NanoInnovation 2016 Rome, 20-23 September
Conference & Exhibition

Faculty of Civil and Industrial Engineering of “Sapienza” University of Rome

Renaissance cloister by Sangallo

PHOTOCATALYTIC NOx ABATEMENT FOR DIESEL ENGINES

TS.I.A3

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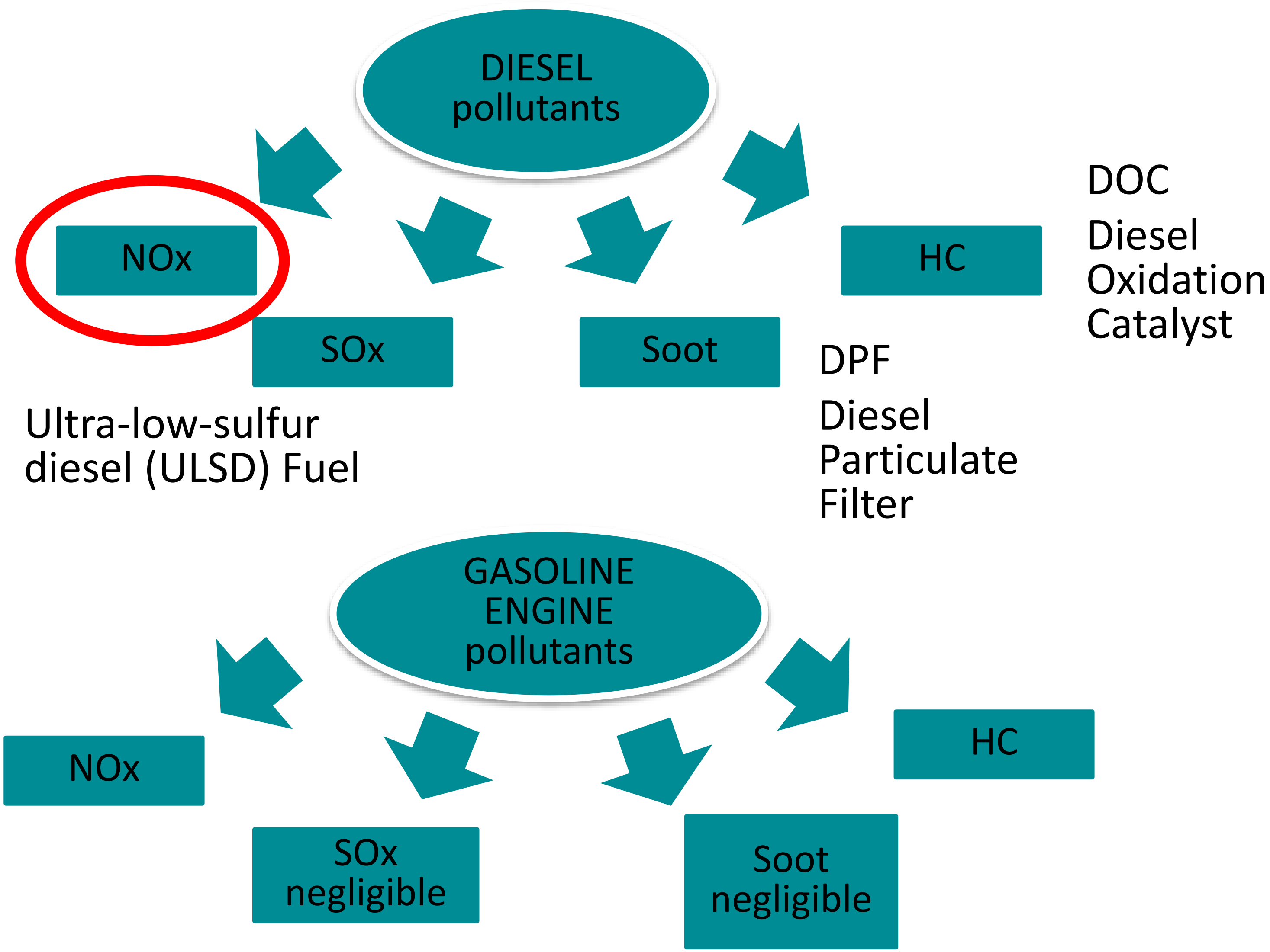
Outline

- Engine pollutant emissions
- NOx abatement techniques
- Preliminary work on photocatalytic NOx Abatement (PON01_01419)
- NanoAPULIA Project
- Simplified NOx storage chemical model on a BaO/γ-Al_2O_3 surface
- Validation against literature data
- Numerical simulation of a real automotive catalyst
- Ongoing activities

