CLEER's 2012:

Challenges and Perspectives on Simulating the Relationship Between Emissions Controls and Fuel Efficiency

Developing Modeling Capabilities for managing Fuel Economy and Tail Pipe Emissions

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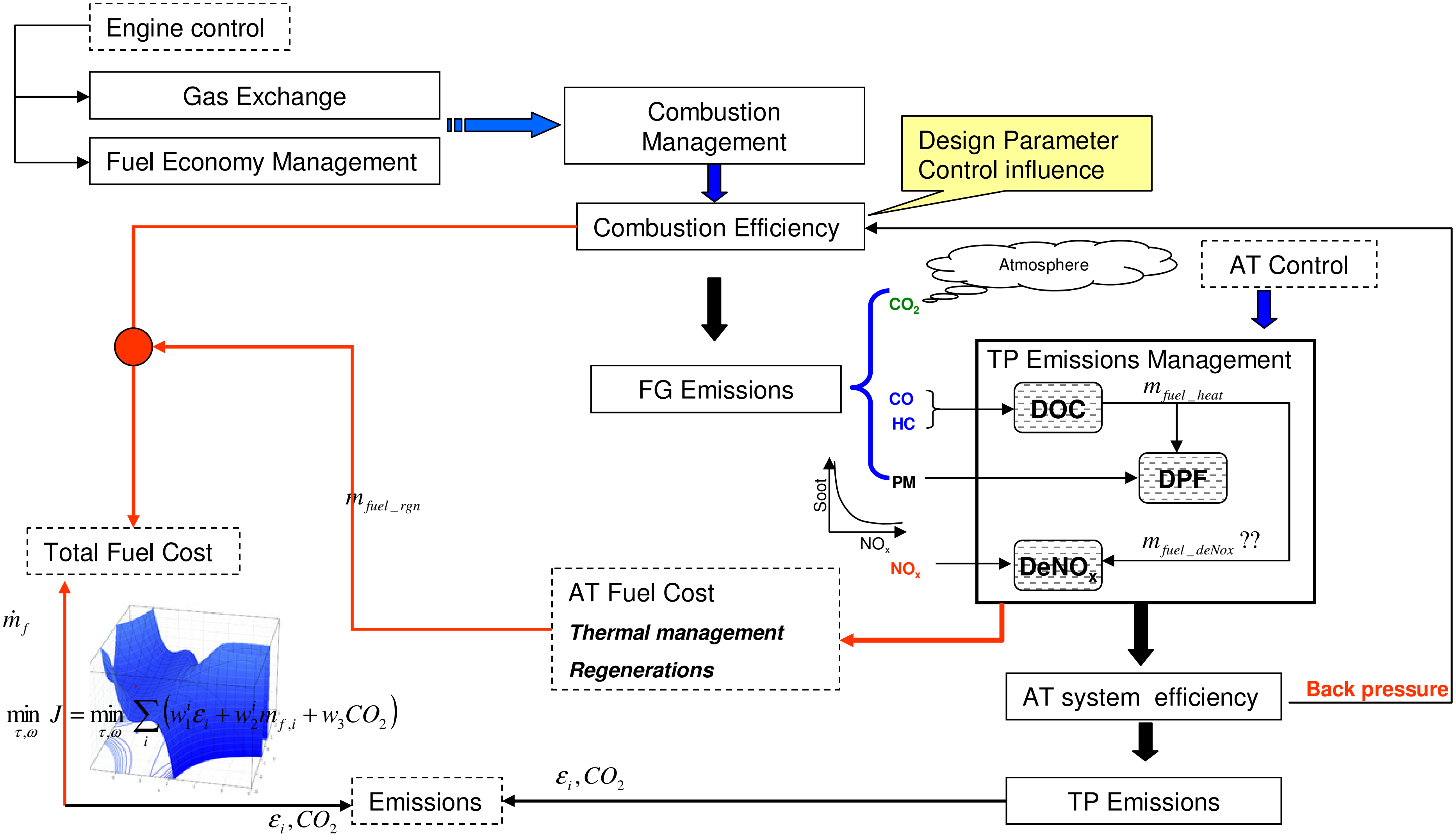
Fuel Economy and Emissions

