VECOM
Vehicle Concept Modelling

Exhaust gas aftertreatment modelling: a focus on the NH_3-SCR of NOx from Diesel vehicles

Massimo Colombo

ESR at LAT/AUTh, Nov. 2010 - June 2011

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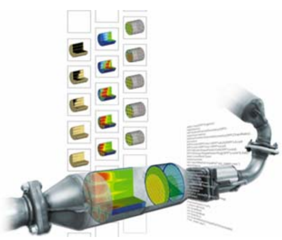
Personal Background

- **Project:** EC Marie Curie FP7 ITN **VECOM** (Oct 2008 - Sept. 2012)
- **Massimo Colombo (ESR, from Italy)** http://www.vecom.org
  - Born on September, 24th 1984
  - M.Sc. in Chemical Engineering at Politecnico di Milano, December 2008;
  - Internship at DAIMLER A.G., Oct. 2007/March 2008 (6 months);
  - Ph.D. Student at Dipartimento di Energia - Politecnico di Milano, Jan.2009/Dec.2011;
  - ESR for **EC Marie Curie FP7 ITN "VECOM" at Laboratory of Applied Thermodynamics, Aristotle University of Thessaloniki, Greece** (Nov. 2010-May 2011)
  - 11 communications to international conferences
  - 4 journal papers
- **Research Topics:**
  - Mechanism, kinetics and modeling of Ammonia Selective Catalytic Reduction (SCR) of NOx from diesel exhausts
  - Diesel exhausts aftertreatment modeling



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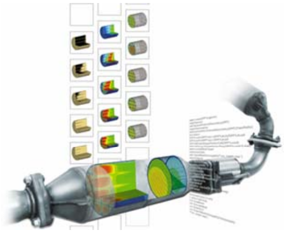
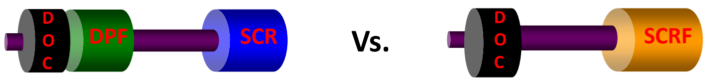
Research activity at LAT

METHODS: Simulation studies by means of an exhausts systems simulation platform, axisuite®, developed at LAT/AUTh over the last 15 years and further developed and supported by Exothermia SA



TOPICS:

- ✓ **Simulation study of Selective Catalytic Reduction on Filters (SCRF) systems**
  → To ZEV symposium (June 9-10, 2011, Turin, Italy):
  Oral Presentation + SAE Technical Paper (2011-37-0031)



- ✓ **Simulation of Ammonia Slip Catalysts (ASC)**
  → 2011 CLEERS workshop (April 19-21, 2011, Detroit – MI, U.S.A.)
  Oral Presentation + future publication in peer-reviewed journal

- ✓ **Modeling of ammonia adsorption over zeolite based catalysts**
  → MODEGAT II (September 19-20th, 2011)
  Poster presentation + eventual publication in peer-reviewed journal

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Outline

- Background
  - NOx & PM emission regulations for Diesel vehicles
  - NH_3-SCR & DPF technologies
- Methods
  - Simulation tools: axisuite®
- Simulation results
  - Selective Catalytic Reduction on Filters (SCRF) systems
  - Dual-Layer Ammonia Slip Catalysts (ASC)

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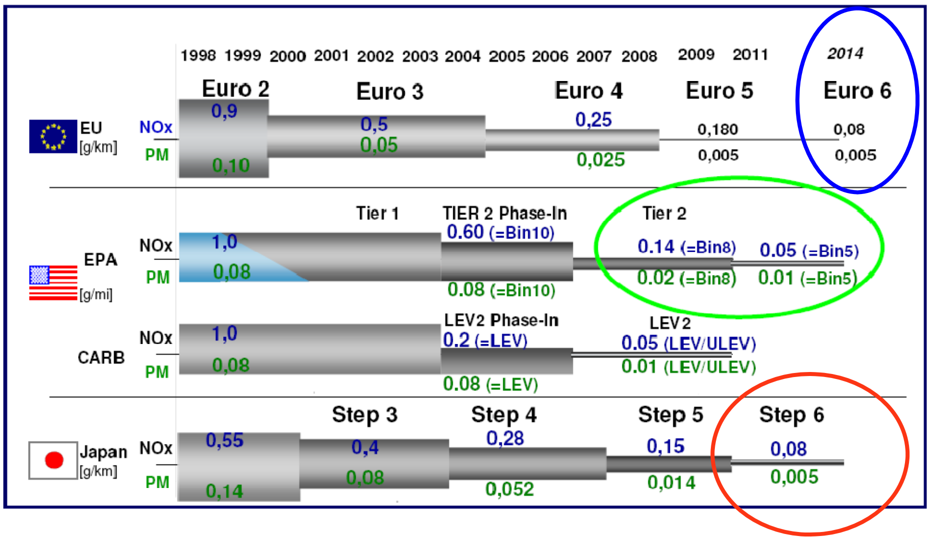
NOx & PM emission standards