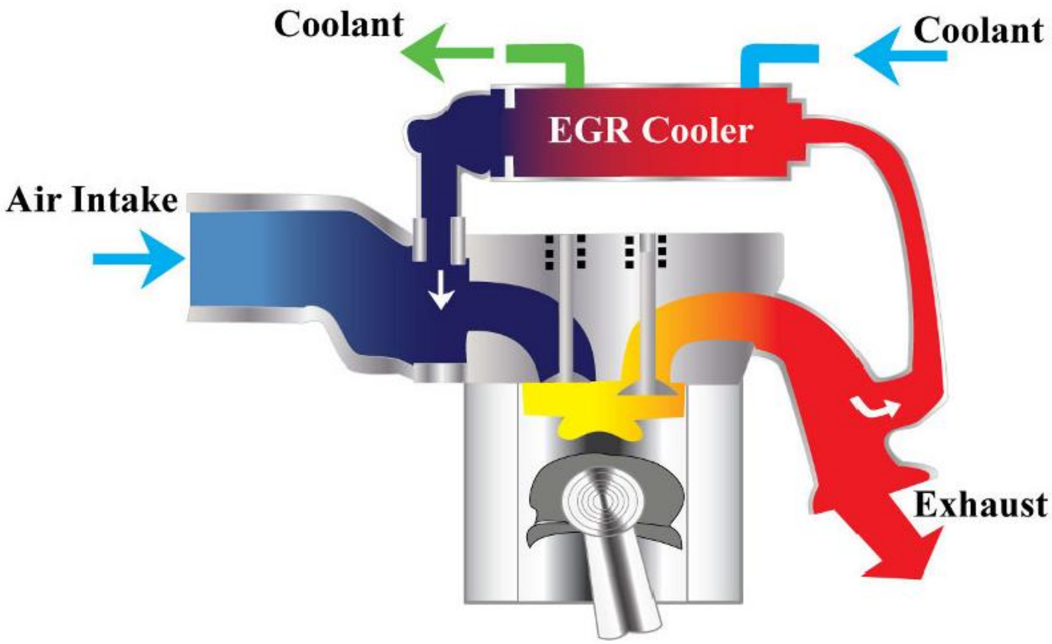
Engine pollutant emissions



NOx abatement techniques

- Exhaust Gas Recirculation (EGR)
- Selective Catalytic Reduction (SCR)
- Nitrogen oxide Storage-reduction Catalyst (NSC)

EGR involves recirculating a controllable proportion of the engine exhaust back into the intake air. A valve is usually used to control the flow of gas, and the valve may be closed completely if required.



NOx abatement techniques

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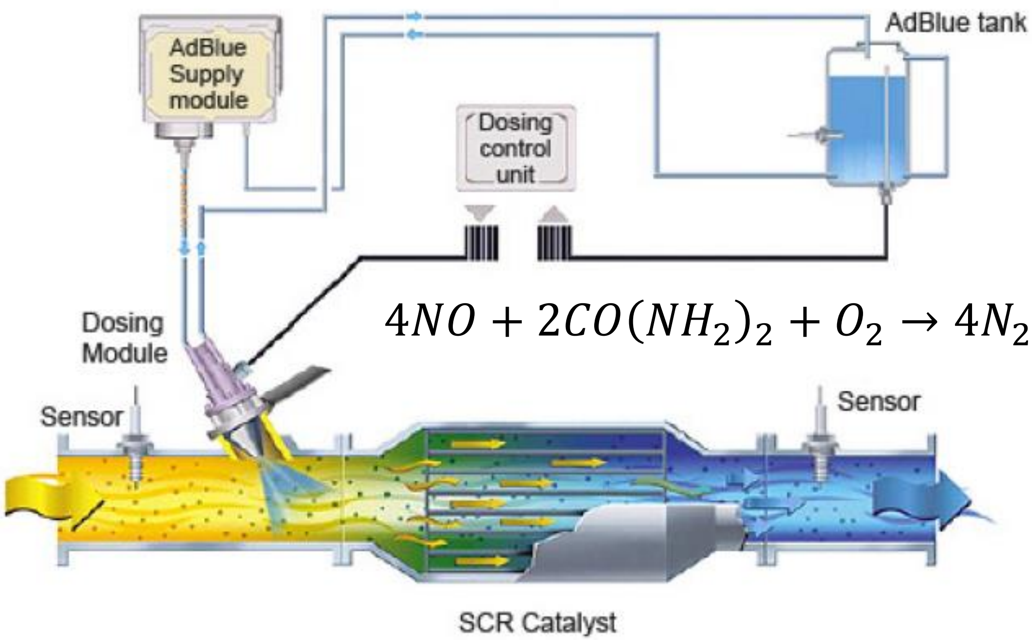
A gaseous reductant, typically anhydrous ammonia, aqueous ammonia or urea, $CO(NH_2)_2$, is added to a stream of exhaust gas and is adsorbed onto a catalyst.