- Two critical requirements define the automotive industry needs
  - Fuel Economy improvement to meet CAFE.
    - Attract customers, here higher is better, CAFE, may only serve as a lower limit.
    - Consequences with projections to national interest issues.
  - Emissions reduction subject to Federal mandates.
    - Typically majority of customers don't care unless obvious (smoke, odor…)
- An optimization problem, complex, multidimensional …
- There is a base emissions penalty even for an engine operating at the Carnot efficiency
  - Products of HC combustion:
    - CO_2 → unavoidable but can be reduced → Got Diesel ?
      - Efficiency and FE implications are first order effects
      - Much larger debate addresses the higher order impacts.
    - CO, HC, Soot → products of combustion inefficiency → must be minimized.
  - Nitrogenous by products → NO_x → direct consequence of type of combustion. After treatment (or pre-Treatment) necessary.
    - May also be managed at the Feed Gas (FG) level.
    - Improved efficiencies → less heat rejection → colder exhaust → AT efficiency ?

The FE, Emissions coupling



$$\min_{\tau,\omega} J = \min_{\tau,\omega} \sum_i \left(w_1^i \varepsilon_i + w_2^i m_{f,i} + w_3 CO_2 \right)$$

Minimize a cost on fuel consumption and emissions over all engine operating points defined by feasible pairs <T,N>

Time varying trade off scenarios must be managed during operation.

Lack of convexity, Realizability is questionable at best.

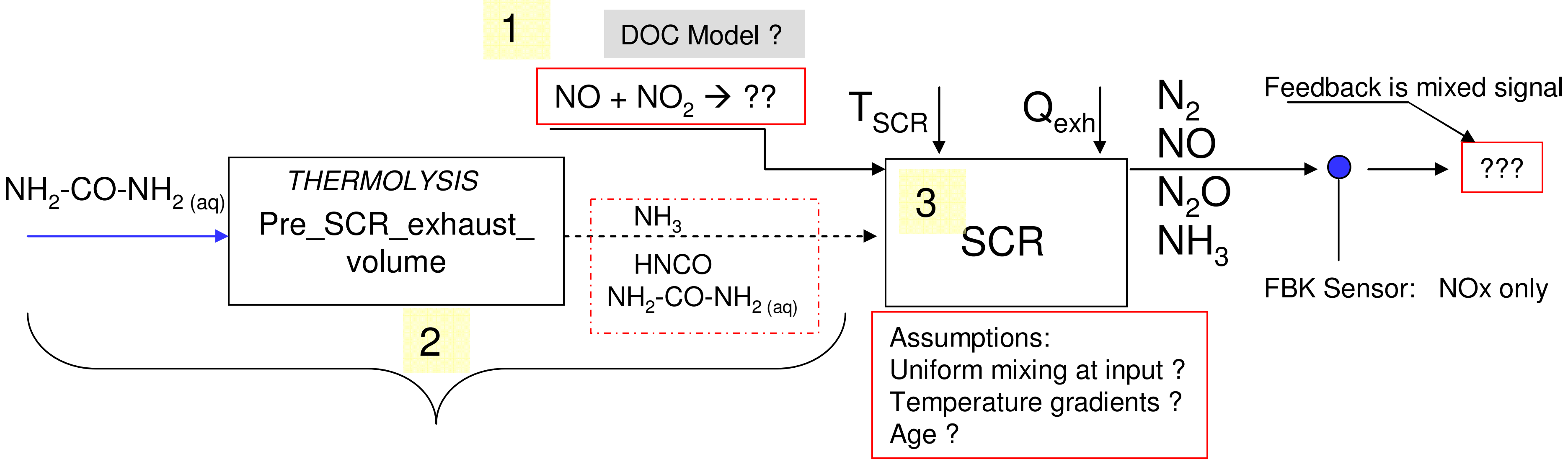
Cost and Performance trade-off

- Cost will often dictate component selection and therefore impact design.
- Example:
  - N sensors Vs (N-n) sensors with n sensors replaced by models, observers, …
    - Note this deletion is not addressing redundancy, … there is NO redundancy in automotive power-train systems !
  - Which design is better ?
  - Not easy to answer, extra sensors come with monitoring burden and therefore warranty costs can creep up, not to mention sensor cost.
  - Less sensors will/may impact performance and may also impact warranty. Long term costs ?
- Several other cost related choices are often subjects of heated debates.
  - Precious metal loading of catalysts
  - Catalyst sizing
  - Cost Reduction wants lower loading and smaller catalysts without reducing AT burden ??? UNREAL …. NO a very Real problem …
- Superficial cost savings will often lead to loss in performance and increased complexity, virtual costs must be understood.
- Comprehensive system level models can help in quantitatively illustrating impacts in terms of Risk migration from such decisions.

