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Simulation and design of emission catalysts for marine applications with green hydrogen, ammonia, methanol, methane and diesel fuels

MODEGAT 8

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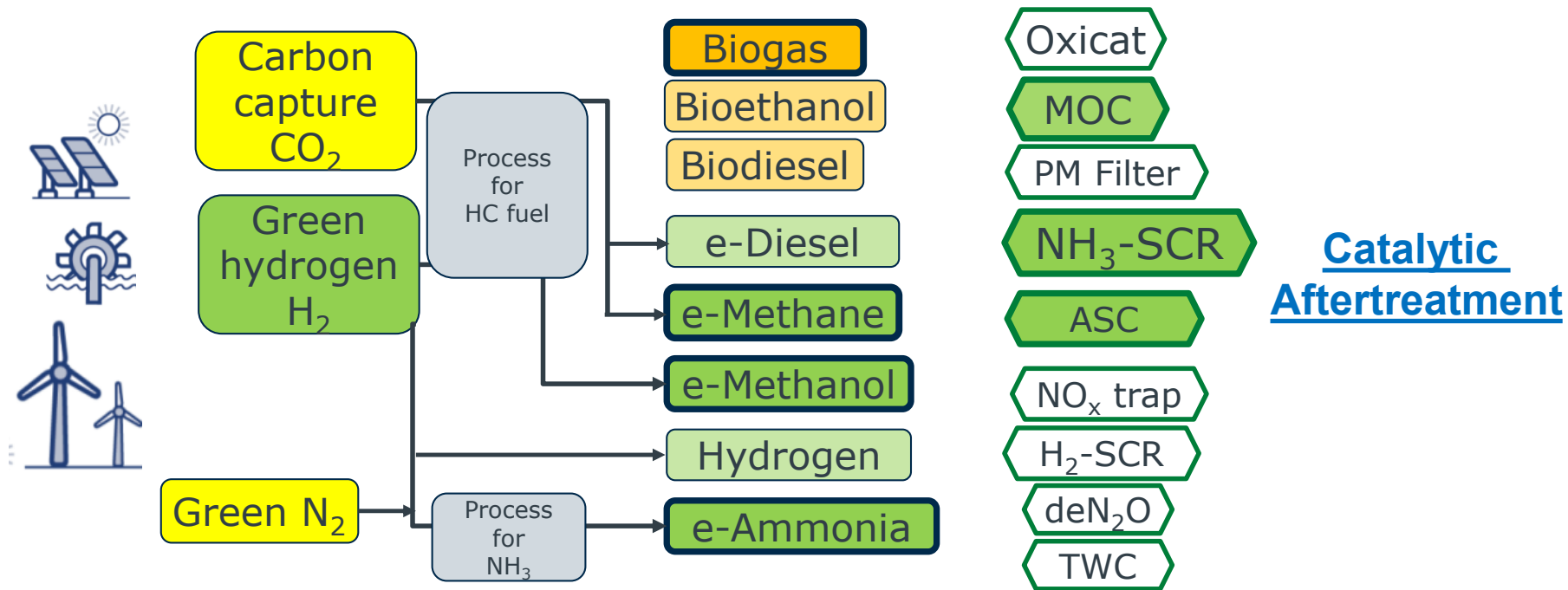
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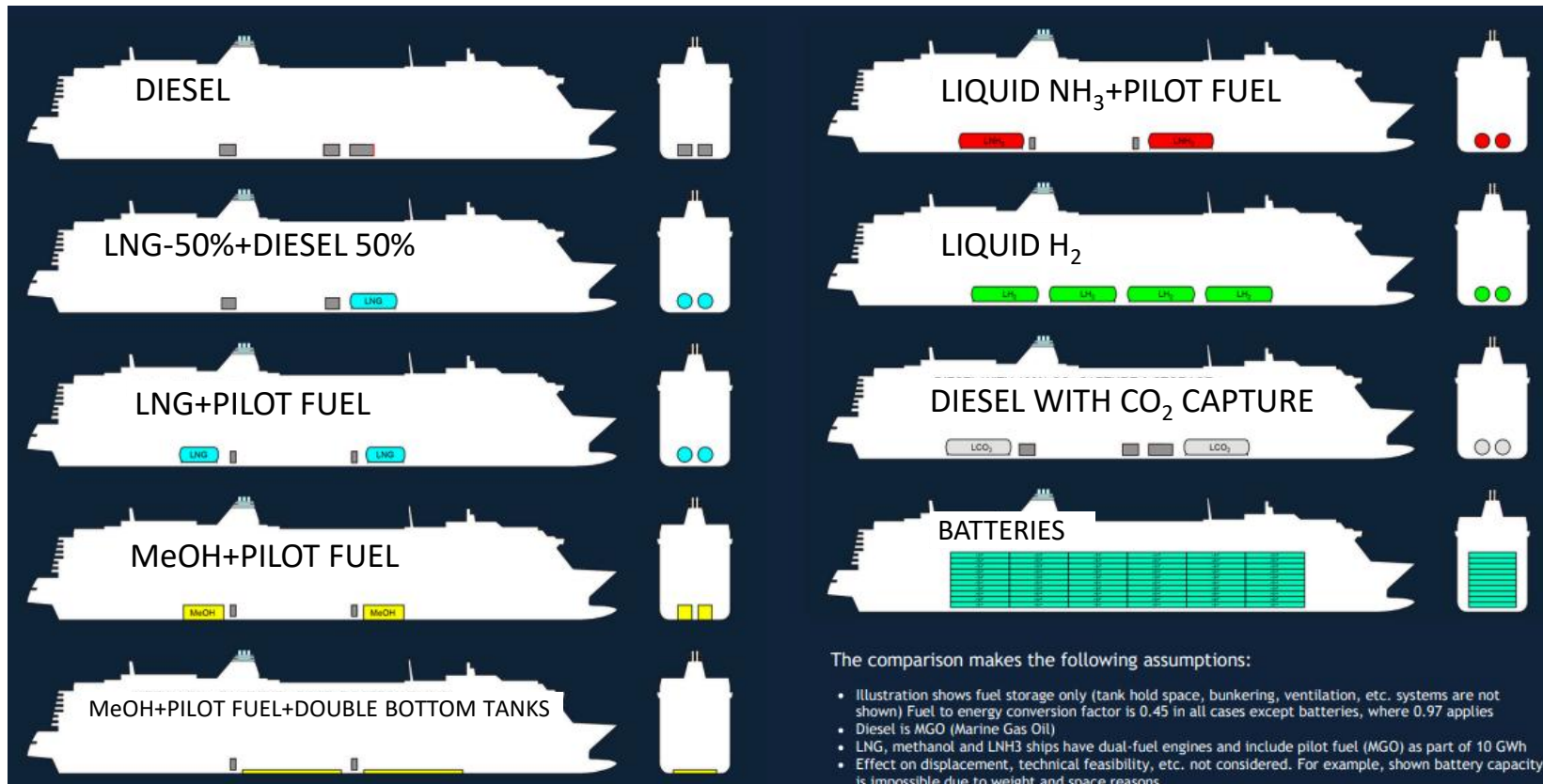
Background

- ▶ The emission focus has moved from harmful-to-health pollutants (CO , HCs, NO_x , SO_x , particulates, NH_3) to green house gases (GHG).
- ▶ Light-duty cars and other applications are moving fast electric or hybrids, but liquid fuels needed in heavy-duty applications
- ▶ Pollutant limits will remain the same or tightened in near future
- ▶ Harmonization: Emission limits independent on fuel or engine type (multi-fuel engines)
- ▶ Green fuels can decrease (NO_x , SO_x , particulates, other poisons) or increase (NO_x , CH_4 , N_2O , NH_3) pollutant emissions
- ▶ Green electricity has a key role in the move to carbon-free fuels and energy



Green fuels for marine applications

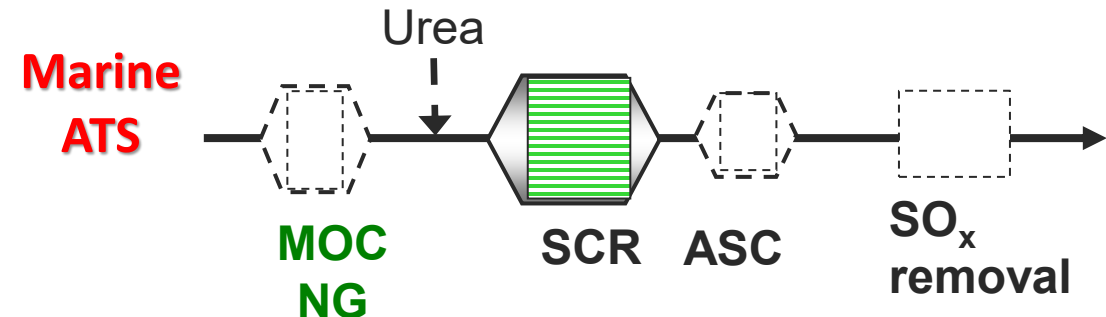
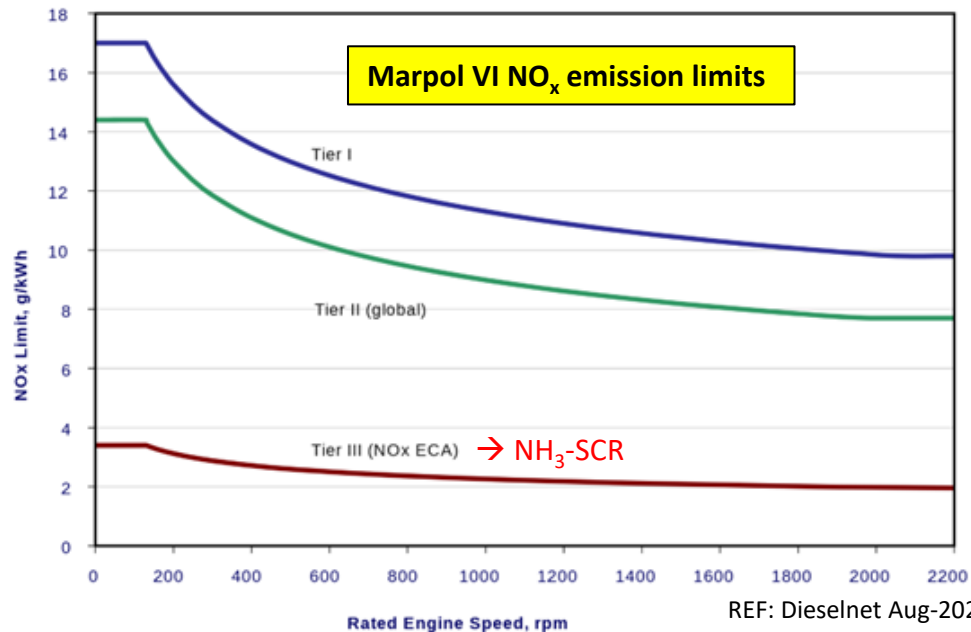
- ▶ Carbon neutral targets for year 2050 in marine field (IMO) in many leading industrial countries
- ▶ No full electrification in near future for heavier ships due to on-board energy storage capacity – partial hybridization possible
- ▶ Energy-dense fuels like liquid **methanol (MeOH)**, **methane (CH₄)** and **ammonia (NH₃)** planned to replace diesel in marine applications.
- ▶ Fuel cost and consumption are driving commercial force in heavy ship applications.
- ▶ Flexible use of fuels necessary by the fuel availability/distribution, engine technology and costs