$$4NO + 2CO(NH_2)_2 + O_2 \rightarrow 4N_2 + 4H_2O + 2CO_2$$

NOx abatement techniques

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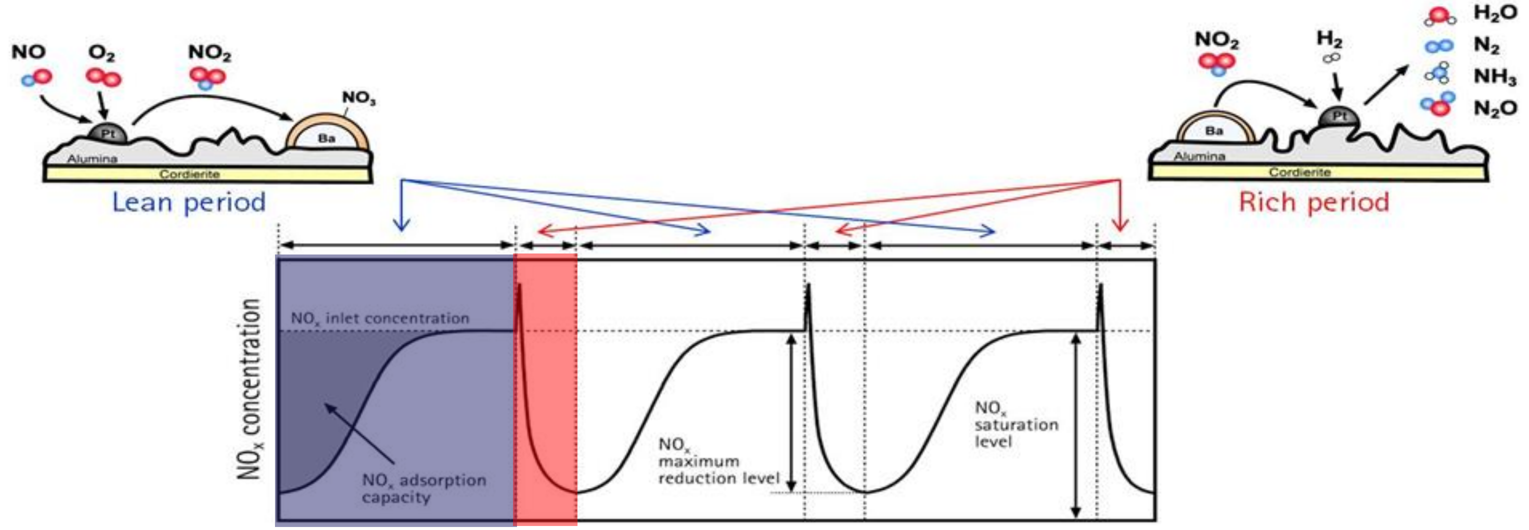


LEAN PERIOD

- **Oxidizing atmosphere**
- **Oxidation of NO to NO_2 on the Pt surface**
- **Adsorption of NOx as barium nitrites and nitrates**

RICH PERIOD

- **Reducing atmosphere**
- **Substitution of barium nitrites and nitrates with barium carbonates**
- **Release of nitrogen species**
- **Reduction of NOx to N_2**

UNIONE EUROPEA
Fondo europeo di sviluppo regionale

PON Ricerca e Competitività 2007-2013

Ministero dell'Istruzione dell'Università e della Ricerca

Ministero dello Sviluppo Economico

"CO2 LIGHT DUTY DEMONSTRATOR"

Strategies and HW/SW measures on the engine, transmission and vehicle in order to achieve a CO_2 reduction to be applied on light duty commercial vehicles (N1/M1 - EURO6) as required by the EU's proposal of 28 October 2009.

BOSCH
CVIT/EVL3

ISTITUTO MOTORI
Consiglio Nazionale delle Ricerche

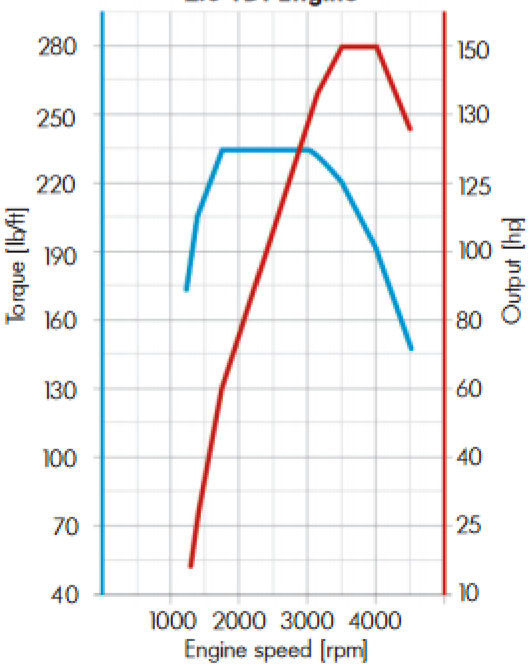
PON01_01419

A first version of a photocatalyst prototype has been built.
To perform the necessary investigations the engine Volkswagen 2.0l (110kW) was used.
This engine is part of the widespread and therefore significant Volkswagen MQB family (modular Der Dieselmotoren-Baukasten von Volkswagen)

Technical Data

Engine Code	CRBC
Design	Four-cylinder inline engine
Engine Capacity	1968 cm^3
Bore	81.0 mm
Stroke	95.5 mm
Valves per Cylinder	4
Compression Ratio	16.2:1
Maximum Output	150 hp (110 kW) from 3500 to 4000 rpm
Maximum Torque	235 lb/ft (320 Nm) from 1750 to 3000 rpm
Engine Management System	Bosch EDC 17
Fuel	Ultra-Low Sulfur Diesel
Exhaust Gas Aftertreatment	Exhaust gas recirculation, oxidizing catalytic converter, diesel particulate filter
Emissions Standard	BIN 5

