Application of an SCR Model

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Overview

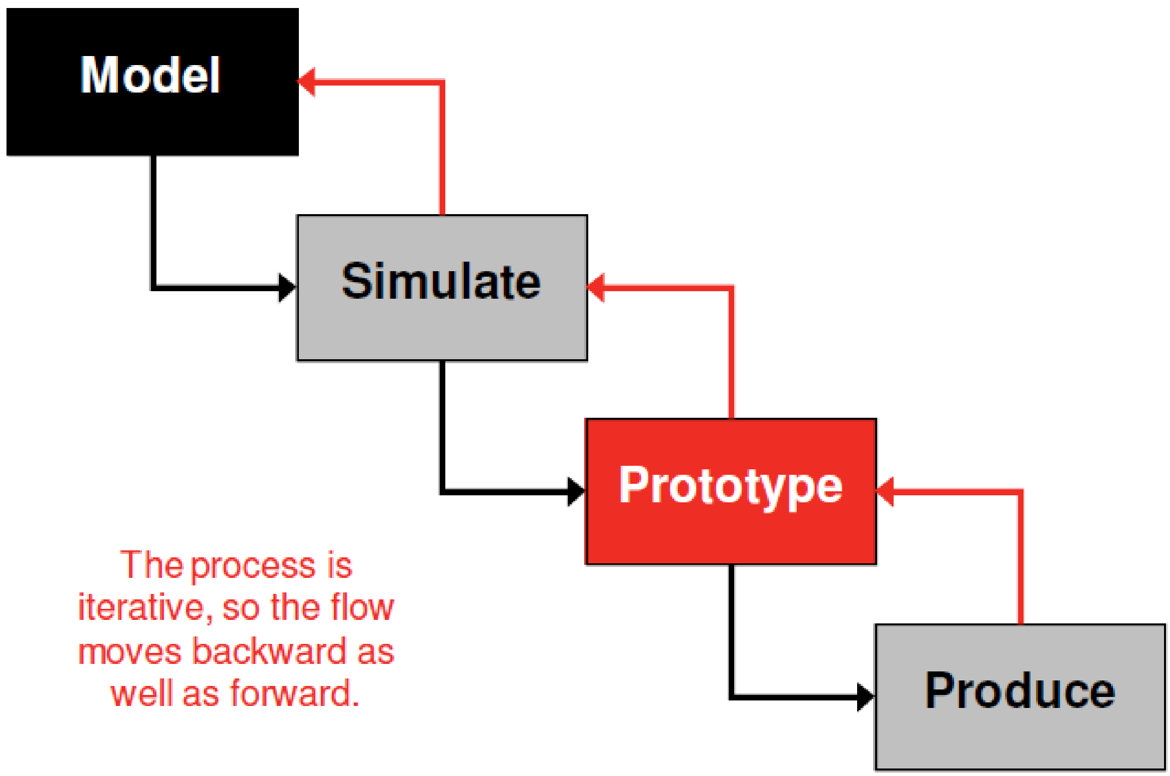
- Product development and design
- Progressive deterioration
- Certification vs Off-cycle
- Catalyst state visualization
- Virtual reactor

Considerations

- Analysis using Dynamic models (Analysis Led Design)
  - Ease of evaluation
    - Including physically difficult, impossible conditions, or nonexistent catalysts
  - Availability of spatially resolved catalyst state
  - Some other synergies – multiple catalyst sizes in a single simulation
- Variables:
  - Architecture (catalyst order, formulations, sizes, loadings)
  - Controls strategy
  - Thermal management
  - Cold start emissions strategies
  - Catalyst initial state (including aging and deactivation)
  - Duty cycle
- Objectives:
  - Determine the sources of performance limitations
  - Evaluate trade offs (*e.g.* fuel economy vs emissions, conversion vs ammonia slip)
  - Determine off-cycle emissions

