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Applications of Kinetic Modeling to H_2-ICE Aftertreatment System Design

Dr. Rajbala

Clean Air, Johnson Matthey

Overview

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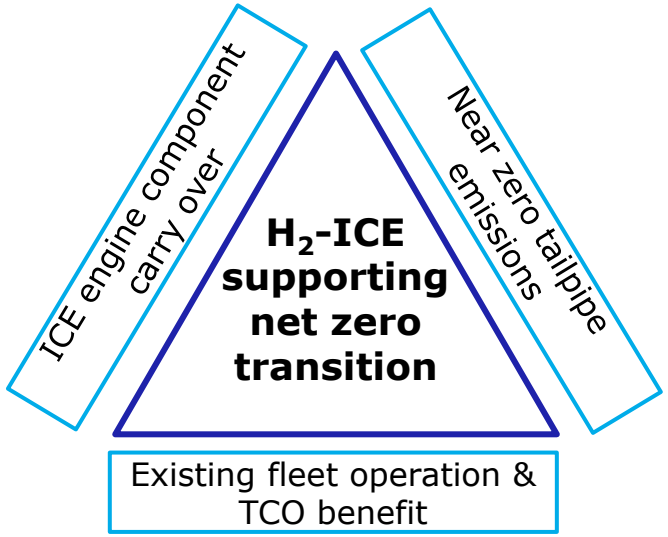
Why H_2-ICE?

H_2-ICE functions very similar to conventional engines running on gasoline, natural gas or diesel, up to 80% components carry over from traditional ICE

- H_2-ICE has a role to play in the decarbonization of the transport sector
- Growing government and OEM interest due to potential classification as a ZEV
- Easily industrialized with TCO benefits, existing manufacturing and vehicle maintenance
- PGM and supply chain benefits as Li, Co, Ni (BEV applications) are in high demand and are less circular, while Pt (H_2 applications) are circular and sustainable



https://auto.economictimes.indiatimes.com/
EU Council, inter-institutional File: 2021/0197(COD): Zero-emission vehicles: BEV, FCEV, other H2-powered vehicles
How hydrogen combustion engines can contribute to zero emissions | McKinsey

H_2-ICE Emissions Control – Requirements & Challenges

Pollutants: ~~CO, CO_2, HC, soot,~~ NOx

- **NOx Emission Control**
  Developed from JM's class leading diesel technology and continuing R&D

- **Excess H_2 Emission Control**
  DOC functionality replaced by H_2 oxidation function

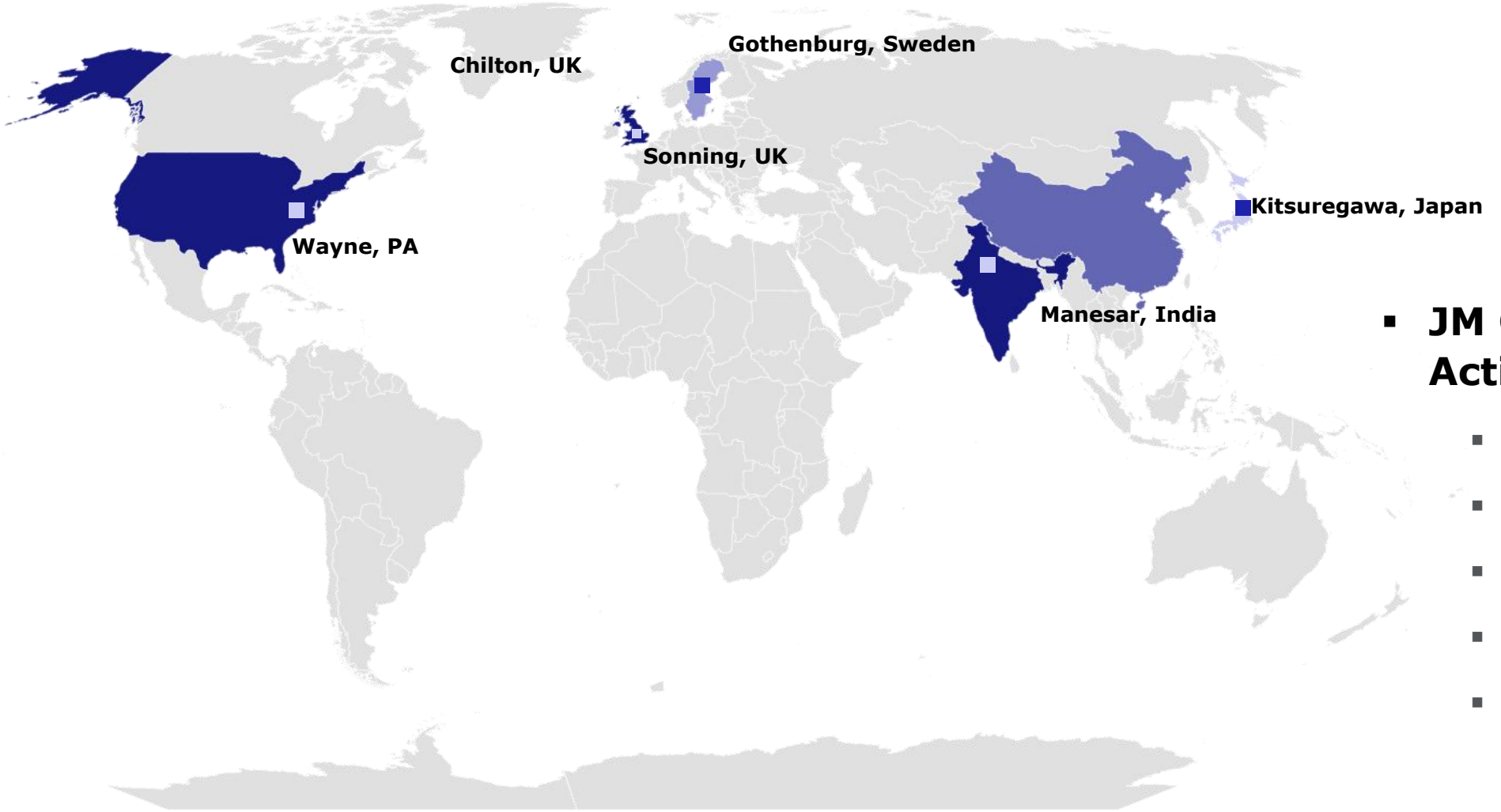
- **High Water Emission**
  Impact on SCR performance