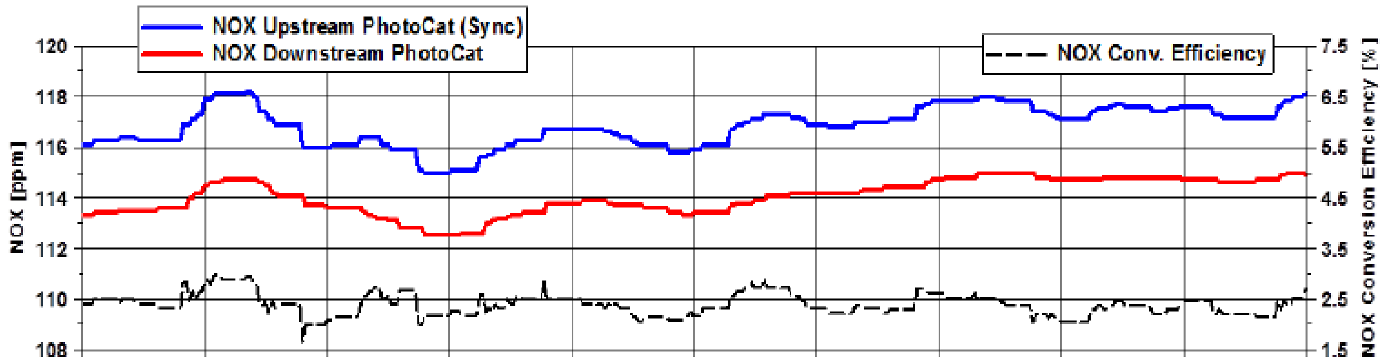
Torque and Power Diagram
2.0 TDI Engine



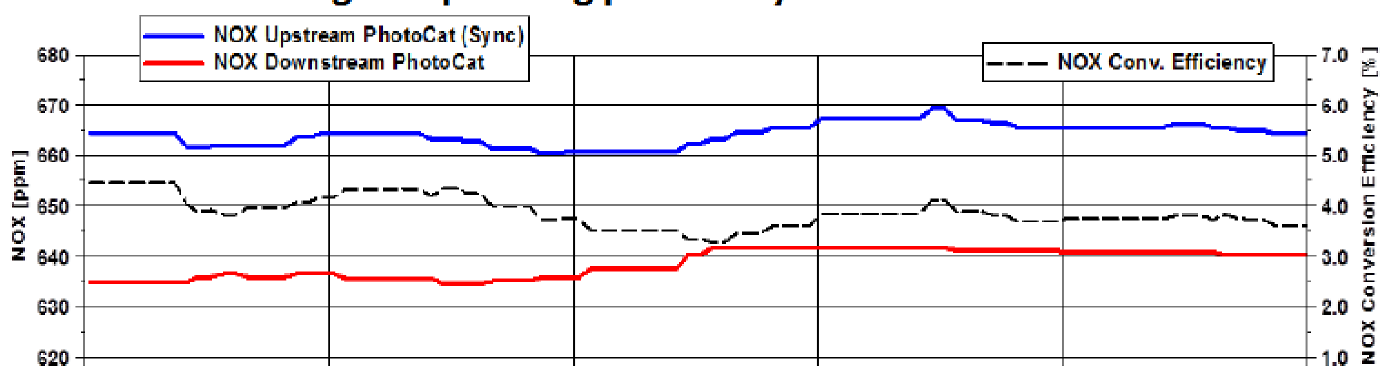
	Engine operation point 1	Engine operation point 2
Engine Speed	1500 rpm	1500 rpm
PME	4.3 bar	4.3 bar
EGR	w	w/o
Air Mass	63 kg/h	104 kg/h

Photo-catalytic NOx Abatement

engine operating point 1: synchronized NOx tracks



engine operating point 2: synchronized NOx tracks



NanoAPULIA Project

UNIONE EUROPEA	MINISTERO DELLO SVILUPPO ECONOMICO	MINISTERO DELL'ISTRUZIONE, DELL'UNIVERSITA' E DELLA RICERCA	REGIONE PUGLIA AREA POLITICHE PER LO SVILUPPO, IL LAVORO E L'INNOVAZIONE

Avviso Aiuti a Sostegno dei Cluster Tecnologici Regionali per l'Innovazione

Progetto Codice MDI6SR1

NANOAPULIA - NANOfotocatalizzatori per un'Atmosfera più PULItA

NANO PHOTOCATALIST FOR A CLEANER ENVIRONMENT

CUP: B38C14001160008
Periodo: Dicembre 2015 – Novembre 2017

Politecnico di Bari

NanoAPULIA Project

The NanoAPULIA project aims to apply **nano-technologies** (KET 2) to **reduce air pollution** from nitrogen oxides (NOx).

The basic idea is to synthesize nano-structured metal oxides with high surface area and high crystallinity and phase purity having photo-catalytic properties (in the visible and the ultraviolet spectra).

Two main sectors are considered:

1) buildings;
2) automotive.

Furthermore, new diagnostic methods are investigated for toxicity of nanostructured photocatalytic materials.