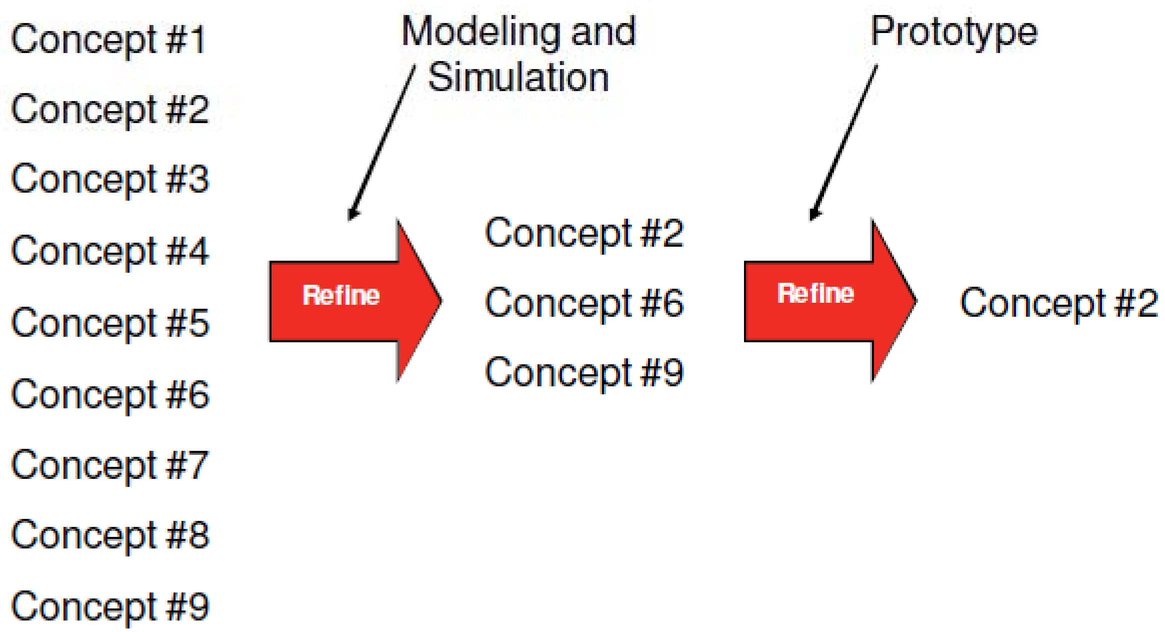
Models in product development

The MSPP Process



- MSPP is not a linear process: there is a lot of iteration.
- The loop around prototyping and simulation is critical for the fast and efficient development of new control systems.
- Effective controls development requires accurate simulation tools.

The modeling step allows evaluation of many alternatives



High fidelity is required in an SCR model

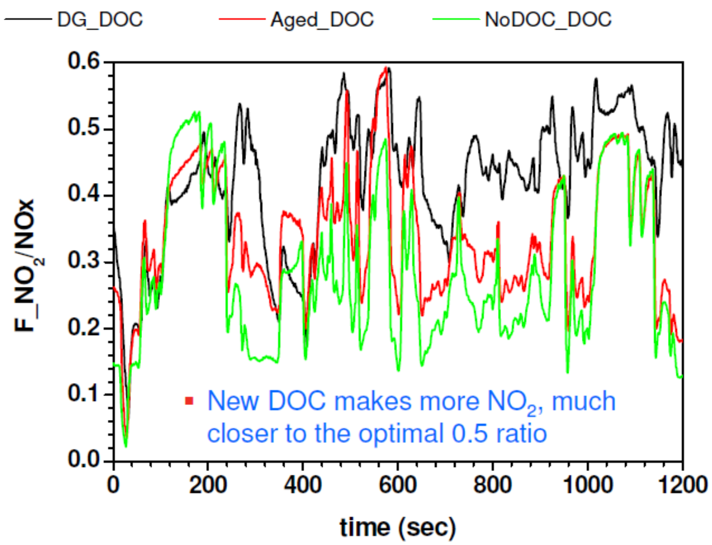
- A key feature of SCR models is ammonia storage.
  - Amount and location are critical.
- The primary difficulty in accurately reflection ammonia storage during a test cycle is cumulative error
  - Significant error can accumulate:
    - over and FTP
    - when there are few “reset events” over the cycle
  - Trends may not even be accurate
  - Comparison of options may be problematic
- Even quite good models fail on this point
  - Lower order models are even worse

