LABORATORY OF APPLIED THERMODYNAMICS
ARISTOTLE UNIVERSITY THESSALONIKI

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4-way Catalyst Modeling in Wall-Flow and Deep-bed Substrates

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Exothermia modeling efficiency

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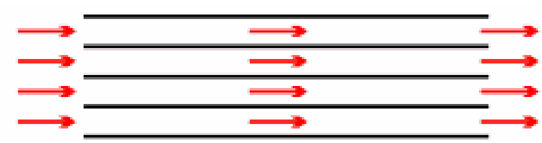
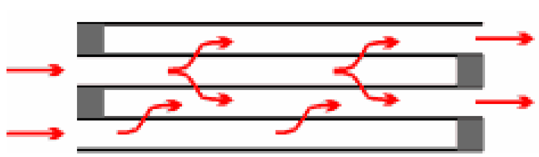
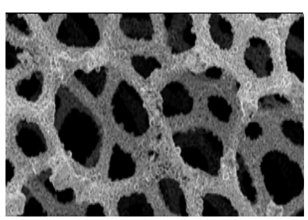
Introduction
4-way catalysis

- The term "3-way" catalysis first introduced for closed-loop control stoichiometric engines (CO, HC, NO_x)
- Until recently, "2-way" catalysis was adequate for lean burn engines (CO, HC)
- Nowadays and in the near future
  - Most diesel engines will be equipped with "4-way" systems
  - Lean burn gasoline engines currently employing "3-way" catalysis. PM aftertreatment may also arise.
- "4-way" catalysis may involve
  - Multiple reactors (e.g. DOC+DPF+SCR/LNT)
  - Single reactor (e.g. DPNR)

Reactor concepts – application areas

	DOC	LNT	SCR	DPF
Flow-through honeycomb, incl. "turbulent substrates" 	Yes	Yes	Yes	No ~30% efficiency with "turbulent" substrates
Wall-flow honeycomb 	Yes	Yes	?	Yes
"Deep-bed" (e.g. fiber, foam) 	Yes At development stage	?	?	Yes ~90% efficiency with metal foams

Content of presentation

Development and application of modeling tools for
System design optimization
Engine / exhaust system calibration

For each possible system (chemistry/reactor concept combination)

Governing Equations → Parameter Calibration → Experimental Validation

Integrated exhaust line simulation

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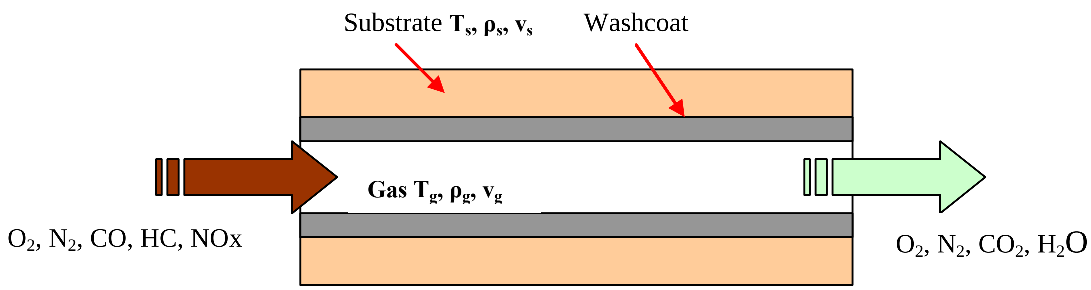
Flow-through catalyst
Model equations

Basic 1-D model equations



Gas energy balance

$$\rho_g v_g \frac{\partial T_g}{\partial x} = -h \cdot \left(\frac{S}{\varepsilon}\right) \cdot \left(T_g - T_s\right)$$

Gas species balance

$$\frac{\partial \left(v_g c_g\right)}{\partial x} = -k_j \cdot \left(\frac{S}{\varepsilon}\right) \cdot \left(c_{g,j} - c_{s,j}\right)$$

Transient energy balance

$$\underbrace{\rho_s C_{p,s} \frac{\partial T_s}{\partial t}}_{\text{Solid heat capacity}} = \underbrace{\lambda_s \frac{\partial^2 T_s}{\partial x^2}}_{\text{Conduction}} + \underbrace{h\left(\frac{S}{1-\varepsilon}\right)\left(T_g - T_s\right)}_{\text{Convection}} - \underbrace{\frac{1}{1-\varepsilon}\sum_{k=1}^{n_k} \Delta H_k R_k}_{\text{Reaction heat}}$$

$$\frac{\rho_g}{M_g} k_j \left(\frac{S}{\varepsilon}\right)\left(c_{g,j} - c_{s,j}\right) = R_j$$

Mass-transfer rate = reaction rate

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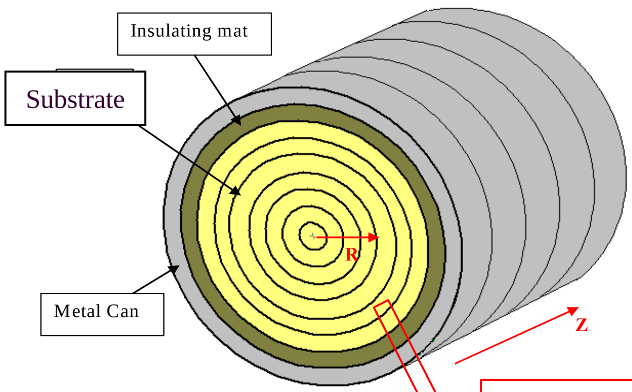
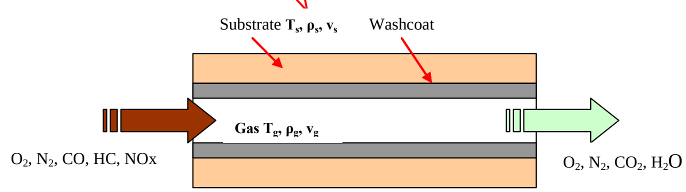
2-D axi-symmetric modeling
Basic concept



Simulation of discrete "representative" channels



Derivation of heat source terms (convection, exothermy)

Energy balance

$$\rho_s \cdot C_{p,s} \frac{\partial T_s}{\partial t} = \lambda_{s,z} \frac{\partial^2 T_s}{\partial z^2} + \lambda_{s,r} \frac{1}{r} \frac{\partial}{\partial r}\left(r \frac{\partial T_s}{\partial r} \right) + S$$

Heat capacity

Axial heat conduction

Radial heat conduction

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DOC modeling

Basic oxidation reactions on Precious Metals NO-NO_2 chemical equilibrium

$$CO + \tfrac{1}{2} O_2 \longrightarrow CO_2$$

$$R_1 = \frac{A_1 \cdot e^{-E_1/RT} \cdot c_{CO} \cdot c_{O_2}}{G_2}$$

$$CH_a + (1 + 0.25a) O_2 \longrightarrow CO_2 + 0.5a H_2O$$

$$R_2 = \frac{A_1 \cdot e^{-E_1/RT} \cdot c_{CH} \cdot c_{O_2}}{G_1}$$

$$NO + \frac{1}{2} O_2 \rightarrow NO_2$$

$$R_5 = \frac{A_5 \cdot e^{-E_5/RT} \cdot c_{NO} \cdot c_{O_2} \cdot Eq_5}{G_5}$$

$$NO_2 \rightarrow NO + \frac{1}{2} O_2$$

$$R_6 = \frac{A_6 \cdot e^{-E_6/RT} \cdot c_{NO} \cdot c_{O_2} \cdot Eq_6}{G_5}$$

L-H reaction rates with inhibition terms

NO/NO_2 thermodynamics are taken into account by the terms Eq_i

$$Eq_i = 1 - K_p(T) \cdot \frac{\prod c_{s,prod}^{\;n}}{\prod c_{s,react}^{\;m}}$$

Chemical equilibrium constant (function of temperature)

Negative value of a parameter Eq_i suggests that the reaction is not thermodynamic possible and the reaction rate in the model is zeroed.

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Adsorption – desorption modeling

- Competitive HC, H_2O, NH_3 adsorption on zeolite
  - *H_2O <--> (H_2O)ads*
  - *C_xH_y <--> (C_xH_y)ads* (toluene)
  - *C_xH_y <--> (C_xH_y)ads* (decane)
  - *NH_3 <--> (NH_3)ads*

Adsorption model
Dubinin-Radushkevich isotherm

- The equation of the DR isotherm gives the adsorbed mass as function of temperature and partial pressure.

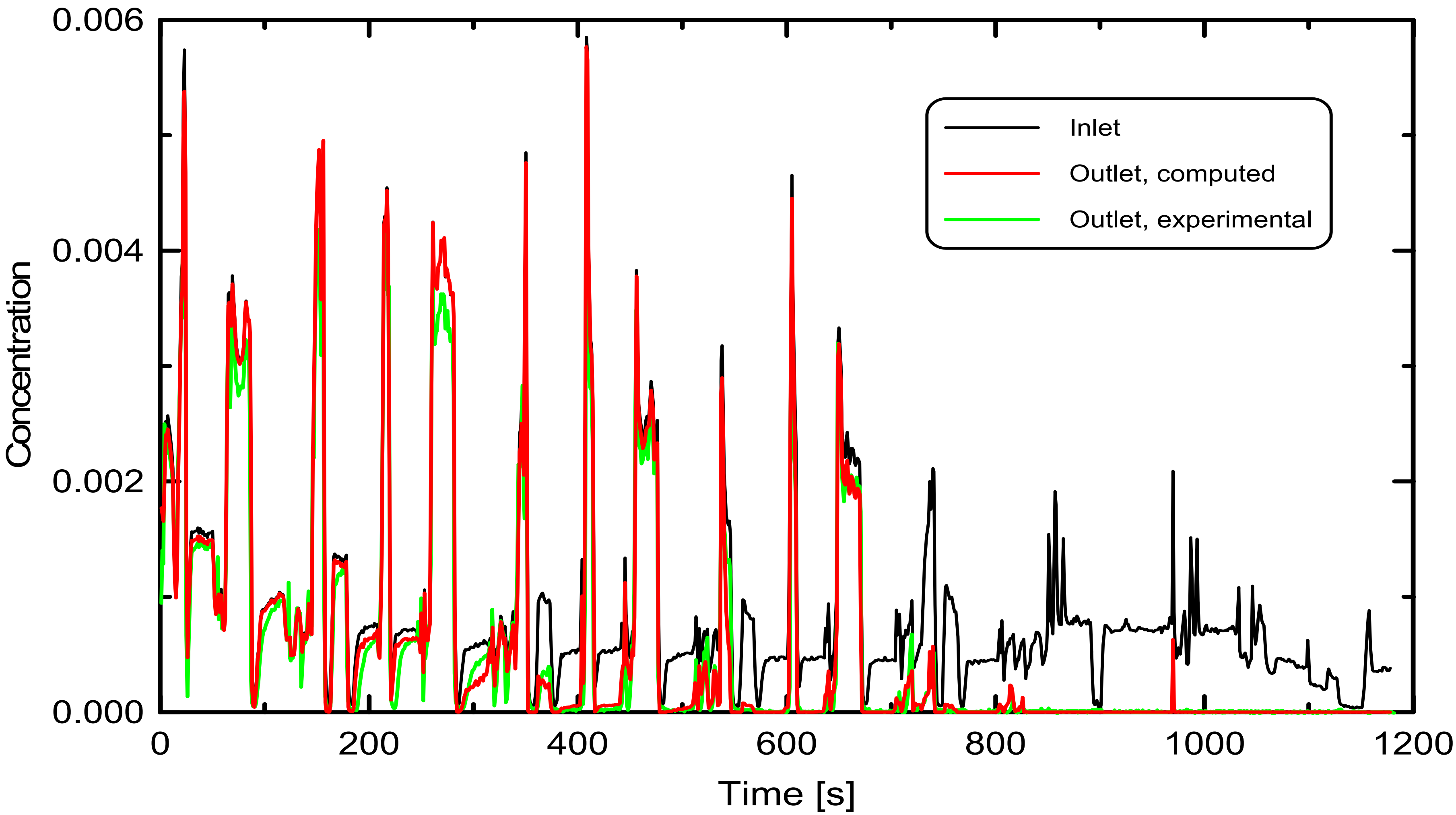
$$\ln x_{eq} = \ln(W_0 \rho) - D\left[\ln\left(\frac{p_0}{p}\right)\right]^2 \qquad D = A\left(\frac{RT}{\beta}\right)^2$$

- A linear «driving force» is assumed to calculate the rates towards equilibrium.

$$R = \frac{\partial x}{\partial t} = k \cdot \left(x_{eq} - x\right)$$

- Adjustable parameters:
  - W_0 (micropore volume)
  - A (micropore size distribution)
  - β (affinity parameter)
  - k (Arrhenius-type parameter)