TCT DIVISIONE NANOTECH

SIPRE Prodotti e Tecnologie per l'edilizia moderna

Italcementi Italcementi Group

BOSCH CVIT/EVL3

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ECHOLIGHT

Politecnico di Bari

UNIVERSITÀ DEL SALENTO

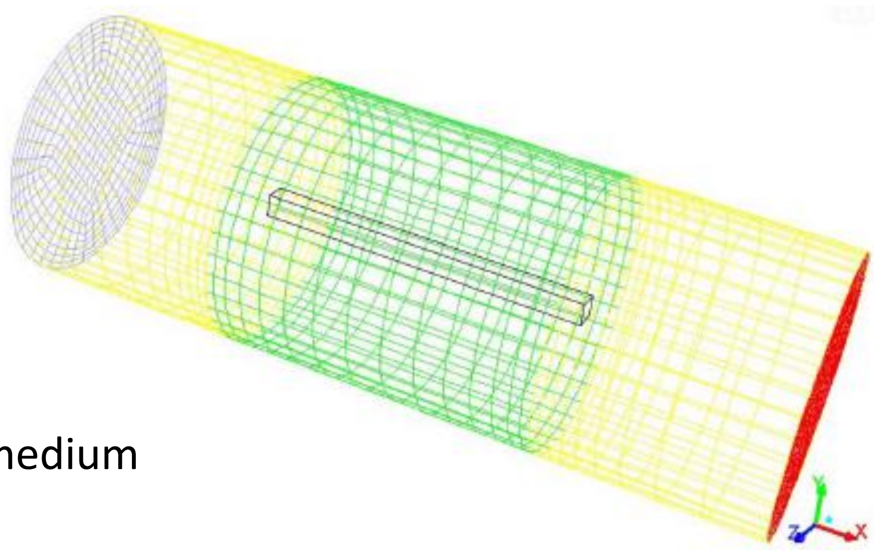
UNIVERSITÀ DEGLI STUDI DI BARI ALDO MORO

Consiglio Nazionale Ricerche

Reference case

Olsson L, Persson H, Fridell E, Skoglundh M, Andersson B, “A kinetic study of NO oxidation and NOx storage on Pt/Al_2O_3 and Pt/BaO/Al_2O_3", Journal of Physical Chemistry B, 2001, 105, 29

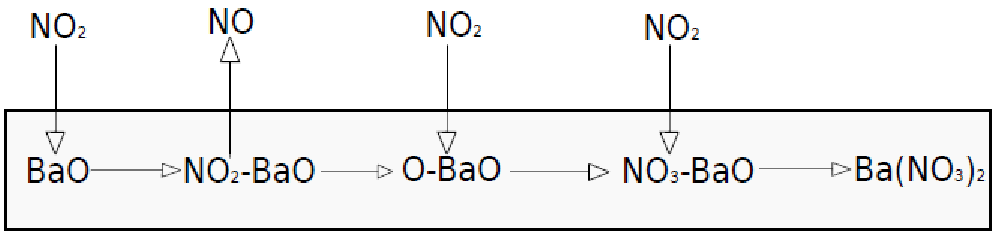
- Cylindrical catalyst, d = 12:34mm, l = 15mm
- 69 square channels (1mmx1mm)
- washcoat weight = 206mg
- 20%wt BaO/γ - Al_2O_3
- flow rate = 2600ml/min



Numerical details:

- The catalyst monolith is treated as a porous medium
- 3D unsteady numerical simulation
- 12540 cells
- 2nd order numerical schemes in space and time

NO_2 Storage Catalyst kinetics model



Global Storage Reaction:

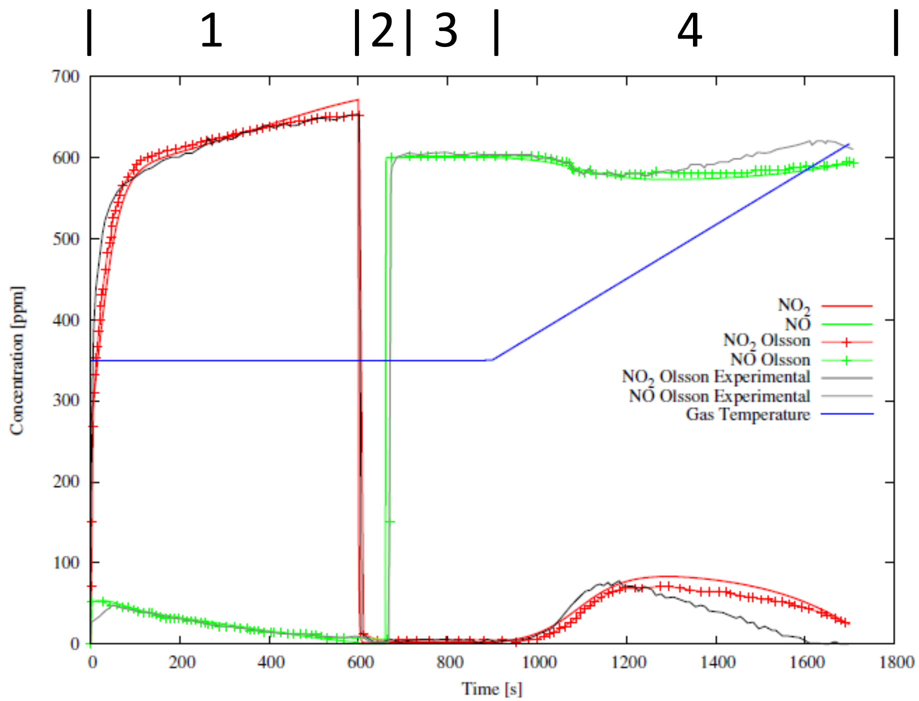
$$BaO + 3NO_2 \rightarrow Ba(NO_3)_2 + NO$$

