Passive NH3 SCR Operation for Lean SIDI: Overview of Modeling Results

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Kevin L. Perry, and Chang H. Kim
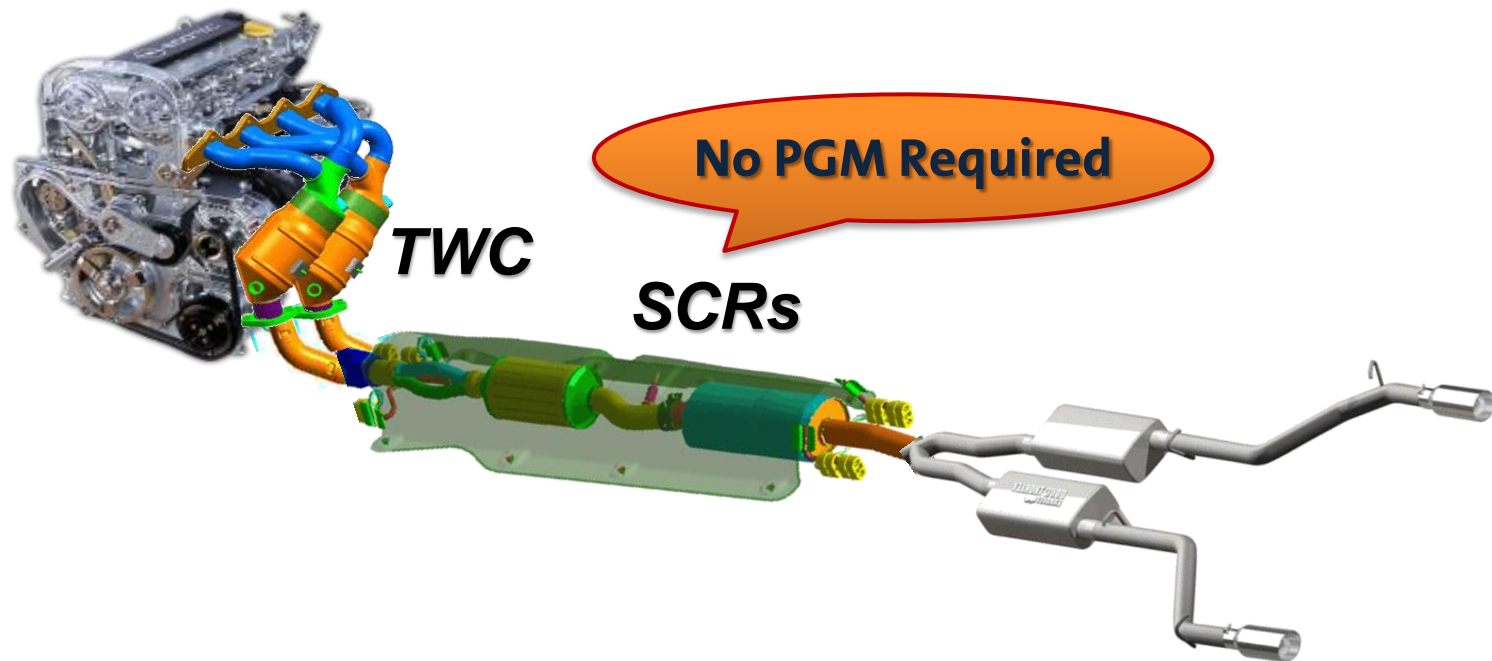
12th DOE CLEERS Workshop

Outline

- Passive NH3 SCR Concept

- Introduction

- Model Validation

- Sample Results

- Summary

Passive NH3 SCR Concept

No PGM Required

TWC

SCRs

- Use rich pulses to generate NH_3 on the TWCs and store it in multiple SCRs

  Rich: $NO_x + H_2/CO \Leftrightarrow NH_3 + CO_2$

- Use the stored NH_3 for lean NO_x conversion

 *Lean:* $NO_x + NH_3 \Leftrightarrow N_2 + H_2O$

Introduction

- Use system level models to explore feasibility of passive SCR operation for lean SIDI operation
  - Explore a range of what-if scenarios
    - SCR type, volume, order
  - Compliment experiments for system optimization
    - Meet emission, thermal management requirements
  - Fine tune a given system for better performance
    - Optimize system for minimal NOx/NH3/CO/UHC breakthrough

- Modeling tools
  - Commercial Cycle Simulation Code
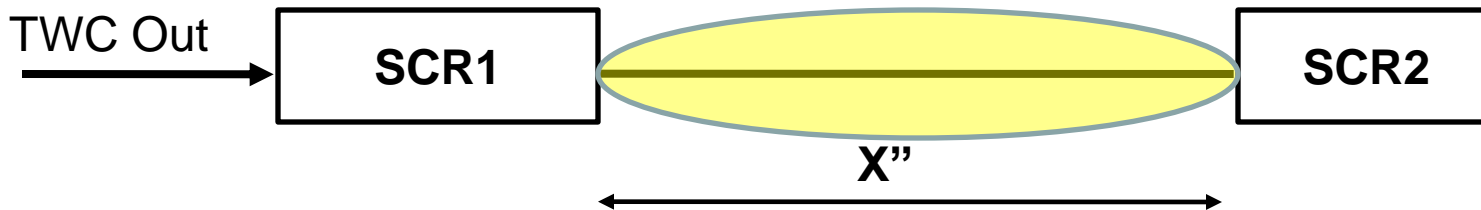 - In-house 1-D Aftertreatment models with relevant kinetics
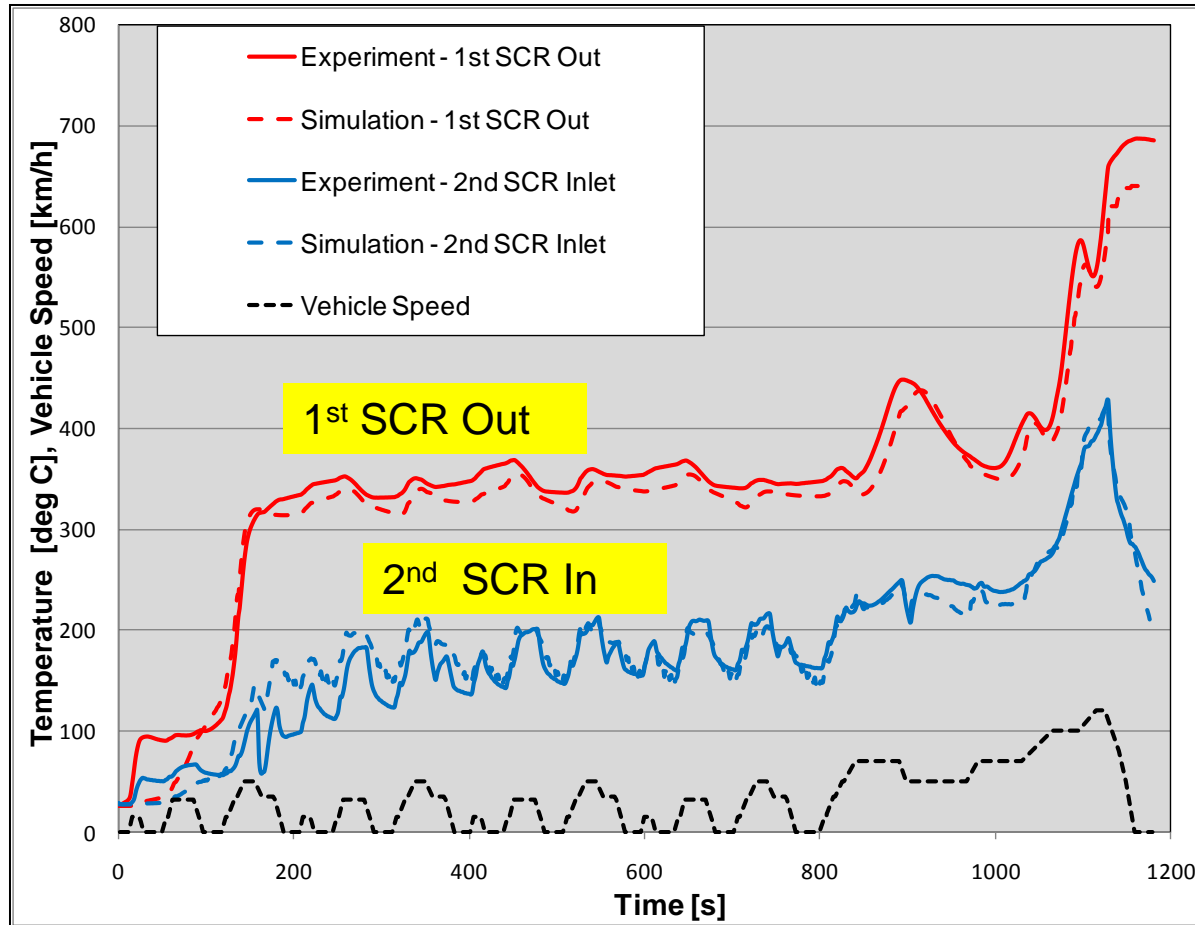 - Standalone or coupled