CO prediction in transient driving cycle instantaneous emissions



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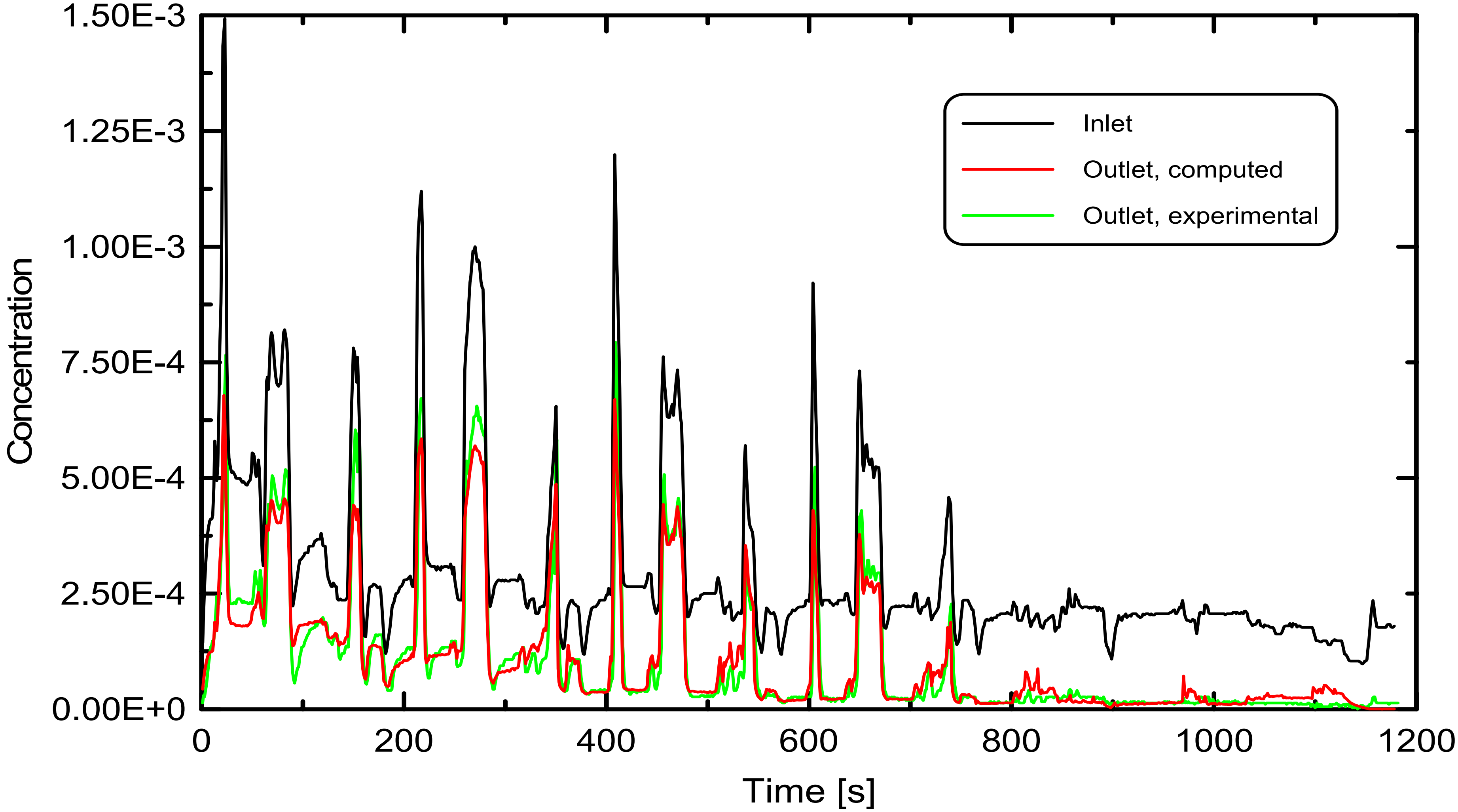
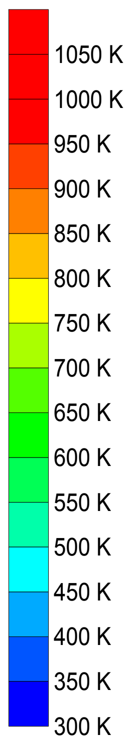
HC prediction in transient driving cycle instantaneous emissions

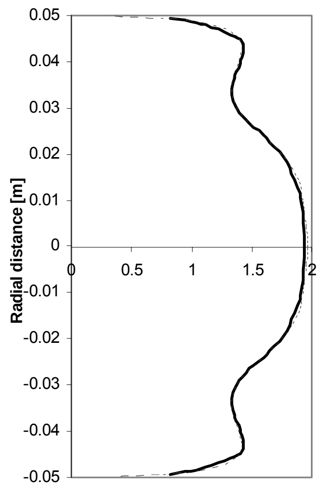


2-d simulation example
Catalyst warm-up behavior



t=5 s

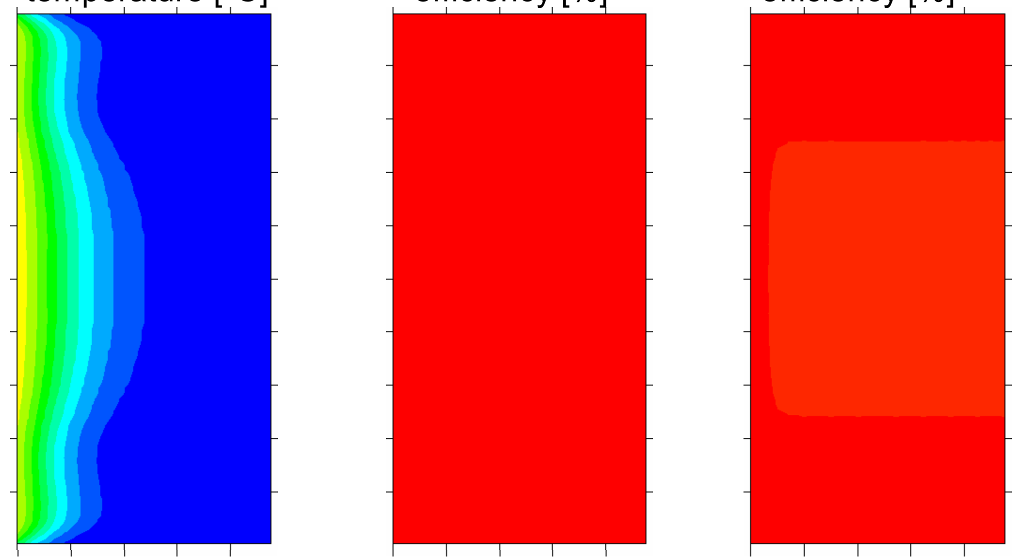
Velocity [m/s]

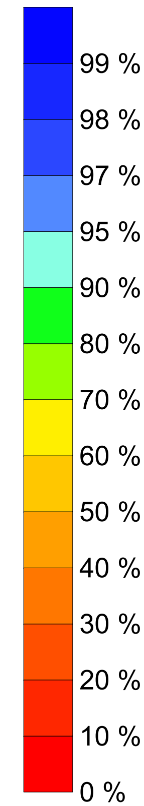


Solid phase temperature [°C]

HC conversion efficiency [%]

CO conversion efficiency [%]





Temperature distribution affected by flow distribution

Too low CO and HC conversion due to low temperature

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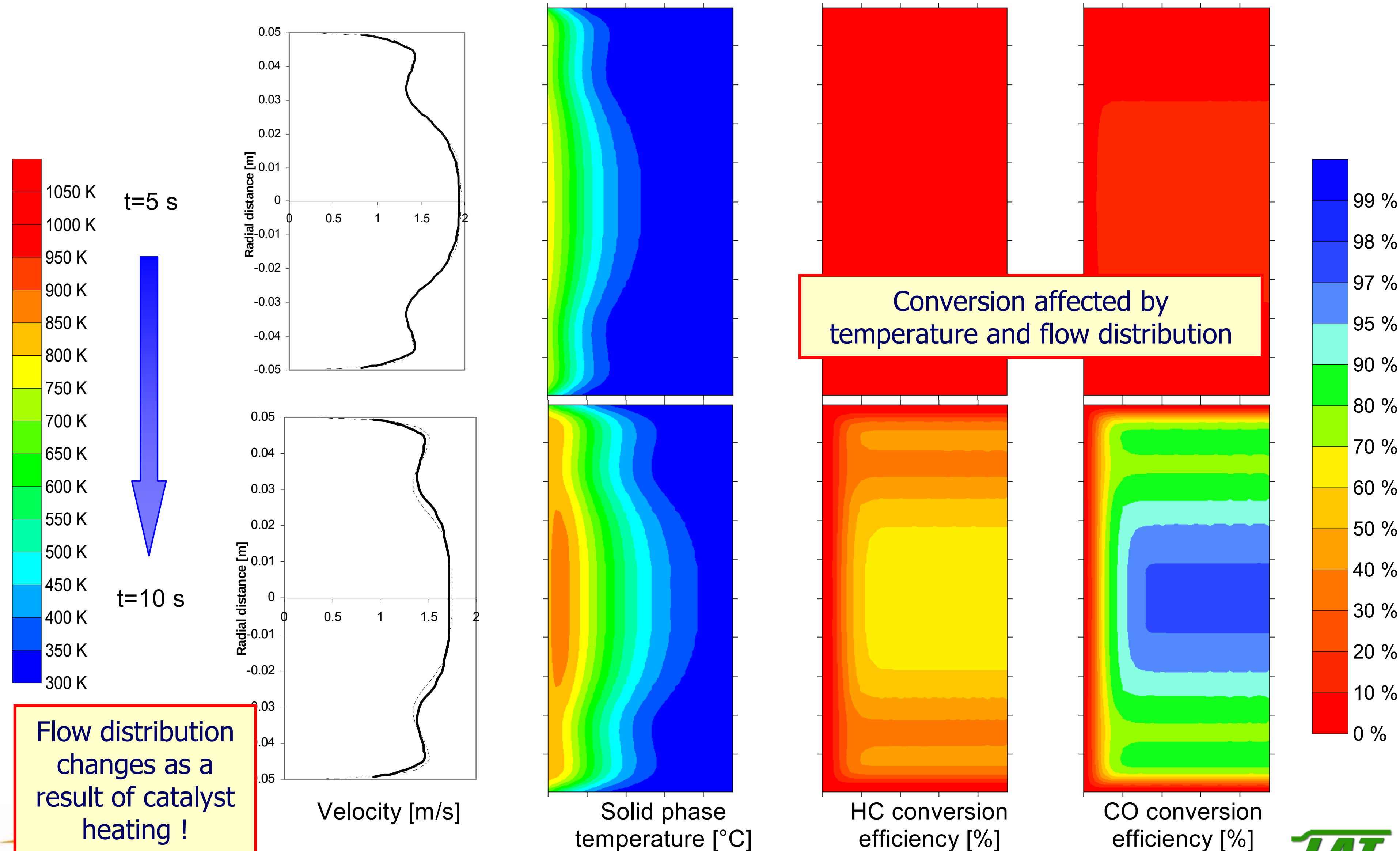
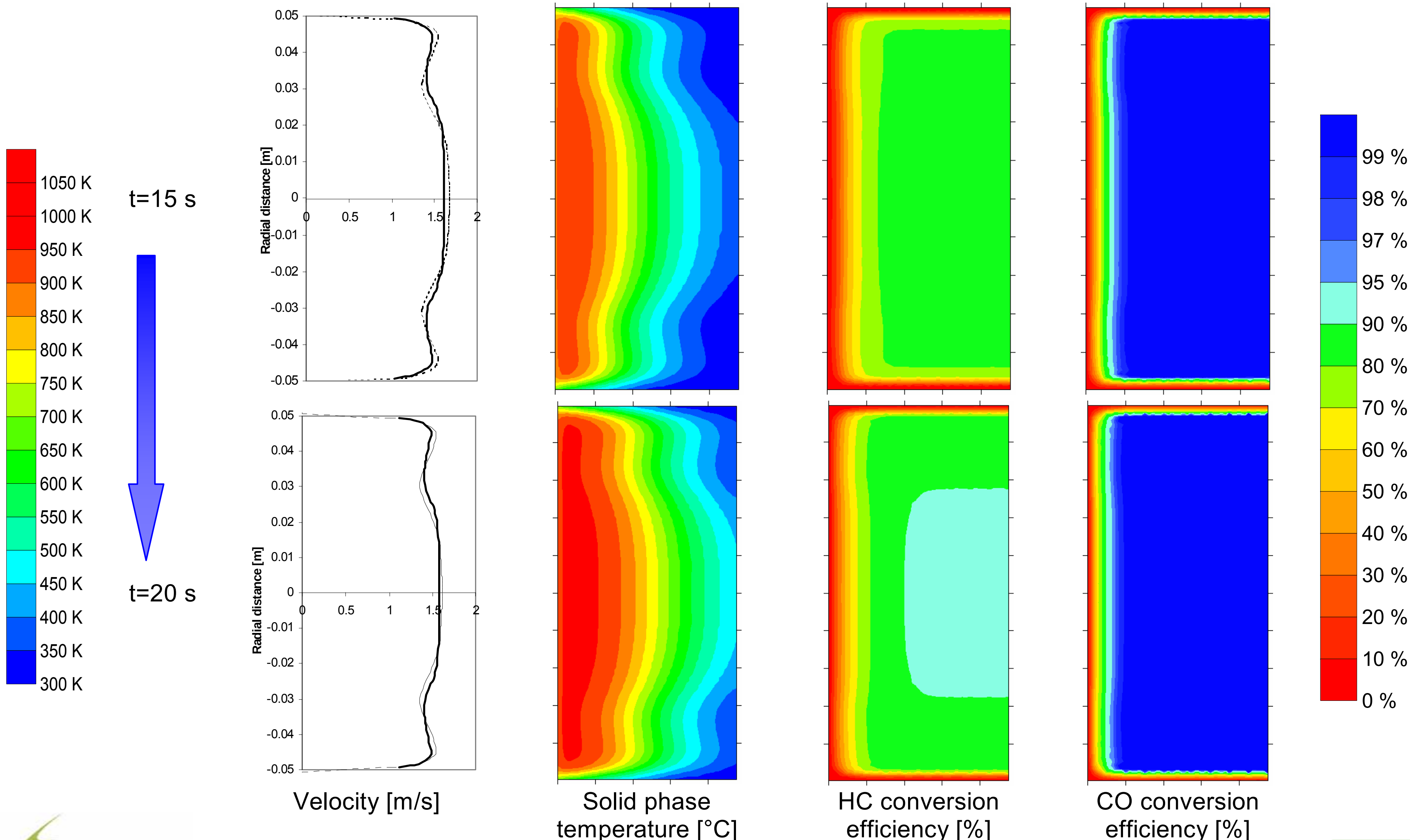
2-d simulation example
Catalyst warm-up behavior



modeling efficiency

2-d simulation example
Catalyst warm-up behavior



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LNT modeling

NO_x Storage reactions

NO, NO_2 storage

$$BaO + 2NO_2 + \frac{1}{2}O_2 \rightarrow Ba(NO_3)_2 \qquad R_4 = A_4 \cdot e^{-E_4/RT} \cdot c_{NO_2} \cdot c_{O_2} \cdot \Psi_{cap} \cdot \psi_{BaO}$$

$$BaO + 2NO + \frac{1}{2}O_2 \rightarrow Ba(NO_2)_2 \qquad R_5 = A_5 \cdot e^{-E_5/RT} \cdot c_{NO} \cdot c_{O_2} \cdot \Psi_{cap} \cdot \psi_{BaO}$$

Nitrate and Nitrite decompositions

$$Ba(NO_3)_2 \rightarrow BaO + 2NO_2 + \frac{1}{2}O_2 \qquad R_7 = A_7 \cdot e^{-E_7/RT} \cdot \Psi_{cap} \cdot \psi_{Ba(NO_3)_2}$$

$$Ba(NO_2)_2 \rightarrow BaO + 2NO + \frac{1}{2}O_2 \qquad R_8 = A_8 \cdot e^{-E_8/RT} \cdot \Psi_{cap} \cdot \psi_{Ba(NO_2)_2}$$

Nitrite to nitrate

$$Ba(NO_2)_2 + 2NO_2 \rightarrow Ba(NO_3)_2 + 2NO \qquad R_6 = A_6 \cdot e^{-E_6/RT} \cdot c_{NO_2} \cdot \Psi_{cap} \cdot \psi_{Ba(NO_2)_2}$$