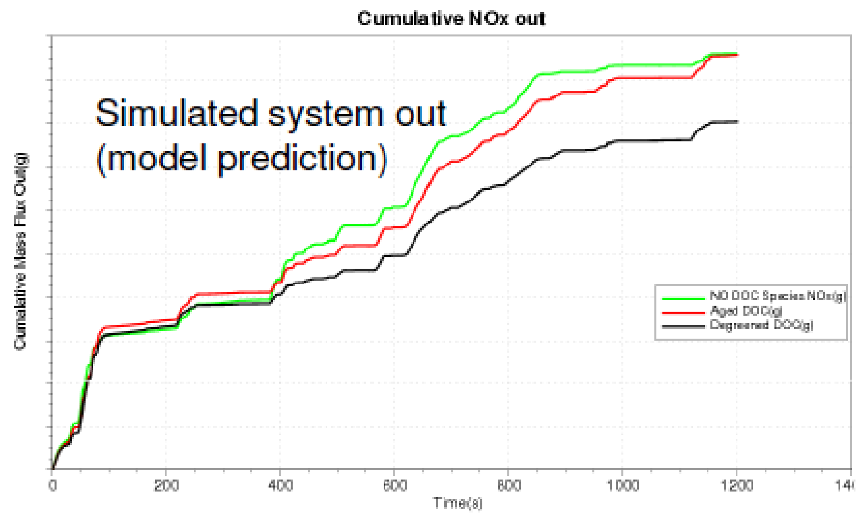
One critical design criteria is OBD

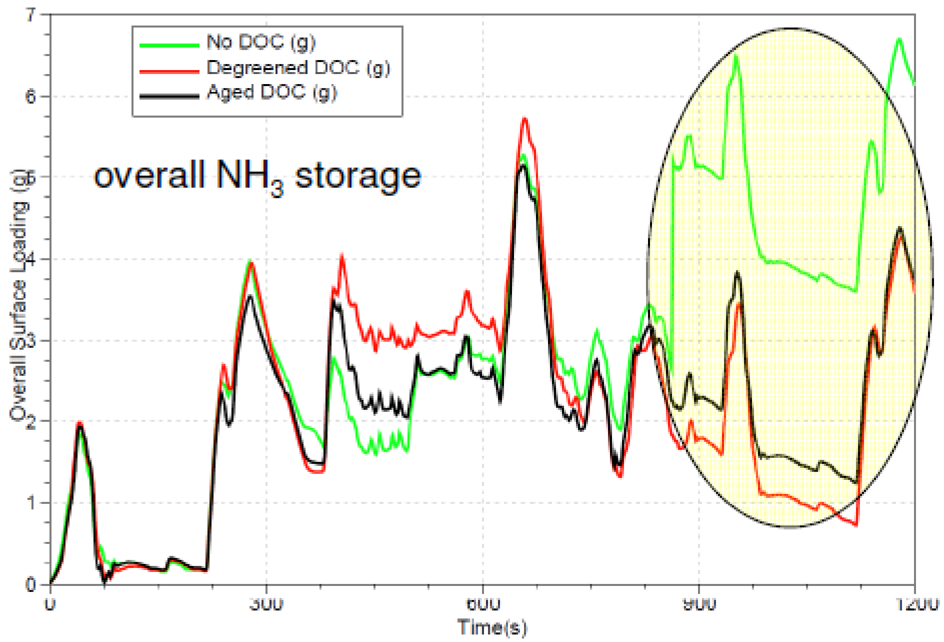
- OBD must identify an underperforming catalysts, BUT it must not misidentify a healthy one
- Using simulation and Monte Carlo analysis, the warranty impact of particular design/control strategy/catalyst or OBD algorithm can be estimated.
- To achieve this, the model must contain all of the catalyst performance traits, including its foibles.