- **Sulphur**
  If grade of H_2 contains S, Cu SCR needs DeSOx, S from lube oil can also have a negative impact long term improved Cu-SCR durability and sulphur tolerance, significant expertise from Diesel development

- **No Soot Emission but PM from Lube Oil & Urea**
  Typical DPF is not required along with regen , but filter may still be required to meet PN10

- **N_2O Emission**
  JM R&D/PGM expertise to customise performance

Modeling at JM – Global Locations

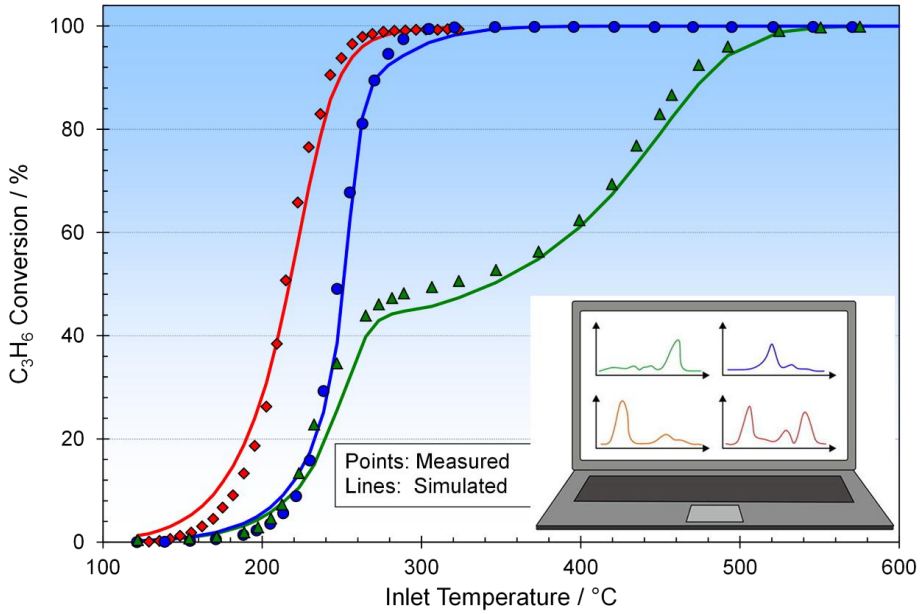


- **JM Global Modeling Activities**
  - Kinetic Modeling
  - Process Modeling
  - Molecular Modeling
  - CFD
  - ML/AI