Perspective on Models for Controls and Diagnostics

- Complex systems such as catalysts must *ideally* be modeled as 2D or 1D+1D for full impact analysis. 1D models may often fill the need (system depenedent).
- However, higher order models must allow *order reduction* guidance and capability for verification of low order models.
- Control oriented models for RT applications, must by necessity, be of low order
  - Lumped parameter (0D) models
  - Essential purpose is to provide an accurate representation of state trajectories for control guidance.
  - There is a growing tendency to adopt distributed 0D models or pseudo 1D models.
- Simplified or Reduced Order models for RT control and diagnostics must:
  - Include an adequacy (accuracy) metric, whereby, the simplified model proposed is considered adequate via considerations like the operator norm or the largest singular value of the operator matrix deviation over a range of operating conditions.
  - Provide state convergence horizons that are compatible with the desired controller bandwidth.
  - Not increase run time or keep alive memory burden.
  - Not increase sensor cost.
  - NOT impact system robustness to the extent that it actually interferes with OBD requirements on Type-I, II error constraints.
  - Be calibration friendly → Nonlinearities must be handled in a way that afford calibration flexibility.

Case-study: Urea SCR based AT control and OBD



1

DOC Model ?

$NO + NO_2 \rightarrow$??

T_{SCR}

Q_{exh}

N_2

NO

N_2O

NH_3

Feedback is mixed signal

???

$NH_2\text{-}CO\text{-}NH_{2\,(aq)}$

THERMOLYSIS

Pre_SCR_exhaust_volume

NH_3

HNCO

$NH_2\text{-}CO\text{-}NH_{2\,(aq)}$

3

SCR

FBK Sensor: NOx only

2

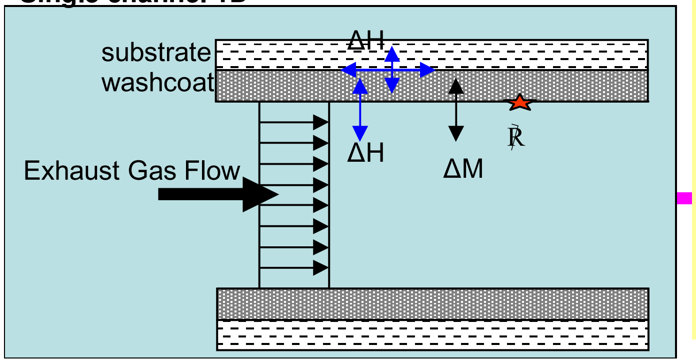
Assumptions:
Uniform mixing at input ?
Temperature gradients ?
Age ?

Model-1: FG NO_x →eliminates sensor cost

Model-2: urea→ NH3 chemistry, spray break-up and distribution are optimized via HW design eliminating the need for targeted modeling in the system context.

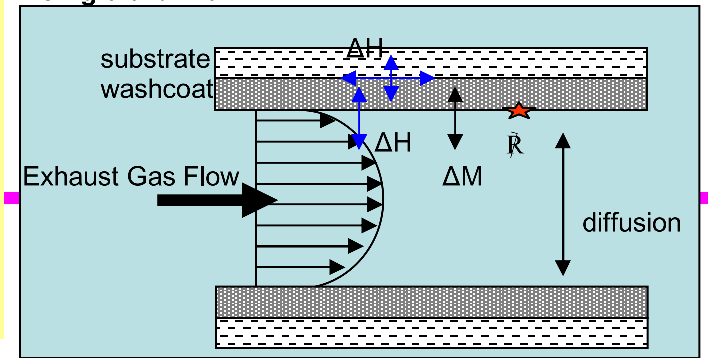
Model-3: urea→ SCR chemistry, the most critical part of the modeling exercise. Internal model necessary for robust control. 1st generation model 0D, new debate on usage of 1D models, most 1D models are however, simply distributed lumped models.