REF: www.foreship.com, Aug 2025

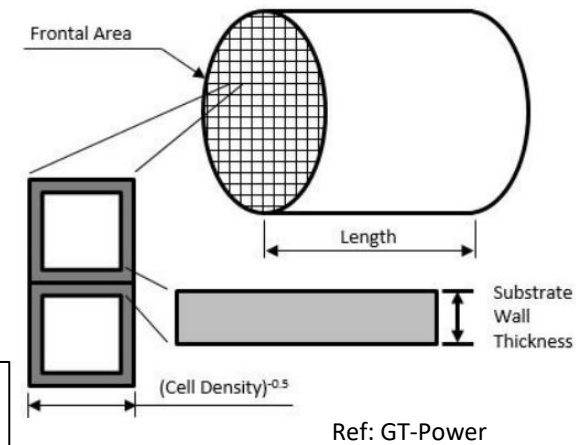
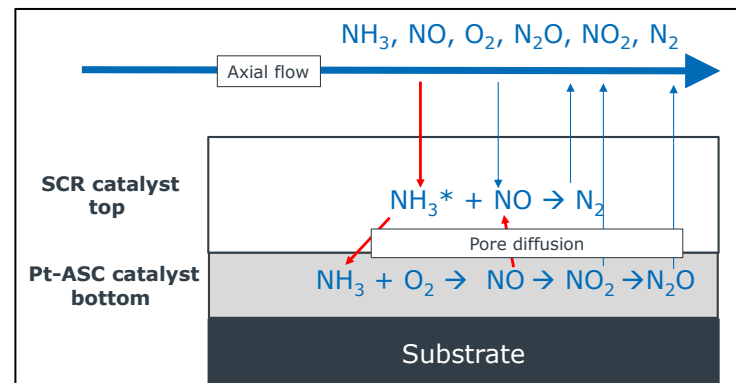
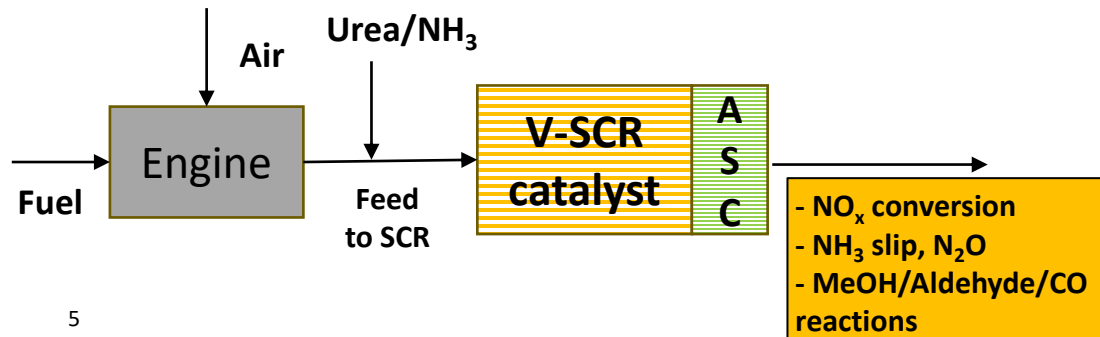
Emission limits and aftertreatment systems

- ▶ Marine emission regulations (Tier III latest) for pollutants are not that strict (focus has been on NO_x and SO_x) as in on-wheel applications but the effect of new fuels on emissions requires development and design for catalytic aftertreatment systems (ATS)
- ▶ In marine applications, extruded vanadium-SCR catalysts with low cell density and thick walls used for NO_x removal
- ▶ **In this study**, improved capabilities to simulate emission catalyst functionality in marine applications
 - ▶ The effect of pore diffusion on catalyst efficiency in extruded V-SCR catalyst
 - ▶ Oxidation of NH_3 , MeOH, formaldehyde (FA), hydrocarbon and CO on V-SCR and Ammonia Slip Catalysts (ASC) in diesel (REF), MeOH, and NH_3 engine exhaust gas conditions
 - ▶ Methane Oxidation Catalysts (MOC) functionality in CH_4 engine exhaust gas conditions.



Methods

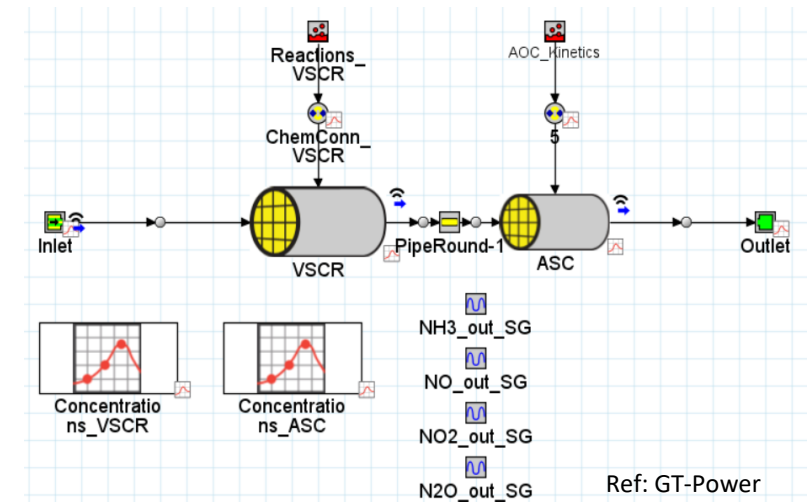
- ▶ Pollutant removal efficiencies on catalysts investigated in single fuel conditions using GT Power program tools.
 - ▶ Ready emission catalyst models using modified parameters
 - ▶ Volumetric active site density defined by the catalyst (SCR) or active metal (PGM) amounts
- ▶ 1D model of flow-through catalysts by defined reactions in GT Power libraries
 - ▶ Mass, energy and momentum balances along the channels, quasi-steady flow solver, assumption of a short residence time
 - ▶ Possible to simulate pore diffusion (d_{50} 0.1–10 μm) in thick coating layers, effects seen best with high SV (short residence time) range
 - ▶ External diffusion built-in (channel diameter/shape in catalyst)
- ▶ ASC model based on 2-layer structure and model (top SCR and bottom Pt-DOC)
 - ▶ Based on Fe-SCR + Pt-DOC kinetics – Pt-layer dominates, thus similar with varying SCR catalysts
 - ▶ Pore diffusion essential in 2-layer ASC models- controlling mass transfer and selectivity in layers
- ▶ In final V-SCR+ASC simulations, pore diffusion included in both units – d_{50} of 0.25 μm for pores



Methods – model validation

- ▶ Emission catalyst models in GT Power applied with partly modified kinetic and mass transfer parameters
 - ▶ Adjusted parameters by available experimental and publication data in experimental conditions (rates, NH_3 adsorption-desorption)
 - ▶ Verification of pore diffusion effects by experimental data with extruded marine V-SCR catalysts (≈ 60 cpsi, $\text{V}_2\text{O}_5/\text{TiO}_2\text{-WO}_3$)
 - ▶ Modification and verification of 2-layer ASC model by experimental data on coated catalysts (400 cpsi)
 - ▶ Defined reactions and kinetic parameters for MeOH, FA and CO reactions on extruded V-SCR and 2-layer Pt-ASC (Top. Catal. On-line 2025)

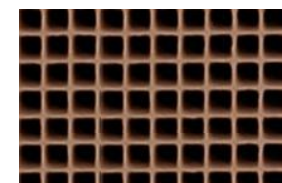
Compound	Engine testing typical	SCR simulations Feed	ASC simulations Feed
NO_x , ppm	1500	1425	0
NO_2 , ppm- 5%/ NO_x	na	75 (set)	0
N_2O , ppm	na	5 (set)	5 (set)
NH_3 , ppm	Varied by ANR	Varied by ANR	100
CO, ppm	~ 90	0*	0*
CO_2 , %	~ 6	0*	0*
HC (C_1) ppm	~ 170	0*	0*
Water, %	~ 5	5	5
N_2	balance	balance	balance
Space velocity (SV), h^{-1}	6000 - 16000	6000 – 60000	100.000-400.000
Flow rate, m^3/h	varied	varied	varied



Extruded



Coated-400 cpsi



Simulation methods

- ▶ Mainly separate simulations for NH_3 -SCR (steady state = SS) and oxidation reactions (light-off) on extruded V-SCR and V-SCR+ASC
- ▶ NH_3 -SCR simulation in SS steps at 200–500 °C for 2–6 min for temperature-ANR (NH_3/NO_x) points → criterion deNO_x (10/5 ppm NH_3)
 - ▶ Additional temperature ramp test with V-SCR and ASC to simulate transient SCR performance with fixed ANR = 0.9
- ▶ MeOH, FA, CO and HC oxidation reactions simulated in a light-off ramp on V-SCR, ASC and MOC at 0 – 500/600 °C by the rate of 5 °C/min
- ▶ A feed matrix to simulate key reactions and pollutant removal in exhaust gas feeds (not connected to exact real-world engine emissions:

Compound	Diesel	MeOH	CH_4	NH_3
NO, ppm	1000	1000	1000	3000
NO_2 , ppm	50	50	50	150
NH_3 , ppm	0	0	0	300
CH_4 , ppm	0	0	1500	0
Ethane, ppm	0	0	300	0
Propane, ppm	0	0	100	0
Propene, ppm	100	0	0	0
Methanol, ppm	0	1200	0	0
Formaldehyde, ppm	20	300	150	0
CO, ppm	500	500	500	0
Oxygen, %	10	10	10	10
Water, %	6	6	8	12
CO_2 , %	6	6	6	0
Nitrogen	bal.	bal.	bal.	bal.

Temp, °C	SV, h-1			
	16000	12000	9000	6000
200	Alfa1	Alfa8	Alfa15	Alfa22
250	Alfa2	Alfa9	Alfa16	Alfa23
300	Alfa3	Alfa10	Alfa17	Alfa24
350	Alfa4	Alfa11	Alfa18	Alfa25
400	Alfa5	Alfa12	Alfa19	Alfa26
450	Alfa6	Alfa13	Alfa20	Alfa27
500	Alfa7	Alfa14	Alfa21	Alfa28

