle experiments

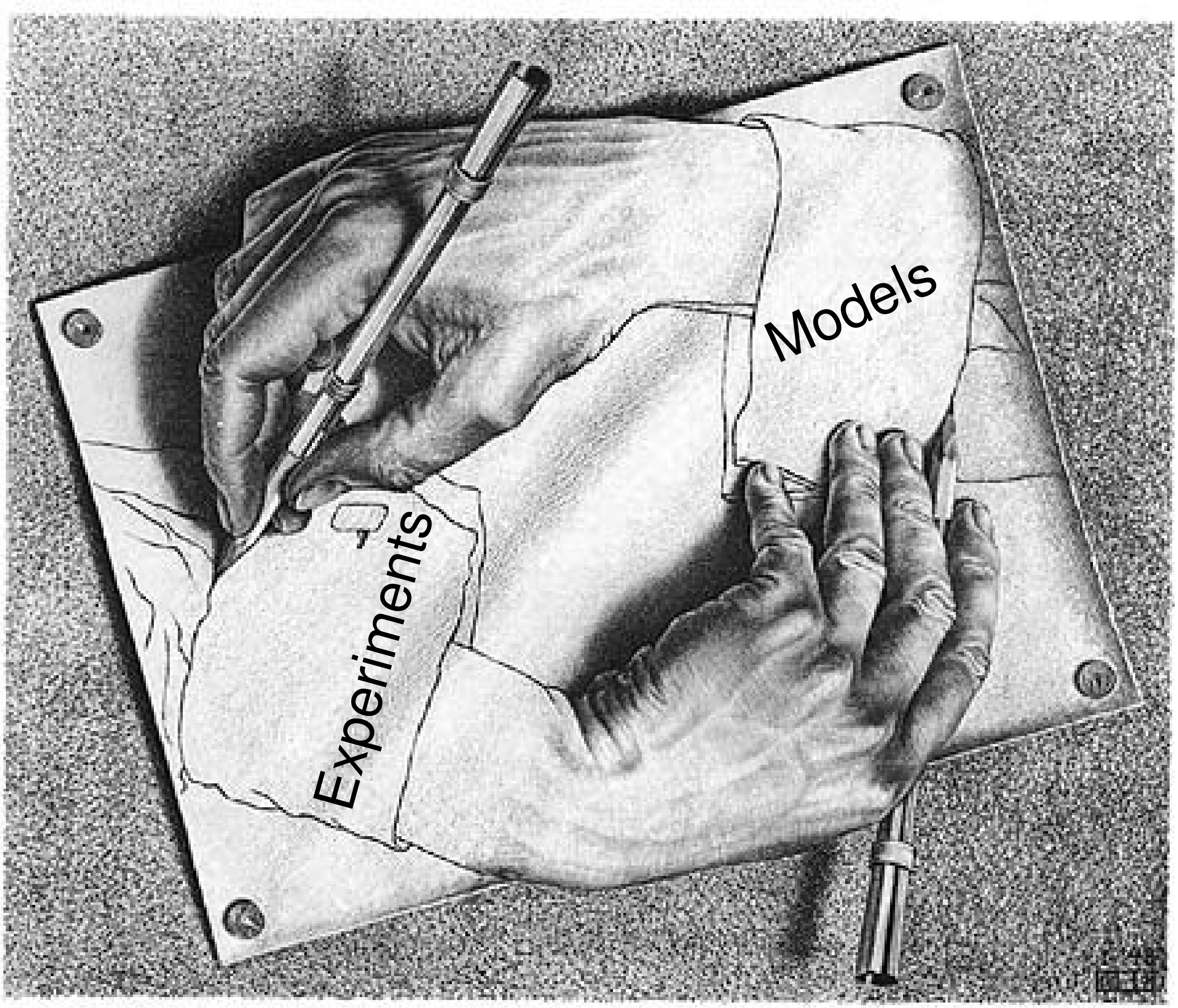
Optimization & statistical tools enhance model development process

DOC model
- Predicted post DOC NO_2 on a vehicle
- Extrapolated fresh catalyst information to predict aged catalyst performance