Single channel 1D



1. **Gas transport → conductive, convective, diffusive.**
2. **Pore diffusion**
3. **Boundary layer transfer**
4. **Surface storage**
5. **Reaction on active sites**

Single channel 2D



Case-study: Urea SCR based AT control and OBD

1. FG NO_x models are in broad use now, errors exist (humidity effect) but are generally considered manageable in the FBK control framework.
2. Need for modeling urea input quality (mixing index) is typically reduced via upfront design (mixers .. etc). May need to however model urea to NH_3 chemistry:
   - First principles or empirically identified.
3. SCR catalyst is a good example of a complex system and a good candidate for MOR. 0-D SCR models are currently widely used in RT applications. However, several issues must be tackled:
   1. Modeling scale up → reactor volume (core, typicall 1”x1”) to full catalyst volume (xx Lit’s)
   2. How do you guarantee a correct value for N_T→ fudge factor ?
   3. Residence time distributions impact species concentrations especially at catalyst exit.
   4. Arrhenious type rate models force asymptotic solutions which cannot always match discontinuity of NH_3 release profiles at slip onset. Additionally transport limited mechanisms cannot be captured.
   5. What are the primary kinetics of interest to be considered → may be dictated by the operating space, eg fast SCR is relevant only for cold SCR. But cold SCR
   6. Catalyst aging is a complex process, can be very distributed (x, r) in nature. What happens to the generic model as the catalyst ages ? Should one model or probe for age ??
   7. From a controls perspective NH_3 storage errors are a primary concern and force adaptation and observer design. However single sided control capability (cannot actively deplete storage) makes plant uncontrollable once in over-stored state. That is one loses reachability with regard to maintaining 0 NH_3 slip !
   8. Model structure can amplify storage error dynamic leading to control instability
      - Asymptotic errors for NH_3 slip onset.

Models and SCR control challenges

- Feed back control is necessary → criticality of coverage forces use of an internal model of storage.
- Model based control related solutions must address the following:
  - NH_3 storage error is a fact of Urea-SCR life (under considerations of system uncertainty), learn to live with it.
    - Ignoring this may make for a good presentation but will not work in real life.
  - Reachability (Realizability) issues must be considered → controllability
  - Output signal disambiguation must be defined in the context of the feedback sensor set.
  - Model based constructs (observers) must address robustness for storage errors.
  - Convergence based schemes (observers, adaptive update laws, on line ID) must address convergence horizons, not only over standard cycles but also for off cycle situations.
  - Robustness demonstration time scales must be compatible with time storage scales storage error may not lead to NH_3 slip in one FTP-75 but back to back repeats WILL lead to NH_3 slip.
- Stability and Optimality are big questions.
  - Optimal → find an optimal strategy to minimize Y_{mes} → keep $Y = Y_{NOx} + \alpha Y_{NH3} \rightarrow 0 \ \forall t$. With constraints on urea usage.
    - Typical storage constraint: $m^{*}_{NH3} \in \left(\left\{m^{stor}_{NH3} \middle| \left(\max\left(m^{stor}_{NH_3}\right) < m^{AS}_{NH_3}(\ )\right)\right\} \cap \left\{\min\left(m^{stor}_{NH3}\right) \middle| \eta = \eta^{*}\right\}\right), \forall t, T_{SCR}.$
  - Stability definition must be reframed under system response time scales.

Conclusions

- Models are essential for design and development *BUT* must be built with a purpose.
- Reduced order embedded models for RT control and OBD are becoming ubiquitous… BUT, generating ROM requires insight into system complexity.
- Control design must be carried out with an understanding of System complexity.
  - Non-linearities must not just be ignored rather they must be managed.
- In general control design for urea SCR's requires some creative approaches, cookie cutter approaches may not provided global desired results.
- Control design without considerations on OBD is an incomplete exercise.
- For validation must have:
  - Repeated on cycle performance
  - Repeated off cycle
  - Include Noise factors