Alfa varied: 0.6, 0.8, 0.9, 1.0, 1.1, 1.2 and 1.4 = ANR

Catalytic reactions

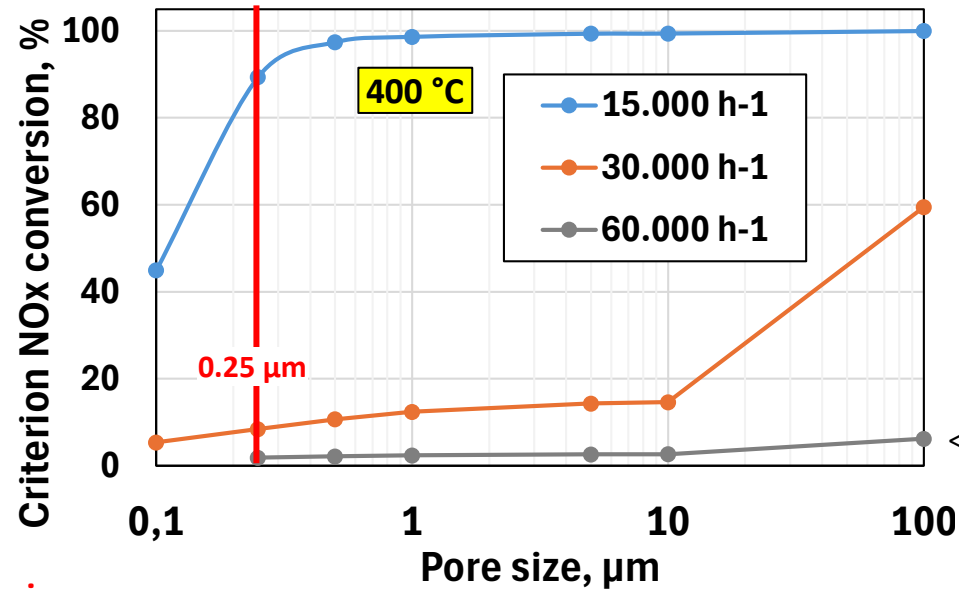
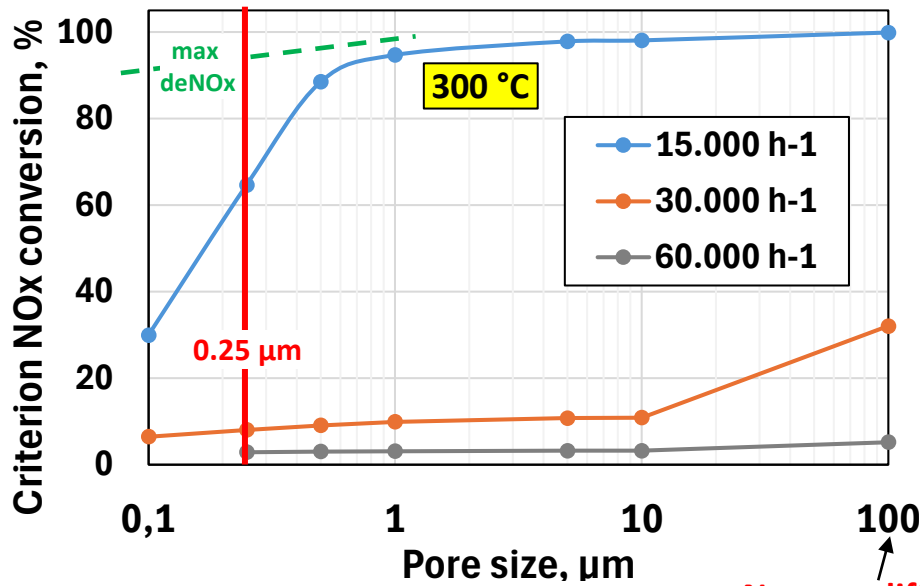
- Catalytic reactions by GT Power library (NH₃ adsorption and metal sites, rate equations, inhibition effects (CO, HC, NO) together with added reactions :

$\text{NH}_3 + \text{S1} \rightleftharpoons \text{NH}_3\text{-S1}$ $\text{NH}_3 + \text{S2} \rightleftharpoons \text{NH}_3\text{-S2}$ $\text{NH}_3 + \text{NO} + 0.25 \text{O}_2 \rightarrow \text{N}_2 + 1.5 \text{H}_2\text{O}$ $\text{NH}_3 + 0.5 \text{NO} + 0.5 \text{NO}_2 \rightarrow \text{N}_2 + 1.5 \text{H}_2\text{O}$ $\text{NH}_3 + 0.75 \text{NO}_2 \rightarrow 0.875 \text{N}_2 + 1.5 \text{H}_2\text{O}$ $\text{NH}_3 + 1.25 \text{NO}_2 \rightarrow 0.875 \text{N}_2 + \text{N}_2\text{O} + 1.5 \text{H}_2\text{O}$ $\text{NO} + 0.5 \text{O}_2 \rightleftharpoons \text{NO}_2$ $\text{NH}_3 + 1.25 \text{O}_2 \rightarrow \text{NO} + 1.5 \text{H}_2\text{O}$ $\text{NH}_3 + 0.75 \text{O}_2 \rightarrow 0.5 \text{N}_2 + 1.5 \text{H}_2\text{O}$	Non-productive adsorption Adsorption enabling SCR Standard SCR Fast SCR Slow SCR N ₂ O formation by NO ₂ promotion NO ₂ formation NH ₃ oxidation to NO NH ₃ oxidation to N ₂	V-SCR catalyst ASC
$\text{CH}_3\text{OH} + \text{O}_2 \rightarrow \text{CO} + 2 \text{H}_2\text{O}$ $\text{CH}_3\text{OH} + \text{O}_2 \rightarrow \text{HCHO} + \text{H}_2\text{O}$ $\text{HCHO} + 0.5 \text{O}_2 \rightarrow \text{CO} + \text{H}_2\text{O}$ $\text{C}_3\text{H}_6 + 3 \text{O}_2 \rightarrow 3 \text{CO} + 3 \text{H}_2\text{O}$ $\text{CO} + 0.5 \text{O}_2 \rightarrow \text{CO}_2$	MeOH oxidation to CO formation MeOH oxidation to formaldehyde FA oxidation to CO Propene (diesel-HC) oxidation to CO CO oxidation	
$\text{CH}_4 + 1.5 \text{O}_2 \rightarrow \text{CO} + 2 \text{H}_2\text{O}$ $\text{C}_2\text{H}_6 + 2.5 \text{O}_2 \rightarrow 2 \text{CO} + 3 \text{H}_2\text{O}$ $\text{C}_3\text{H}_8 + 3.5 \text{O}_2 \rightarrow 3 \text{CO} + 4 \text{H}_2\text{O}$ $\text{CO} + 0.5 \text{O}_2 \rightarrow \text{CO}_2$	CH ₄ oxidation to CO and CO ₂ on MOC Ethane oxidation to CO on MOC Propane oxidation to CO on MOC CO oxidation on MOC – fast	MOC

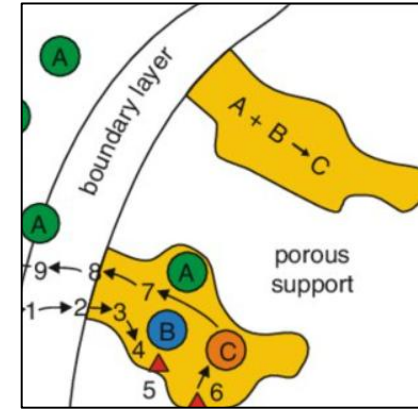
Extruded V-SCR catalyst

- Effect of pore size on diffusion in **extruded V-SCR catalyst** (60 cpsi / 360 μm walls, catalyst 380 g/L)

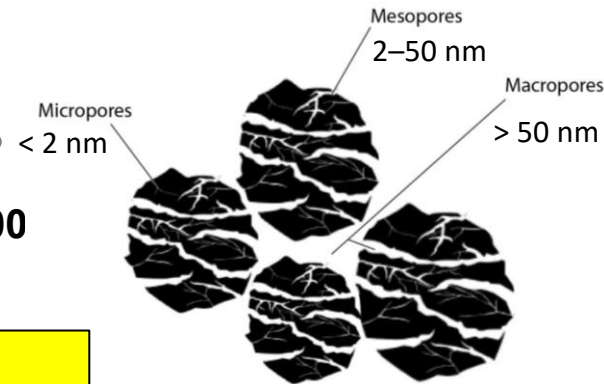
Criterion $\text{deNO}_x\%$ by 10 ppm NH_3 in ANR window



No pore diffusion



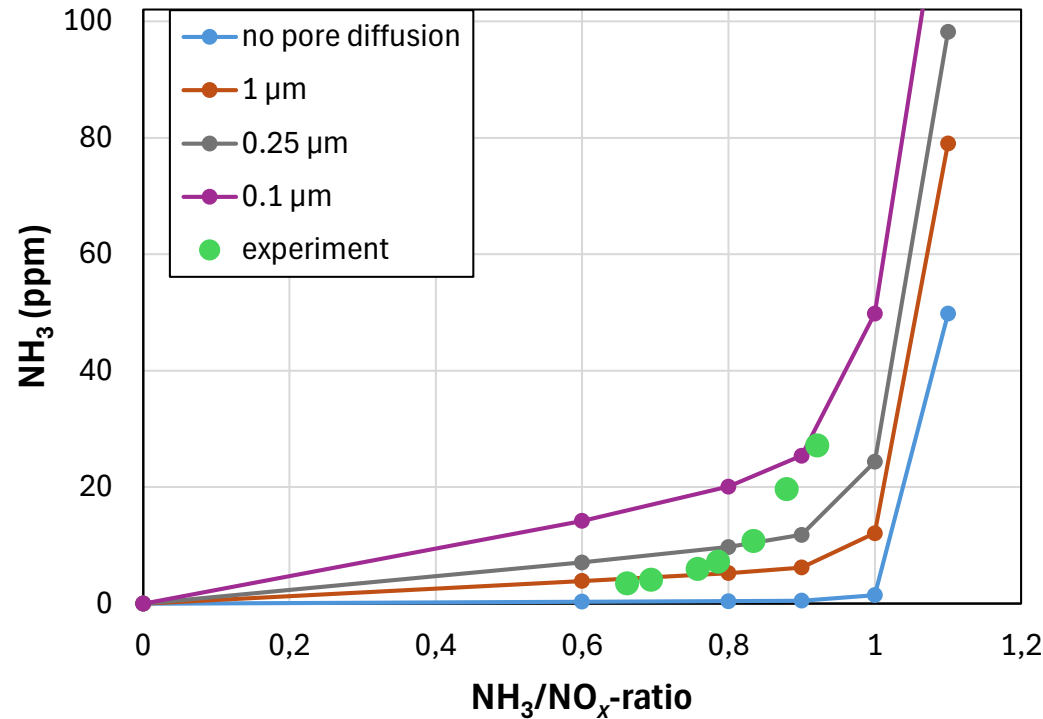
Heterogenous catalytic reactions in porous catalysts (a set of macro-, meso- and micropores)



- Pore diffusion more meaningful in thick catalyst walls of extruded SCR catalysts
- SV (space velocity (s^{-1}), residence time (s) = $1/\text{SV}$) is the primary variable
- Compared simulations with 30,000 and 15,000 h^{-1} , when reaction times limited
- Possible to reach high NO_x conversions with 30,000 h^{-1} and $d=0.25 \mu\text{m}$ but then high NH_3 slip ($>10 \text{ ppm}$)
- Pore diffusion limits clearly when pore sizes below $1 \mu\text{m}$ with 15,000 $\text{h}^{-1} \rightarrow 0.25 \mu\text{m}$ used in later simulations

Extruded V-SCR catalyst

Verification of pore diffusion parameters: Experimental vs simulations



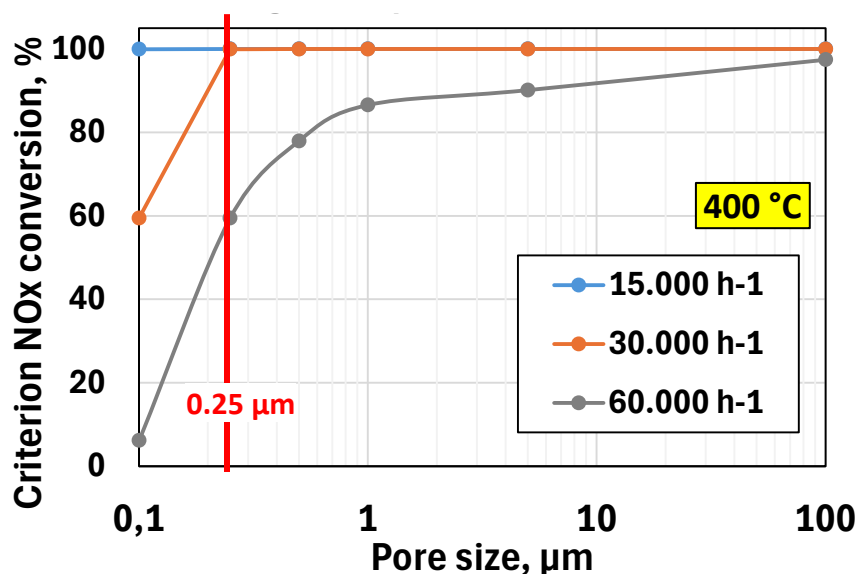
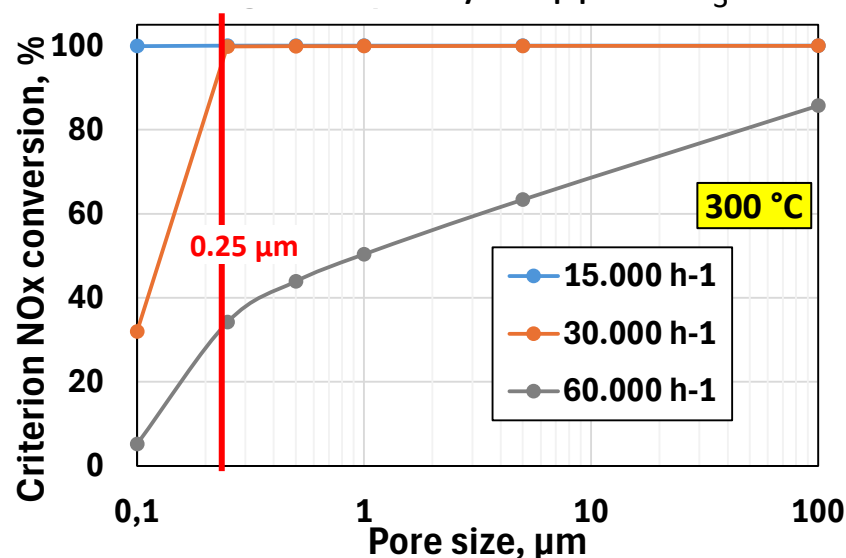
- Extruded V-SCR, 60 cpsi
- SV ~ 15.000 h⁻¹ (high range to see effects)
- Temperature ~ 350°C