LNT Regeneration reactions

Regeneration with CO

$$Ba(NO_3)_2 + 3CO \rightarrow BaO + 2NO + 3CO_2 \qquad R_9 = A_9 \cdot e^{-E_9/RT} \cdot c_{CO} \cdot \Psi_{cap} \cdot \psi_{Ba(NO_3)_2}$$

$$Ba(NO_2)_2 + CO \rightarrow BaO + 2NO + CO_2 \qquad R_{12} = A_{12} \cdot e^{-E_{12}/RT} \cdot c_{CO} \cdot \Psi_{cap} \cdot \psi_{Ba(NO_2)_2}$$

Regeneration with H_2

$$Ba(NO_3)_2 + 3H_2 \rightarrow BaO + 2NO + 3H_2O \qquad R_{10} = A_{10} \cdot e^{-E_{10}/RT} \cdot c_{H_2} \cdot \Psi_{cap} \cdot \psi_{Ba(NO_3)_2}$$

$$Ba(NO_2)_2 + H_2 \rightarrow BaO + 2NO + H_2O \qquad R_{13} = A_{13} \cdot e^{-E_{13}/RT} \cdot c_{H_2} \cdot \Psi_{cap} \cdot \psi_{Ba(NO_2)_2}$$

Reduction of released NO – NH_3 production / oxidation

$$CO + NO \rightarrow CO_2 + \frac{1}{2}N_2 \qquad R_{11} = \frac{A_{11} \cdot e^{-E_{11}/RT} \cdot c_{CO} \cdot c_{NO}}{G_6}$$

$$H_2 + NO \rightarrow H_2O + \frac{1}{2}N_2 \qquad R_{14} = \frac{A_{14} \cdot e^{-E_{14}/RT} \cdot c_{H2} \cdot c_{NO}}{G_6}$$

$$NO + 2.5H_2 \rightarrow NH_3 + H_2O \qquad NH_3 + 1.25O_2 \rightarrow NO + 1.5H_2O$$

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Sulfation / desulfation model

$$SO_2 + \frac{1}{2}O_2 \rightarrow SO_3 \qquad R = (A \cdot e^{-E/RT} \cdot c_{SO_2} \cdot c_{O_2} \cdot Eq)/G_1$$

$$SO_3 \rightarrow SO_2 + \frac{1}{2}O_2 \qquad R = (A \cdot e^{-E/RT} \cdot c_{SO_3} \cdot Eq)/G_1$$

$$BaO + SO_3 \rightarrow BaSO_4 \qquad R = A \cdot e^{-E/RT} \cdot c_{SO_3} \cdot \Psi_{cap} \cdot \psi_{BaO} \cdot Eq$$

$$BaSO_4 \rightarrow BaO + SO_3 \qquad R = A \cdot e^{-E/RT} \cdot \Psi_{cap} \cdot \psi_{BaSO_4} \cdot Eq$$

$$BaSO_4 + CO \rightarrow BaO + SO_2 + CO_2 \qquad R = A \cdot e^{-E/RT} \cdot c_{CO} \cdot \Psi_{cap} \cdot \psi_{BaSO_4} \cdot Eq$$

$$BaSO_4 + H_2 \rightarrow BaO + SO_2 + H_2O \qquad R = A \cdot e^{-E/RT} \cdot c_{H_2} \cdot \Psi_{cap} \cdot \psi_{BaSO_4} \cdot Eq$$

$$BaSO_4 + 4H_2 \rightarrow BaO + H_2S + 3H_2O \qquad R = A \cdot e^{-E/RT} \cdot c_{H_2} \cdot \Psi_{cap} \cdot \psi_{BaSO_4} \cdot Eq$$

$$H_2S + \frac{3}{2}O_2 \rightarrow SO_2 + H_2O \qquad R = (A \cdot e^{-E/RT} \cdot c_{H_2S} \cdot c_{O_2})/G_1$$

O_2 storage submodel – Ceria based mechanism

O_2 "storage"

$Ce_2O_3 + ½ O_2 \rightarrow 2CeO_2$

$Ce_2O_3 + NO \rightarrow 2CeO_2 + ½ N_2$

O_2 "release"

$CO + 2CeO_2 \rightarrow Ce_2O_3 + CO_2$

$H_2 + 2CeO_2 \rightarrow Ce_2O_3 + H_2O$

Ce oxidation state

$$\psi = \frac{2 \times \text{moles}\,\text{CeO}_2}{2 \times \text{moles}\,\text{CeO}_2 + moles\,\text{Ce}_2 O_3}$$

$$\frac{d\psi}{dt} = -\frac{1}{\Psi_{cap}}\left(R_{ox} - R_{red}\right)$$

Oxygen storage/release phenomena strongly affect
reductants availability and NO release during regeneration

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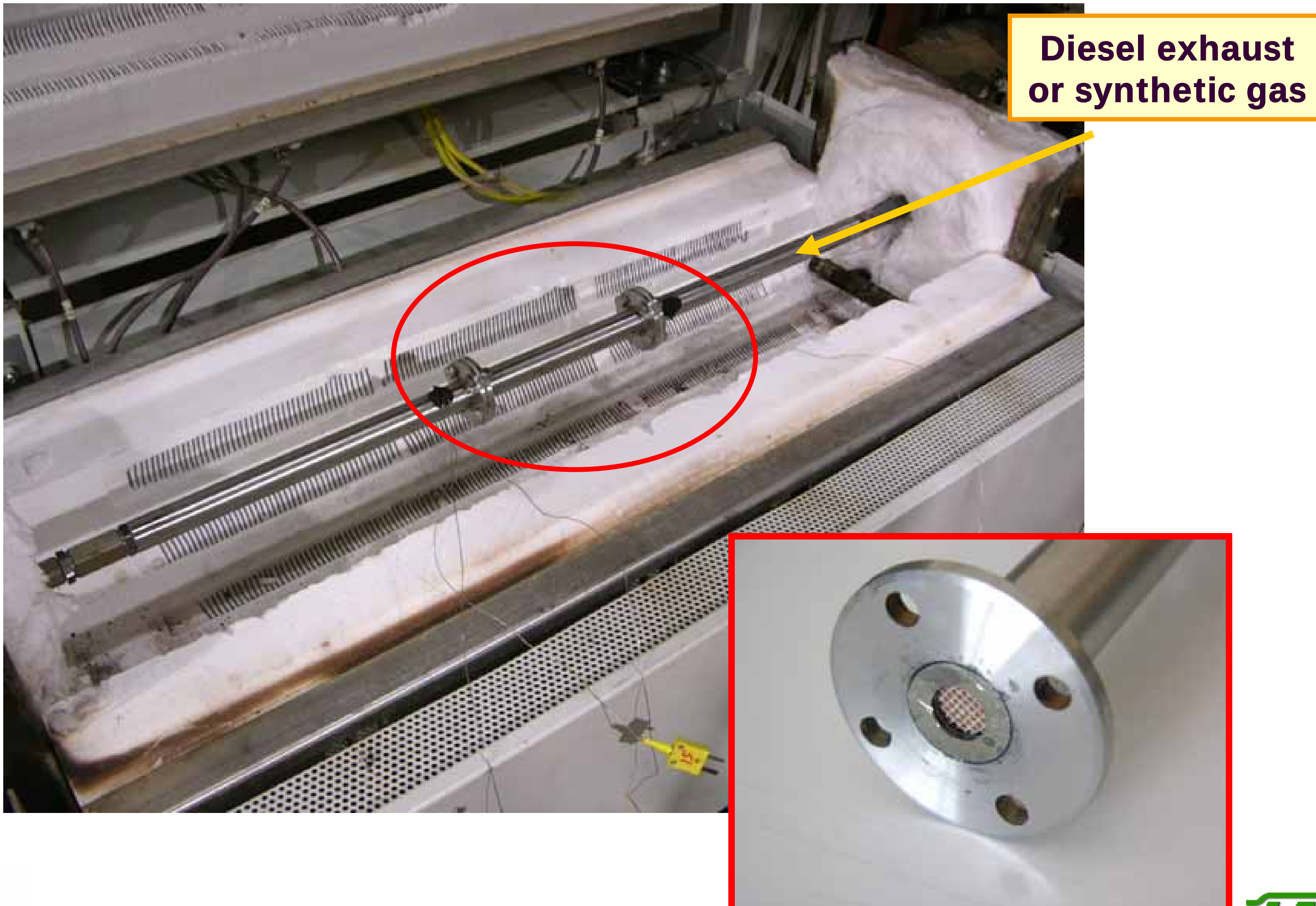
LNT model parameter calibration
Tube reactor placed in an electrically heated tube furnace



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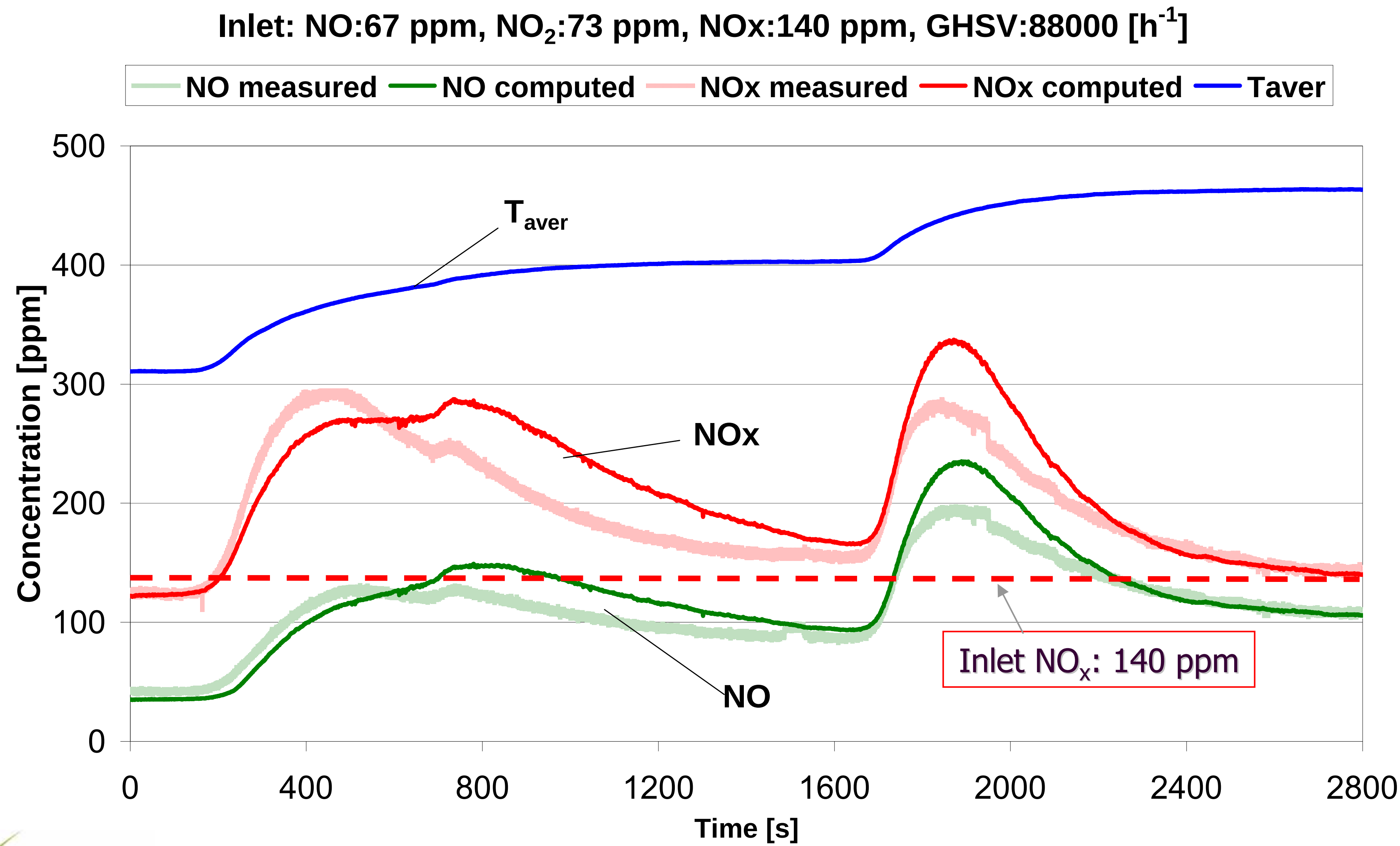
“Spontaneous” (thermal) NO_x release during temperature increase in lean operation



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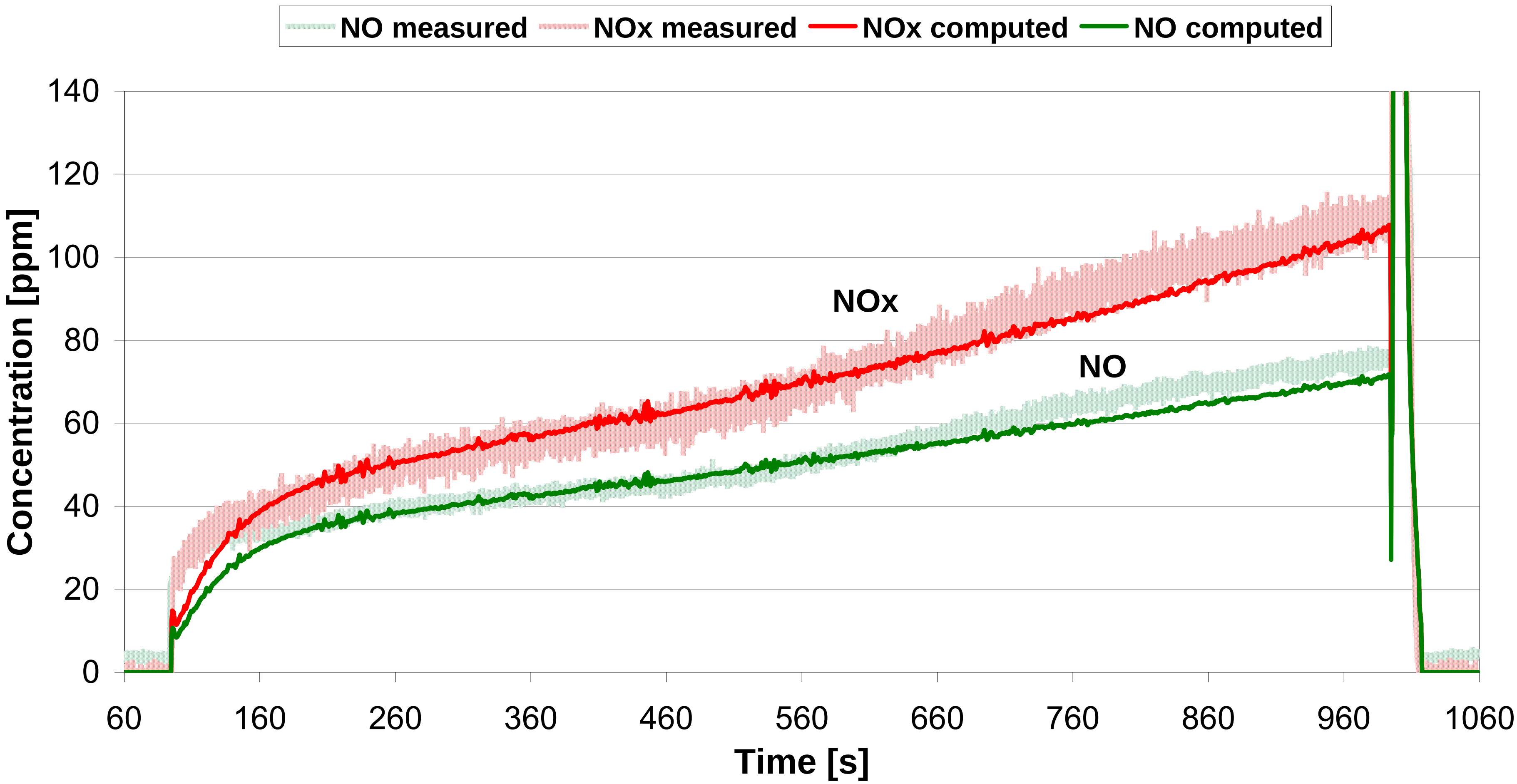
Storage experiment at 400°C with diesel exhaust