Simplified Reaction model:

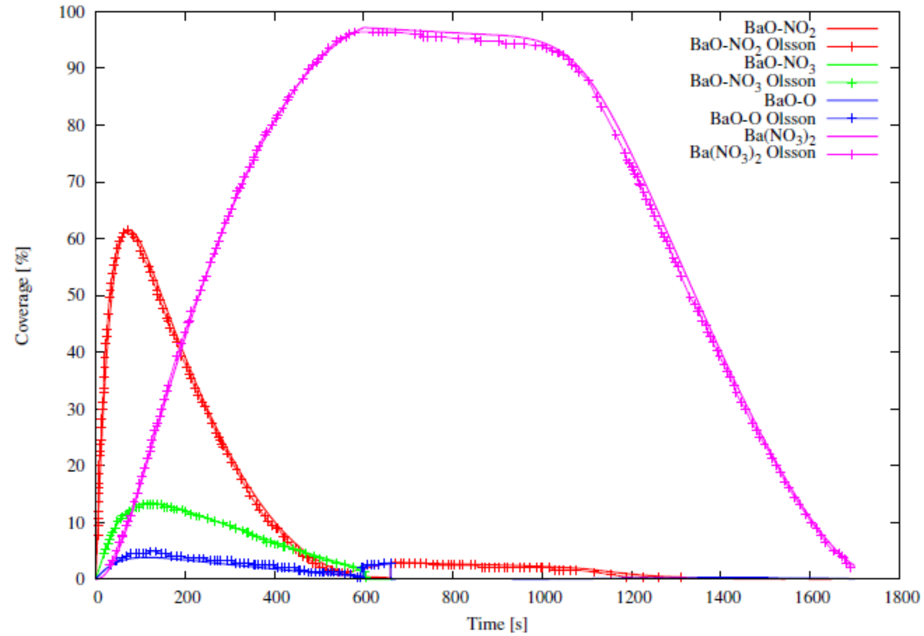
R1	$NO_{2(g)} + S$	$\rightleftharpoons$	$NO_2 - S$
R2	$NO_2 - S$	$\rightleftharpoons$	$O - S + NO_{(g)}$
R3	$NO_{2(g)} + O - S$	$\rightleftharpoons$	$NO_3 - S$
R4	$NO_{2(g)} + NO_3 - S$	$\rightleftharpoons$	$Ba(NO_3)_2$
R5	$2S - O$	$\rightleftharpoons$	$2S + O_{2(g)}$