Kinetic Modeling at JM

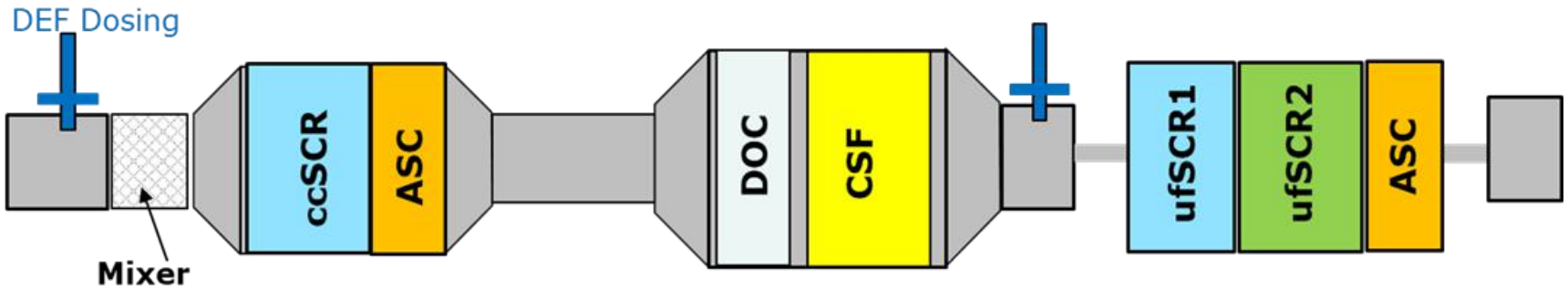
Continuous improvement to meet customer requirements

- High fidelity kinetics models, developed based on reactor data, validated against engine data
- Models are available on two different platforms, Matlab/Simulink and AVL Boost
- Models can be used to make predictions of TP NOx, N_2O, and NH_3 for different duty cycles
- Models can be also used to simulate the impact of
  - PGM loading, Dosing strategy, Catalyst sizing, Aging, Chemical poisoning, Dry gain, feed gas conc.



JM Model Library for Emission Aftertreatment

CO/HC Removal	PM Removal	NOx Removal	NH_3 Removal	CO/HC/NOx Removal
DOC	DPF	SCR	ASC	TWC
	CSF	LNT		
	GPF	PNA		
	SCRF®			