	Concept #1	Concept #2	Concept #3
Added OBD Burden per Engine ($)	250	10	< 2
Repair per Hundred (RPH)	50	2	< 0.1
Percentage of Unresolved Cases (%)	3	0.04	< 0.0001

Progressive Deterioration

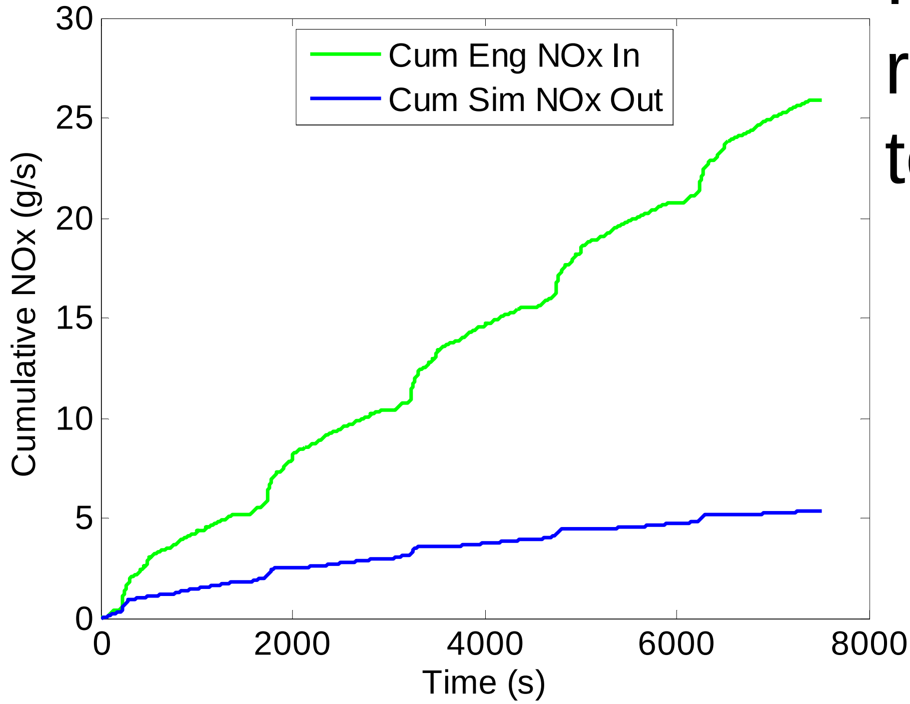






- Beyond system performance, access to the catalyst state indicates potential hazards that may not show up on a particular cycle performance.
- In this case, excessive ammonia storage.