- When including pore diffusion with smaller pore sizes (100-250 nm) in modelling, NH₃ slip near to experimental
- In addition: tolerances in modelling (kinetic parameters, pores) and experiments (uniformity of NH₃/NO_x, analysis, other)?
- Instead of pore diffusion, possible to adjust active site densities (lumped parameters)

Coated V-SCR catalyst

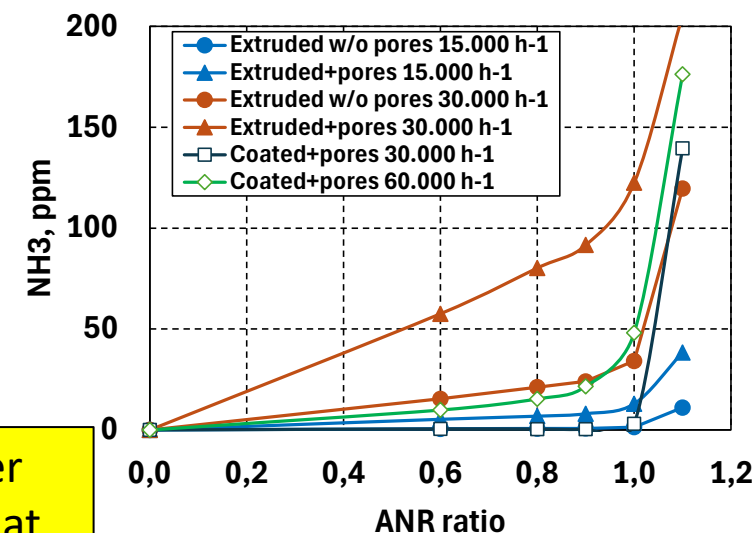
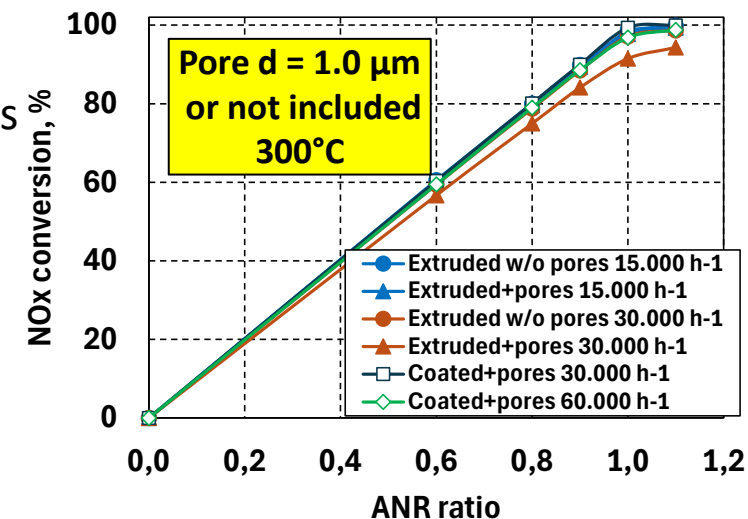
- ▶ Effect of pore diffusion on **coated V-SCR catalyst** performance – same catalyst kinetics
- ▶ 400 cpsi cordierite / 100 μm walls + 50 μm coating (250 g catalyst/L)

Criterion deNO_x% by 10 ppm NH₃ in ANR window



- Pore diffusion has low effects on a coated substrate of 400 cpsi with 50 μm catalyst layer
- Pore diffusion has small effects on modelling of coated SCR catalyst – limitation started at around 60.000 h⁻¹ → **often lumped in kinetic parameters in mobile applications**

Effect of pores on NO_x conversion and NH₃ slip with extruded or coated SCR catalyst



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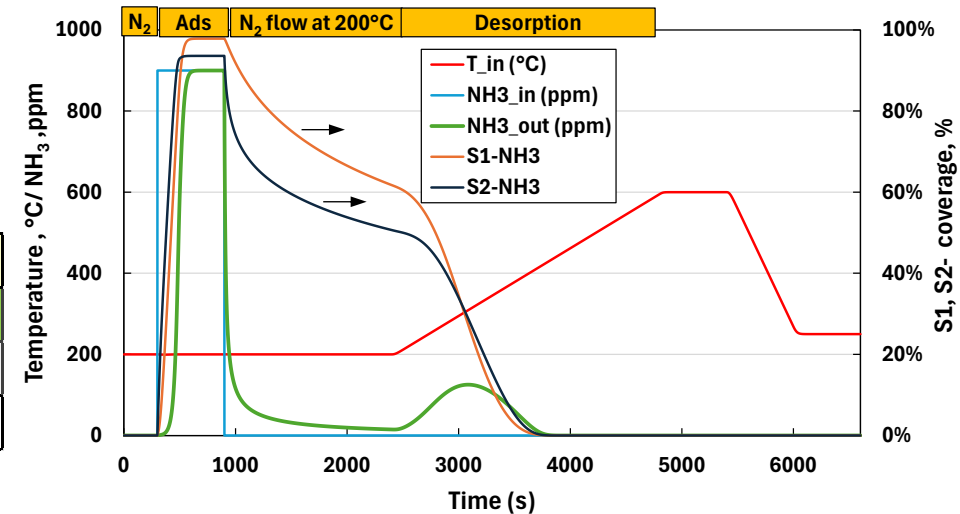
Extruded V-SCR catalyst – NH₃ adsorption capacity

Confirmed NH₃ adsorption capacity (GT Power library) on the V-SCR catalyst (60 cpsi) simulating a NH₃ adsorption-desorption detection method (15.000 h⁻¹)

NH₃ adsorption capacity (μmol/g) on S1+S2 sites by temperatures at 200-600 °C

← Increasing capacity Low, decreasing capacity →

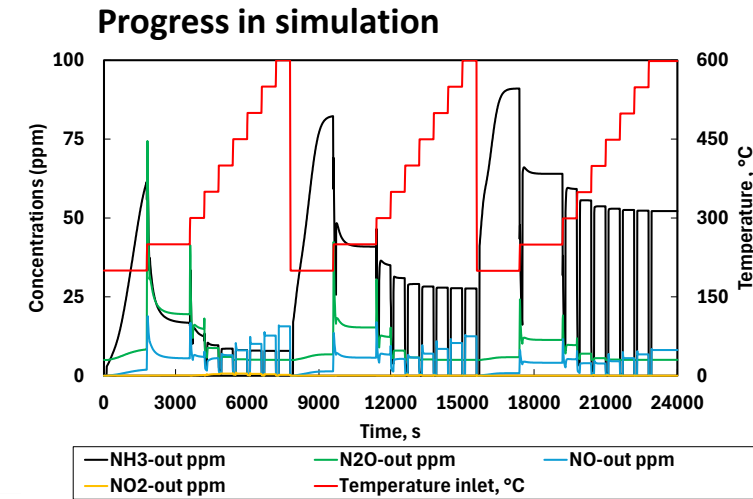
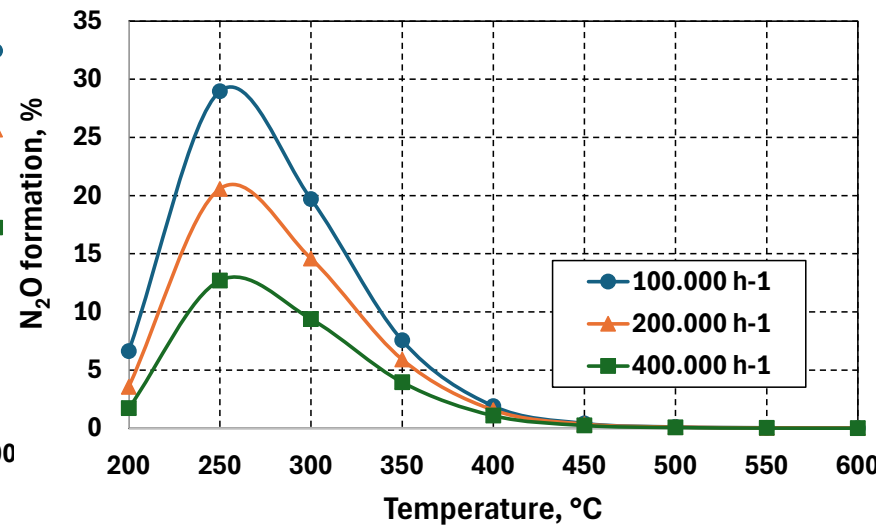
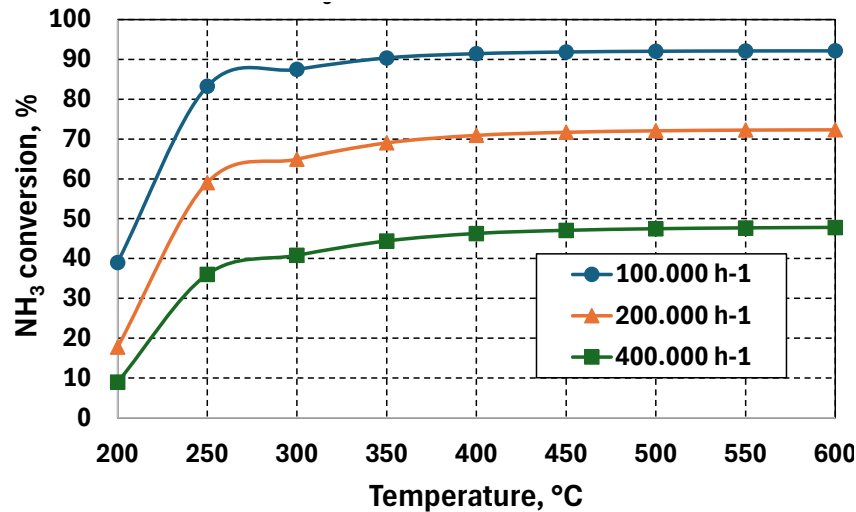
Temperature, °C	200	250	300	350	400	450	500
By desorption	47	42	27	10	1	0	0
In NH ₃ /N ₂ flow	78	69	54	37	23	13	7
Ads step	81	not calculated					