Inlet: NO:90 ppm, NO_2:75 ppm, NOx:165 ppm



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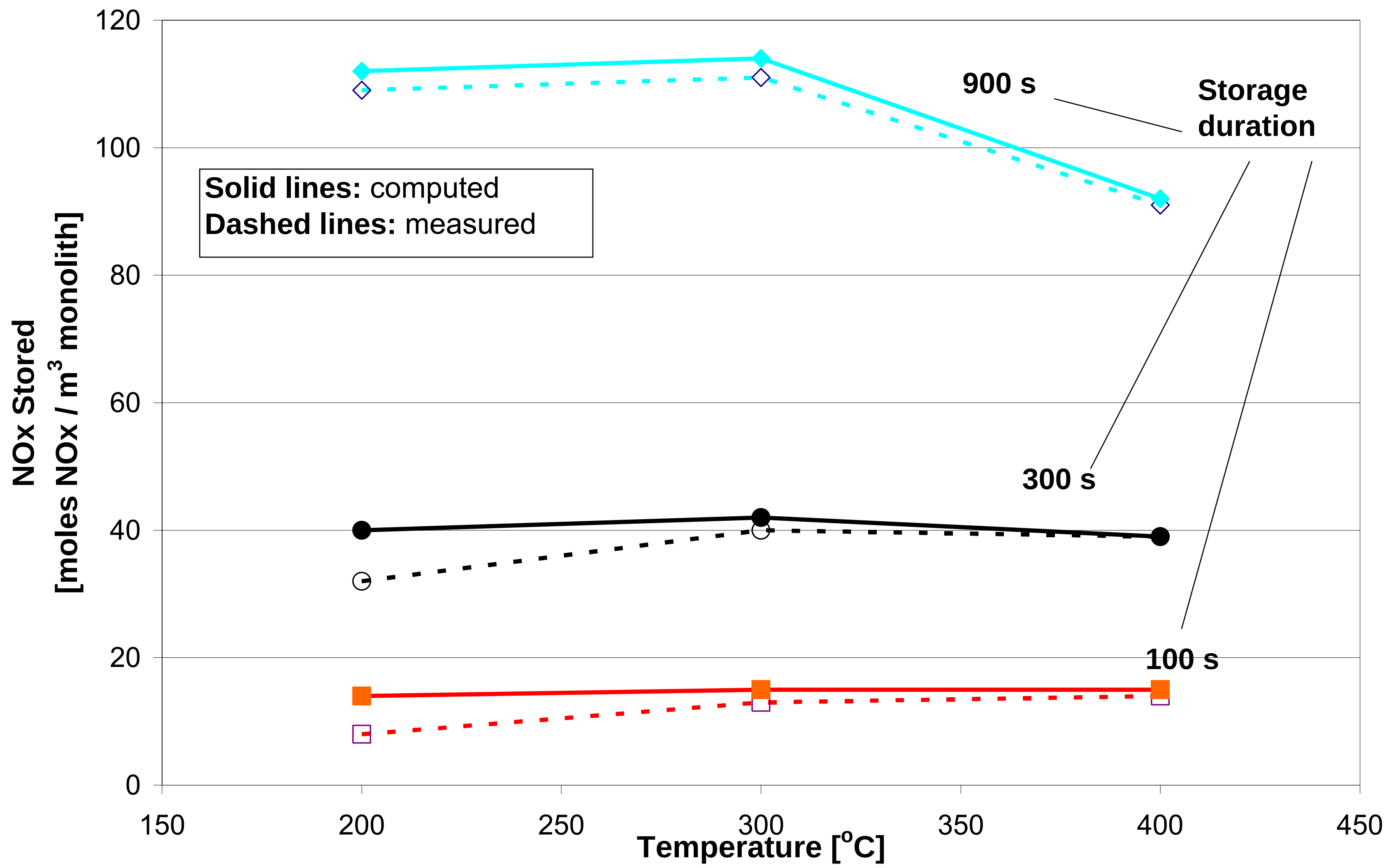
Stored NO_x at different temperatures



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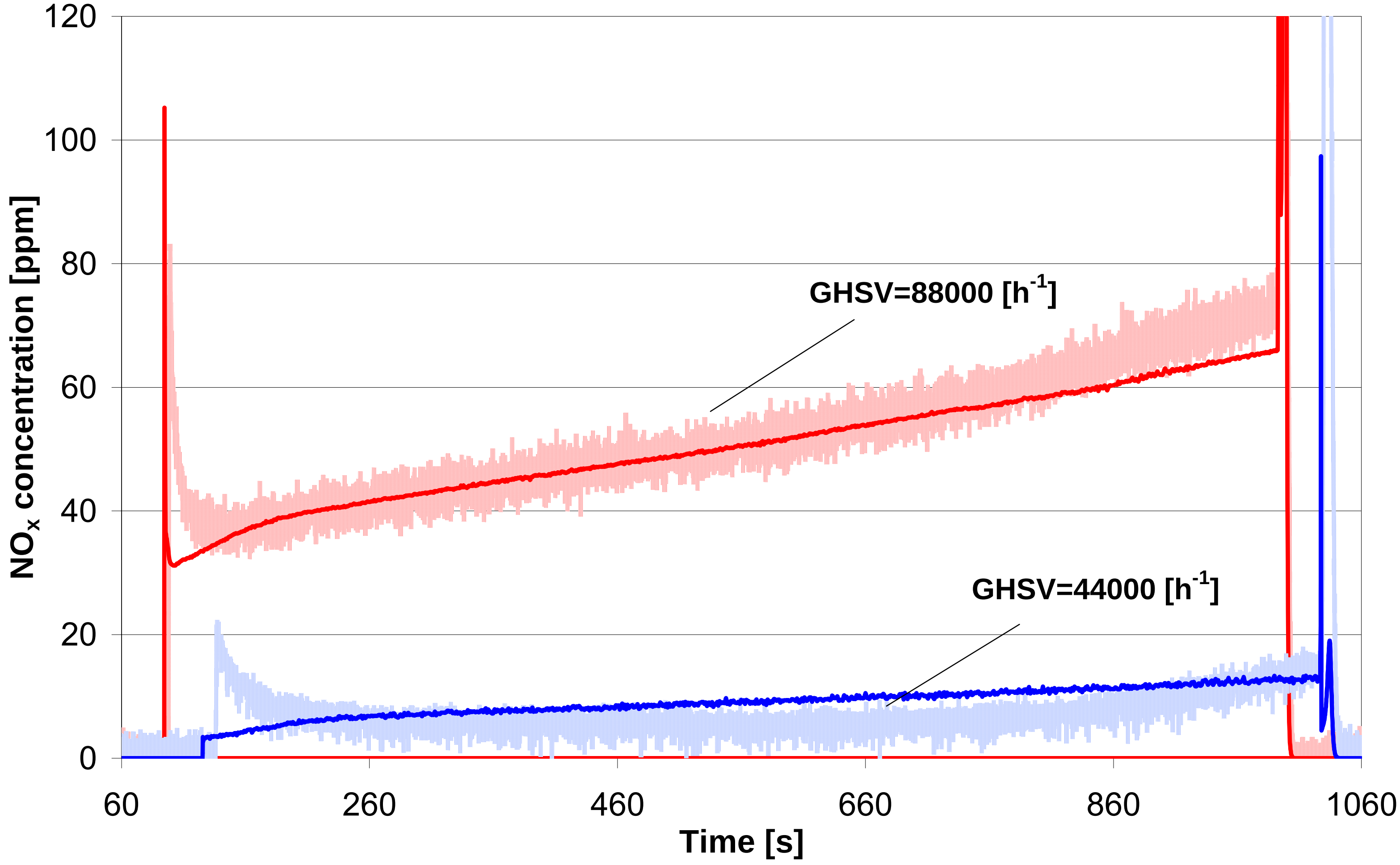
Model validation at different flow rate at 300°C



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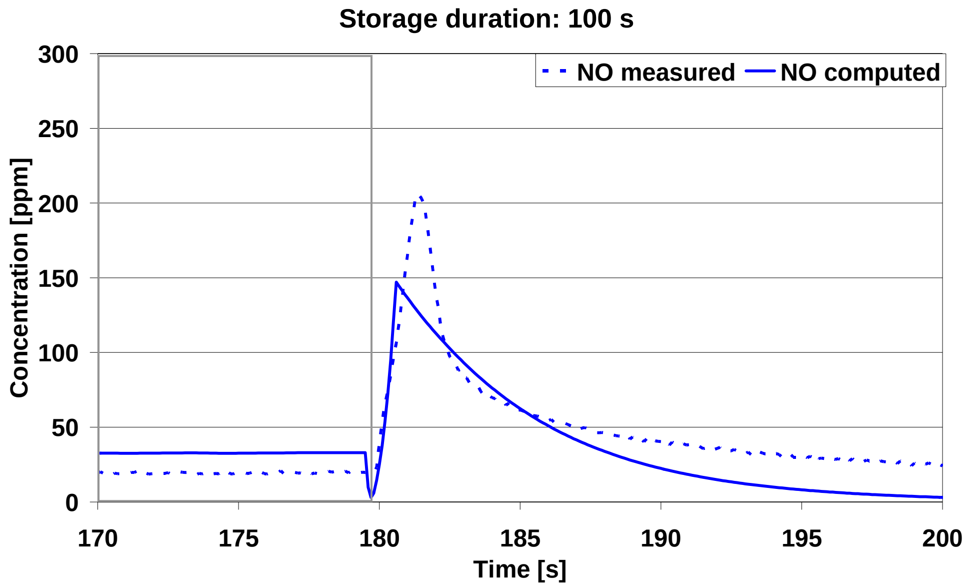
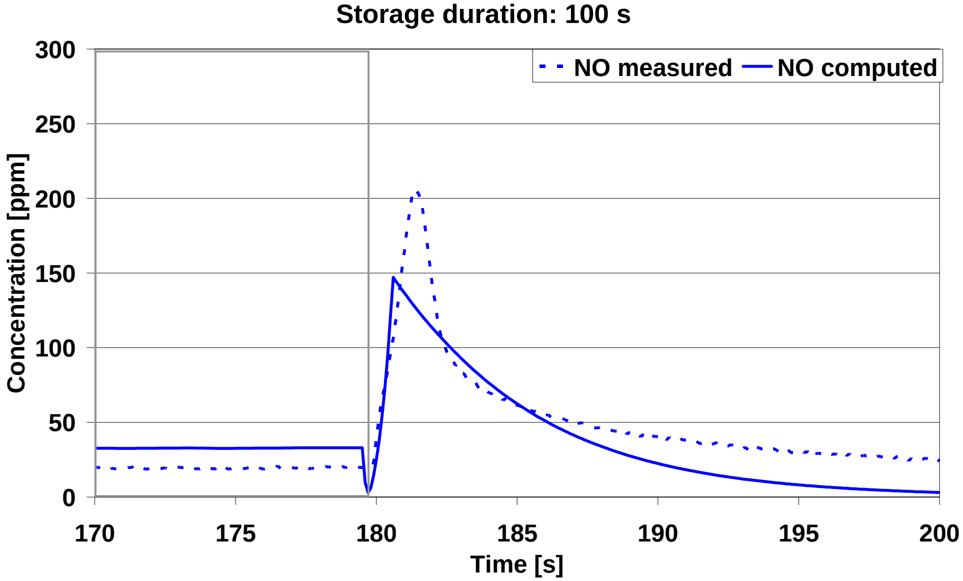
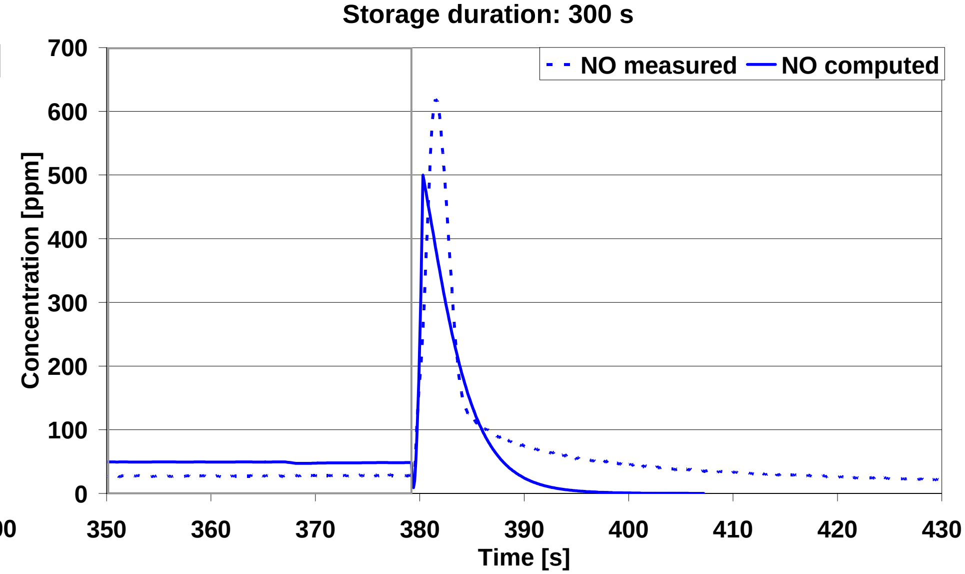
NO emissions during regeneration at 200˚C



During regeneration NO_2 is negligible (not favored thermodynamically)