SCR model
- Motivated the need for analyzing SCR performance = f (NH_3 storage)
- Predicted vehicle NOx conversion and NH_3 slip

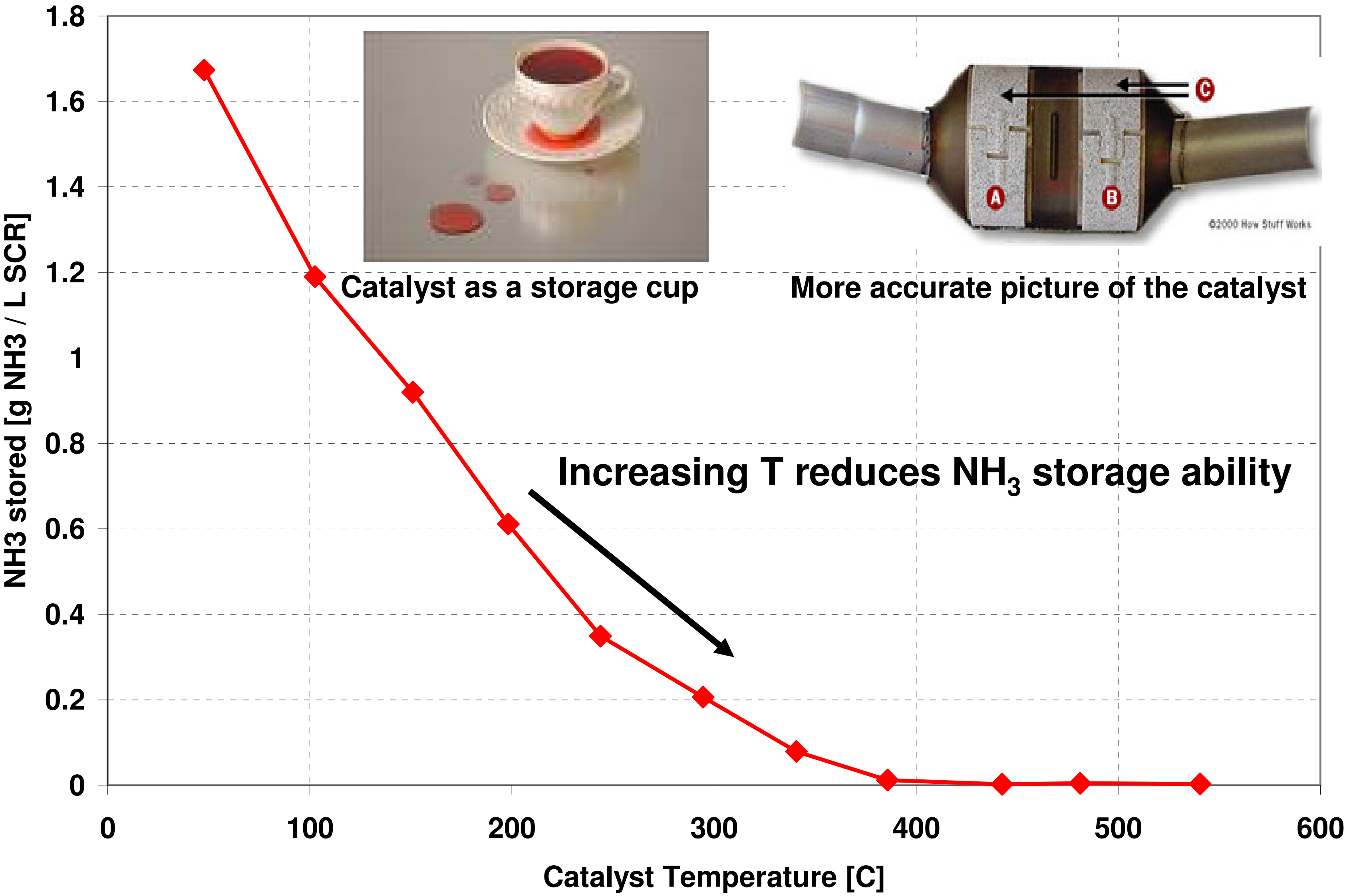
DOC+SCR system analysis
- Highlighted importance of NO_2/NOx from DOC for SCR performance
- Optimization of the urea injection strategy
  (trade-off between NOx conversion & NH_3 slip)