- Adsorption on two sites (S1, S2) in the model and calculated the adsorption capacity and coverage
- Adsorption capacities (μmol/g) matched well to experimental detections on stable V₂O₅/TiO₂-WO₃ catalysts
- It exists **three types of NH₃ adsorption strength**: 1) Strongly bound (N₂ in gas phase), 2) Strongly + weakly bound (NH₃ in gas phase), 3) NH₃ adsorbed in reaction conditions (NH₃ + NO_x in gas phase) → **included in models**
- NH₃ adsorption capacity by desorption relates to strongly (chemically) bound NH₃
- NH₃ adsorption capacity promotes SCR activity at low temperatures
- High volumetric adsorption capacity in extruded V-SCR catalysts (catalyst ≈ 350-500 g/L)

Coated Ammonia Slip Catalyst - verification

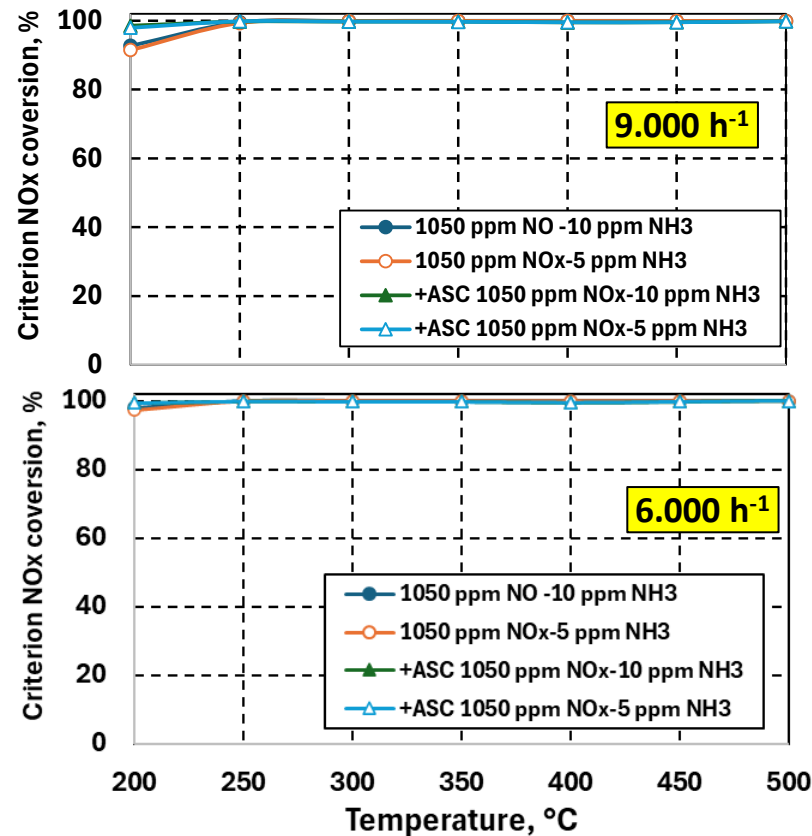
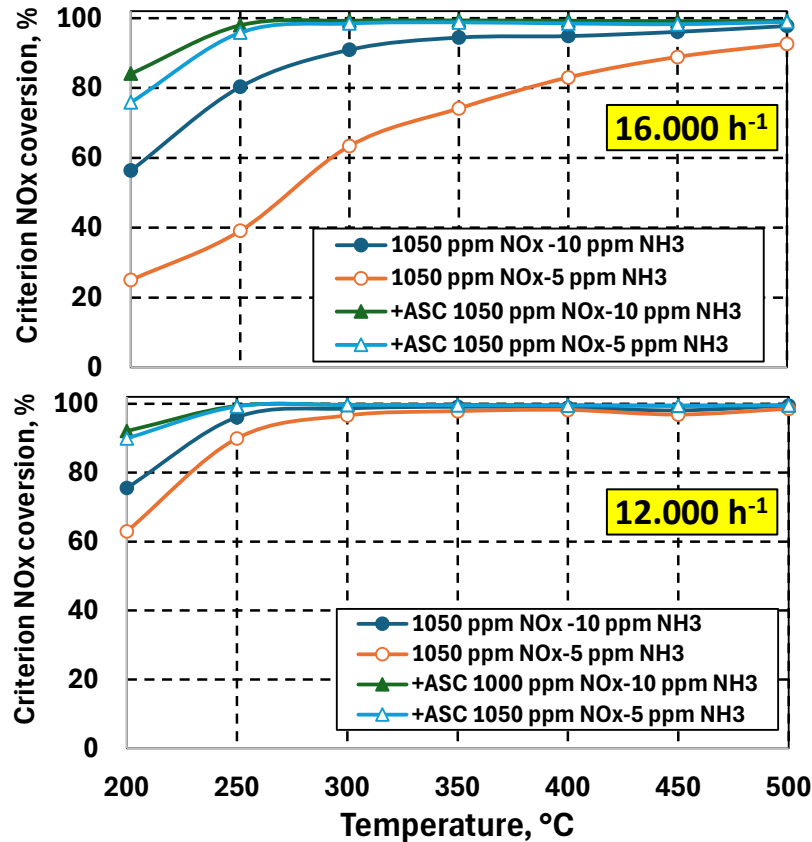
- ▶ Modified library parameters (Scheur et al., Appl. Catal. 111-112(2012) 445) to match better to recent experimental results with 2-layer coated metallic/500 cpsi/50 μm (Maunula 2020 Emission Contr. Sci. Tech. 6(2020) 390)
- ▶ Simulated first ASC to calibrate NH_3 conversions and selectivity (N_2 , NO , NO_2 , N_2O) with 100 ppm NH_3 only in ASC feed



- NH_3 conversions similar as detected in experimental conditions, e.g. with 2-3 g/cft Pt based on 2-layer ASC – very low volume and Pt loading limits the NH_3 conversion but keep $\text{NO}_x/\text{N}_2\text{O}$ formation acceptable
- N_2O formation range and magnitude realistic for aged ASC – GHG formation risk!
- NO_x (mostly NO) had a maximum of 16% at high temperatures with 100.000 h^{-1}

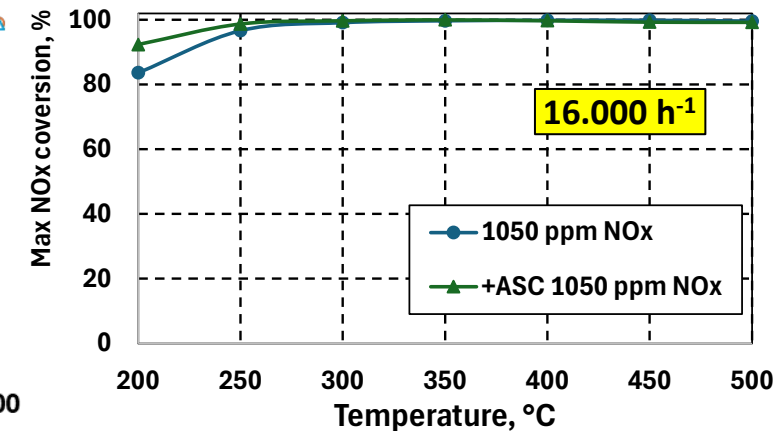
NO_x removal on extruded V-SCR and ASC - simulations

- Comparisons by criterion NO_x conversion in SS, when reached 5 or 10 ppm NH₃ slip in SS by SV of 6.000 – 16.000 h⁻¹



- Extruded V-SCR: 60 cpsi
- Coated ASC: 400 cpsi
- pores $d = 0.25 \mu\text{m}$
- Inlet 1050 ppm NO_x, NO₂/NO=0.05

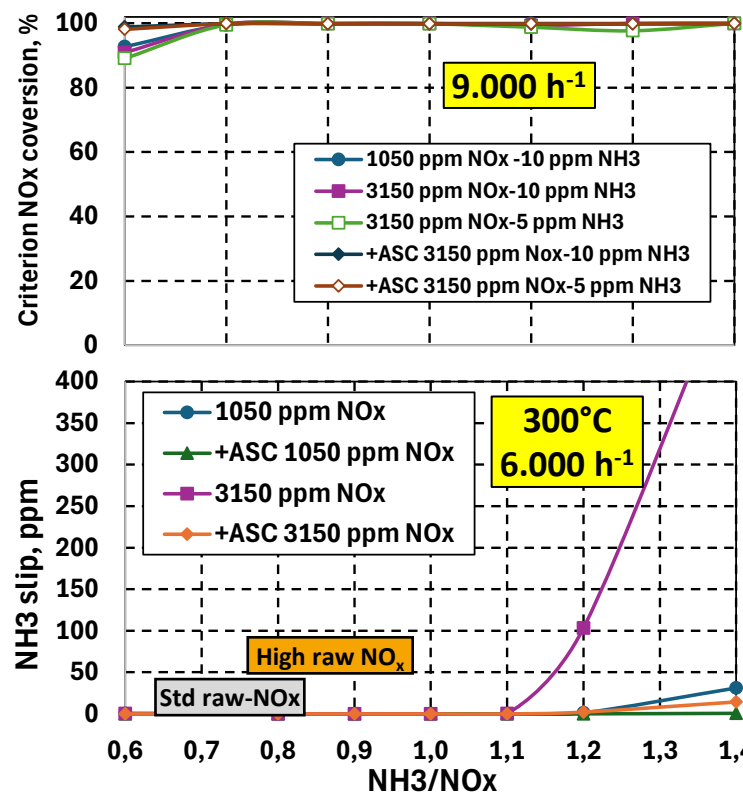
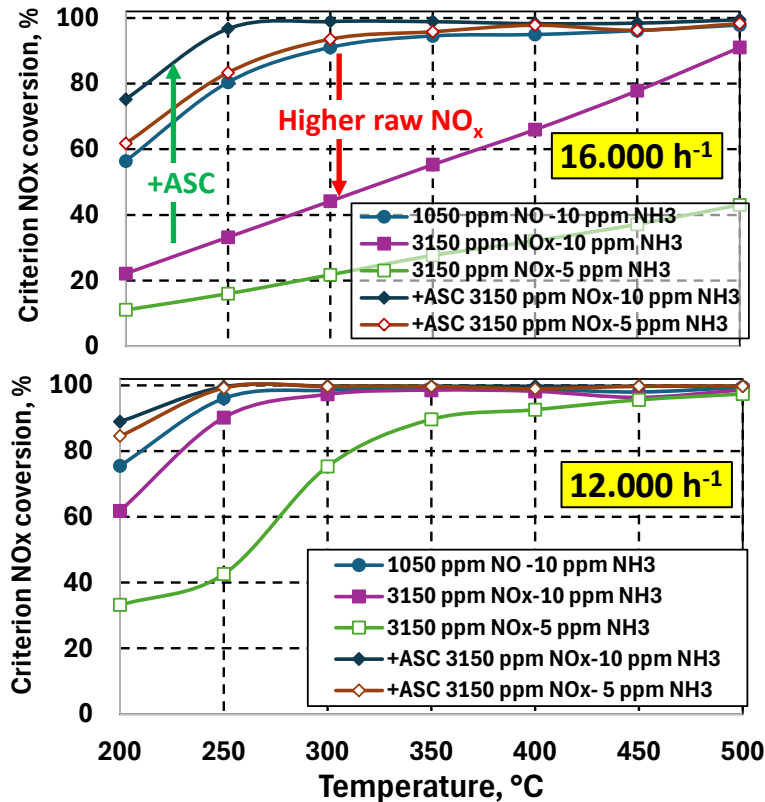
Maximum NO_x conversion in SS



- The range of 6000 – 16.000 h⁻¹ is the design range for extruded SCR by experiments and simulations
- 5 ppm NH₃ slip criterion shows the sensitivity by SV, a better support to SCR design
- ASC promotes to reach high NO_x conversion with high SV conditions (small SCR catalyst or high flow rate)
- Possible to reach high NO_x conversion with high SV but NH₃ slip start to limit (design, control)