NO emissions during regeneration at 200˚C

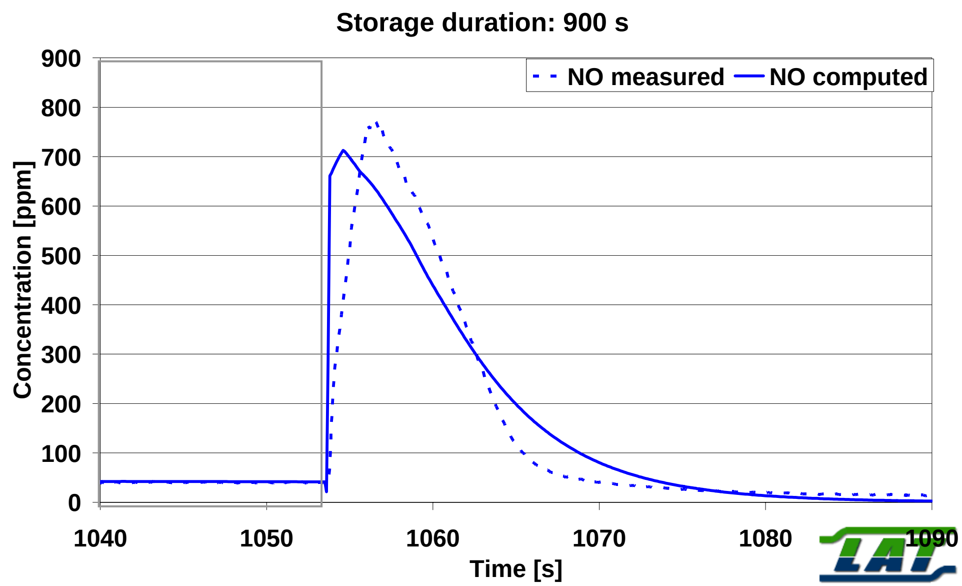




During regeneration NO_2 is negligible (not favored thermodynamically)

Note the different peak NO levels

NO release duration: 5 - 10 s



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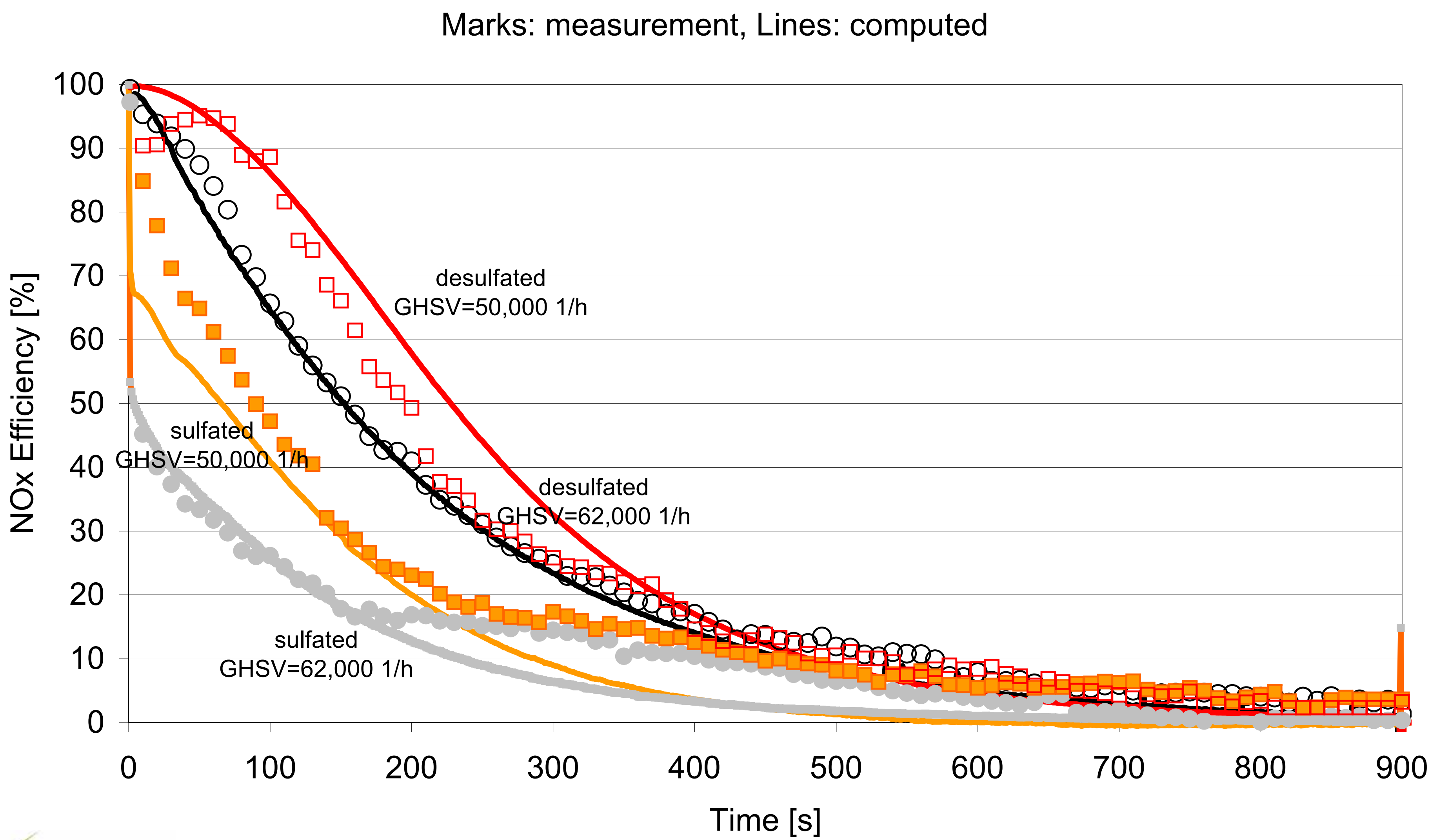
Sulfur effects

Sulfation model validation at two different space velocities



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SCR catalyst modeling

Main SCR reactions

- Reaction scheme:
  - SCR reactions

$$4\ NH_3 + 4\ NO + O_2 \rightarrow 4\ N_2 + 6\ H_2O$$

$$2\ NH_3 + NO + NO_2 \rightarrow 2\ N_2 + 3\ H_2O$$

$$4\ NH_3 + 3\ NO_2 \rightarrow 3.5\ N_2 + 6\ H_2O$$

  - Alternatively, "direct NH_3 + NO_2" reaction is split in 2 reactions:

$$2\ NH_3 + 2\ NO_2 \rightarrow N_2O + N_2 + 3\ H_2O$$

$$2NH_3 + 3N_2O \rightarrow 4\ N_2 + 3\ H_2O$$

  - NH_3 oxidation reaction

$$NH_3 + 5/4\ O_2 \rightarrow NO + 3/2\ H_2O$$

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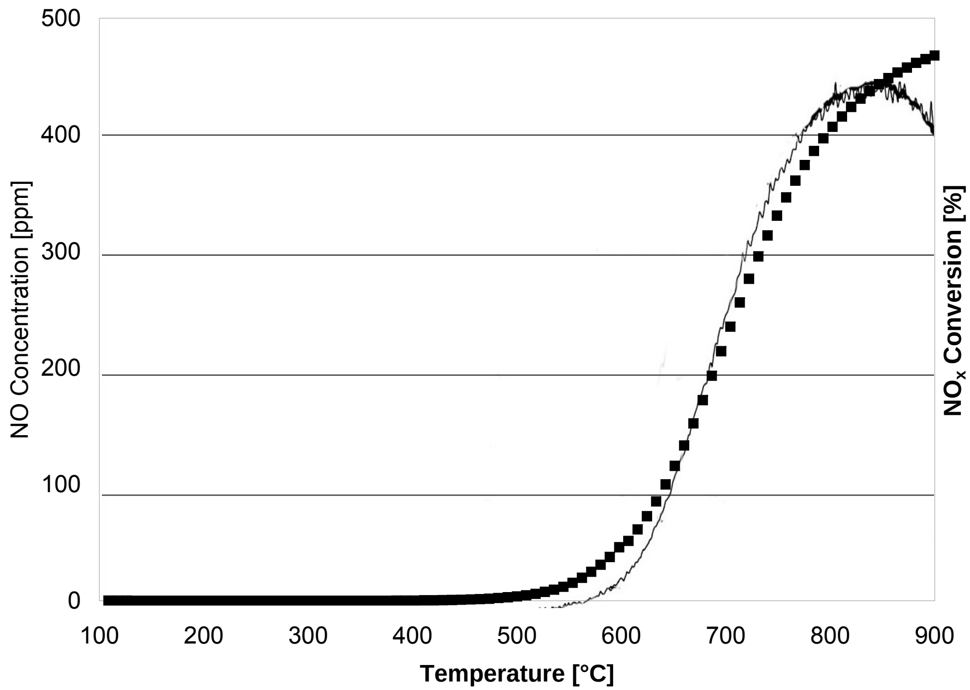
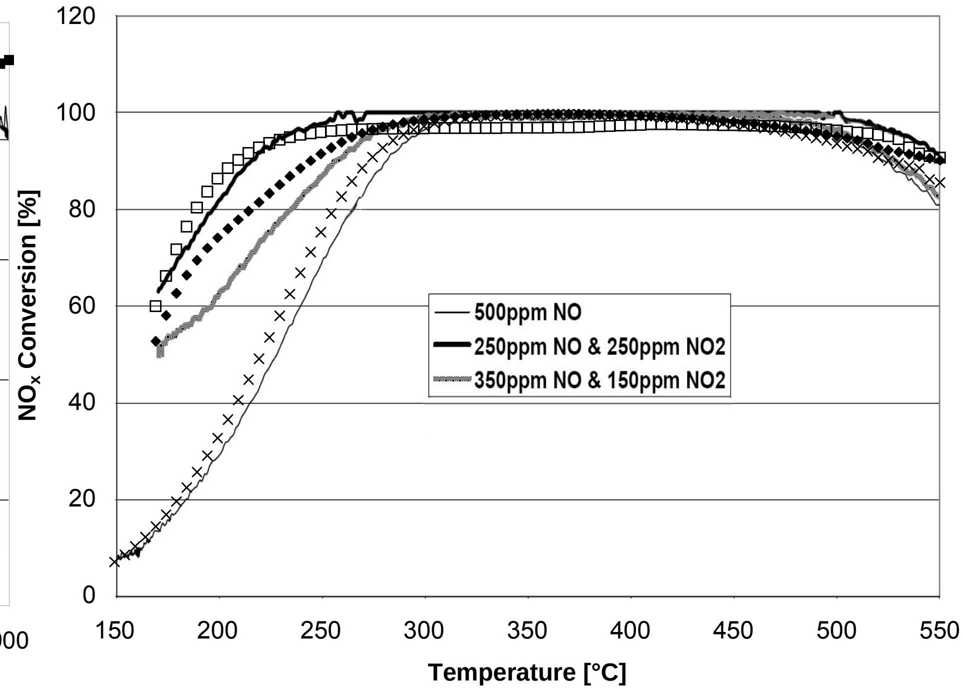
SCR
Parameter calibration example

NH_3 oxidation



Effect of NO / NO_2 ratio



Lines: Experimental, symbols: simulation.

Experimental Data Source: *Winkler et al., Modeling of SCR DeNOx Catalyst – Looking at the Impact of Substrate Attributes, SAE Paper 2003-01-0845*

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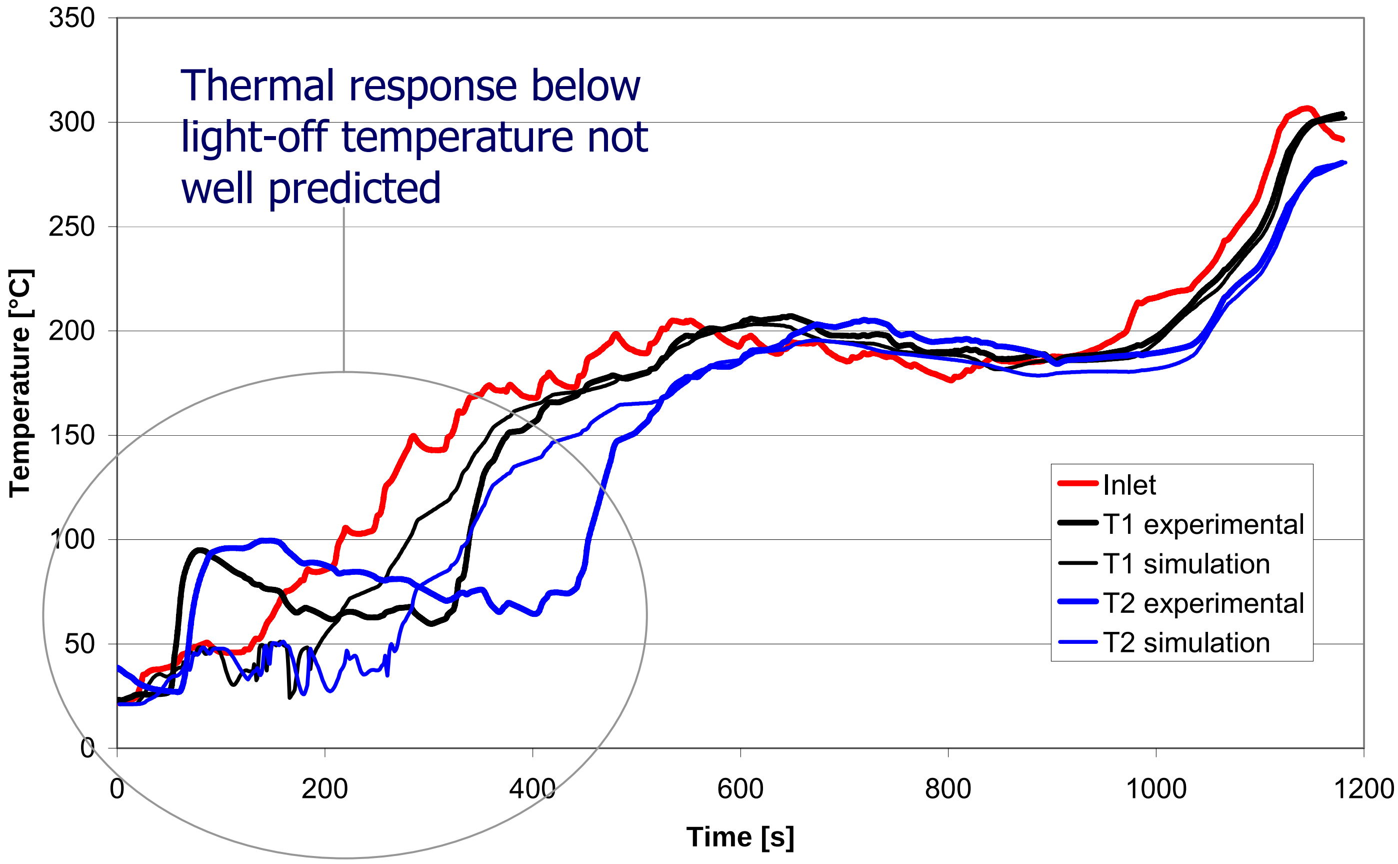
Experimental validation
SCR simulation in transient cycle