Impact of NO_2/NOx on recovery after High temperature shut-down



NO2/NOx = measured values

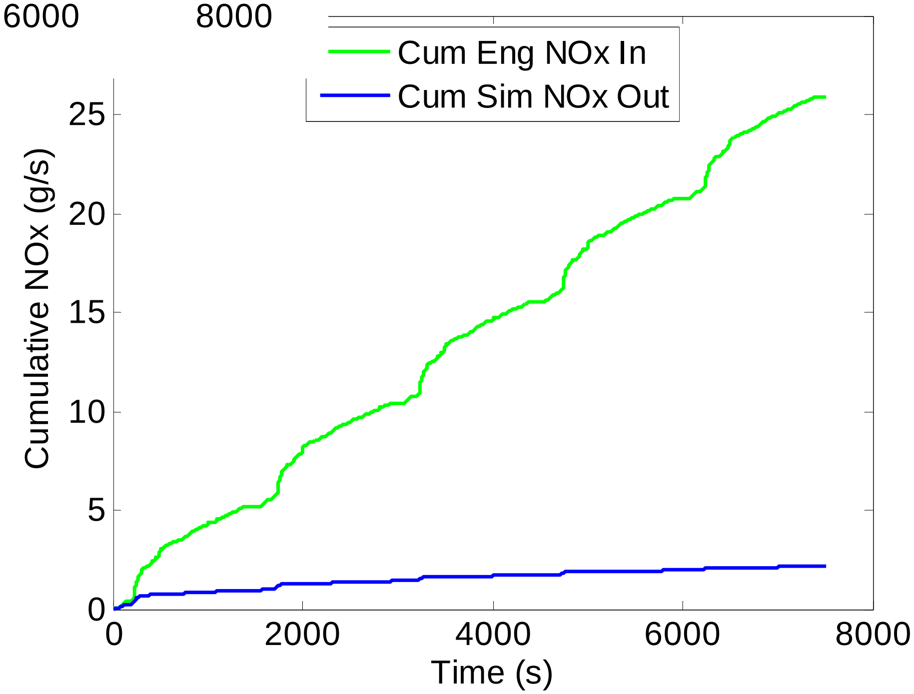
NOx conversion efficiency:

Simulation = 79.30 %

NO2/NOx = 0.5

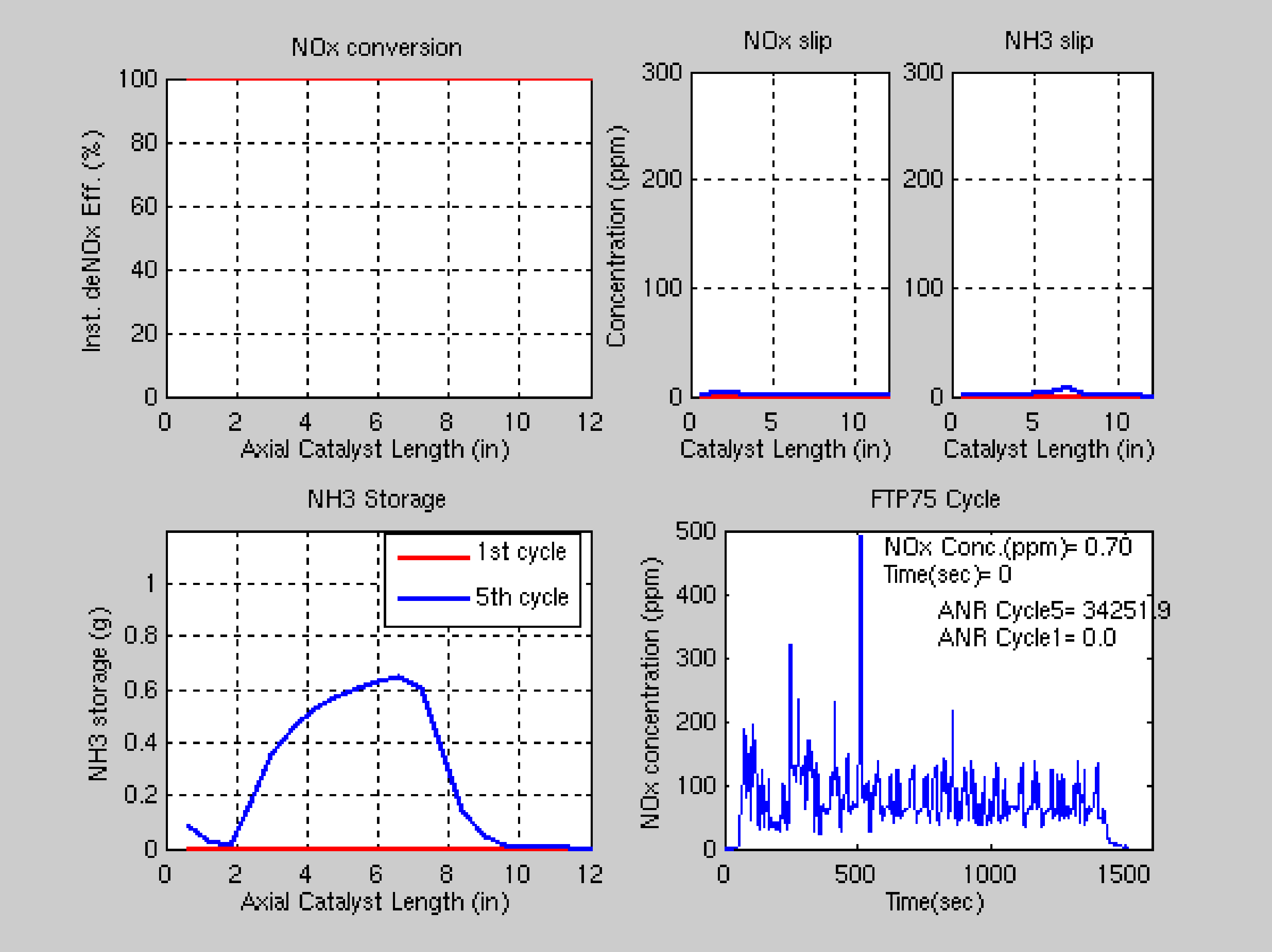
NOx conversion efficiency:

Simulation = 91.69 %



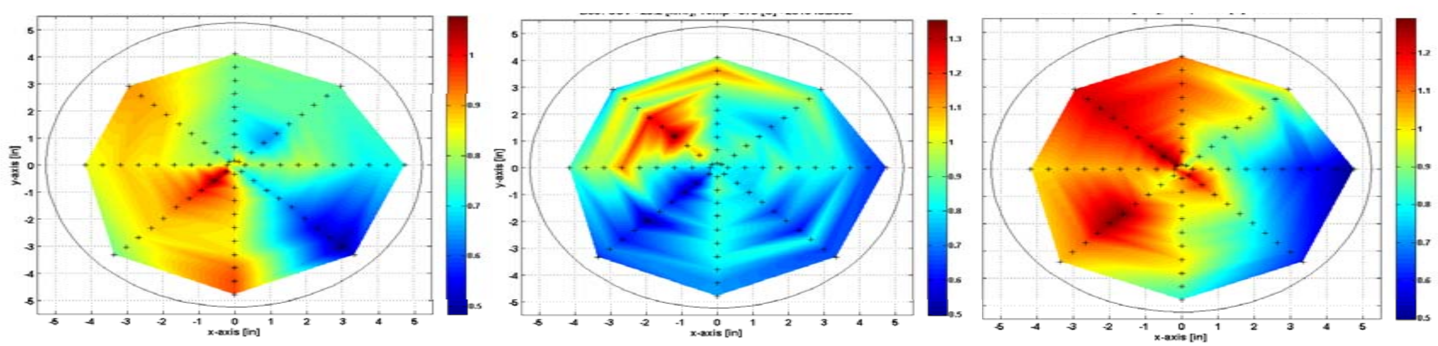
Dynamic Behavior Visualization

- Visualization of the temporal and spatial performance and state of the catalyst can be quite useful.



Virtual Reactor

- Substituting for lab reactors, in some cases.
  - Reducing the need for physical reactors
  - Take less time – for models running faster than real time
  - Evaluate non-existant catalyst structures
- Establishing the level of uniformity of ANR and flow distributions.



Summary

- Although we often think of catalyst models in the context of cycle simulations and system performance evaluations:
  - Their applications are many and varied.
  - Fidelity is always the goal, but not necessarily to the primary characteristics of the catalysts
  - The word “fidelity” related to catalyst models is context sensitive.
  - An ideal model is based on the physics and chemistry of the catalyst not just its behavior in a given engine or laboratory test.