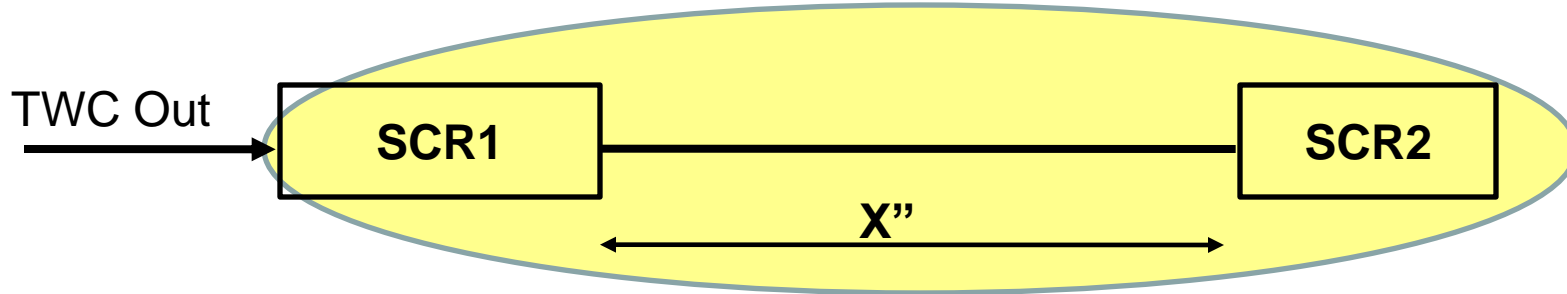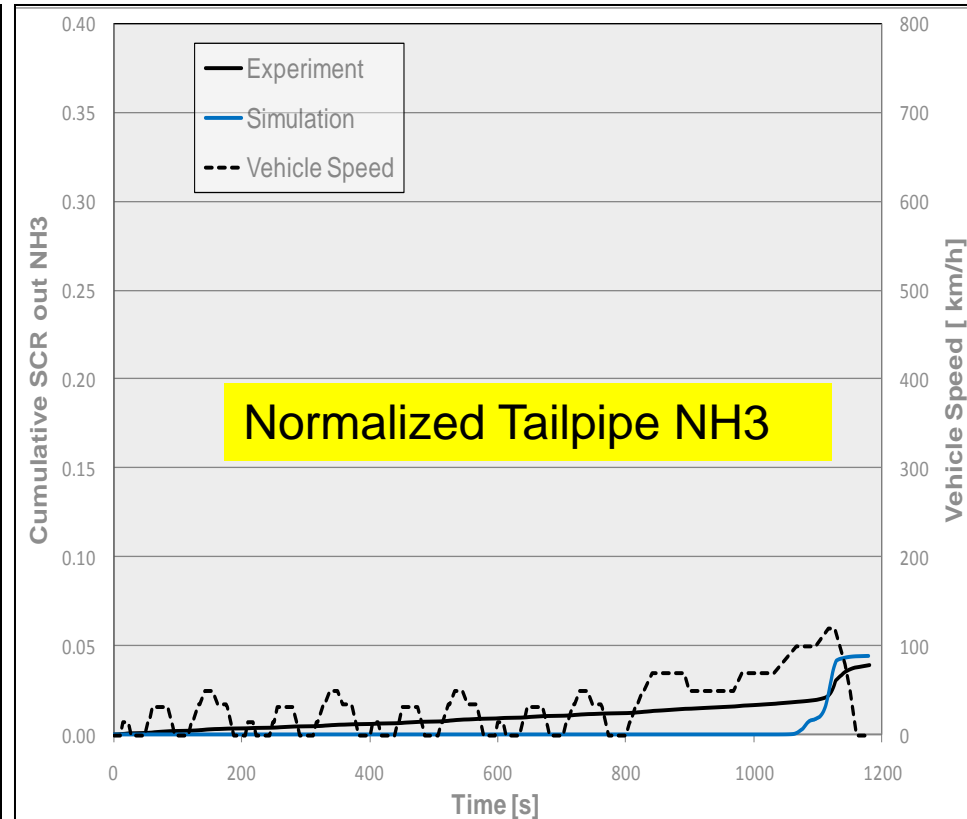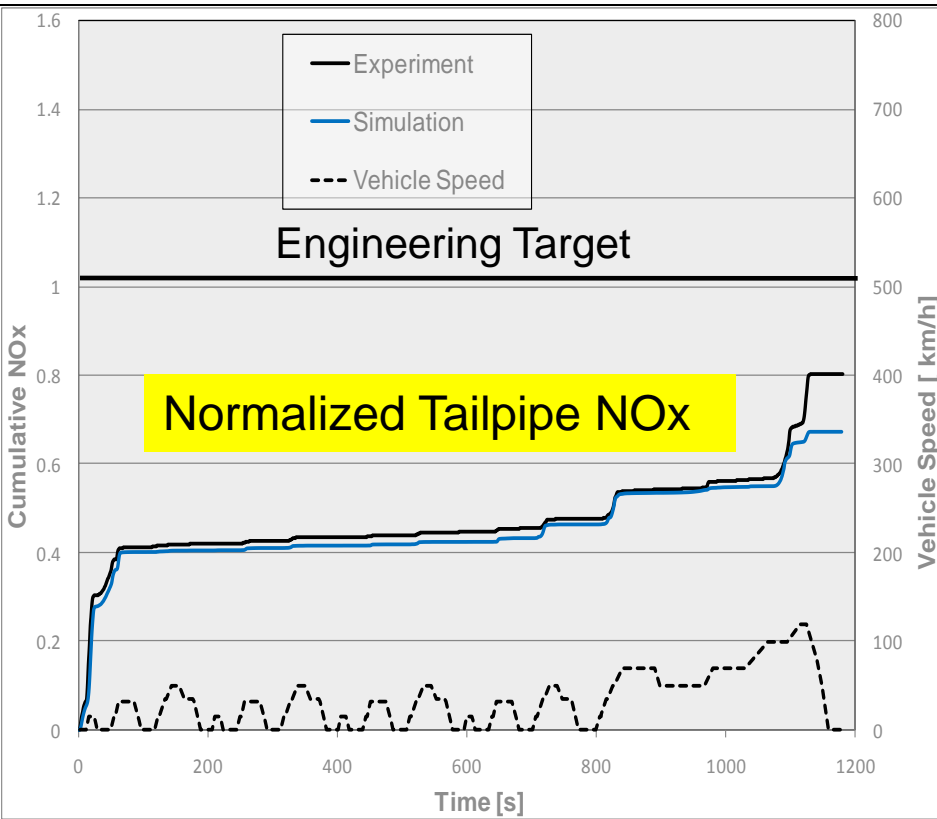# Model Validation – SCR Configuration