Experiments and models drive each other leading to insight



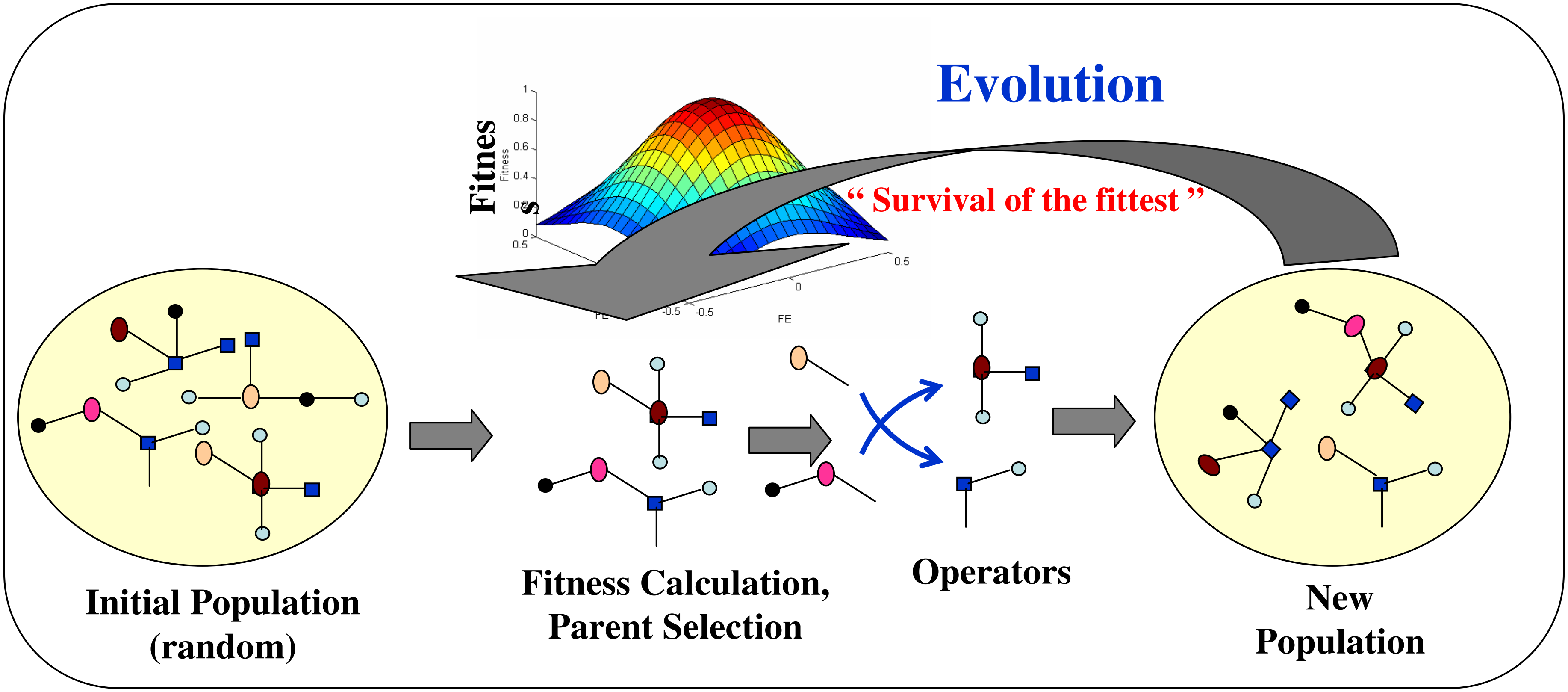
Adapted from “Drawing Hands”, M C Escher, 1948

NH_3 storage decreases with increasing temperature



Model calibration with NH_3 storage information required

AT models are nonlinear and multi-dimensional
Local optimizers may not be efficient