- **Water adsorption neglected!**



Experiments conducted at an engine test bench of IAV GmbH

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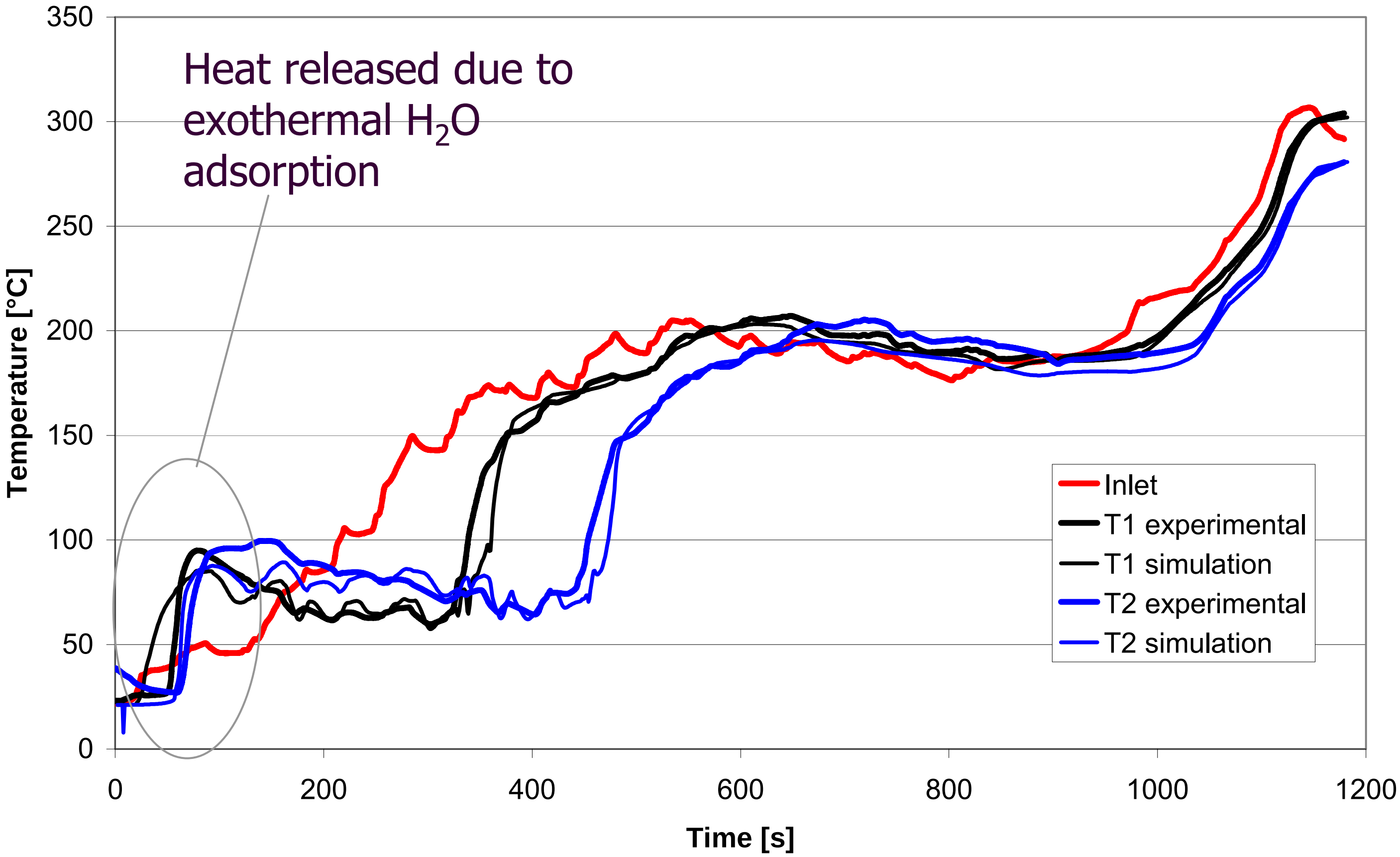
Experimental validation
SCR simulation in transient cycle

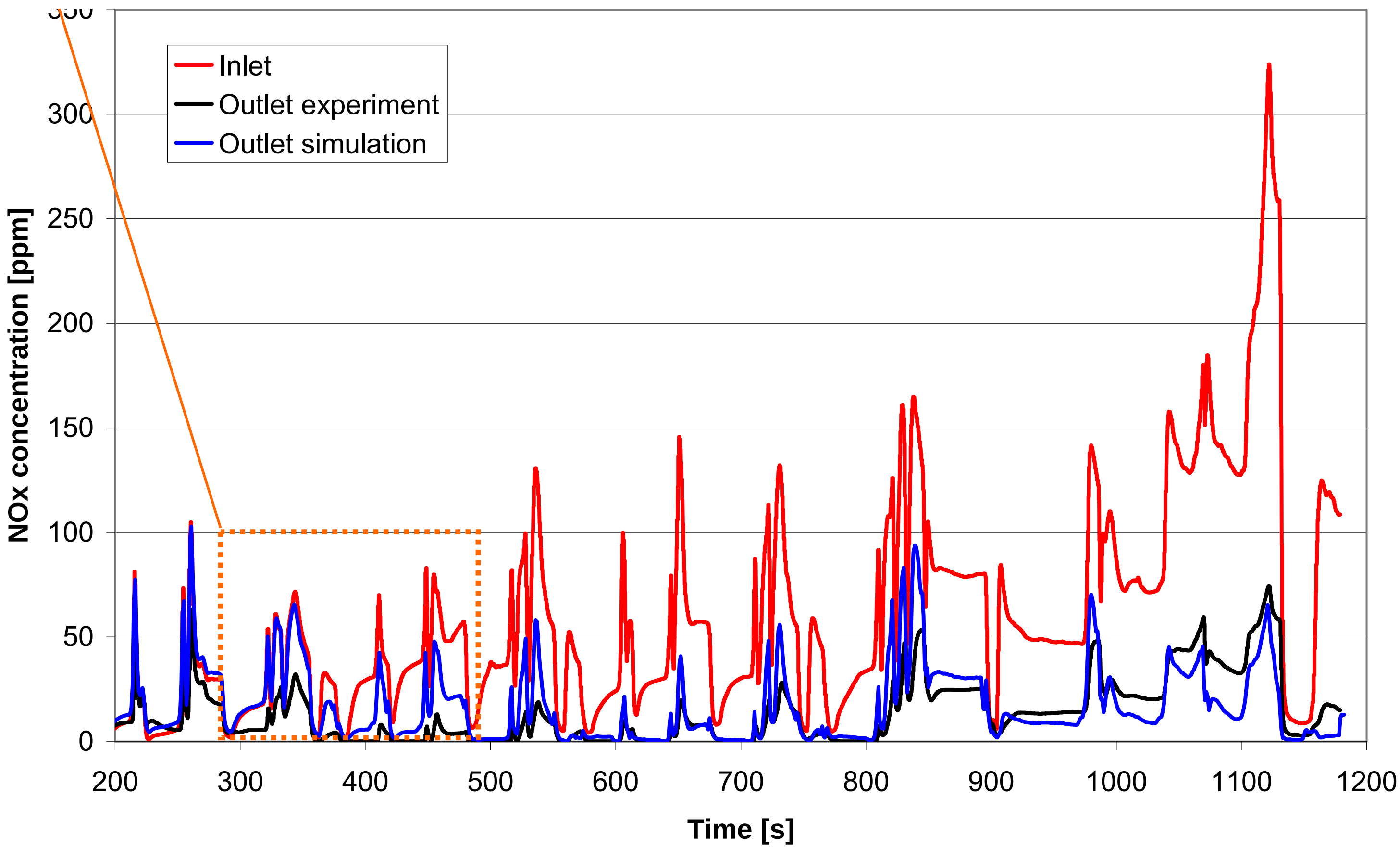
Water adsorption included!



Experiments conducted at an engine test bench of IAV GmbH

Experimental validation
SCR simulation in transient cycle

NOx conversion measured and simulated, as a result of SCR reaction with previously adsorbed ammonia



Experiments conducted at an engine test bench of IAV GmbH

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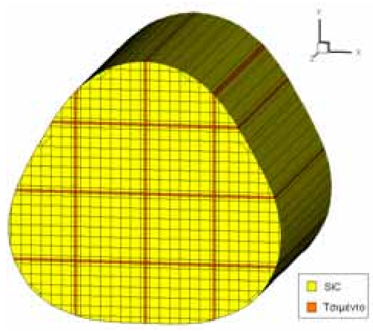
Wall-flow reactor modeling

Wall-flow Reactor Modeling
Modeling levels

<u>Filter scale</u>

- 3D heat transfer
- Inlet flow distribution
- Diffuser effects
- Soot non-uniformities

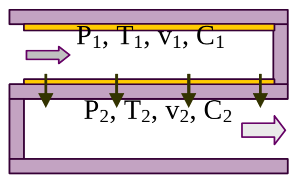


<u>Equations</u>

- Solid energy balance
- Mass balance
- Diffuser pressure drop

<u>Channel scale</u>

- Heat convection
- Wall velocity profile
- Mass convection

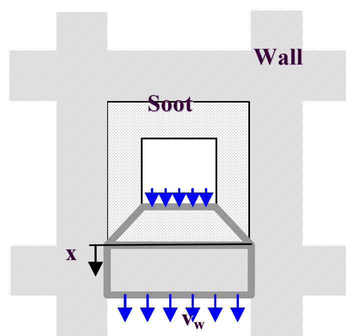


<u>Equations</u>

- Gas energy balance
- Mass balance
- Momentum balance
- Species balance

<u>Wall scale</u>

- Intra-layer reaction
- Intra-layer diffusion
- Intra-layer velocity and density variation



<u>Equations</u>

- Species balance
- Soot mass balance
- Soot layer pressure drop

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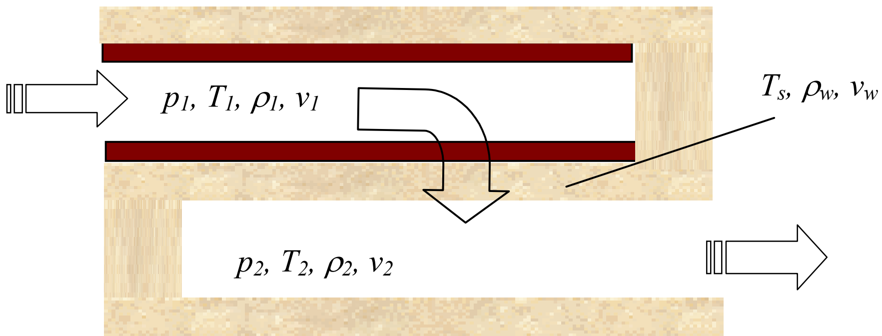
Channel scale (1-d modeling)
Equations



Gas phase

Mass

$$\frac{\partial}{\partial z}\left(d_i^{\,2}\rho_i v_i\right) = (-1)^i 4 d \rho_w v_w$$

Momentum

$$\frac{\partial p_i}{\partial z} + \frac{\partial}{\partial z}\left(\rho_i v_i^2\right) = -\alpha_1 \mu v_i / d_i^{\,2}$$

Energy

$$C_{p,g}\rho_1 v_1\big|_z \frac{\partial T_1}{\partial z} = h_1 \frac{4}{d_1}\left(T_s - T_1\right)$$

$$C_{p,g}\rho_2 v_2\big|_z \frac{\partial T_2}{\partial z} = \left(h_2 + C_{p,g}\rho_w v_w\right)\frac{4}{d}\left(T_s - T_2\right)$$

Wall – Energy balance

$$\frac{\partial}{\partial t}\left(\rho_p C_{p,p} T_w + \rho_s C_{p,s} T_w\right) = h_1\left(T_1 - T_w\right) + h_2\left(T_2 - T_w\right)$$
$$+ \rho_w v_w C_{p,g}\left(T_1 - T_w\right) + H_{react} + H_{cond}$$

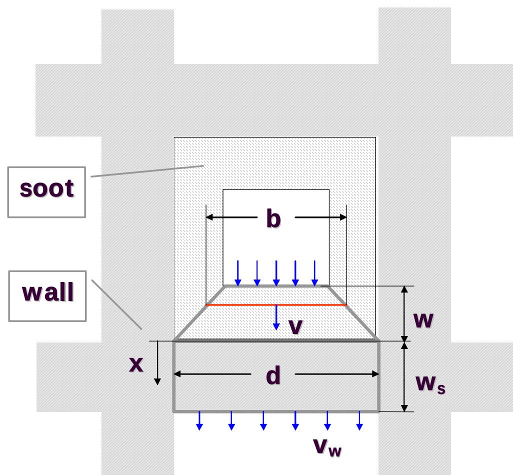
Soot – Mass balance

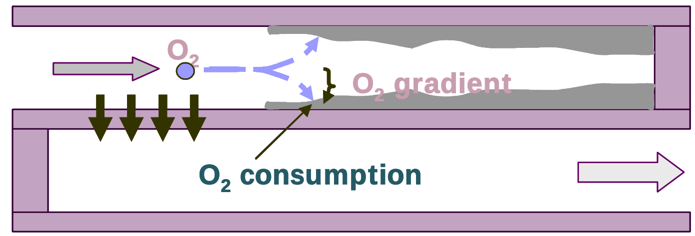
$$\rho_p \frac{dw}{dt} = -\left(\frac{M_c}{M_{O_2}}\right)\rho_w v_w y \frac{1}{a}\left(1 - \exp\left(-\frac{S_p k_1(T_w) w}{v_w} a\right)\right)$$

Exothermia modeling efficiency

Ref: Koltsakis, Stamatelos, Ind. Eng. Chem. Res. 1997

Transport-reaction “coupling”