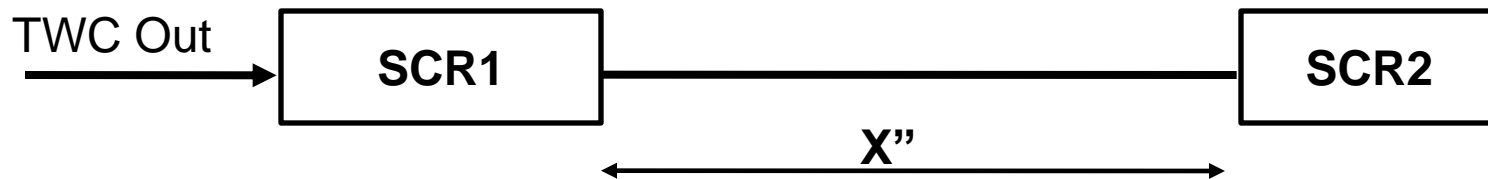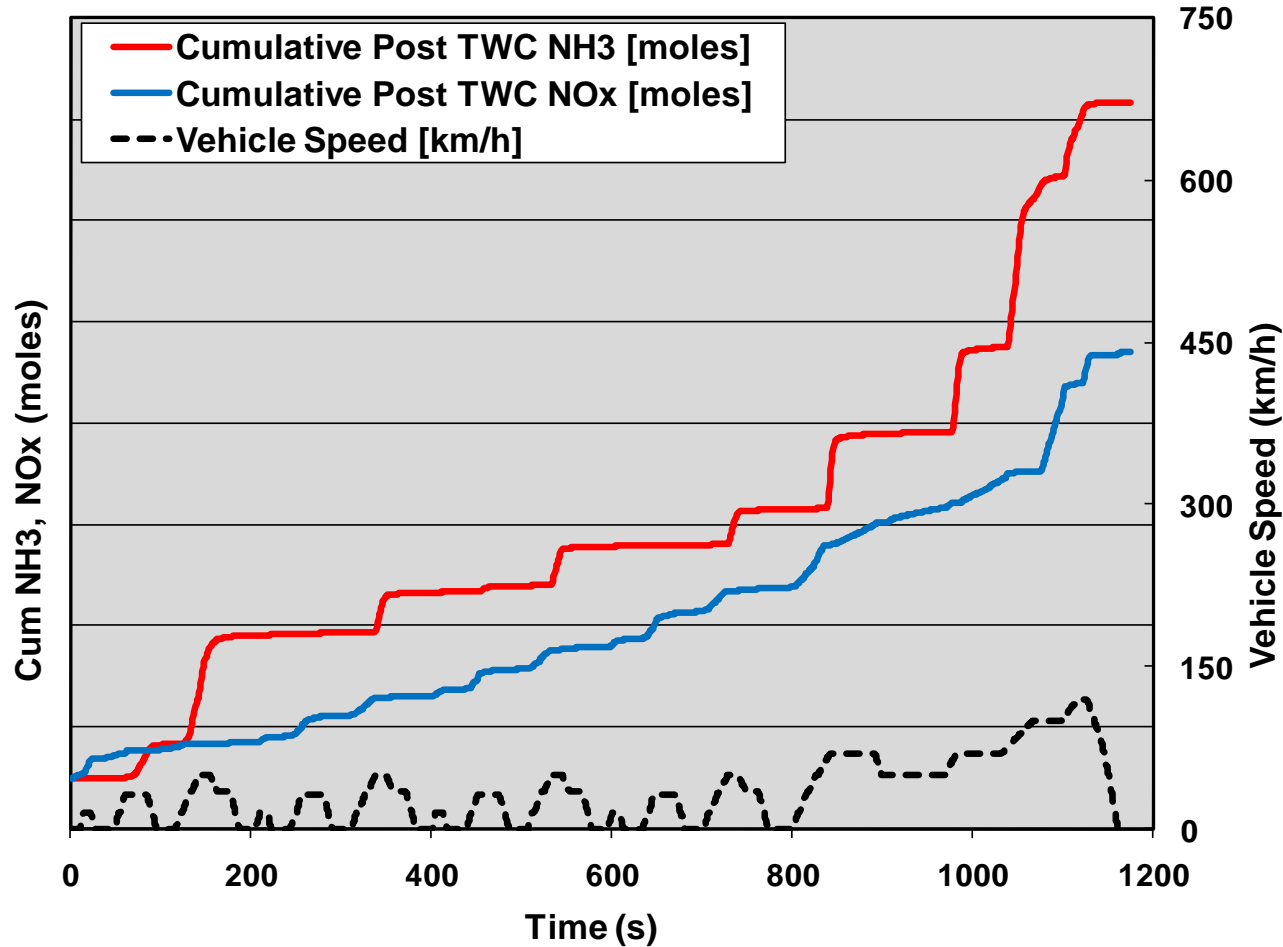
Normalized NOx & NH3 Breakthrough Across