- Capable of optimizing complex system to meet target emission limits

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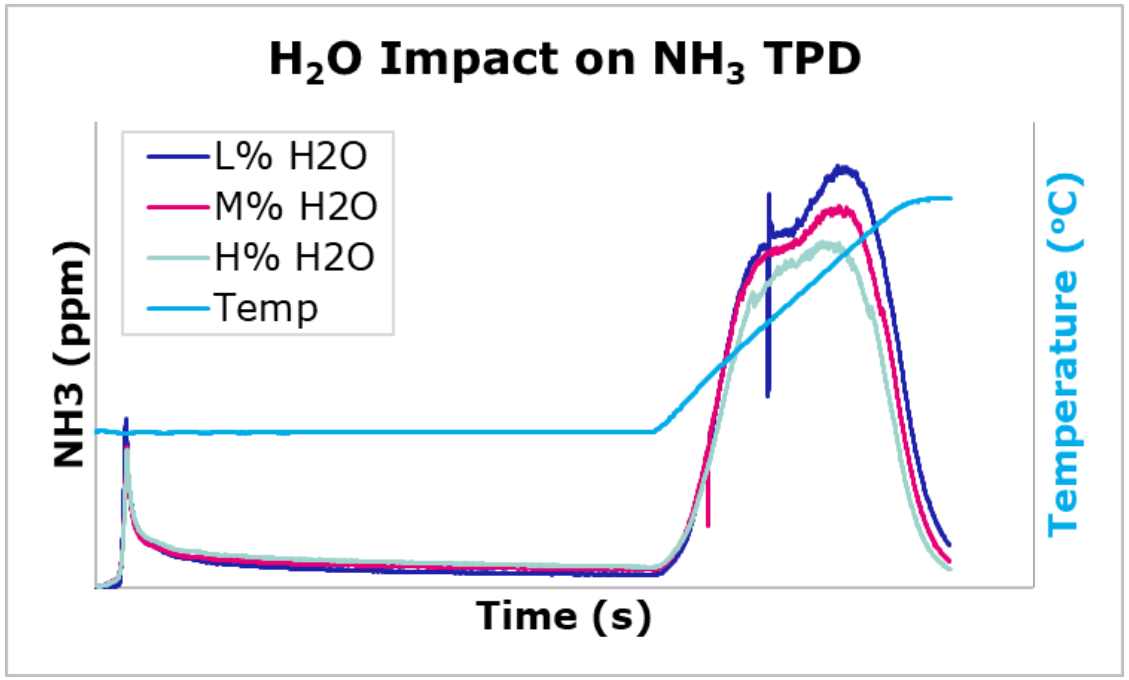
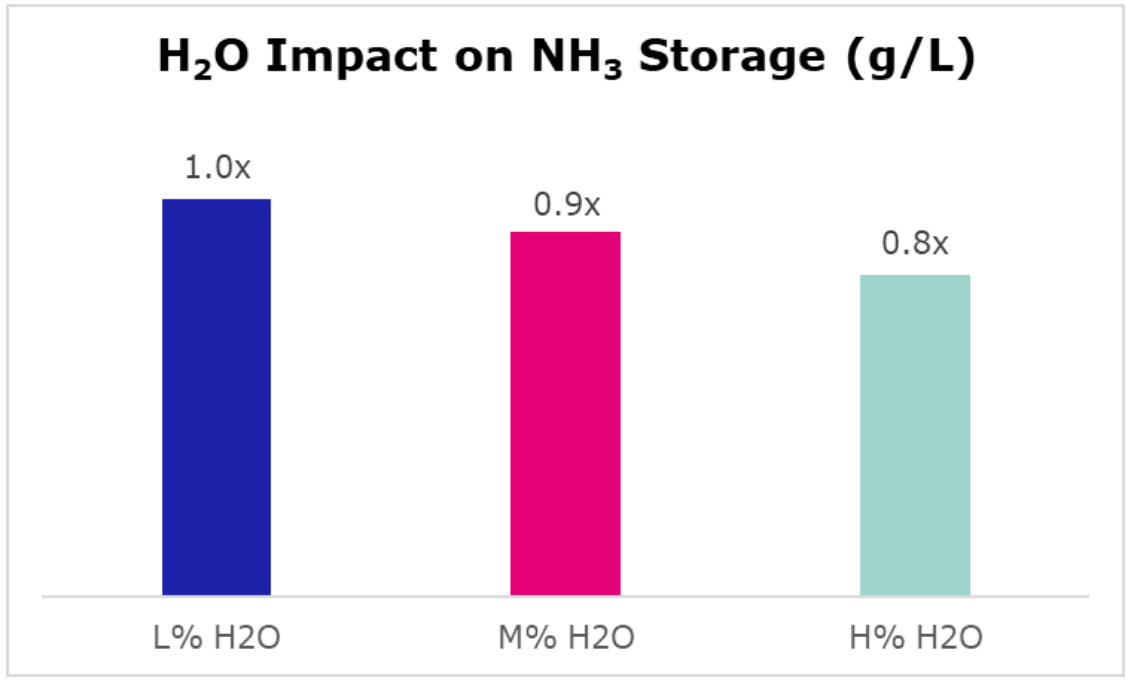
H_2O Impact on SCR NH_3 TPD and Storage

Lower storage at higher H_2O conc.