Note: *S* represents the *BaO* site

Comparison of the results



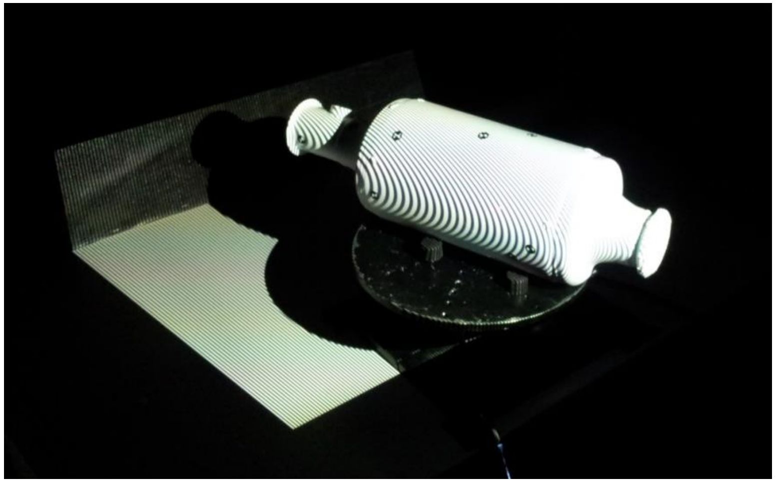
concentration of volumetric quantities

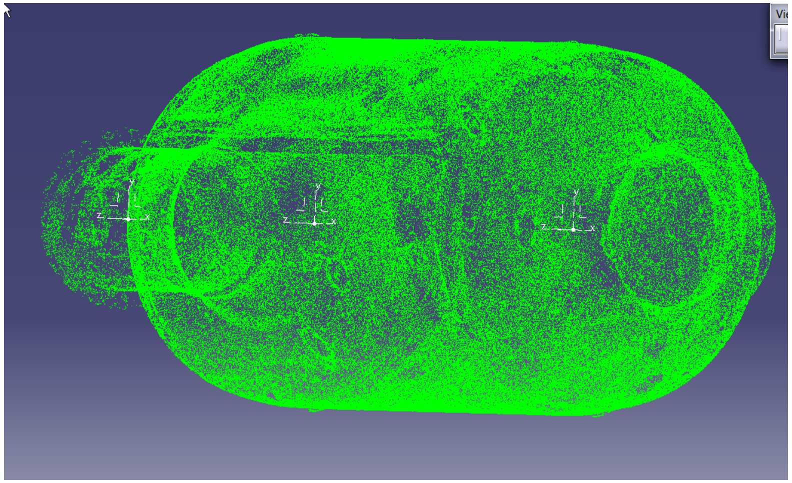


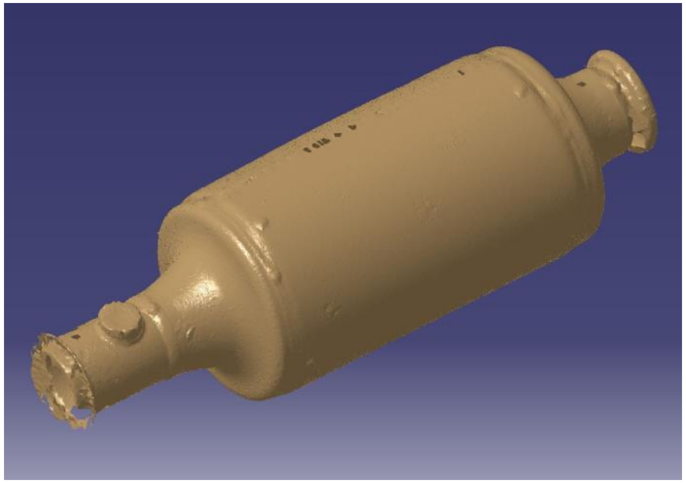
surface coverage percentage

1. 680ppm of NO_2 in N_2 at 350°C for 10 minutes
2. N_2 for 1 minute
3. 600ppm of NO in N_2 at 350°C for 4 minutes
4. temperature increase (20°C/min) up to 600°C