SCR1 – Standalone SCR
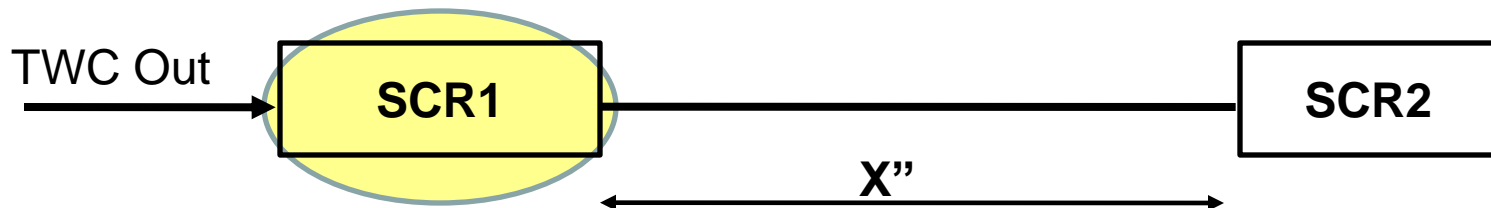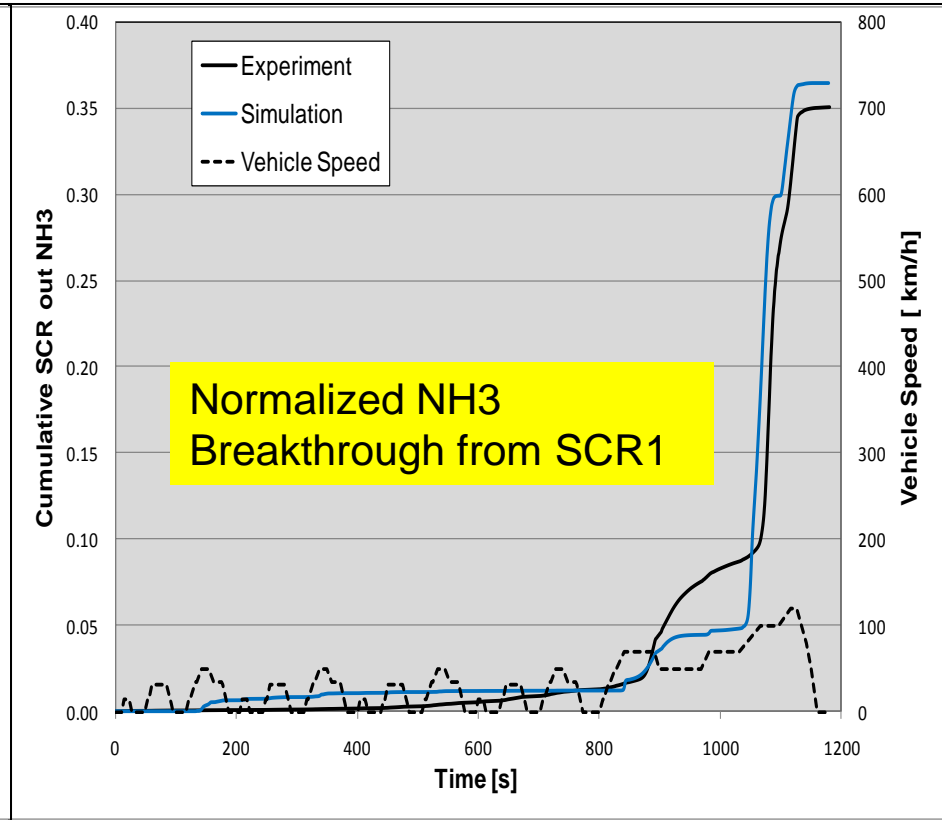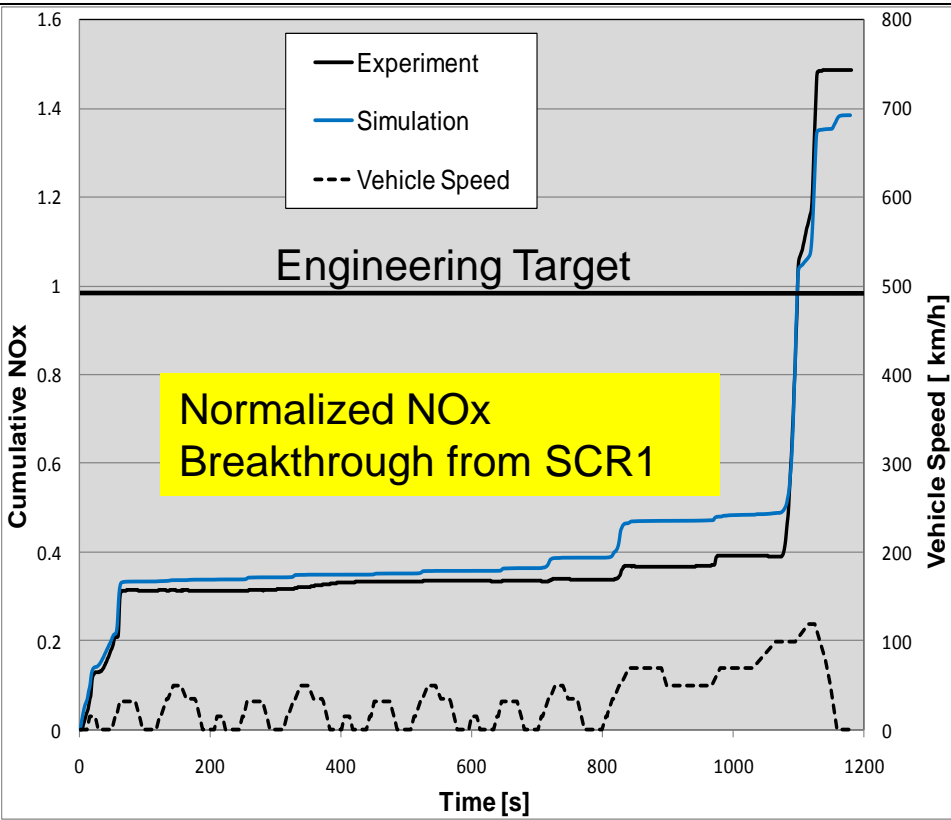