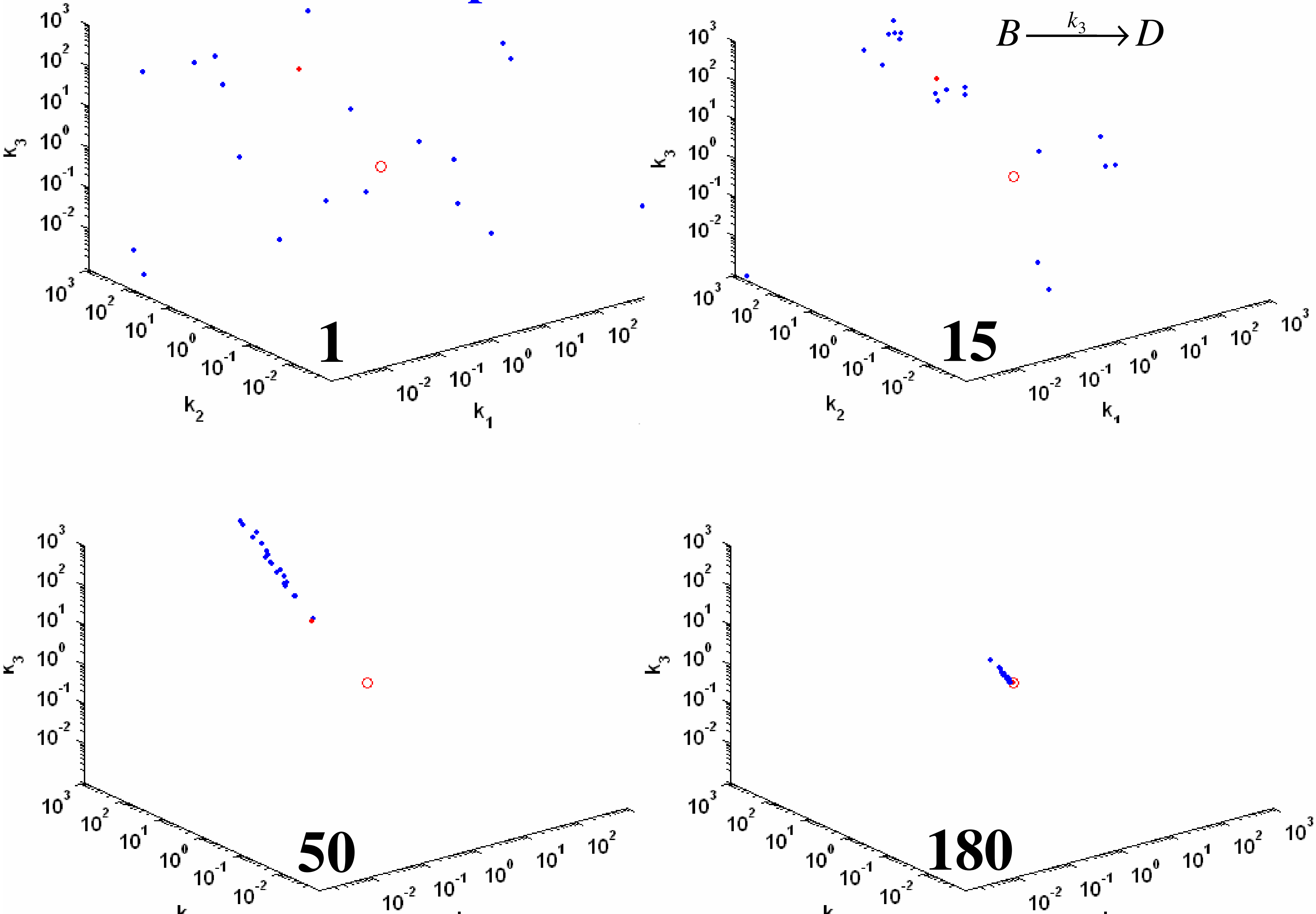
- Do not get trapped in local optima – more robust and efficient than a local optimizer
- Examples: Genetic algorithms, Particle swarm optimization, Differential evolution