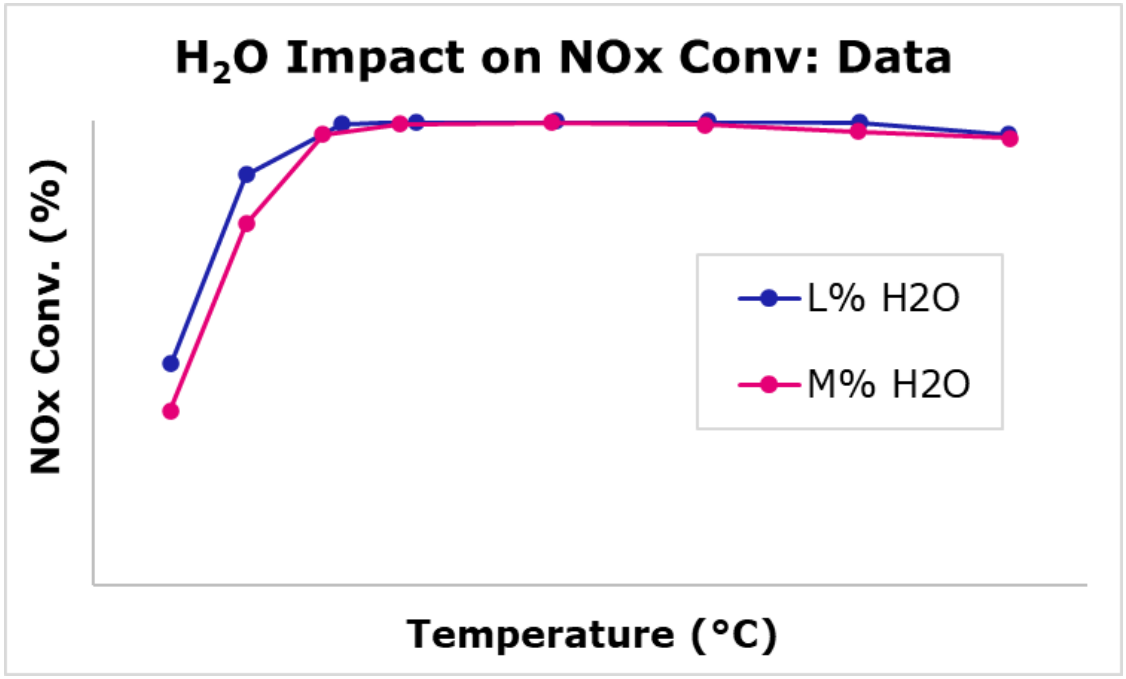


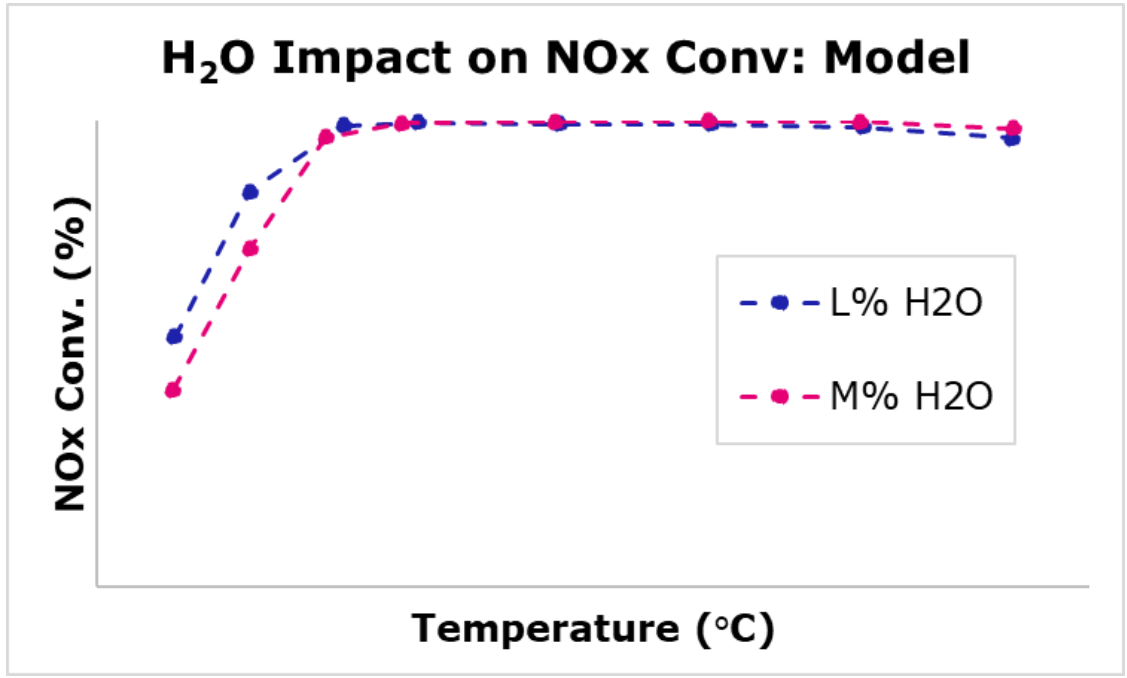


- NH_3 storage decreases with increase in H_2O concentrations
- Dual NH_3 adsorption sites, one site sees more H_2O impact than other