NO_x removal on extruded V-SCR and ASC - simulations

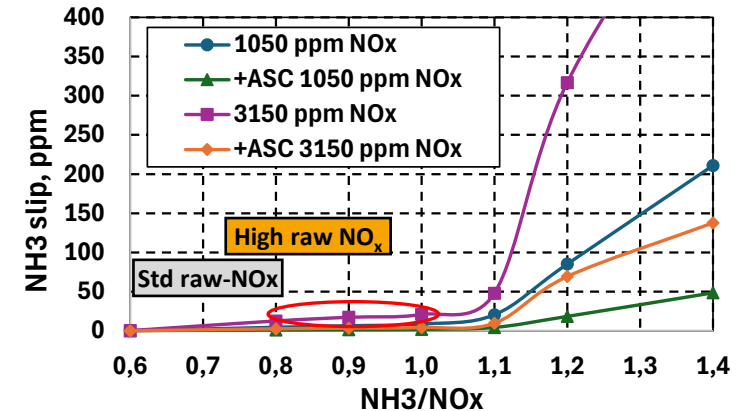
- Criterion NO_x conversion in SS, when reached 5 or 10 ppm NH₃ slip in SS - Effect of inlet NO_x concentration



- Extruded V-SCR: 60 cpsi,
- Coated ASC: 400 cpsi
- pores $d = 0.25 \mu\text{m}$
- SCR/ASC = 10
- Inlet 1050 ppm or 3150 ppm NO_x with NO₂/NO=0.05

300°C
16.000 h⁻¹

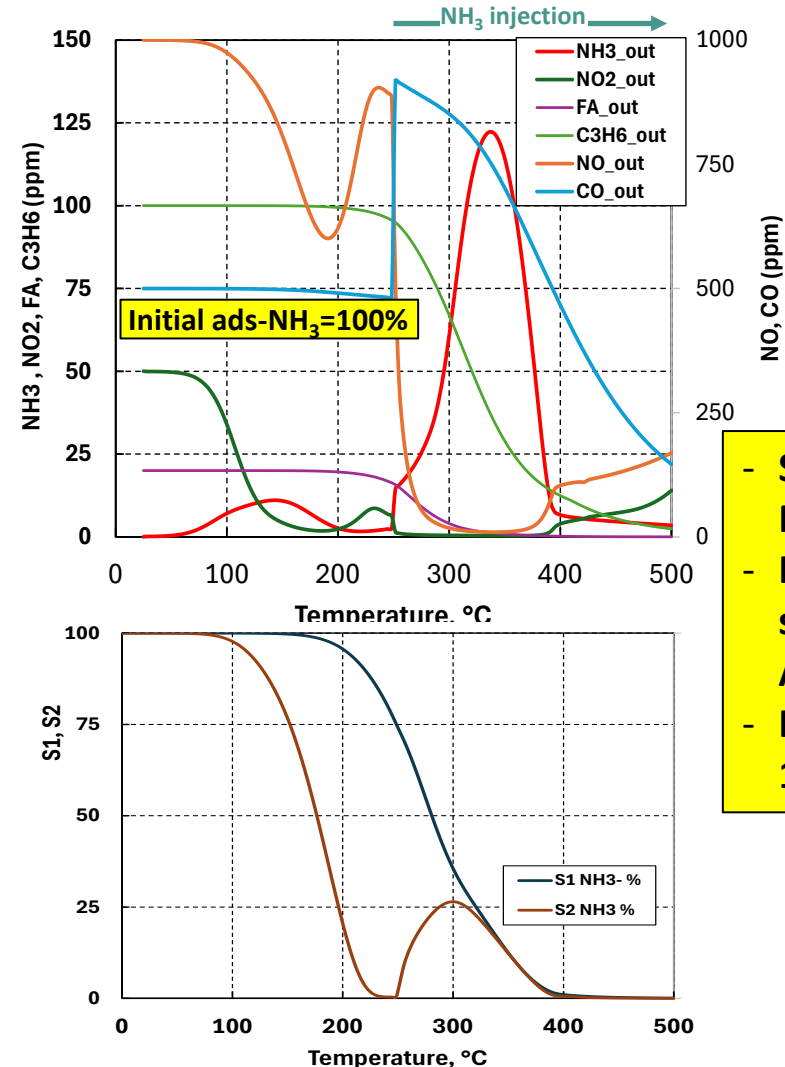
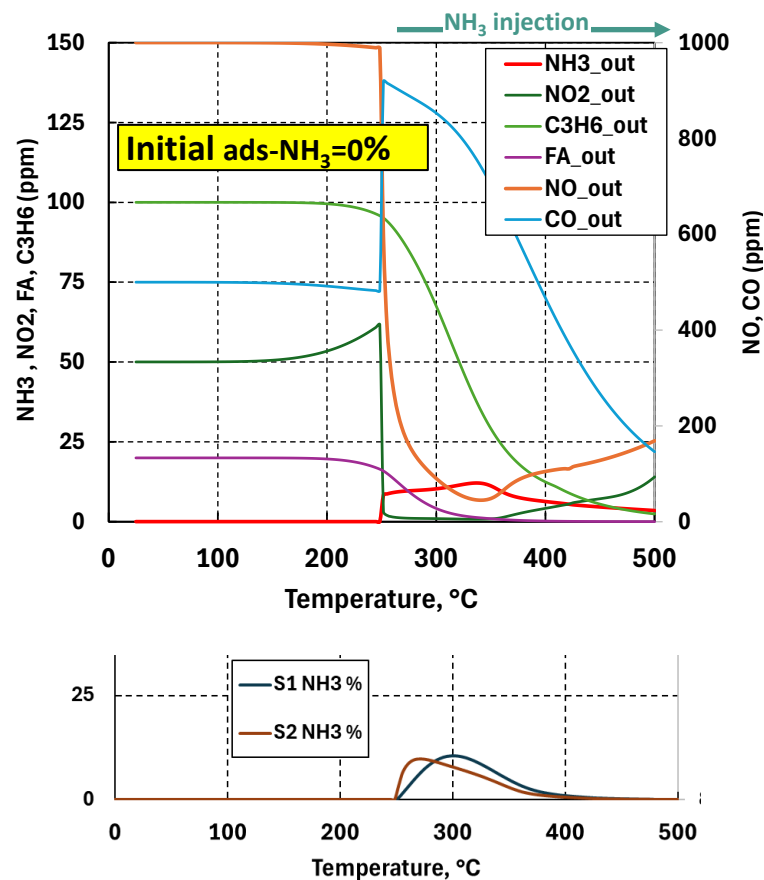
NH₃ slip in ANR window



- Higher raw NO_x emissions (e.g. 3×) reported for NH₃ engines, which will require higher SCR efficiency (deNO_x e.g. 80 → 95 %)
- A promotion by a small ASC enables to reach high NO_x conversion and NH₃ slip targets with high SVs

NO_x removal on extruded V-SCR – transient simulation

- Transient study with V-SCR: **Diesel engine** exhaust gas at 50–500 °C with 20 °C/min, NH₃ injection at 250 °C with **ANR = 0.9**. Two extreme initial states: NH₃ sites empty × NH₃ sites full.

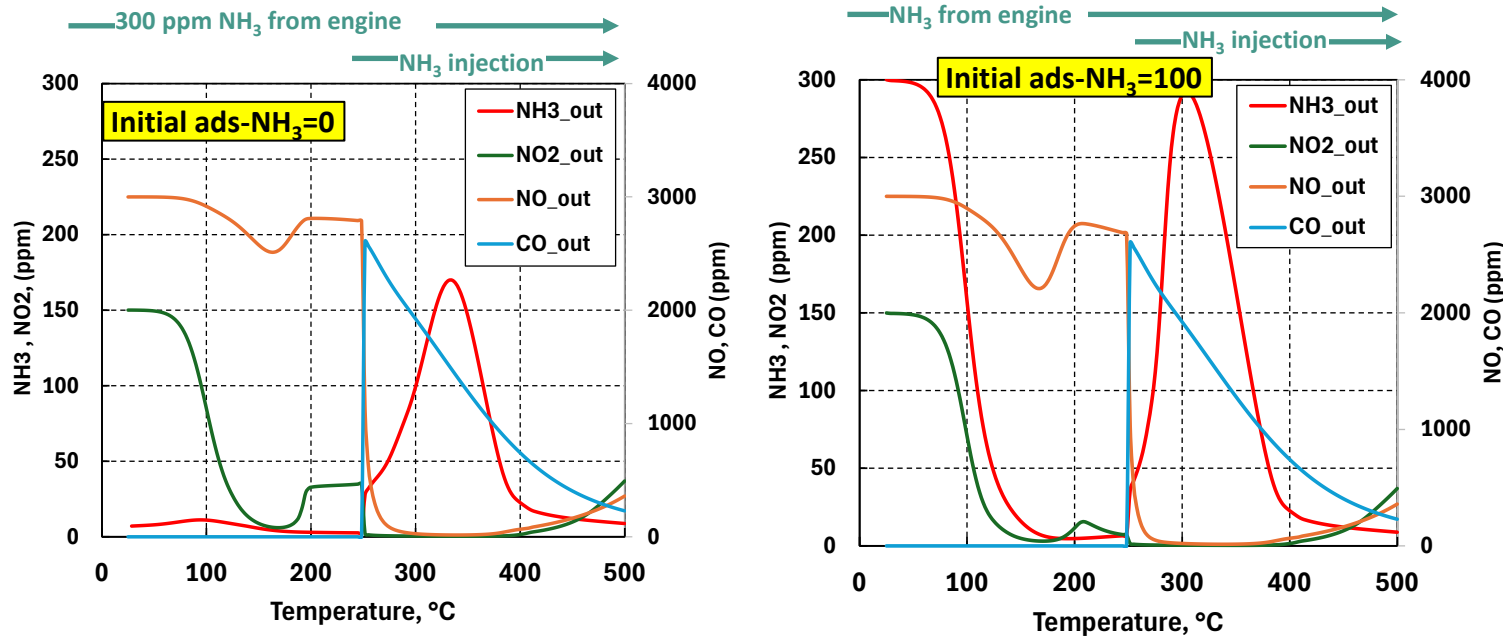


- Extruded V-SCR: 60 cpsi,
- Pore $d = 0.25\mu\text{m}$
- SV 16.000 h⁻¹
- Inlet 1050 ppm NO_x with NO₂/NO=0.05

- Simulation in transients showed the effects of NH₃ adsorption and desorption in a heating ramp
- If SCR catalyst full filled with NH₃, quite high NH₃ slip (max 120 ppm) in the heating ramp when ANR = 0.9 starts at 250 °C
- If SCR empty from NH₃ at 50 °C, max NH₃ slip was 10 ppm in this ramp test

NO_x removal on extruded V-SCR – transient simulation

- Transient study with V-SCR: **Ammonia engine** exhaust gas at 50–500 °C with 20 °C/min, NH₃ injection at 250 °C with **ANR = 0.9**. Two extreme initial states: NH₃ sites empty × NH₃ sites full.

