PACCAR H2 SCR Understanding

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Background/Intro

- PACCAR is investigating the use of **hydrogen internal combustion engines** (H2ICE) in heavy-duty trucks to reach carbon emissions sustainability goals.
- Hydrogen vehicles still **produce NOx**, a pollutant subject to emission regulation. Diesel vehicles have a selective catalytic reduction (SCR) system that reacts with NOx and urea-based Diesel Exhaust Fluid (DEF) to form environmentally safe nitrogen (N2) and oxygen (O2).
- While the DEF-based SCR may be applied for H2ICE emission after treatment, **hydrogen-based SCR (H2SCR) is a promising alternative that could utilize H2 fuel as a reductant.**

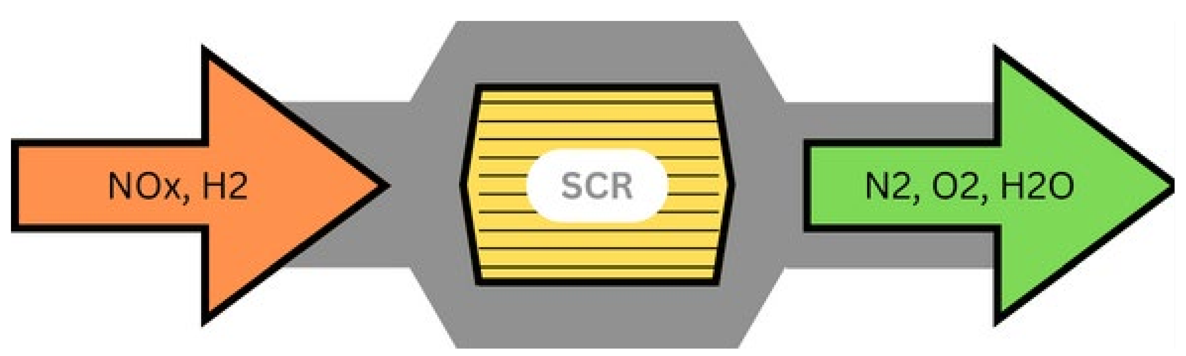

Fig. 1.. Diagram of SCR Systems in Automobile Applications

Impact of Switching from Diesel to Hydrogen Trucks

- Current Diesel Trucks need to use ammonia-based SCR.
- The ammonia is used as a reductant for the SCR catalyst.
- The ammonia needs to be filled up separately from the fuel, which introduces added complexity.
- New hydrogen trucks can potentially use hydrogen SCR.
- The hydrogen fuel can be used as a reductant for exhaust aftertreatment.
- This can save drivers time and bring convenience.

Fundamental Science

Catalyst Structure

- Substrate: Bulk material of the catalyst. Most species that react are adsorbed onto the substrate.
- Active site: Metal particles that sit on top of the substrate. These play an important role in speeding up chemical reactions.

Catalyst Properties

- Activity: How quickly chemical reactions occur on the catalyst.
- Selectivity: How quickly one reaction occurs relative to all reactions.
- Temperature-performance curve: Selectivity and activity are heavily influenced by temperature. Good performance is required across a large temperature range.

$$2NO + 2H_2 \rightarrow N_2 + 2H_2O$$

$$2NO + H_2 \rightarrow N_2O + H_2O$$

$$2NO + 5H_2 \rightarrow 2NH_3 + 2H_2O$$

$$2NO + O_2 \rightarrow 2NO_2$$

$$2H_2 + O_2 \rightarrow 2H_2O$$

Fig. 2. Main reactions occurring in an H2SCR system[1]