H_2O Impact on SCR NOx Performance

Lower conversion at higher H_2O conc., specially at low T

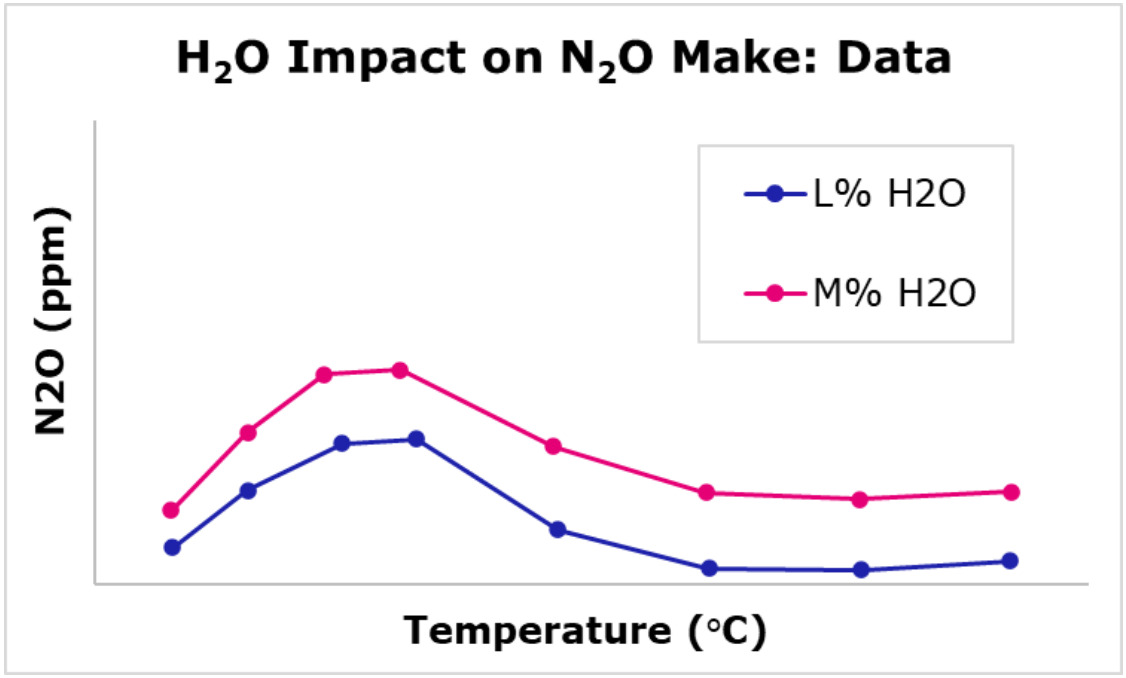


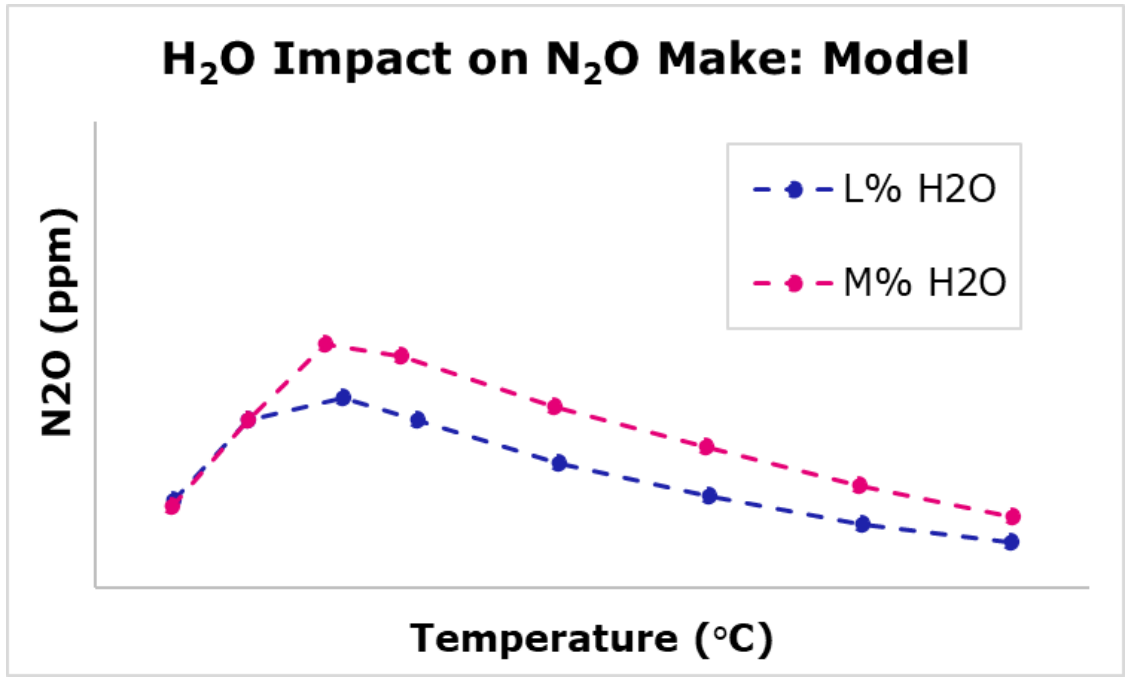


- Model applicability extended to H_2-ICE conditions; update completed to better predict the impact of H_2O content in exhaust gas mix on NOx conversion

H_2O Impact on N_2O Formation in SCR

More N_2O formation at higher H_2O conc.