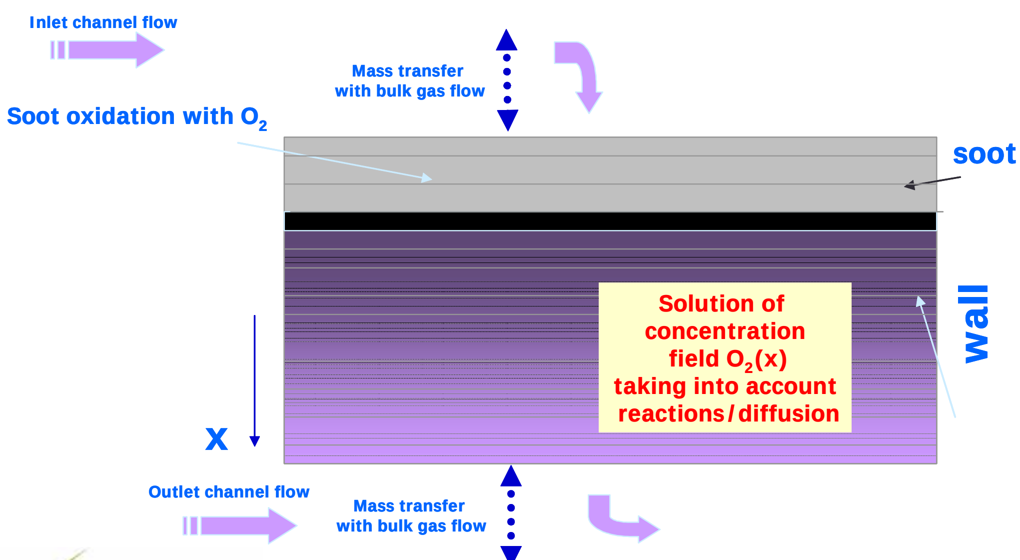




Convective mass transfer in channels

$$\frac{\partial}{\partial z}\left(v_1 y_{1,j}\right) = -\frac{1}{df_{-w}^{\,2}} v_w y_{1,j} + \frac{1}{df_{-w}} k_{1,j}\left(y_{1s,j} - y_{1,j}\right)$$

$$\frac{\partial}{\partial z}\left(v_2 y_{2,j}\right) = \frac{1}{df_{w_s}^{\,2}} v_w y_{2s,j} + \frac{1}{df_{w_s}} k_{2,j}\left(y_{2s,j} - y_{2,j}\right)$$



Intra-layer reaction-diffusion coupling

$$v_w \frac{\partial y_j}{\partial x} - D_j \frac{\partial}{\partial x}\left(f_x \frac{\partial y_j}{\partial x}\right) = \frac{f_x}{c_m} \sum_k c_{j,k} R_k$$

Intra-layer soot mass balance

$$\frac{d\hat{m}_p}{dt} = -\hat{m}_p \sum R'_k + s_F \rho_w v_w \mu_p$$

Intra-layer Δp law

$$\frac{dp}{dx} = \frac{\mu v(x)}{k_p}$$

Ref: Haralampous et al., 2004-01-0696

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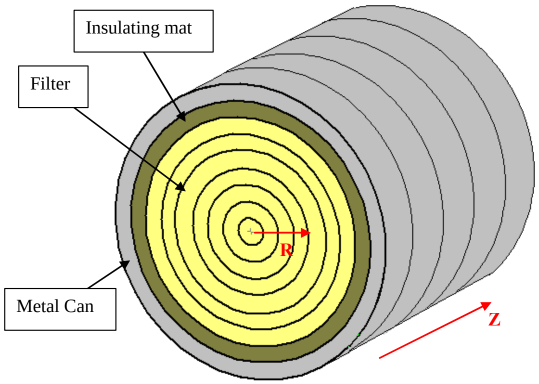
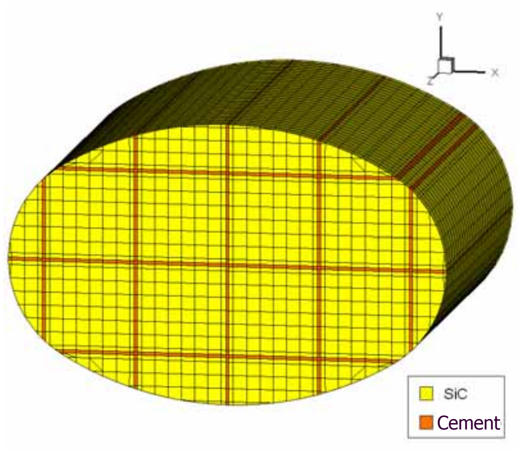
2-d & 3-d extension



2-d Transient Heat Transfer

$$\rho_s \cdot C_{p,s} \frac{\partial T_s}{\partial t} = \lambda_{s,z} \frac{\partial^2 T_s}{\partial z^2} + \lambda_{s,r} \frac{1}{r} \frac{\partial}{\partial r}\left(r \frac{\partial T_s}{\partial r} \right) + S$$

$$S = H_{conv} + H_{wall} + H_{react} + H_{rad}$$



3-d Transient Heat Transfer

$$\rho_s \cdot C_{p,s} \frac{\partial T_s}{\partial t} = \lambda_{s,z} \frac{\partial^2 T_s}{\partial x^2} + \lambda_{s,r} \frac{\partial^2 T_s}{\partial y^2} + \lambda_{s,r} \frac{\partial^2 T_s}{\partial z^2} + S$$

$$S = H_{conv} + H_{wall} + H_{react} + H_{rad}$$

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Wall-flow DOC

Model Reactions

Soot layer

Carbon oxidation

$$C + \alpha_1\, O_2 \rightarrow 2\left(\alpha_1 - \frac{1}{2}\right) CO_2 + 2(1-\alpha_1)\, CO$$

$$C + \alpha_2\, NO_2 \rightarrow \alpha_2\, NO + (2-\alpha_2)\, CO + (\alpha_2 - 1)\, CO_2$$

Catalyzed wall:

basic reactions for Noble Metals coatings

Bi-directional NO oxidation

$$NO + \frac{1}{2} O_2 \leftrightarrow NO_2$$

CO oxidation

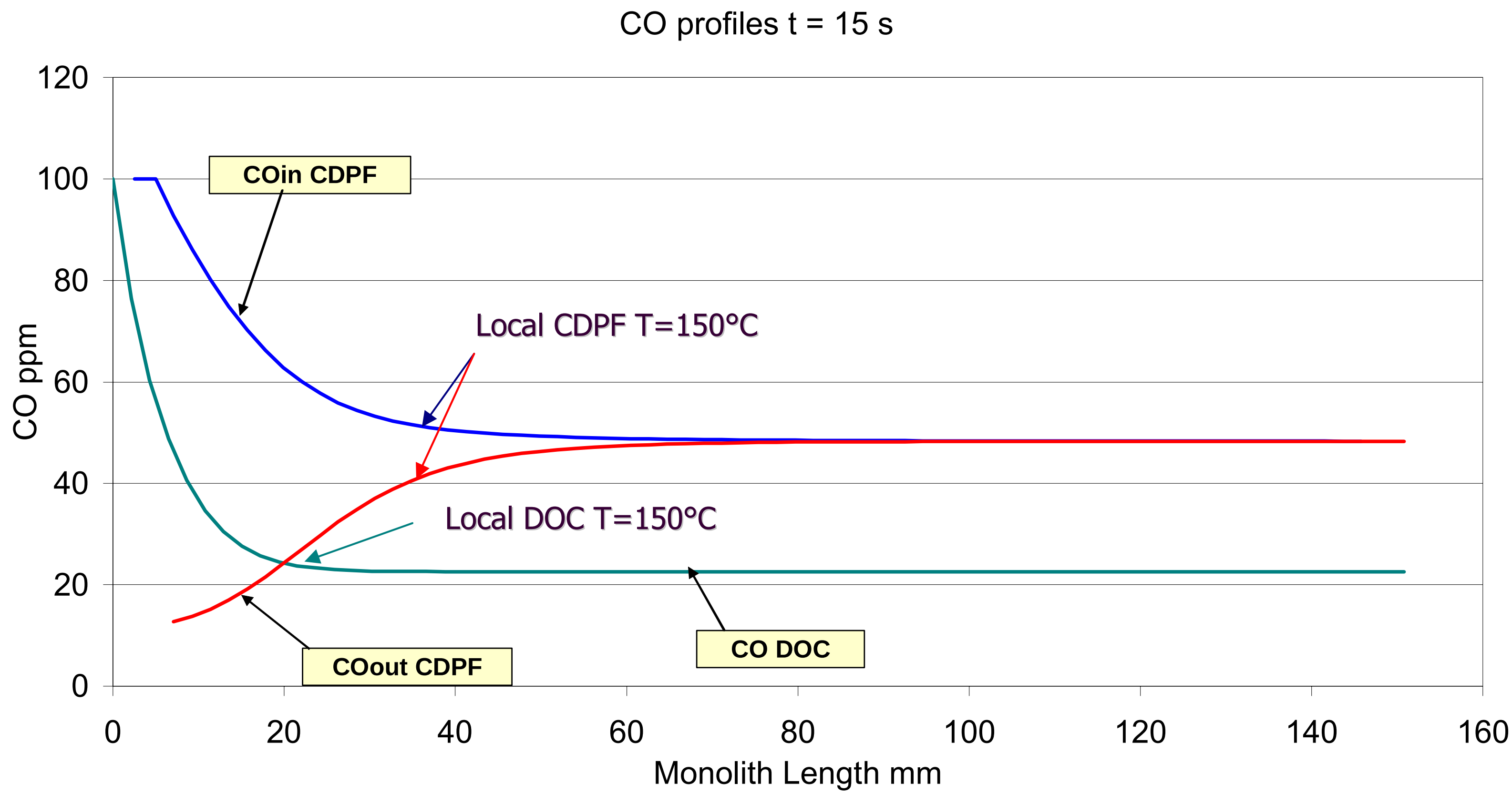
$$CO + \frac{1}{2} O_2 \rightarrow CO_2$$

HC oxidation

$$C_x H_y + \alpha\, O_2 \longrightarrow \beta\, CO_2 + \gamma\, H_2O$$

CO profiles in DOC and CDPF during warm-up

“Active length” (T>150°C): DOC: 25 mm, CDPF: 35 mm



Due to the lower axial gas velocities in the DOC the conversion is higher despite the shorter “active length”

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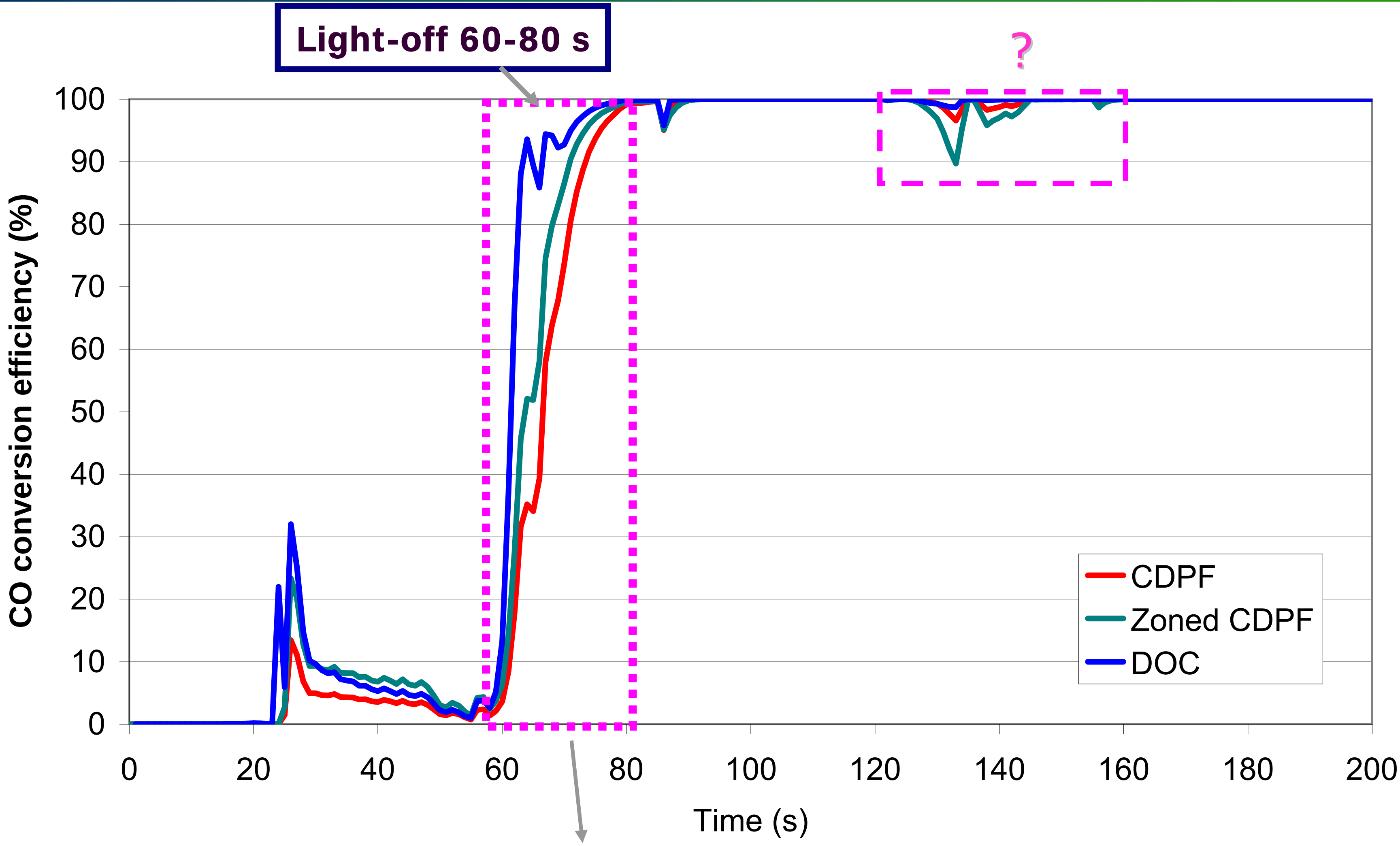
Wall-flow reactor performance in driving cycle
Effect of catalyst zoning