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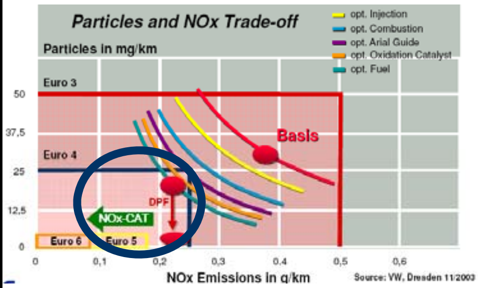
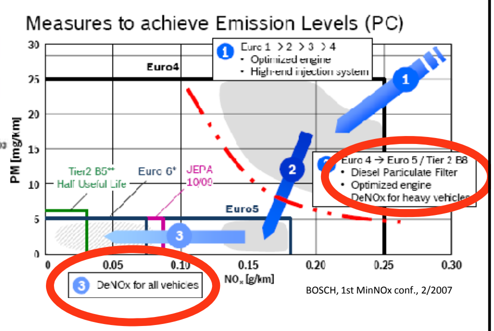
How do we get there?





Improvements in the combustion engine technologies can help…
but they are not sufficient…**DPF and deNOx systems are mandatory!**

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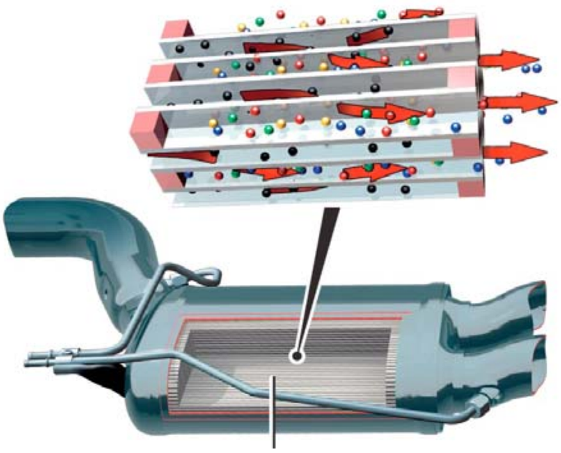
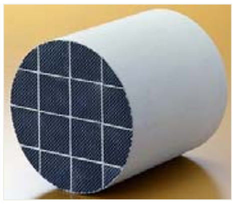
DPF systems





- Plugs at channel outlets
- Wall porosity

Cyclic operation: filtration & regeneration

http://www.ngk.co.jp, http://www.theautochannel.com

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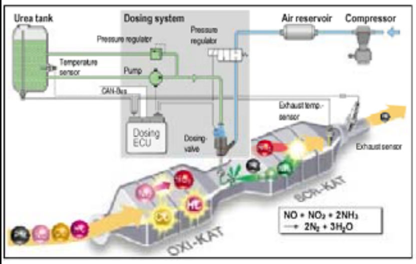
NH_3-SCR systems



$4NH_3 + 4NO + O_2 \rightarrow 4N_2 + 6H_2O$ **Standard SCR**

$2NH_3 + NO + NO_2 \rightarrow 2N_2 + 3H_2O$ **Fast SCR**

$4NH_3 + 3\,NO_2 \rightarrow 3.5\,N_2 + 6H_2O$ **NO_2 – SCR**

- On-board NH_3 source → aqueous solution of **urea**
- DOC upstream of the SCR converter (NO->NO_2)