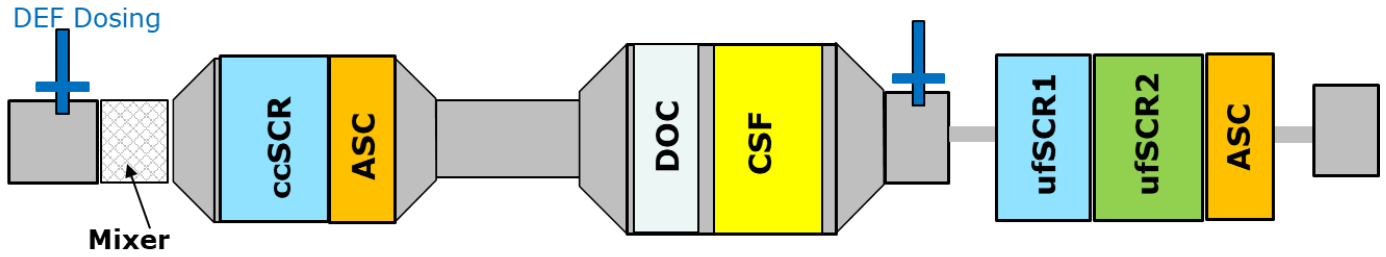


- Model applicability extended to H_2-ICE conditions; update completed to better predict the impact of H_2O content in exhaust gas mix on N_2O selectivity

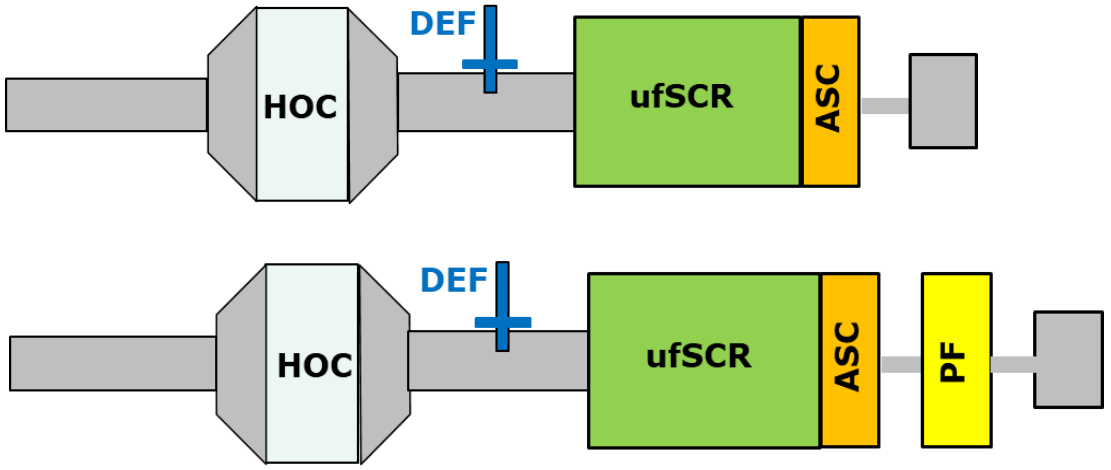
Examples of Potential H_2-ICE Aftertreatment System