NSC Reverse Engineering







Prof. Michele Fiorentino

NSC Mesh Generation

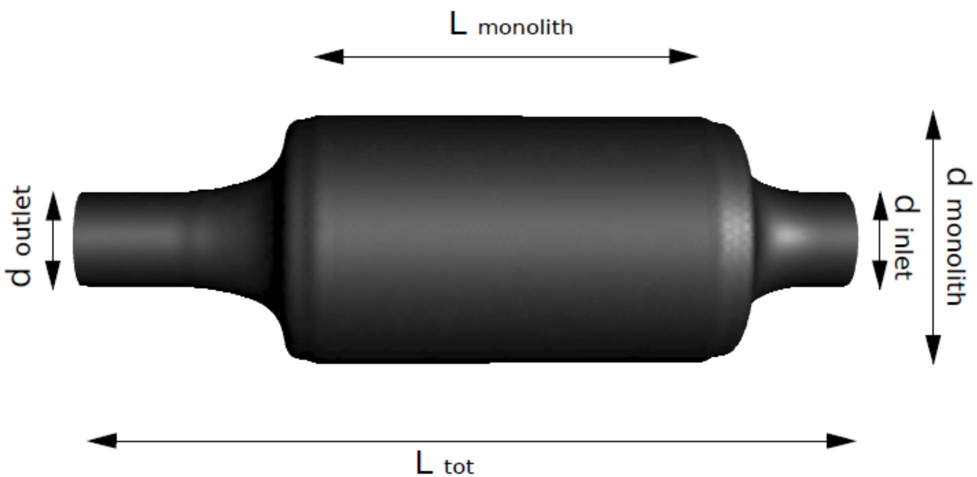
L_{tot} = 486mm

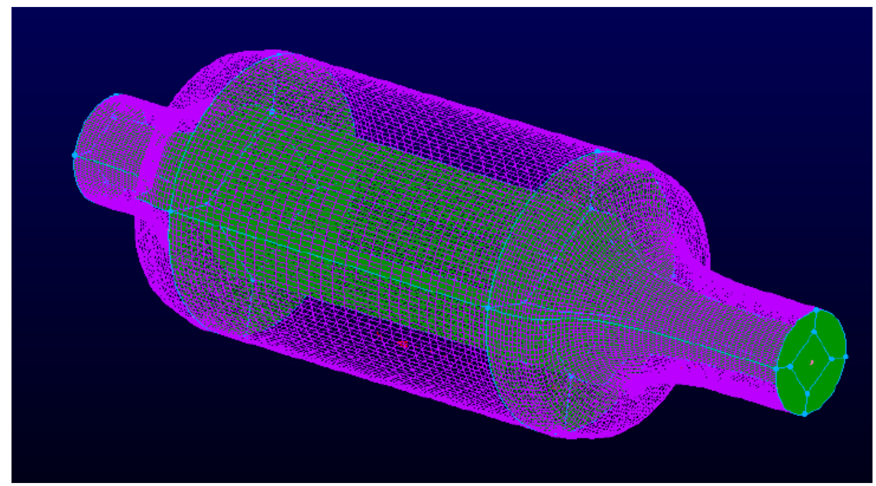
$L_{monolith}$ = 221mm

d_{inlet} = 59mm

d_{outlet} = 57mm

$d_{monolith}$ = 152mm

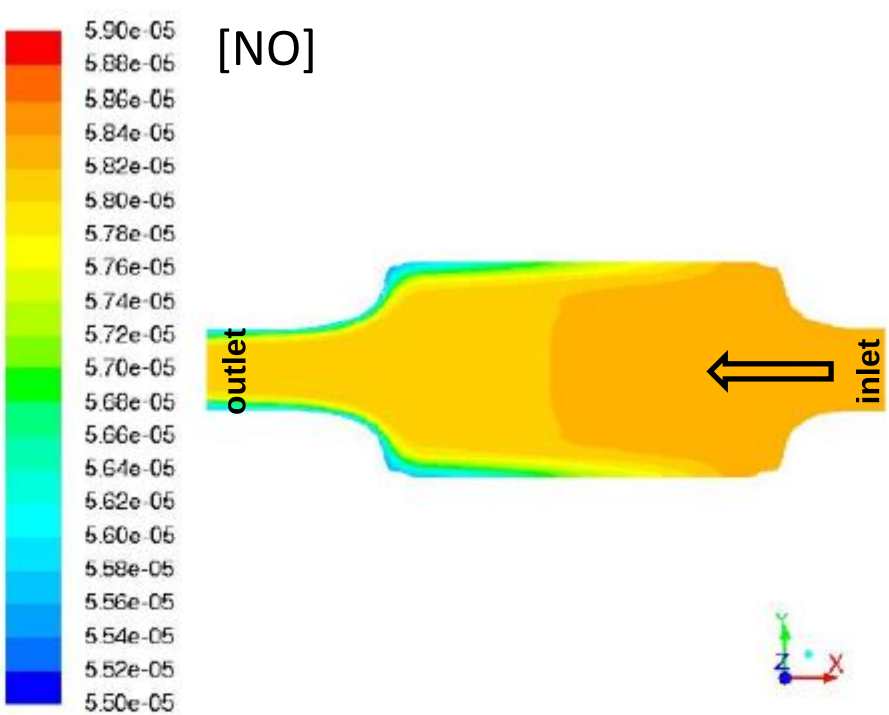


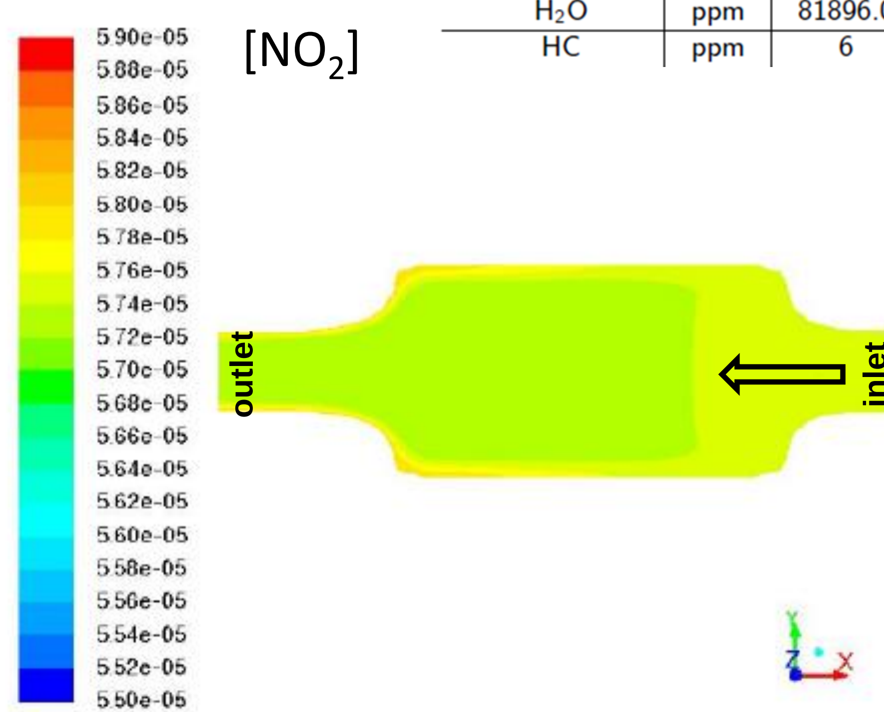


Preliminary results (Lean Period)

Instantaneous contours of the spatial distribution of NO and NO_2 mole fractions in a meridian section of the catalyst

Working point	Units	
Flow Rate	kg/h	200
Temperature	°C	336
CO	ppm	1.52
CO_2	ppm	83519
NO_x	ppm	125.21
NO	ppm	63.07
O_2	ppm	93890.9
N_2	ppm	822457.4
H_2O	ppm	81896.0
HC	ppm	6





t = 2.1 s

Ongoing activities

Implementation in the CFD code of the following models:

- NO oxidation on Pt/Al_2O_3;
- regeneration phase;
- photocatalytic reactions.

Thanks for your attention!