Open issues

1) **Enhanced Low-T activity of the SCR reactions → NEW CATALYSTS**
2) **Reaction pathways, catalytic mechanism, kinetics, role of NO_2**
3) **Integration with other aftertreatment technologies (e.g. SCR on Filters)**
4) **Ammonia slip from SCR converters**

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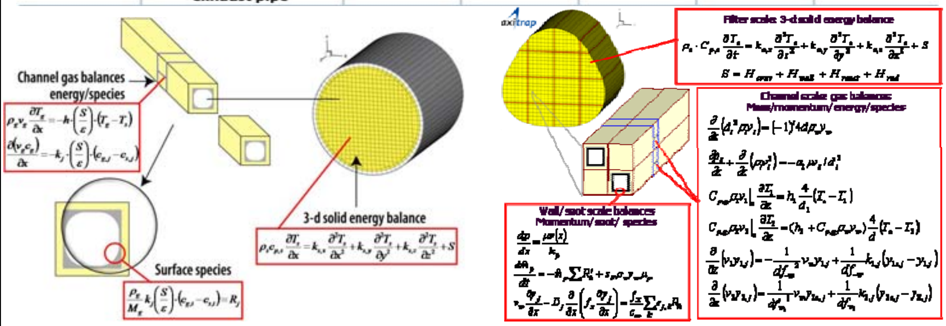
Aftertreatment converters models

axisuite						
software module	functionality / reactor type	3-way catalyst	diesel oxidation catalyst	lean NO_x trap	selective catalytic reduction	diesel particulate filter
axicat	flow-through	✓	✓	✓	✓	n/a
axitrap	wall-flow	n/a	✓	✓	✓	✓
axiheat	exhaust pipe	single-wall	double-wall	insulating material	flanges	reacting flow



Koltsakis & Stamatelos A. M., *Appl. Catal B.*, 1997.
Pontikakis et al., Top. In Catal, 2001
Tsinoglou & Koltsakis, Proc. IMechE, 2007

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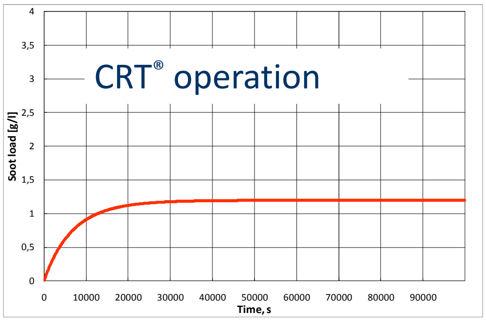
Simulation Results

A modeling study of soot and de-NOx reaction phenomena in SCRF systems

SAE Technical Paper 2011-37-0031

Concept analysis of CRT® operation



CRT®:

- Continuously Regenerating Trap
- DOC + DPF system
- NO_2 from the DOC continuously regenerates the filter

Is CRT® applicable also for SCRF systems?

SAE Technical Paper 2011-37-0031

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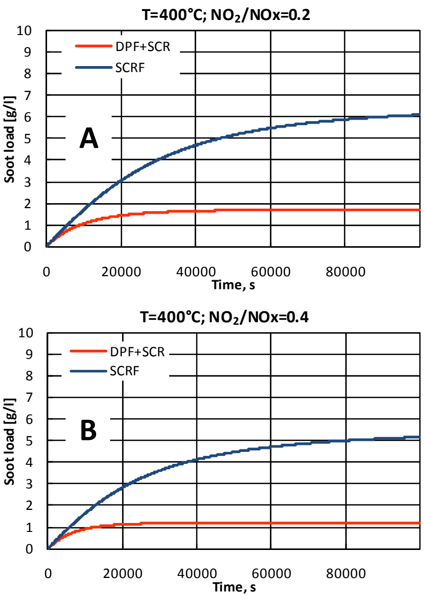
Concept analysis of CRT® operation



Simulated conditions:
500 ppm NH_3, 500 ppm NOx, NO_2/NOx= 0.2, 0.4;
8%O_2, 8%H_2O,
soot emissions= 1e-5 $kg_{PM}/kg_{exhausts}$
mass flow rate=0.2235 kg/s
NO_2/soot mass ratio=16.5, 33
Temperature: 400°C