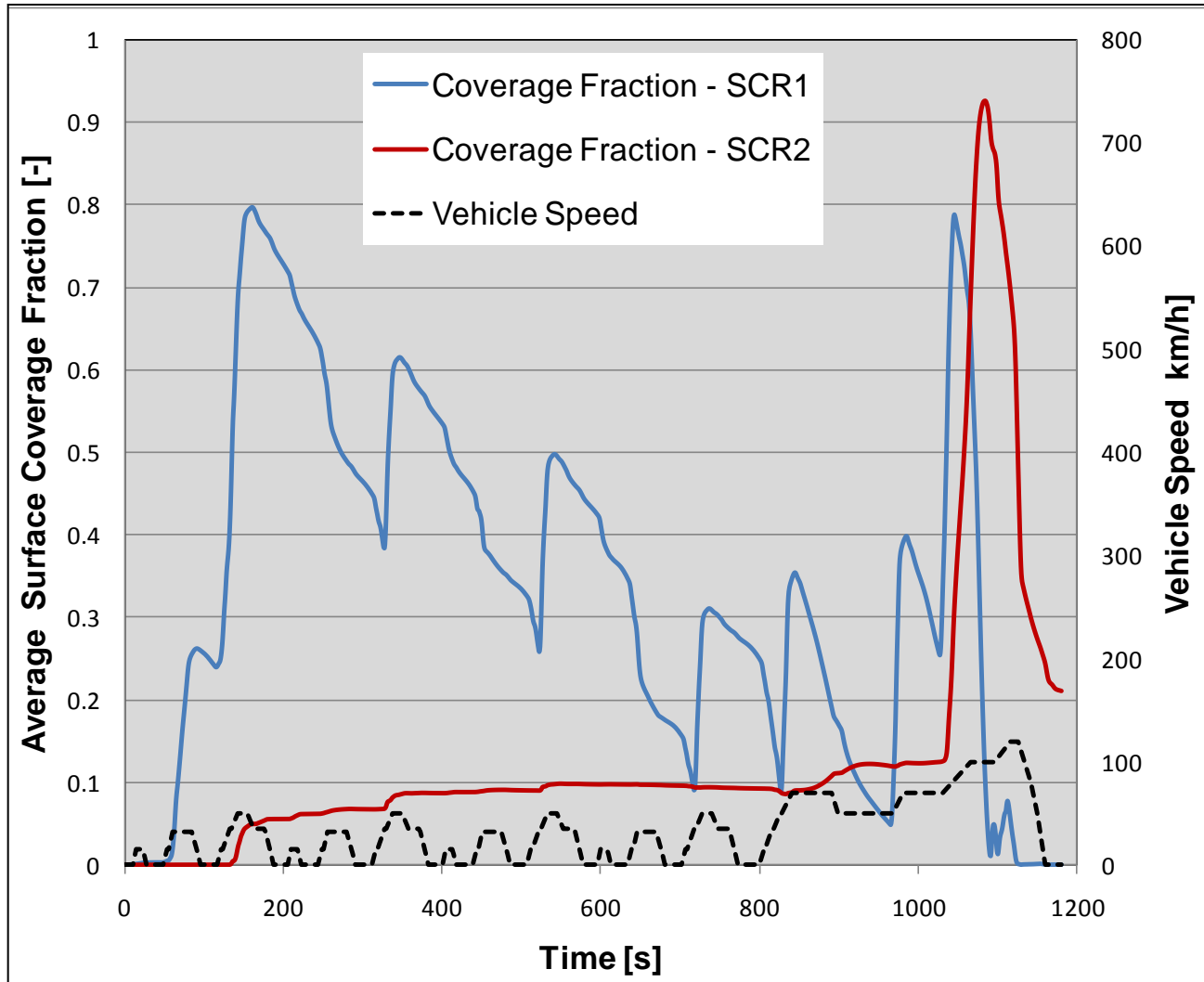
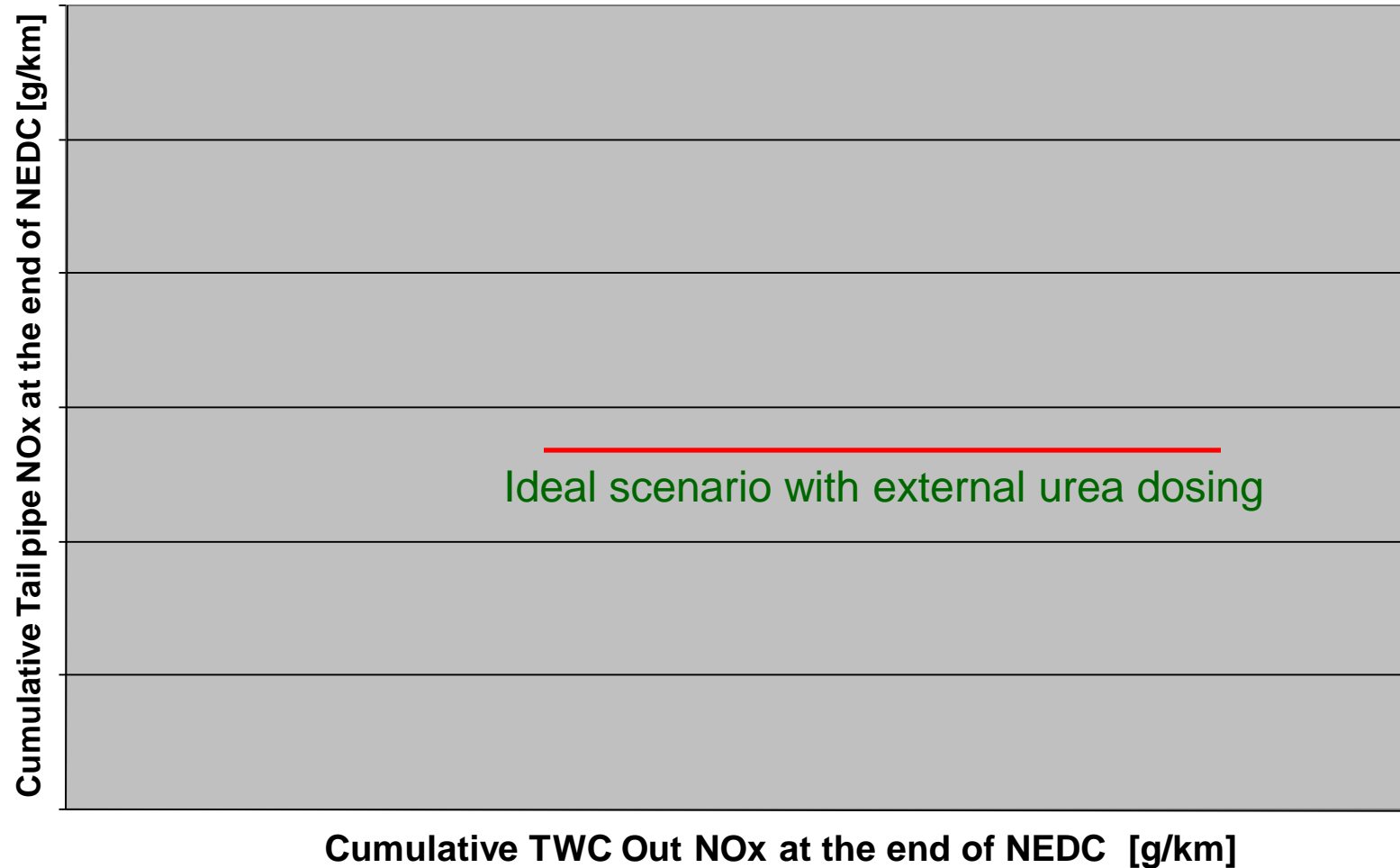# Temperature at Representative Locations – Thermal Model