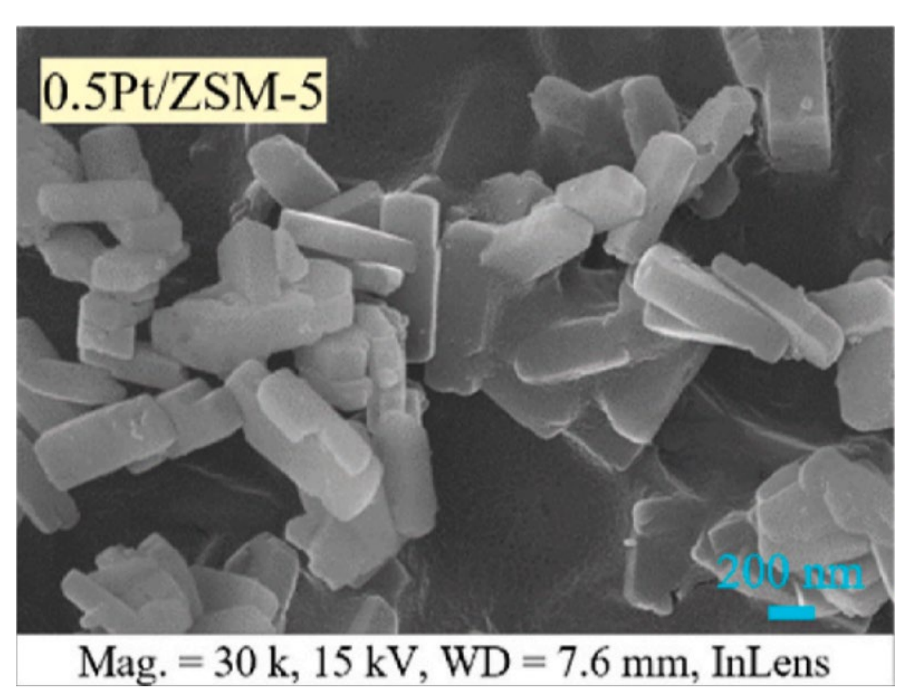

Fig. 3. SEM image of a zeolite-supported platinum catalyst[2]

Methods

1. **Literature Review:** Develop a comprehensive review of existing H2 and NH3 SCR.
2. **Pairwise Matrix:** Determine criteria to evaluate catalysts in the decision matrix. See Table 1.
3. **Catalyst Decision Matrix + Selection:** Evaluate the best of each catalyst type investigated (Pt, Pd, bimetallic). See Table 2.
4. **In-Depth Catalyst Analysis:** Gather more comprehensive information on selected catalysts. Includes system sizing, performance evaluation, and economics.

	NOx Reduction Activity	Temperature Range	Range of Reported Temperatures	N2 Selectivity	Totals	Rank
NOx Reduction Activity		5	5	3	13	1
Temperature Range	1		5	1	7	3
Range of Reported Temperatures	1	1		1	3	2
N2 Selectivity	3	5	5		13	1

Table 1. Finalized pairwise matrix

		Catalyst		
Criterion	Weight	Pt-Cr/ZSM-35 Pt(.5%)-Cr(1%)	Pd/ZrO2-CeO2	Pt/ZSM-5
Catalyst Type	N/A	Bimetallic Zeolite	Pd Based Metal Oxide	Pt Based Zeolite
NOx Reduction Activity	13	7	1	9
Temperature Range	7	5	9	5
dT for Temperature Range (C)	0	100	300	50
T1/2 for Temperature Range (C)	0	85	65	60
Range of Reported Temperatures	3	5	9	9
N2 Selectivity	13	3	9	7
Total	36	5.00	6.11	7.50

Table 2. Top three catalysts selected in the decision matrix

Results/Findings

Promising catalysts investigated:

- Bimetallic Platinum and Chromium catalysts on Zeolite Substrate (Pt-Cr/ZSM-35 Pt(.5%)-Cr(1%))
- Platinum Catalysts on Zeolite Substrate (Pt/ZSM-5)
- Palladium Catalysts on a Zeolite and Metallic Substrate (Pd/ZrO2-CeO2)

Discussion

While multiple catalysts are promising candidates for H2-SCR, **experimental validation is needed to determine performance under typical dynamic engine conditions.**

Conclusion

- **H2-SCR is being actively investigated** by academic and industry researchers.
- In optimal operating conditions, **several catalysts can reduce NOx emissions well below the regulation limit.**
- **Noble metal catalysts (Pt, Pd) and mixed-metals** display the best performance.
- Choice of **substrate has a significant impact** on reaction rate and selectivity.
- **Zeolite-supported** catalysts are typically **more active and selective**, but they have **narrow optimal temperature ranges.**
- **Metal oxide-supported** catalysts display much **wider temperature-performance curves.**

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References

[1] Borchers M et al, Industrial & Engineering Chemistry Research, vol. 60, 6613-6626.

[2] Lee, K et al, Journal of Cleaner Production, vol. 434, 140333.