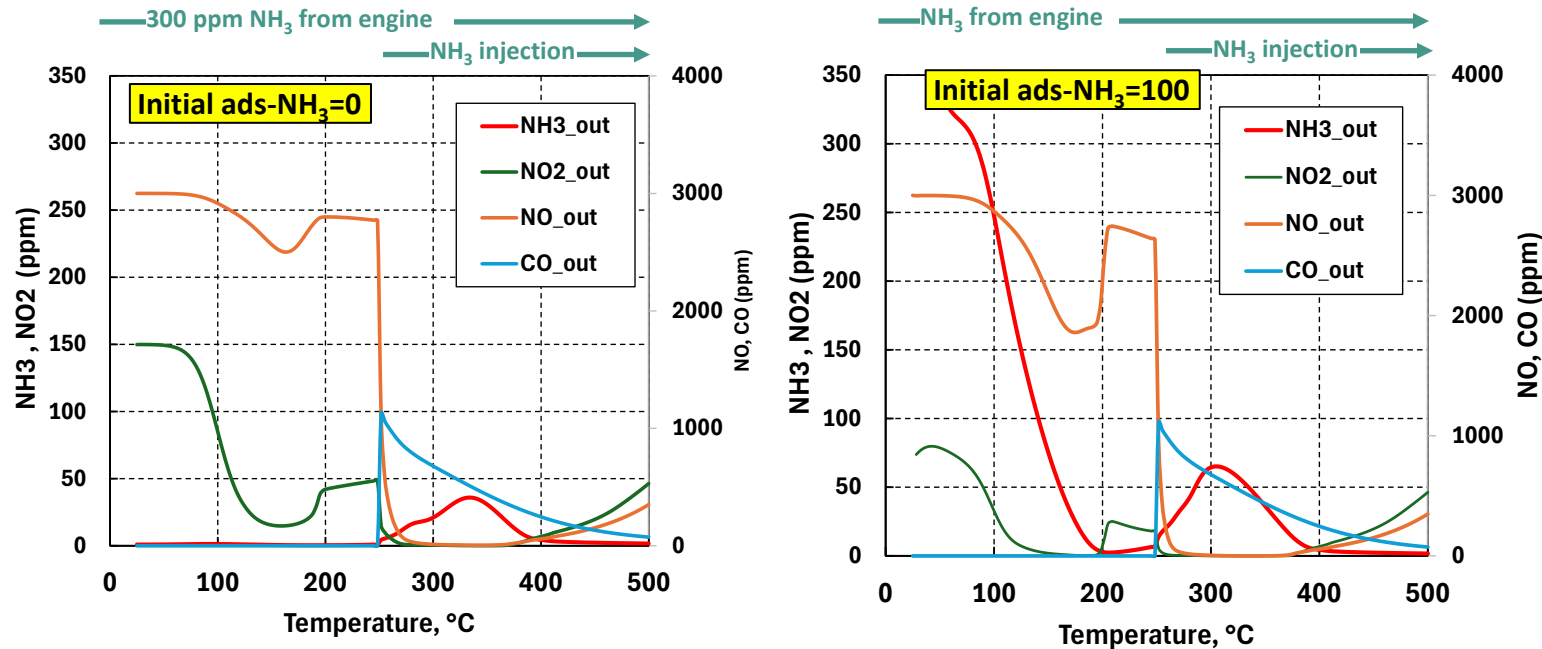


- Extruded V-SCR: 60 cpsi
- Pore $d_{50} = 0.25 \mu\text{m}$
- SV 16.000 h⁻¹
- Inlet 3150 ppm NO_x with NO₂/NO=0.05

- A higher risk for NH₃ slip when NH₃ from engine and urea injection → SCR control to prevent this
- Max NH₃ slip a 165 ppm with zero initial NH₃ and 295 ppm with full-load SCR catalyst
- NH₃-SCR reaction with feed NH₃ starts also before the NH₃ injection at 250 °C

NO_x removal on extruded V-SCR and ASC – transient simulation

- Transient study with V-SCR: **Ammonia engine** exhaust gas at 50-500°C with 20°C/min, NH₃ injection at 250°C with ANR=0.9. Two extreme initial states: NH₃ sites empty - NH₃ sites full.



- Extruded V-SCR: 60 cpsi
- Coated ASC: 400 cpsi
- Pore $d = 0.25\mu\text{m}$
- SV 16.000 h⁻¹
- SCR/ASC = 10
- Inlet 3150 ppm NO_x with NO₂/NO=0.05

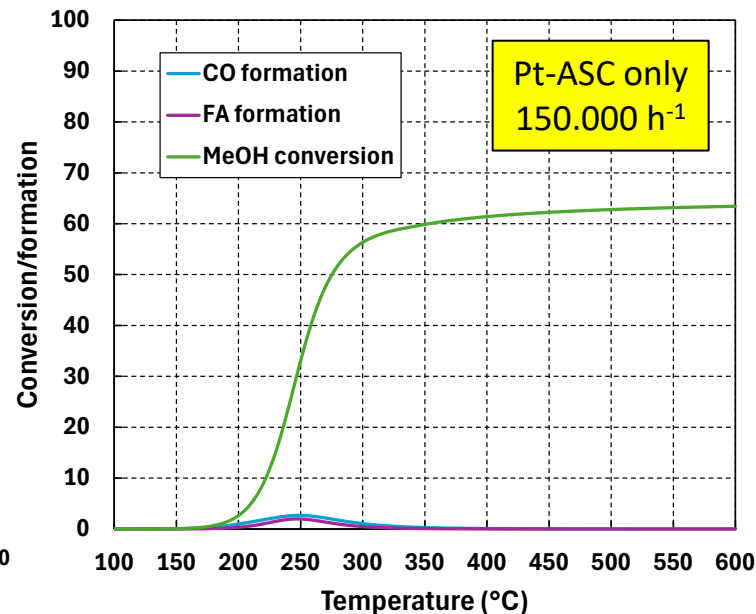
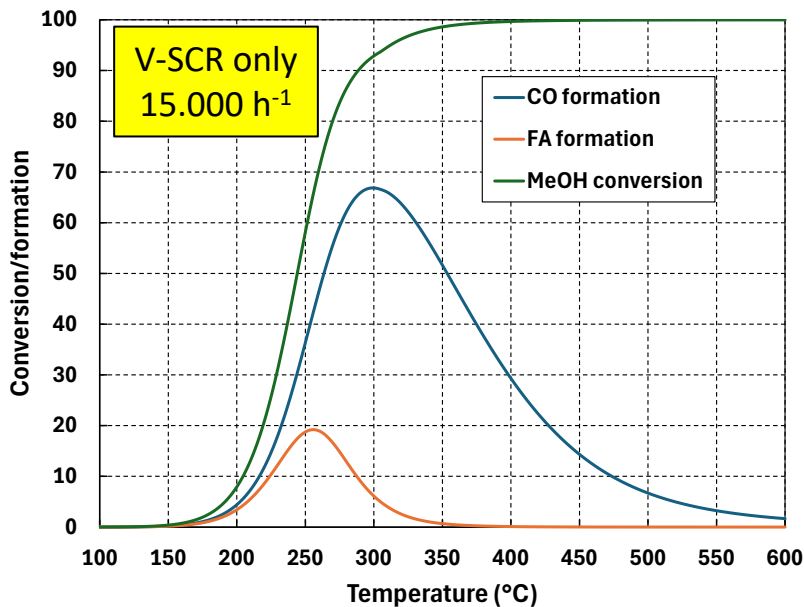
- The presence of ASC prevented well NH₃ and CO slip above 200 °C
- Max NH₃ slip about 60 ppm after NH₃ injection start-up
- “Empty” V-SCR has a good buffering ability to prevent NH₃ emission at low temperatures
- Additional NH₃ adsorption capacity on the zeolite in ASC

Extruded V-SCR catalyst in MeOH application

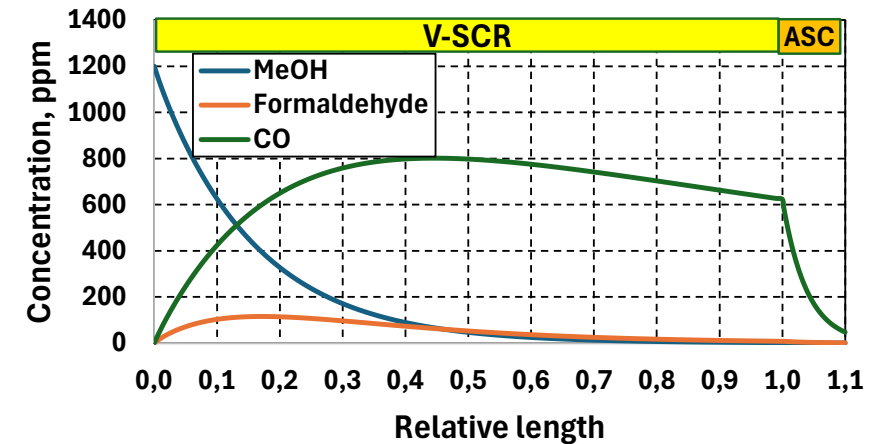
- MeOH, formaldehyde (FA, HCHO) and CO oxidation reactions added for the V-SCR model

Simulated reactions on extruded V-SCR (60 cpsi, 15.000 h⁻¹) and Pt-ASC (400 cpsi, 150.000 h⁻¹) in MeOH engine exhaust gas, temperature ramp 5 °C/min, **1200 ppm MeOH in feed – no FA/CO**

- All MeOH and FA reacts through CO to CO₂
- V-SCR catalysts are good in partial HC oxidation and poor in CO oxidation → net CO formation



MeOH reactions over the catalyst lengths (V-SCR+ASC) at 300°C

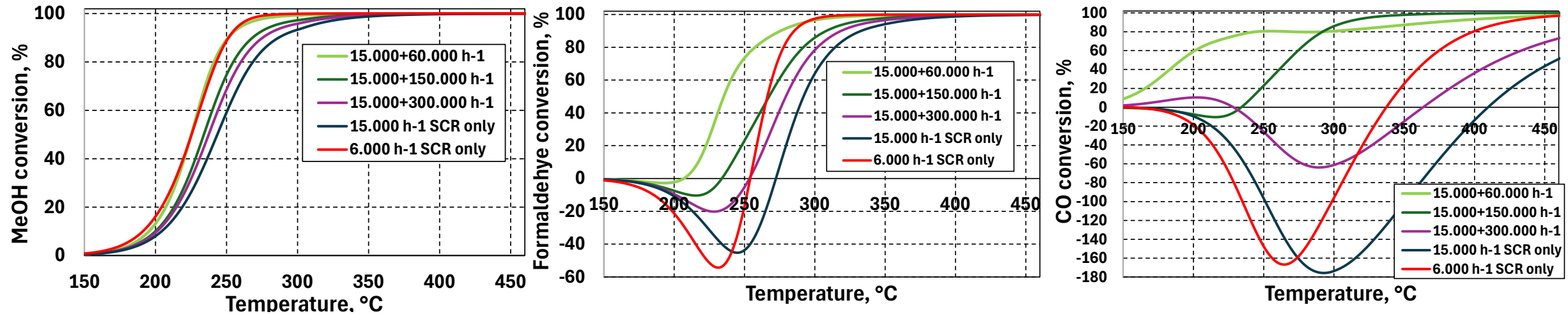


- Investigated MeOH conversion and selectivity separately on V-SCR and ASC
- Small Pt-ASC can prevent well the formation of side reaction products (FA, CO)
- High SV, low Pt loading and pore diffusion prevent to reach near-100% conversions on ASC
- SCR catalyst: ASC = 10 in this verification state

Extruded V-SCR catalyst in MeOH application

- Simulation with extruded V-SCR (60 cpsi, 15.000 or 6.000 h⁻¹) and coated ASC - pore diffusion by d_{50} 0.25 μ m

Simulated reactions on extruded V-SCR (60 cpsi) and Pt-ASC (400 cpsi) in MeOH engine exhaust gas, temperature ramp 5 °C/min, 1200 ppm MeOH, 500 ppm CO and 300 ppm FA in feed