In-house built optimizer – can be customized

Optimizer Iterations

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

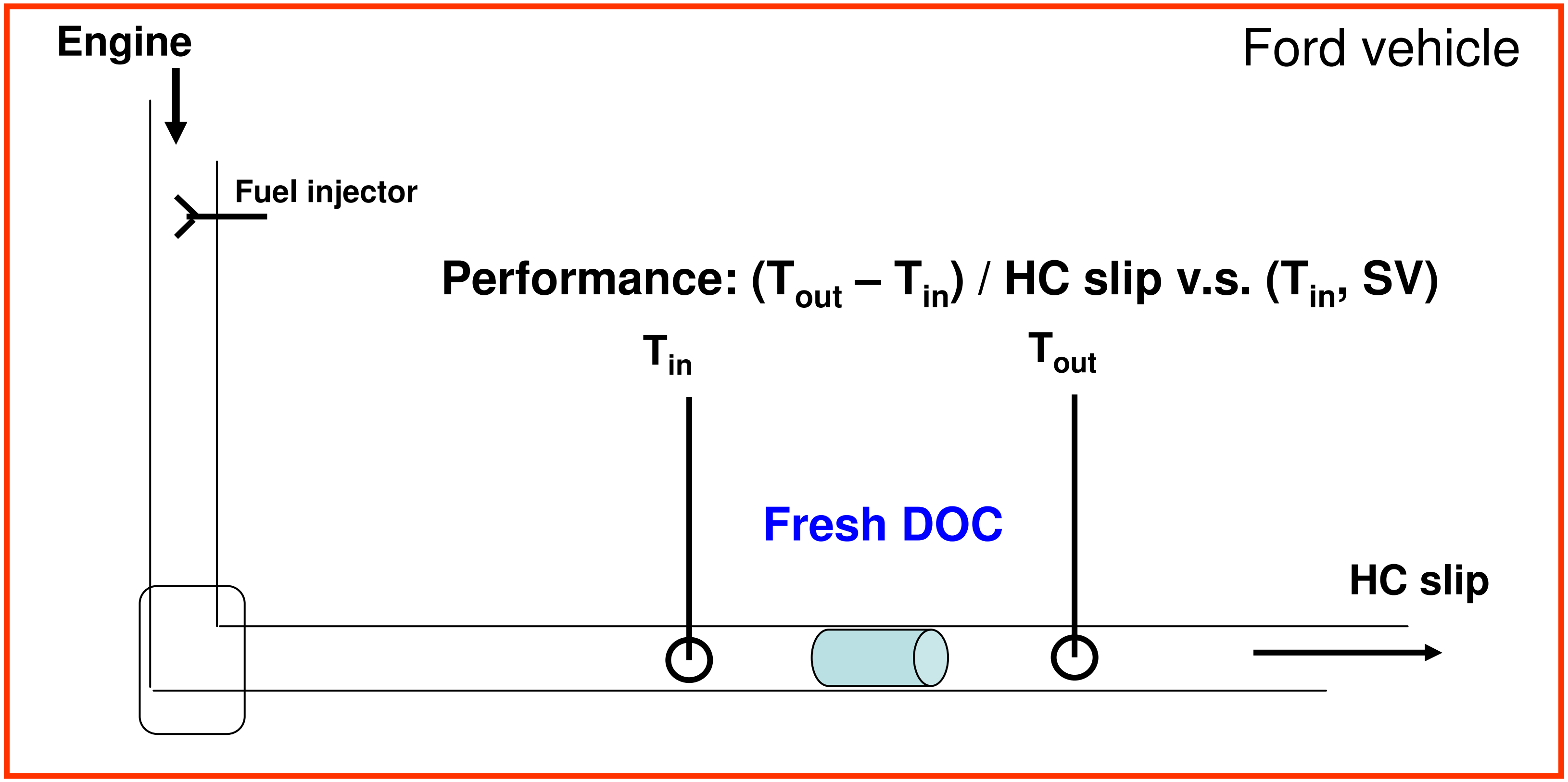
$$B \xrightarrow{k_3} D$$