Asymptotic value of soot load:

- Approached for the DPF+SCR configuration
- Approached also for SCRF

BUT high soot load → too high ΔP

Different operating conditions required for CRT® operation over SCRF

SAE Technical Paper 2011-37-0031

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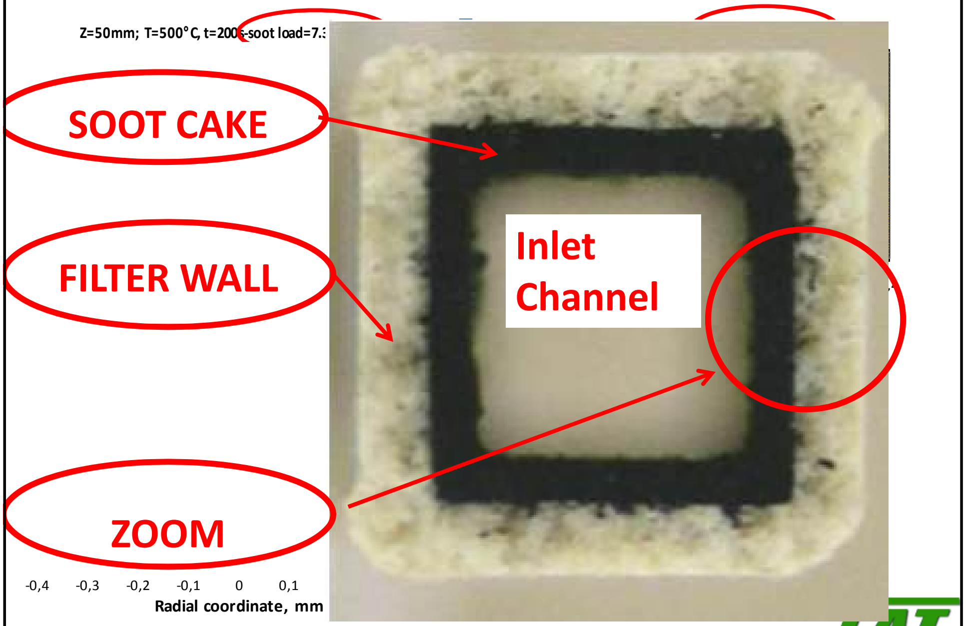
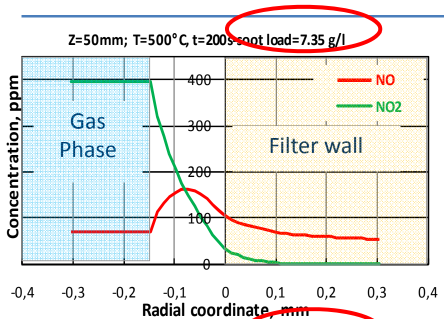
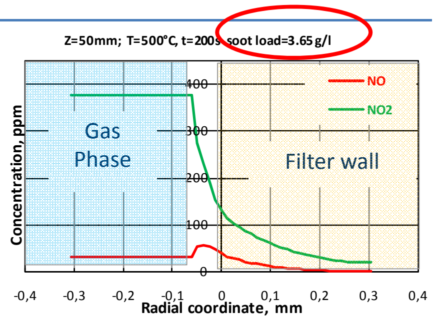
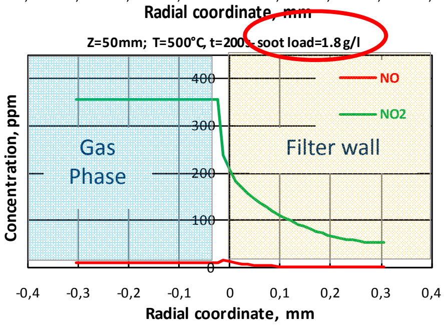
NH_3/NO_2: radial concentration profiles



NH_3/NO_2: radial concentration profiles







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SAE Technical Paper 2011-37-0031