Tailpipe NOx & NH3 Breakthrough – System Model

Average NH3 Coverage Fraction Across Each SCR

Model Application 1 – SCR Catalyst Screening

Ideal scenario with external urea dosing

Y-axis: **Cumulative Tail pipe NOx at the end of NEDC [g/km]**

X-axis: **Cumulative TWC Out NOx at the end of NEDC [g/km]**

Model Application 1 – SCR Catalyst Screening

Cumulative Tail pipe NOx at the end of NEDC [g/km] (y-axis)

For a given SCR catalyst volume/location(temperature)

1.75 * Baseline

1.5 * Baseline

1.25 * Baseline

Baseline

0.75 * Baseline

Ideal scenario with external urea dosing

Fe   Fe

Cumulative TWC Out NOx at the end of NEDC [g/km]

Model Application 1 – SCR Catalyst Screening

Cumulative Tail pipe NOx at the end of NEDC [g/km] (y-axis)

For a given SCR catalyst volume/location(temperature)

1.75 * Baseline

1.5 * Baseline

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Baseline

0.75 * Baseline

Ideal scenario with external urea dosing

Explore ways to lower the slope of the curve

Fe | Fe

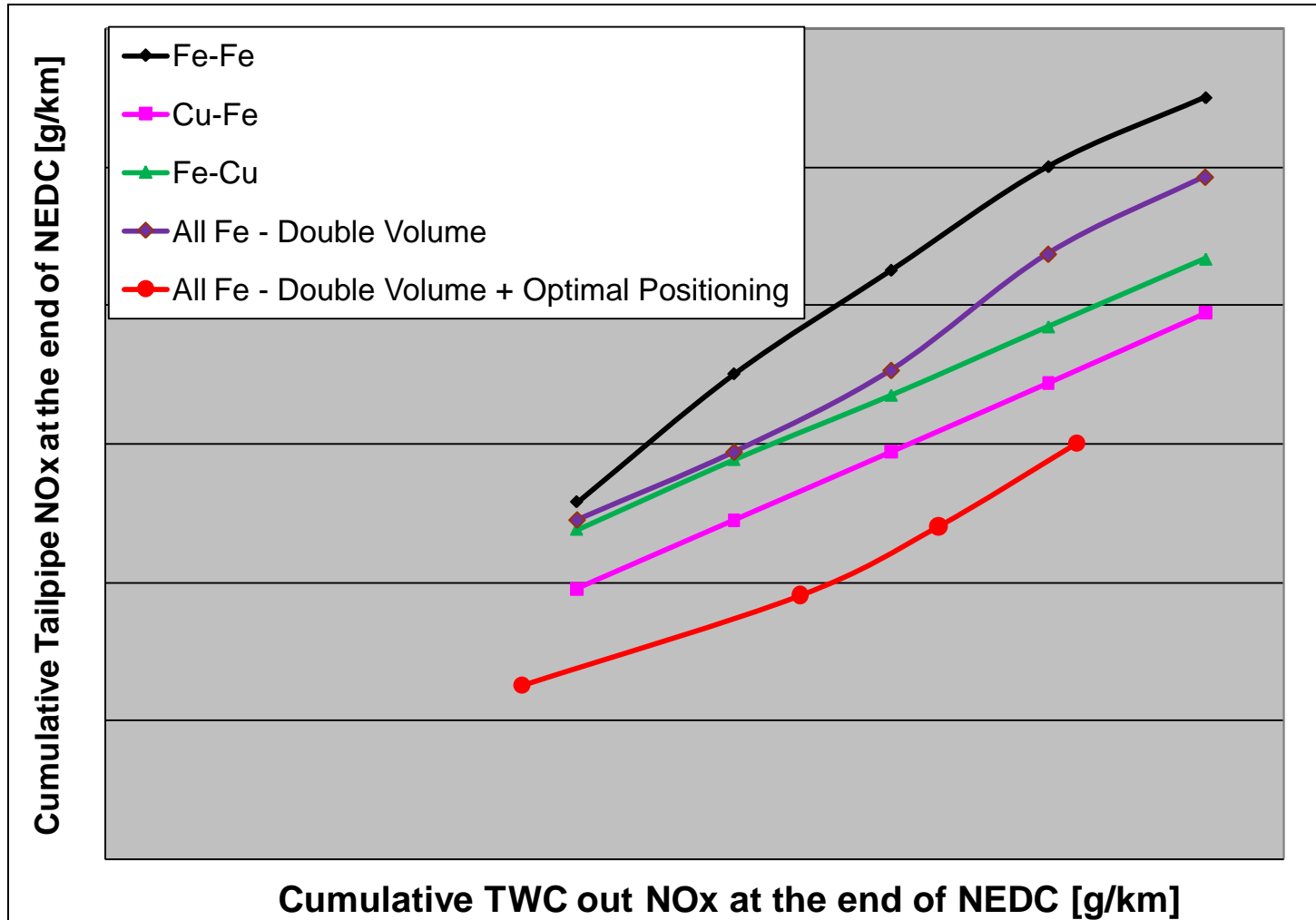**Cumulative TWC Out NOx at the end of NEDC [g/km]**
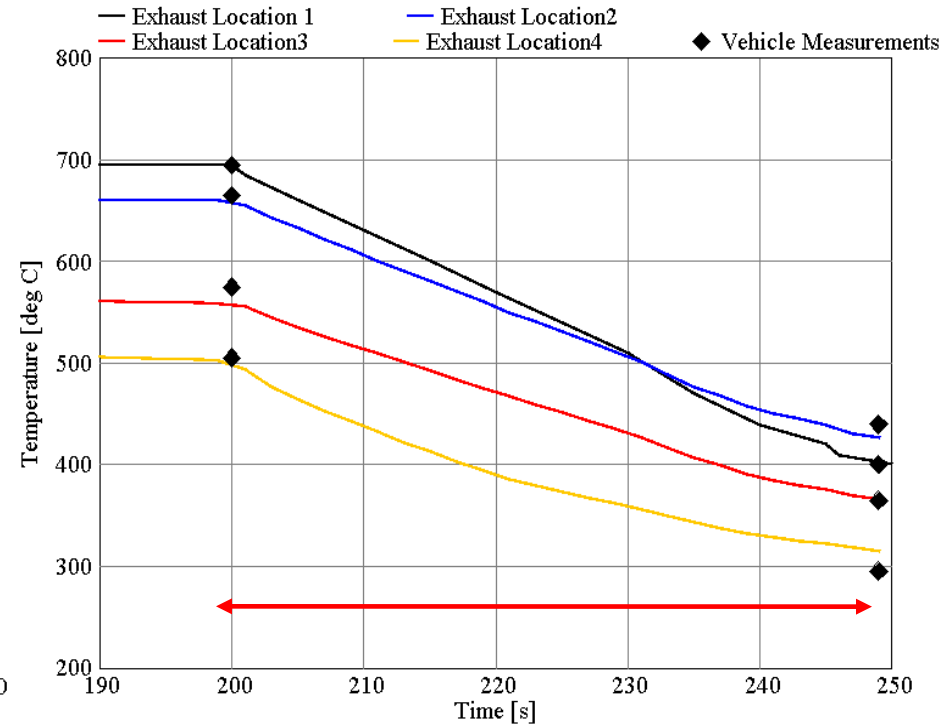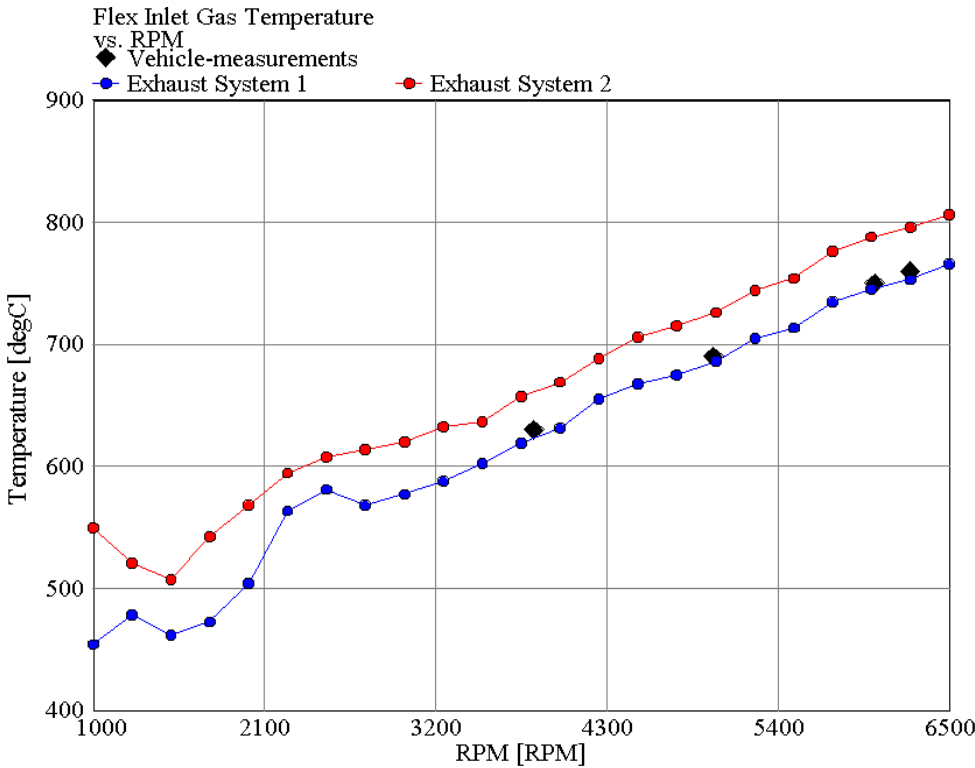
Comparing Fe-Fe vs Cu-Fe