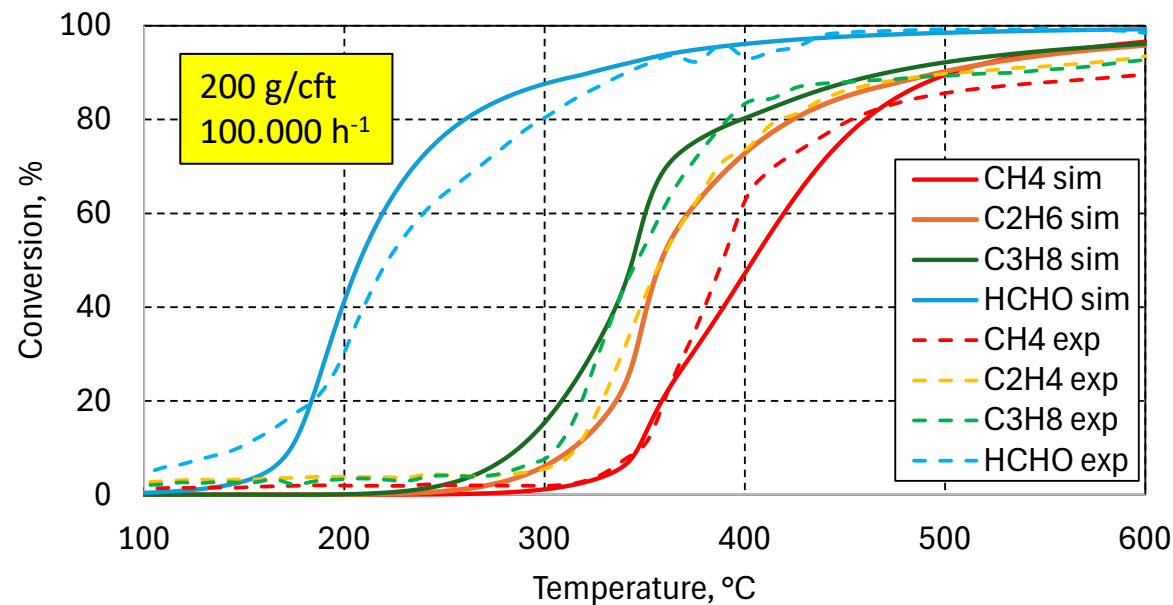


- Investigated the oxidation activities on V-SCR catalyst and ASC by SVs
- T_{50} with 15.000/6.000 h⁻¹ about 245/225°C for MeOH, 295/265°C for FA and 455/365°C for CO on V-SCR only
- Net formation of FA and particularly CO typical on V-SCR- Max CO formation about same with 6.000 and 15.000 h⁻¹
- Pt-ASC (SCR/ASC = 4–20) able to cut efficiently FA and CO → SCR/ASC ratio of 4 was very efficient

Methane oxidation catalyst (MOC)- model verification

Model modification, verifications and simulation with coated, cordierite supported PtPd catalysts (400 cpsi, 50.000 – 150.000 h⁻¹, 100–200 g/cft PtPd (1:4, hydrothermally aged at 700°C/20h)

Simulated reactions in CH₄ engine exhaust gas, temperature ramp 5 °C/min, 1500 ppm CH₄, 300 ppm C₂H₆, 100 ppm C₃H₈, 150 ppm FA, 500 ppm CO and 1050 ppm NO_x in feed)



- All CH₄ reacts through CO to CO₂
- FA also from CH₄ engine
- $\text{CH}_4 + 1.5 \text{O}_2 \rightarrow \text{CO} + 2 \text{H}_2\text{O}$ (CO formation)
- $\text{CO} + 0.5 \text{O}_2 \rightarrow \text{CO}_2$ Fast at CH₄ oxidation T
- $\text{HCHO} + 0.5 \text{O}_2 \rightarrow \text{CO} + \text{H}_2\text{O}$ (FA oxidation)

High-PGM MOC required to activate CH₄, C₂H₆, C₃H₈ oxidation, formed CO oxidized very fast.

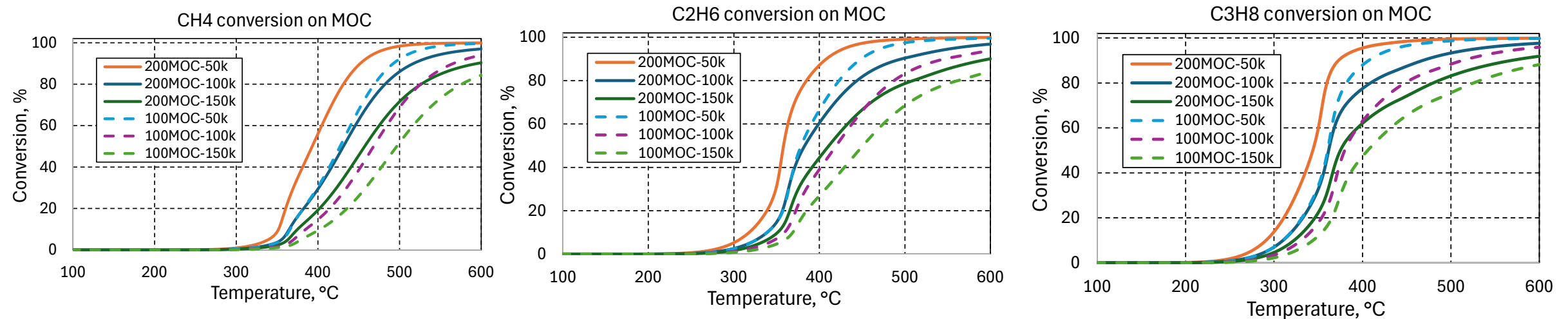
Experimental data: Top. Catal. 59(2016) 1049 and 62(2019) 315

- Methane removal very challenging – most difficult HC to oxidize → high PtPd loadings and catalyst volumes required
- Pore diffusions with the pore size of 0.1 µm included in modelling (alumina-based catalyst)
- MOC removed efficiently CO, FA well but more limited for non-methane saturated HCs

Methane oxidation catalyst (MOC)- simulations

Effect of PtPd(1:4) loading and space velocity (SV) on CH₄, C₂H₆ and C₃H₈ oxidation with MOC (400 cpsi)

Simulation with CH₄ engine exhaust gas, temperature ramp at 50–600 °C by 5°C/min, 1500 ppm CH₄, 300 ppm C₂H₆, 100 ppm C₃H₈, 500 ppm CO, 150 ppm FA and 1050 ppm NO_x in feed (g/cft MOC-SV, k=000)

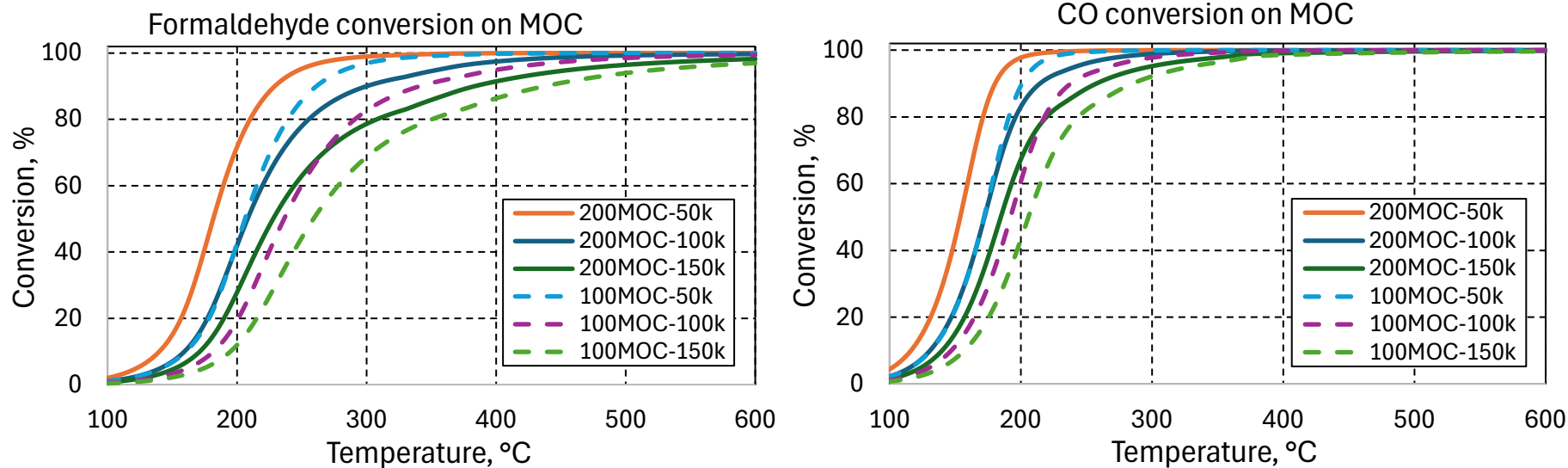


- Methane oxidation light-off (T_{50}) at 395–500 °C – high SV and PtPd loading required reach higher efficiency
- SVs related to the catalyst with 400 cpsi, if lower cell densities, correspondingly lower SVs needed (challenges to add high PtPd in low density catalysts and low volumetric coating amount)
- The light-off temperature T_{50} of saturated HCs with 200 g/cft and 50.000 h⁻¹: CH₄ (395°C) > C₂H₆ (360°C) > C₃H₈ (340°C)
- The PtPd loading controls the light-off but large volumes are required to promote high- T conversions

Methane oxidation catalyst (MOC)- simulations

Effect of PtPd(1:4) loading and space velocity on **formaldehyde and CO oxidation** with MOC (400 cpsi)

Simulation with CH₄ engine exhaust gas, temperature ramp at 50–600 °C by 5 °C/min, 1500 ppm CH₄, 300 ppm C₂H₆, 100 ppm C₃H₈, 500 ppm CO, 150 ppm FA and 1050 ppm NO_x in feed (g/cft MOC SV, k=000)



- Formaldehyde oxidation light-off (T_{50}) at 180-260°C
- CO oxidation light-off (T_{50}) at 150-205°C
- Formaldehyde and CO oxidized easily but larger catalyst volumes enable to reach conversions above 90%
- Even lower Pt and Pd loadings can be applied for FA and CO removal (see ASC simulations)

Summary and conclusions

- ▶ In this study, tailored emission catalyst modelling and simulations for future marine ATS applications
- ▶ Extruded vanadium-SCR catalysts have been applied traditionally for NO_x removal in marine applications
- ▶ In addition to external diffusion, it is important to include pore diffusion in modelling of extruded SCR catalysts and 2-layer ASCs
- ▶ The change from diesel (MGO, LFO) to methanol, ammonia or methane fuels changes significantly the exhaust gas composition:
 - + no/low SO_x, low particulates, less heavy HCs, no/less CO₂
 - Higher water, increasing risks for pollutant or GHG emissions like formaldehyde, methanol, ammonia, methane, N₂O
 - +/- Temperatures, raw-NO_x
- ▶ V-SCR catalyst catalyzes MeOH and C₃H₆(diesel) oxidation to CO, which is oxidized slowly to CO₂
- ▶ ASC after the SCR catalyst removes efficiently ammonia but also remaining methanol, formaldehyde, diesel-HCs and CO above 250°C
- ▶ Extruded V-SCR has a high ammonia adsorption ability, which can prevent ammonia emissions from NH₃ engines at low temperatures
- ▶ Higher raw-NO_x emissions (e.g. from NH₃ engines) demand re-design or reserve for SCR functionality due to higher targets for NO_x and NH₃ conversions – small ASC promotes significantly
- ▶ High loadings like 100–200 g/cft PtPd (1:4) required in MOC to reach methane light-off around 400 °C – sulfation and desulfation experiments exists and will be included next into these models
- ▶ These reaction and parameter calibrations for various pollutants give a good base for the future case studies with green fuels

Thank You

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