Optimizing the diesel oxidation catalyst for fuel diversification
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Agenda

• Background
• My project
• Main takeaways from literature study
• Experimental approach
Pollutants from diesel trucks

- Nitrogen oxides (NO$_x$)
- Particulates
- Hydrocarbons
- CO
- CH$_4$
- CO$_2$
- N$_2$O

Regulated pollutants

Greenhouse gases
European emission legislation

Emissions cut by over 90 % compared to 2000

Euro 6 introduces particle number limits
Scania’s aftertreatment – summary
Example of a Euro 6 aftertreatment system

DOC Oxidizes hydrocarbons and CO into CO₂ and H₂O

Oxidizes NO into NO₂

Pt-Pd/Al₂O₃ typically used
Example of a Euro 6 aftertreatment system

DPF traps particulates

NO₂ generated in the DOC helps burn away trapped soot
Example of a Euro 6 aftertreatment system

In the SCR catalyst $\text{NO}_x$ reacts with $\text{NH}_3$

Increasing the $\text{NO}_2/\text{NO}_x$ ratio from engine-out levels increases activity

Excess $\text{NH}_3$ is taken care of in the ASC
The DOC plays a central role in the system

- Takes care of CO and hydrocarbons
- Oxidizes NO into $\text{NO}_2$
- Facilitates particle filter regeneration
- Increases $\text{NO}_x$ removal activity
- However, its position close to the engine exposes it to various poisons
  - Is performance and longevity affected by fuel substitution?
How does fuel substitution affect exhaust chemistry?

- Changed relative composition of main components
- Other hydrocarbons
- Trace elements that may act as catalyst poisons
  - From feedstock
  - From catalysts used in production process
My project

• Development of an oxidation catalyst
  • which optimizes the performance of the entire aftertreatment system
  • Which is optimized for fuel diversification
• Verify on lab scale its effect on the rest of the aftertreatment system
• Map the effects of poisoning on catalyst performance for different fuels
Three main areas to study

- Fuels
- Catalyst materials
- Poisons

How are they connected?
Kinetics
- Catalytic activity
- Lab set-ups used to study activity and kinetics
- Temperature
- Gas composition
- Hysteresis

Fuels
- Diesel
- FT-diesel
- Biodiesel/FAME
- HVO
- ED95
- DME
- Biogas (CH₄)
- Natural gas

Properties
- Boiling point
- Fuel specifications
- Molecular formula
- Chemical composition
- Trace components

Production processes

Exhaust composition

Catalyst materials
- Different active metals
- Different supports
- Different promoters

Characterization

Deactivation
- Thermal deactivation
- Poisoning
- Other?

Poisons
- Sulphur
- Phosphorus
- Chloride
- Alkali metals
- Zink
- Hydrocarbons
- CO
- Others

Lab set-up

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Hysteresis effect for NO oxidation

The catalyst is reversibly deactivated at high temperatures due to oxide formation from reaction with formed NO₂.

NO oxidation: reverse hysteresis

The reverse hysteresis effect is a transient effect.

DOC kinetics

CO + \frac{1}{2} O_2 \rightarrow CO_2
NO + \frac{1}{2} O_2 \rightarrow NO_2
HC + O_2 \rightarrow CO_2 + H_2O

The different reactions influence each other
Reactant mixture effects: NO, CO and HC co-oxidation

NO oxidation starts after CO and HC have already been oxidized

Reactant mixture effects: HC and CO can act as reductants of NO₂

Because of oxidation of HC and CO by NO₂, with high NO₂ outputs from the engine, the DOC may actually be a net consumer of NO₂

CO inhibition

Inhibition by water

HC oxidation: reactant mixture effects

Benzene (○), o-xylene (■), and styrene (△)

Conclusions

• There are considerable inhibition effects between the different reactants
• A decrease in oxidation activity for one reactant may affect conversion of the other reactants
• To understand the deactivation process you want to be able to study oxidation of each reactant individually
• Using only $\text{C}_3\text{H}_6$ to model all hydrocarbons may not give accurate results
• Flexibility in mind when designing the experiment rig
Experimental set-up

Monolith dimensions: 
D = 2 cm, L = 3 cm

Space velocity:  
80000 – 200000 h⁻¹
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