Leeway for higher EO NOx cal. → Decouple combustion and aftertreatment system

Summary – Catalyst Screening

Model Application 2 - Catalyst Locations

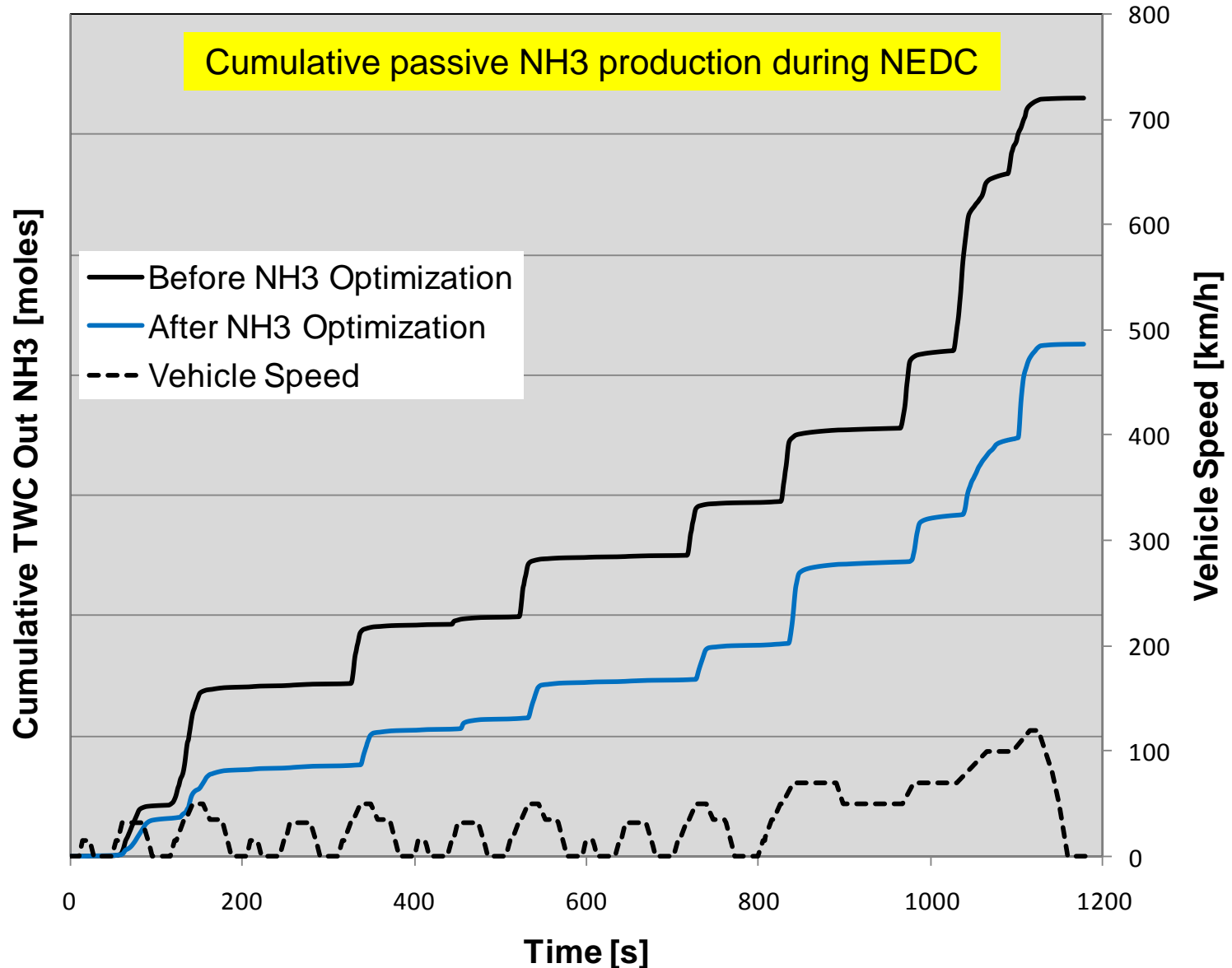Flex Inlet Gas Temperature vs. RPM

Steady State WOT @ a given location
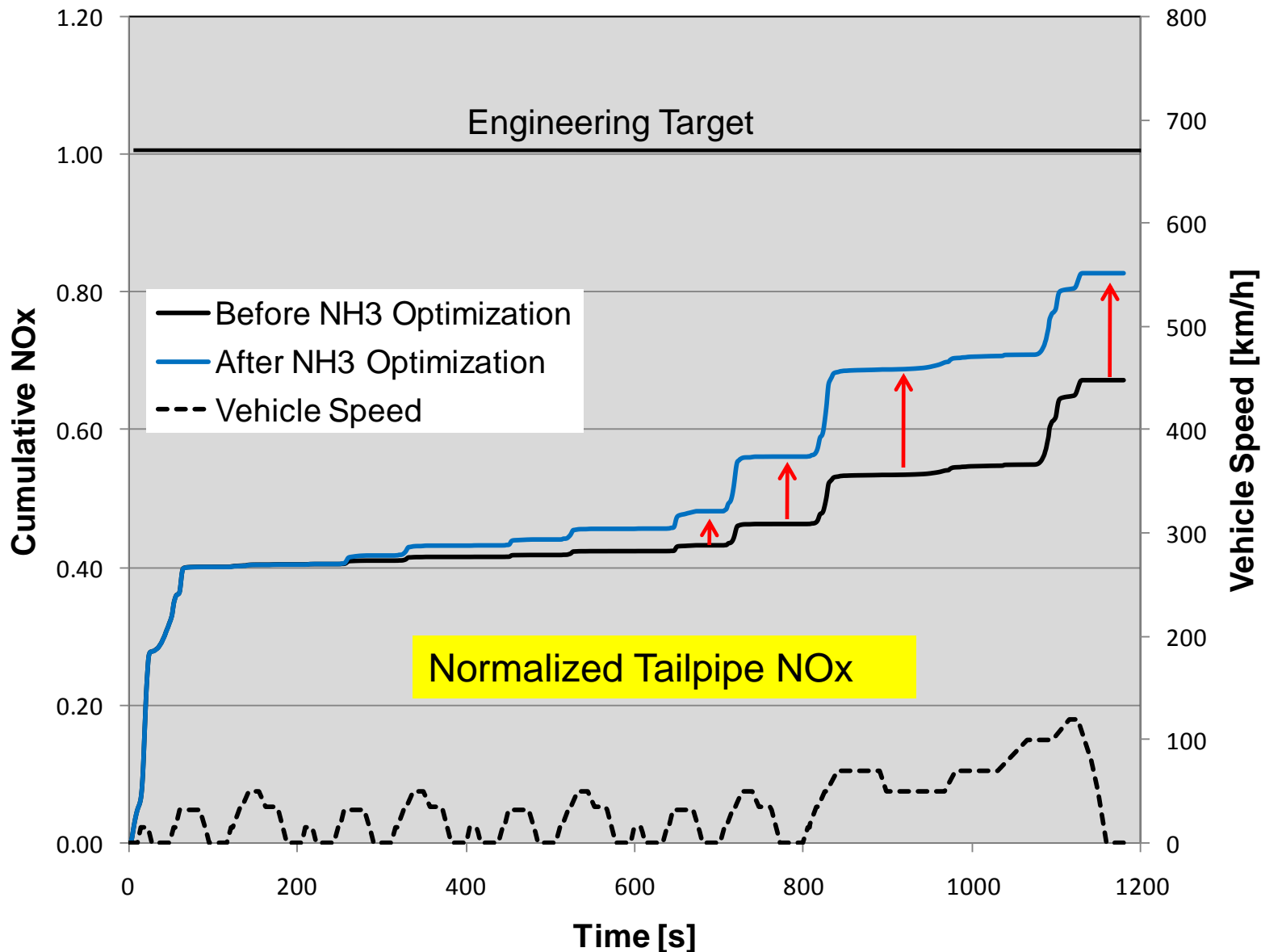
Deceleration @ different exhaust locations

- Calibrate WOT conditions (using full engine model) to get steady state thermal behavior

- Calibrate transients to get thermal response (using standalone exhaust system models)

- Explore catalyst positioning for various configurations (active/passive thermal management)