Relatively simple compared to heavy duty diesel system

Heavy Duty Diesel



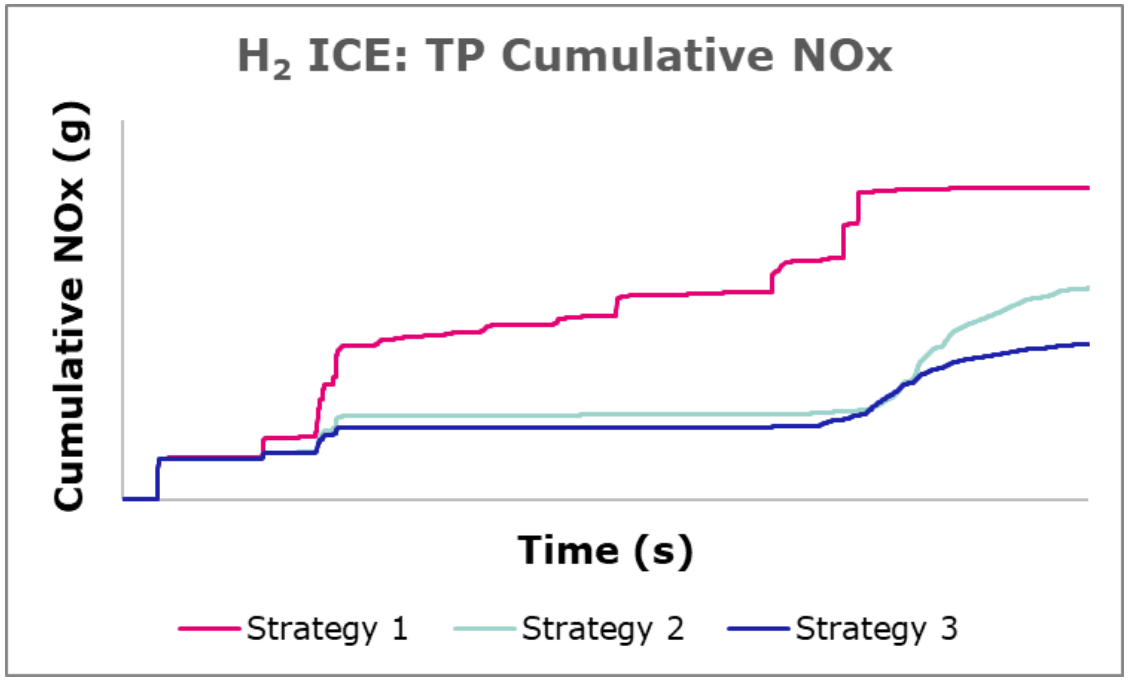
H_2-ICE

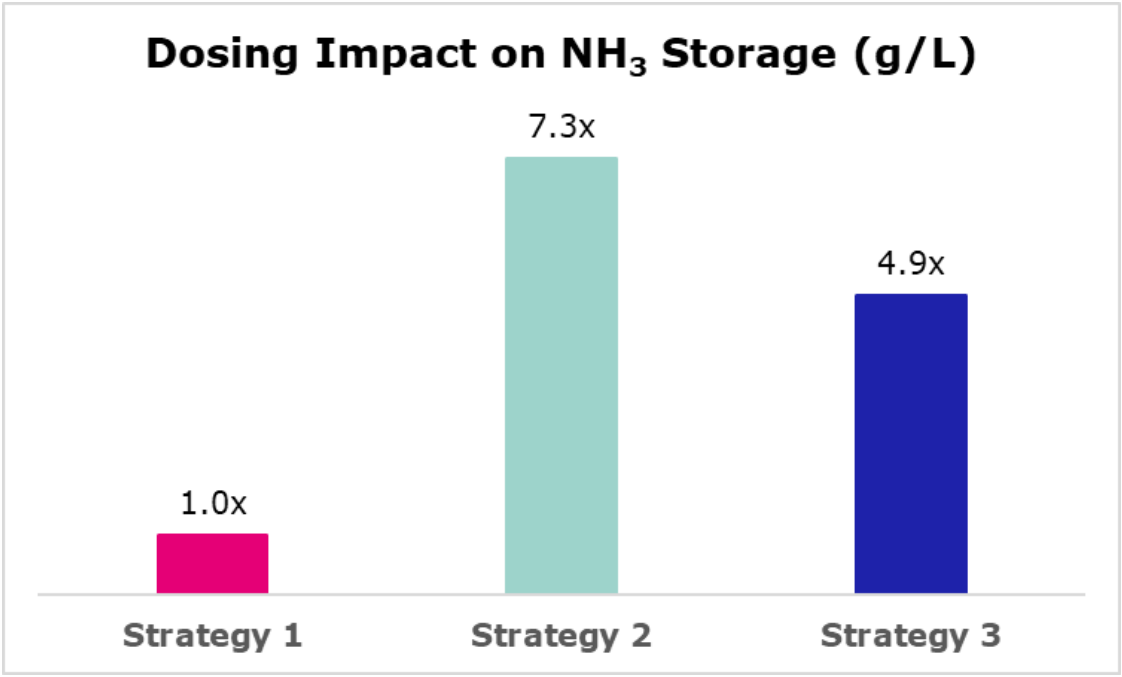


- Although no CO/HC, oxidation catalyst may still require to provide sufficient NO_2 for better SCR performance and/or H_2 oxidation
- Although no soot, filter may still require to capture particles from lube oil and urea dosing

Impact of Urea Dosing Strategy on TP NOx

Optimized dosing strategy works better





- Optimized dosing strategy results in better NOx conversion
- Modeling provides unique advantage as measuring instant NH_3 level in real system is difficult

Summary

JM invested significant resources to build kinetic model library for emission catalysts

Models are useful to design system prototypes, resulting in significant cost and time savings for OEMs

Models are also useful for post design verifications and optimizations

Models are being updated to capture H_2-ICE specific feed conditions

Preliminary system simulations suggest an alternative dosing strategy may be more effective for H_2-ICE system

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