Simulation Results

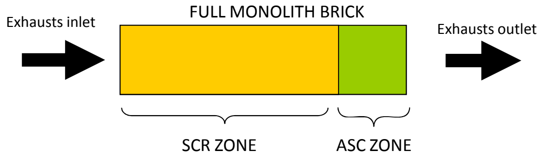
A novel approach to the modeling of dual-layer ammonia slip catalysts

CLEERS Workshop 2011,

In collaboration with Politecnico di Milano

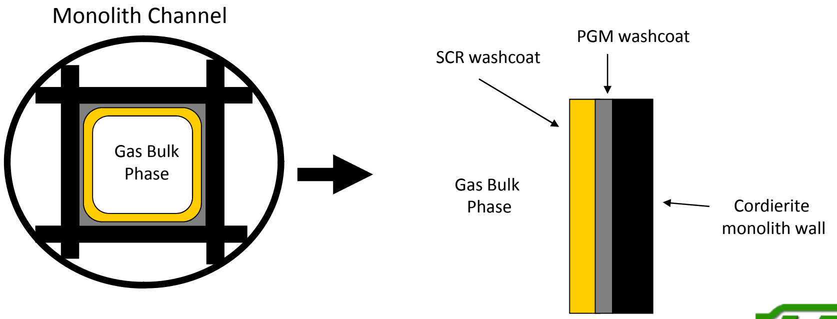
Dual Layer ASCs concept*

System configuration



ASC ZONE → double coated : SCR + PGM

→ Improvement of NH_3 conversion & N_2 selectivity with SCR layer



* Scheuer et al. ICEC 2010, Beijing,China, September 12th-15th 2010

How to model Dual-Layer ASC??

Is it necessary to model reaction/diffusion in both catalytic layers?

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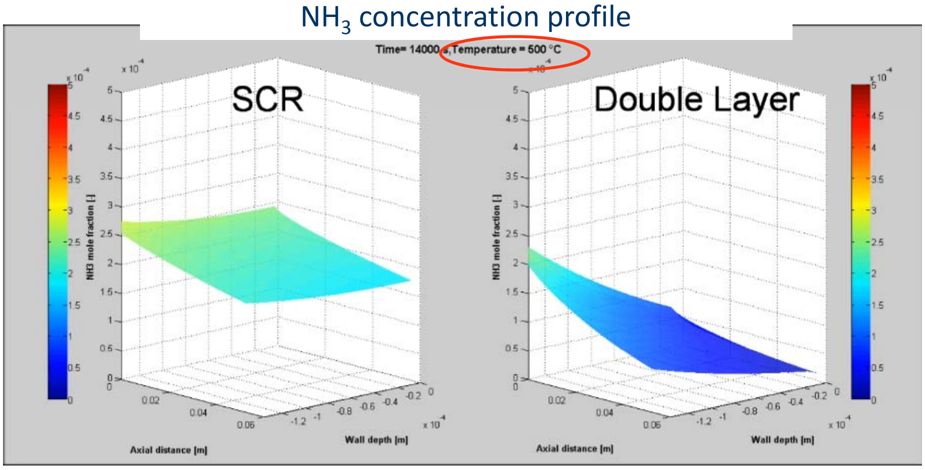
SCR layer: effect of PGM addition

$NH_3/NO/O_2$ reacting system

NH_3 concentration profile



Colombo, Nova, Tronconi: Paper in preparation

Inlet conditions:

300 ppm NH_3, 300 ppm NO, 5%O_2, GHSV = 300’000 h^{-1}

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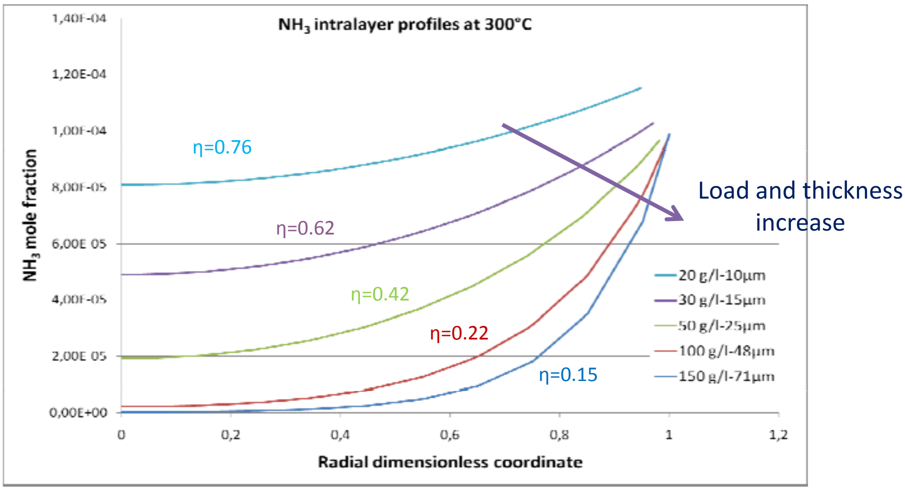
PGM layer: catalyst effectiveness



Internal diffusion control for higher washcoat loads/thickness

Inlet conditions:

300 ppm NH_3, 5%O_2, GHSV = 300'000 h^{-1} ;PGM only catalyst

VECOM Vehicle Concept Modelling

Is it necessary to model reaction/diffusion in both catalytic layers?

SCR layer → YES!!!

PGM layer → NO???

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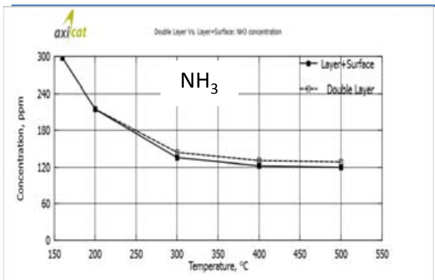
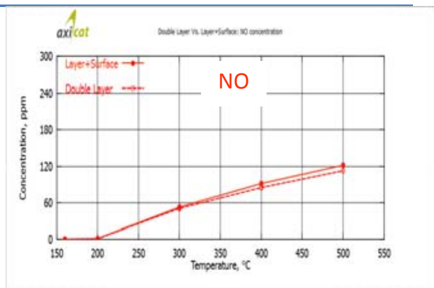
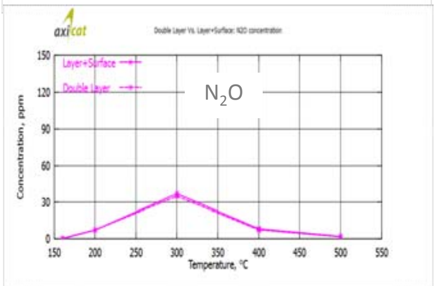
Layer+Surface (LS) approach

LAT

LS Vs. DL simulation results: NH_3/O_2







Negligible deviations between LS & DL simulations

Inlet conditions:
300 ppm NH_3, 5%O_2, GHSV = 300’000 h^{-1}

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SEVENTH FRAMEWORK PROGRAMME

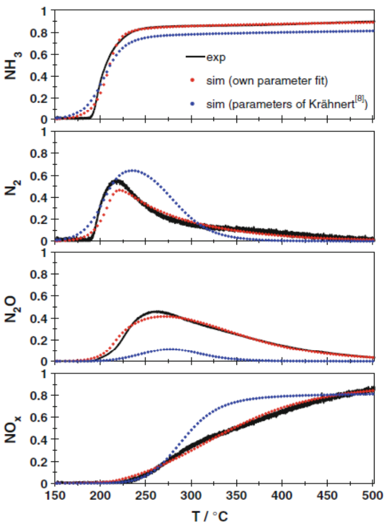
MARIE CURIE ACTIONS

Thank you for your kind attention

mcolombo@aut.gr

Dual layer ASCs concept

Why a dual layer system?



PGM catalysts have poor selectivity to N_2

↓

The unselective oxidation products are N_2O and NOx, which have to diffuse back in the SCR layer

↓

NOx can react with NH_3 over the SCR catalyst to give N_2!!!

↓

Both NH_3 conversion & selectivity to N_2 increase

- Scheuer et al. Top.Catal. 52-2009-1847
- Scheuer et al. ICEC 2010, Beijing,China, September 12th-15th 2010

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