Research and Development

28th April 2009

Model Application 3 - Optimize NH3 Production

Cumulative passive NH3 production during NEDC

Legend:
- Before NH3 Optimization
- After NH3 Optimization
- Vehicle Speed

Y-axis (left): Cumulative TWC Out NH3 [moles]
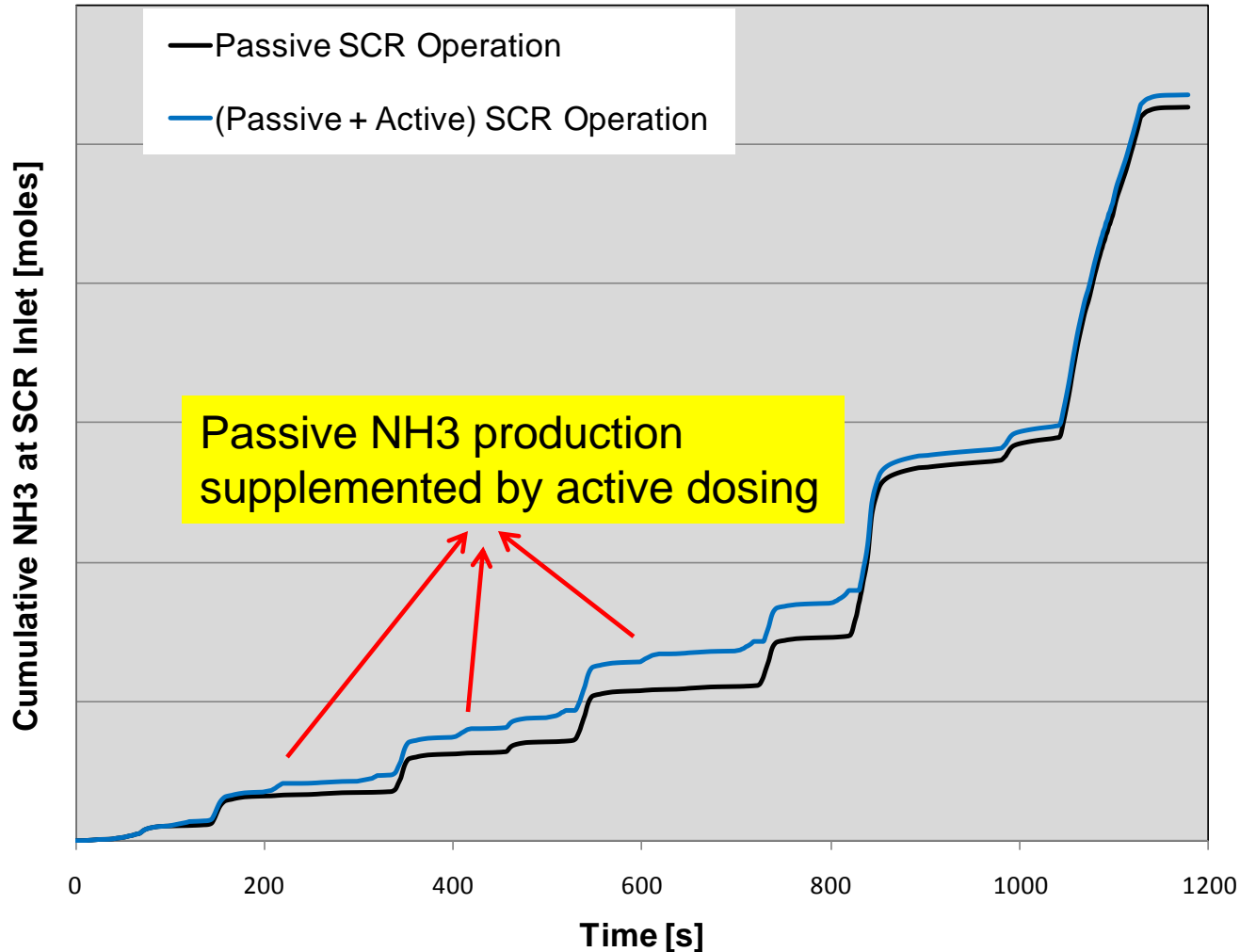Y-axis (right): Vehicle Speed [km/h]
X-axis: Time [s]

Normalized TP NOx – Before & After NH3 Optimization

Normalized TP NOx – Before & After NH3 Optimization
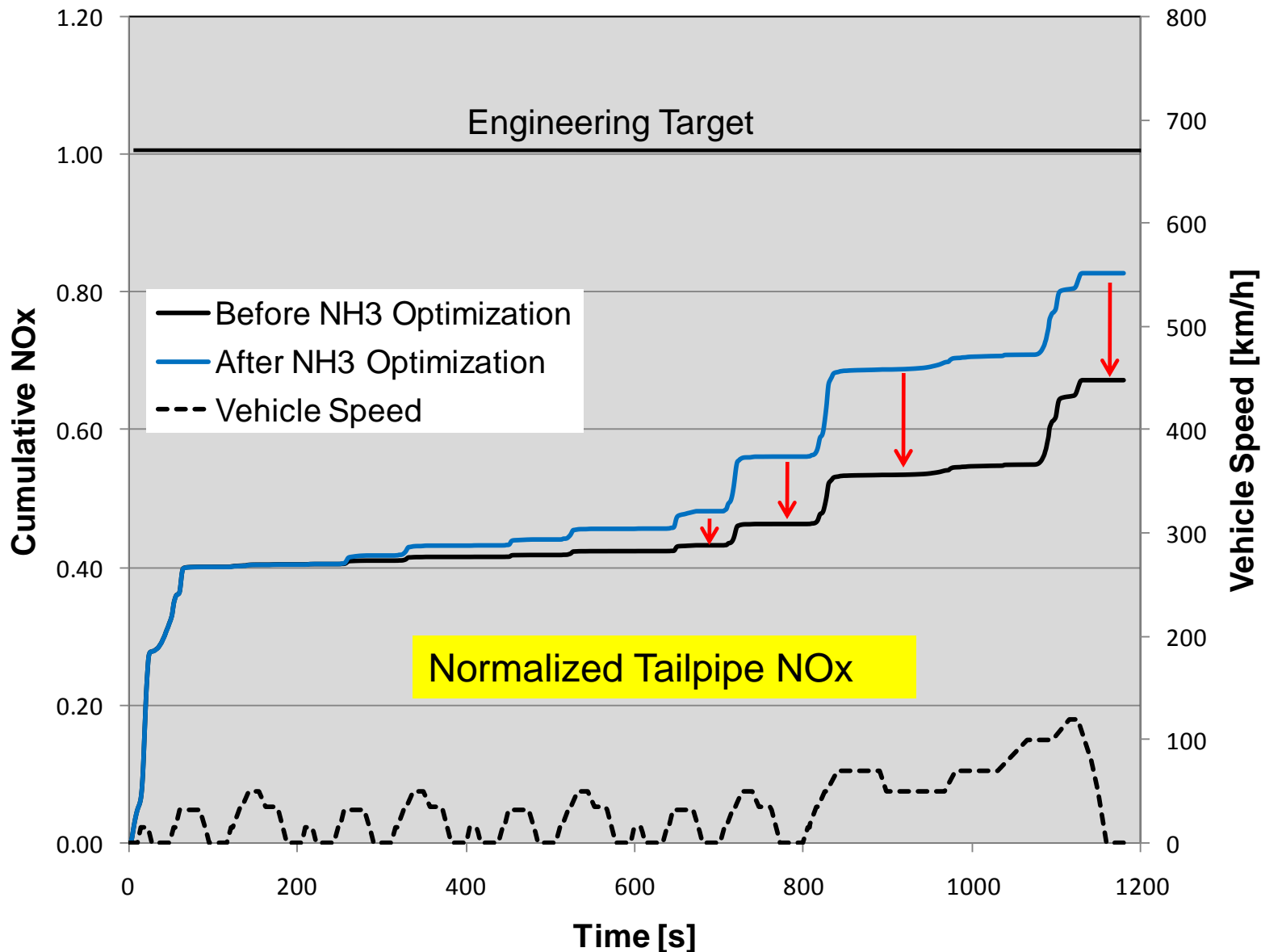
Combined (Passive + Active) SCR Operation

For similar TP NOx, ~33% savings in active reductant usage during NEDC

Summary

- Passive NH3 SCR operation – a very promising aftertreatment concept for lean SIDI

- Models complimenting the experiments has enabled
  - To explore a range of what-if scenarios
  - Accentuate the system optimization process
  - Fine tune a given system for better performance