Katare, SAE 2006-01-069

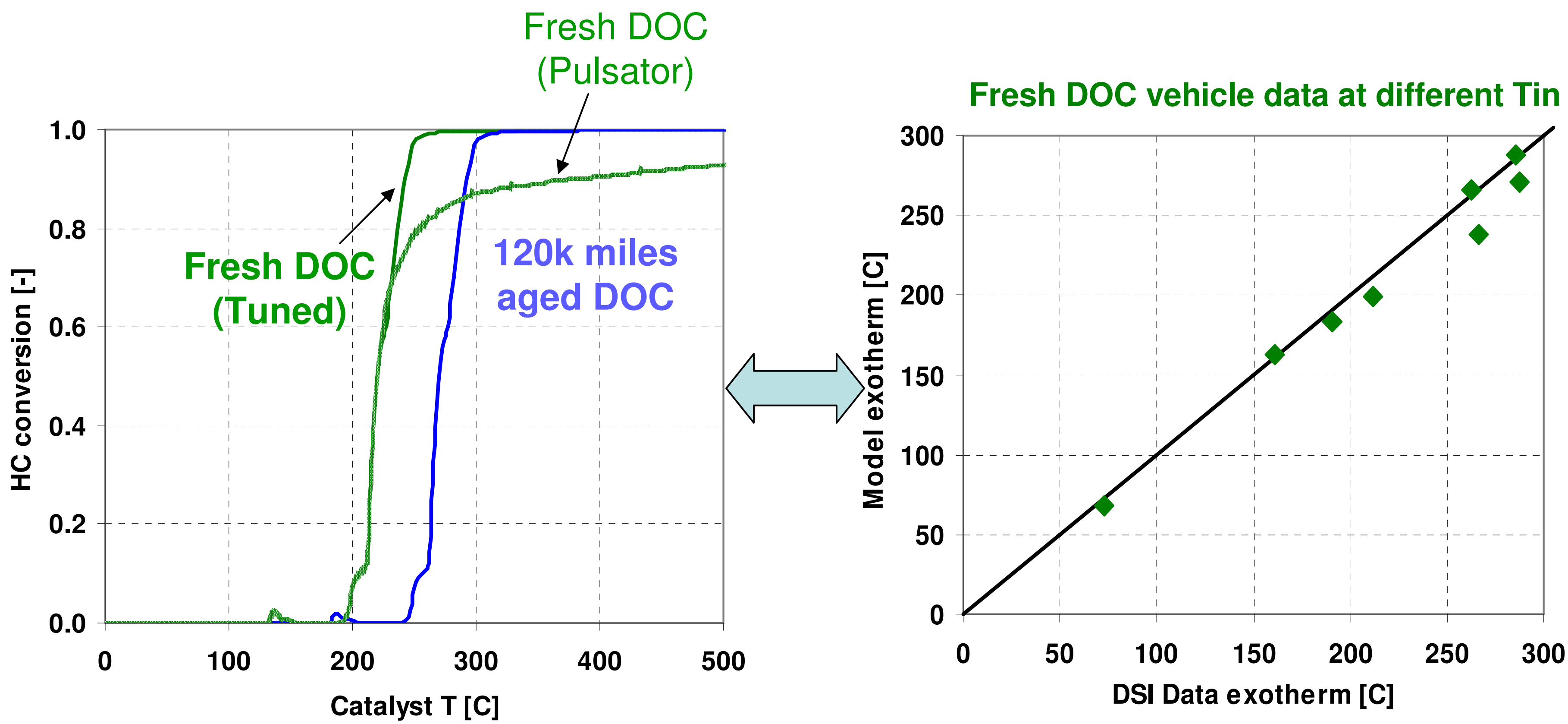
Practical utility of the model: Case study

Burn soot off DPF by down stream injection of fuel (HC)



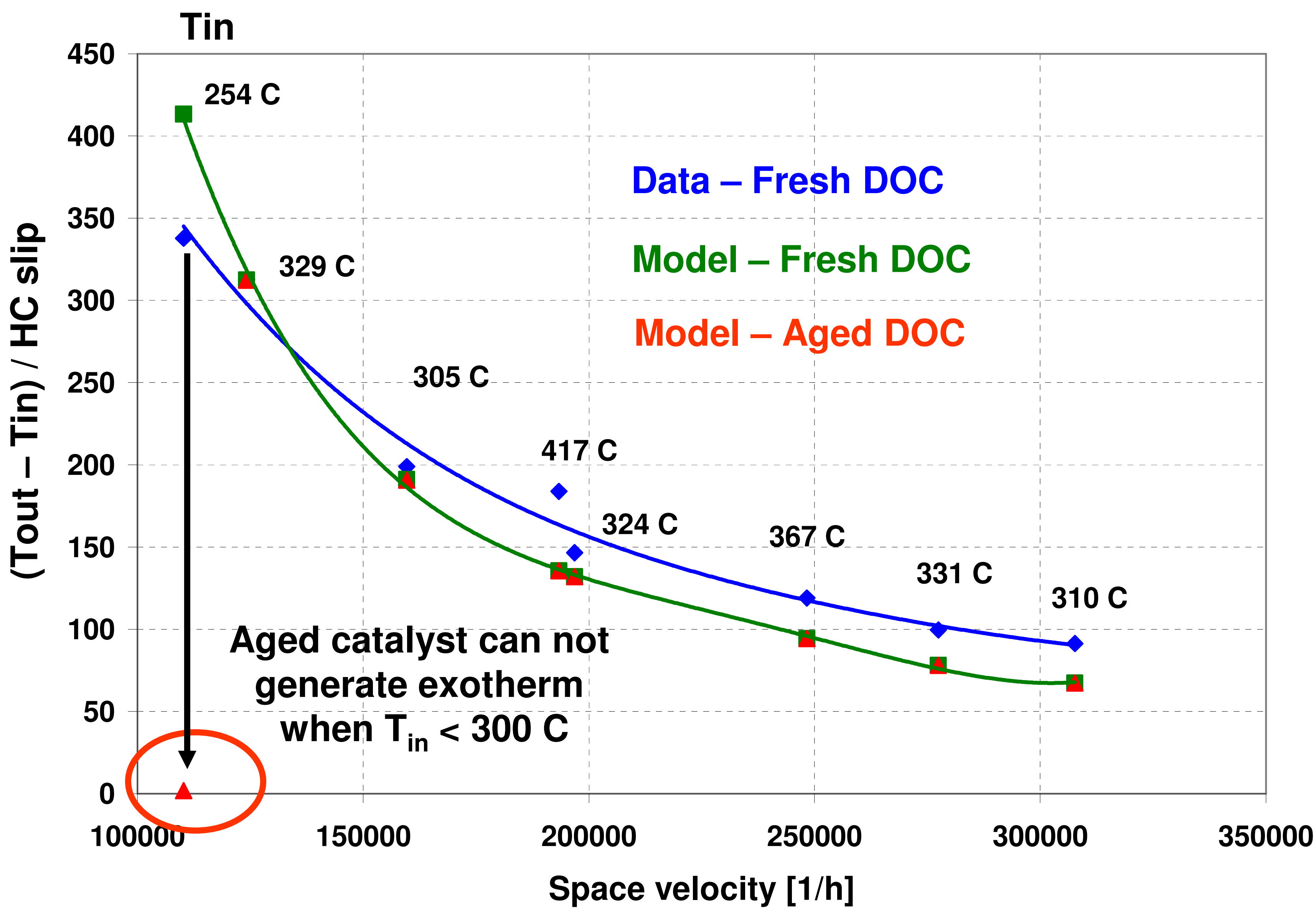
Aged DOC inlet T for exotherm generation given fresh DOC data ?

Calibrating model to fresh DOC data using pulsator map



Model calibrated with “fresh” DOC data Predict “aged” DOC performance

Extrapolating model to predict performance of aged DOC



Model established limits to exotherm generation strategy