Light-off phase: DOC better than CDPF
zCDPF better than CDPF

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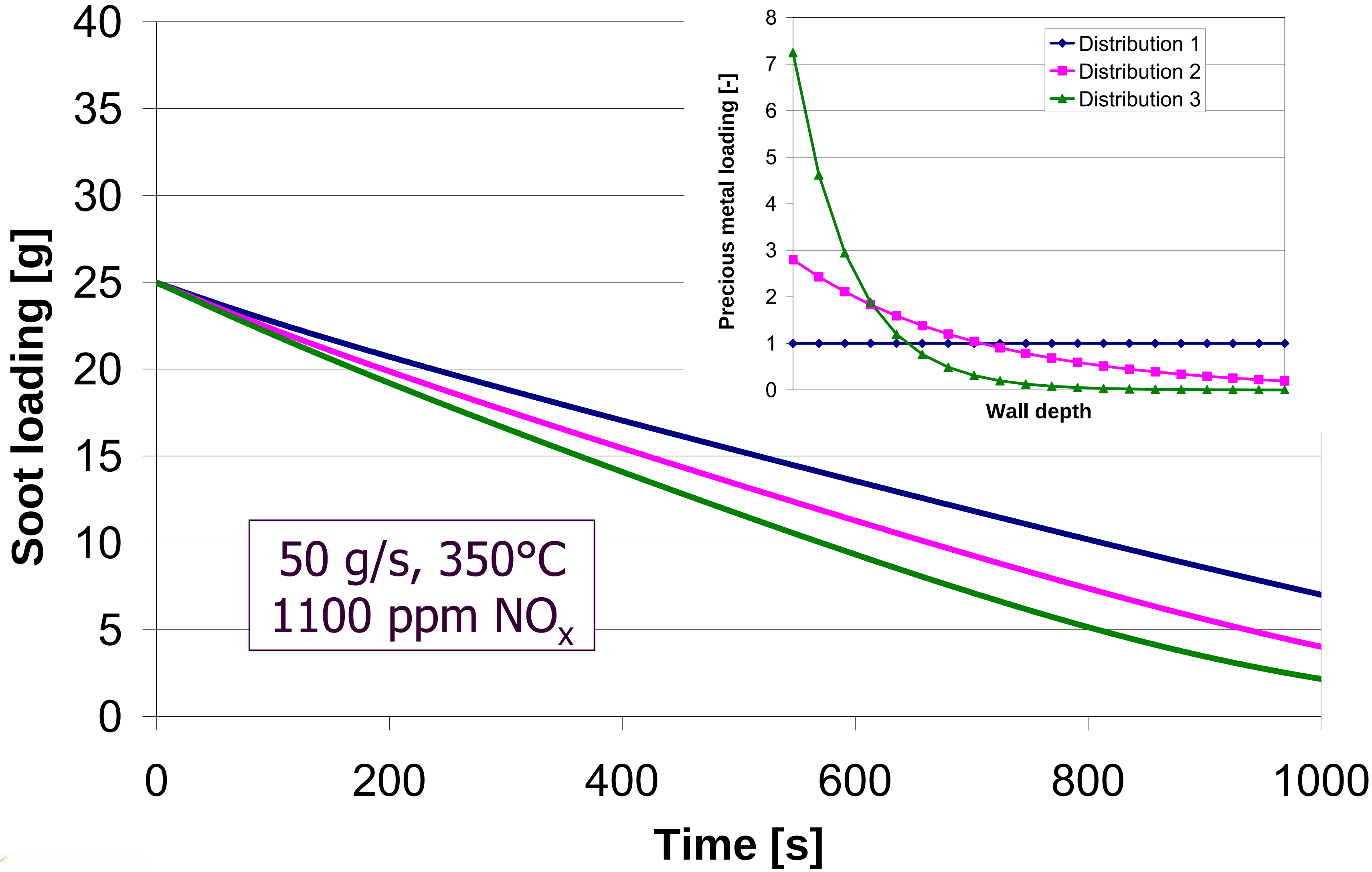
Effect of intra-wall catalyst distribution
CDPF regeneration rate



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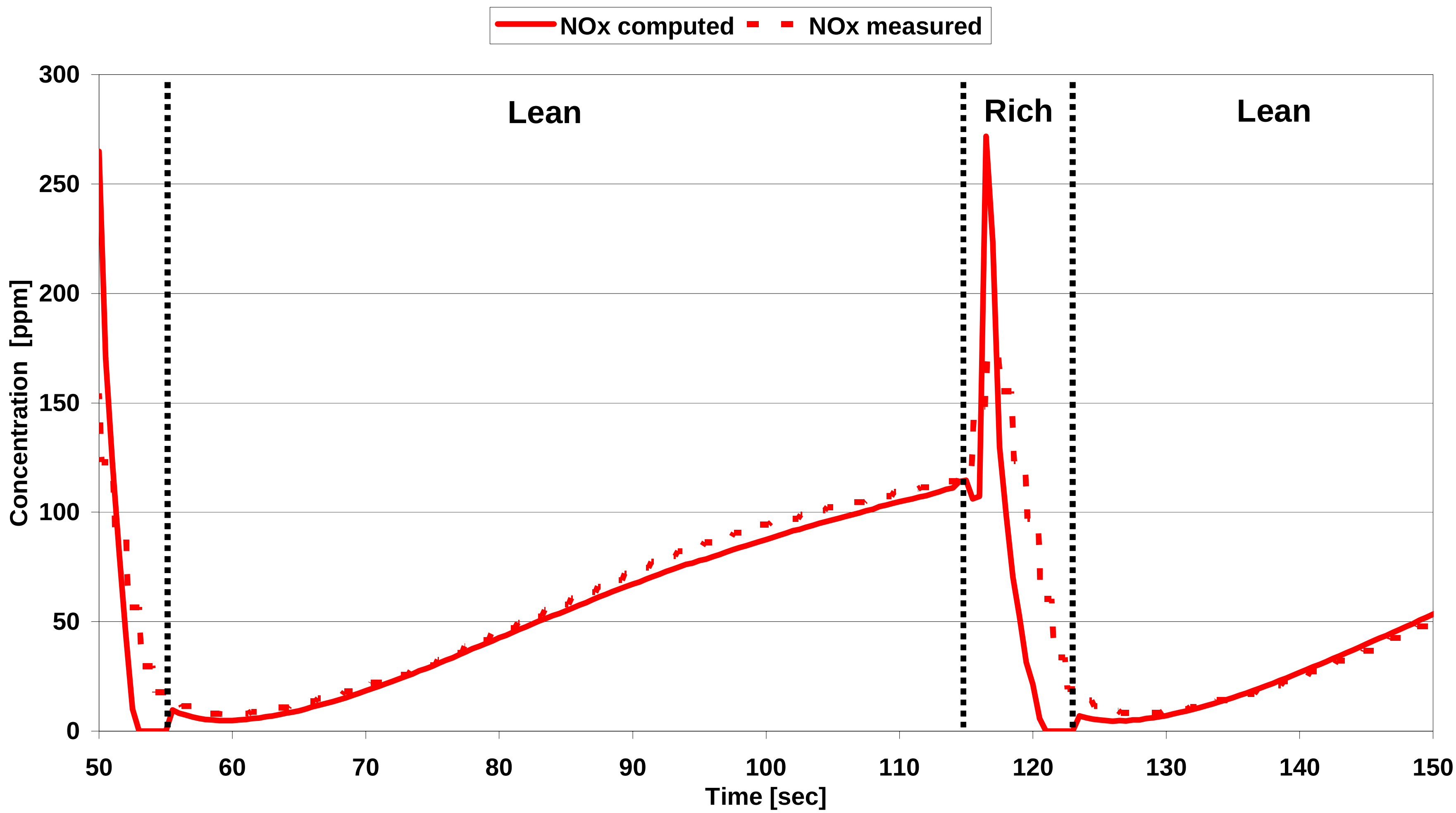
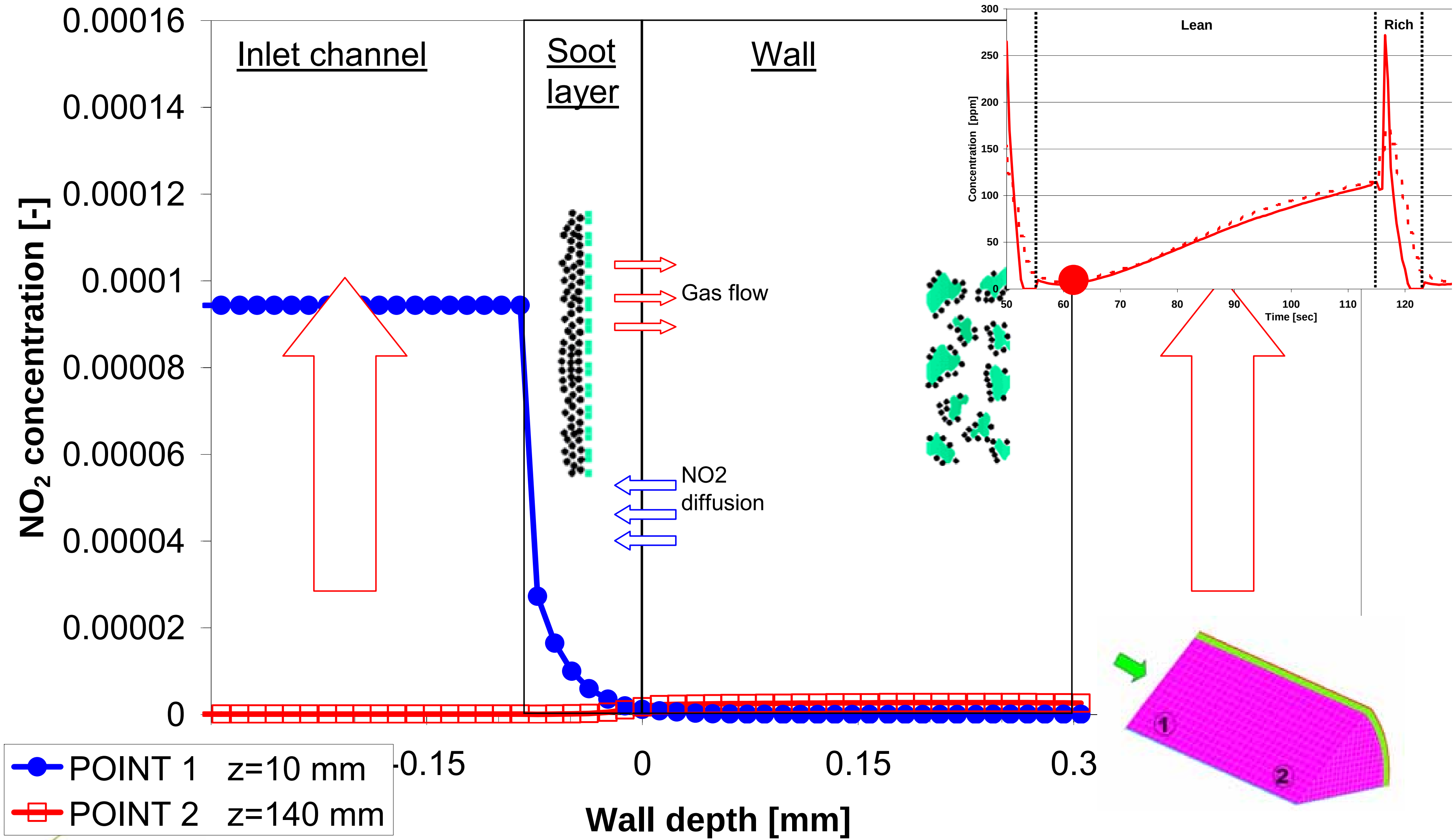
Wall-flow LNT
(DPNR)

DPNR simulation example
Lean-rich cycle at 350°C



Experiments conducted at an engine test bench of IAV GmbH

Intra-layer NO_2 profiles
t=60 s



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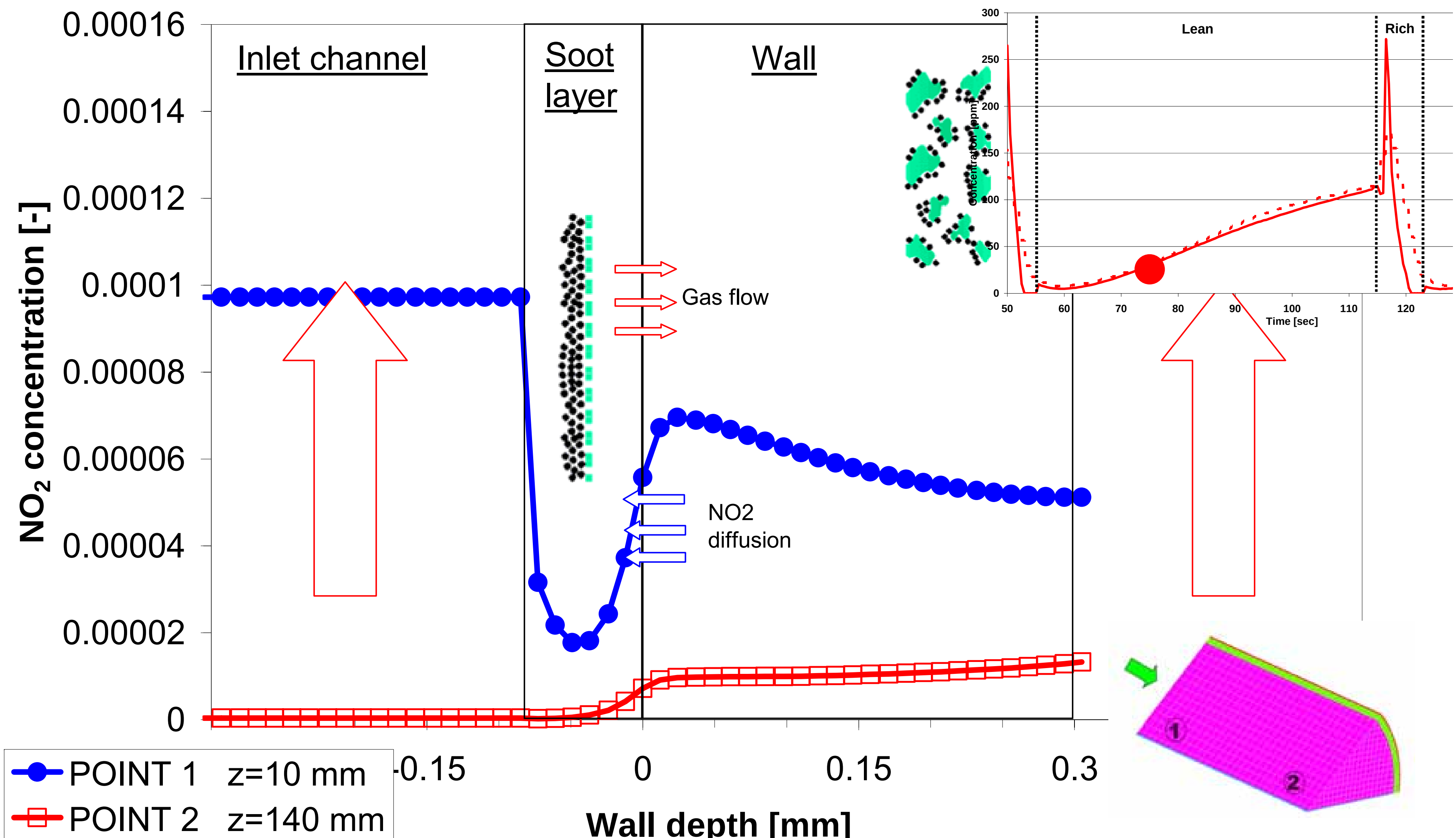
Intra-layer NO_2 profiles
t=75 s



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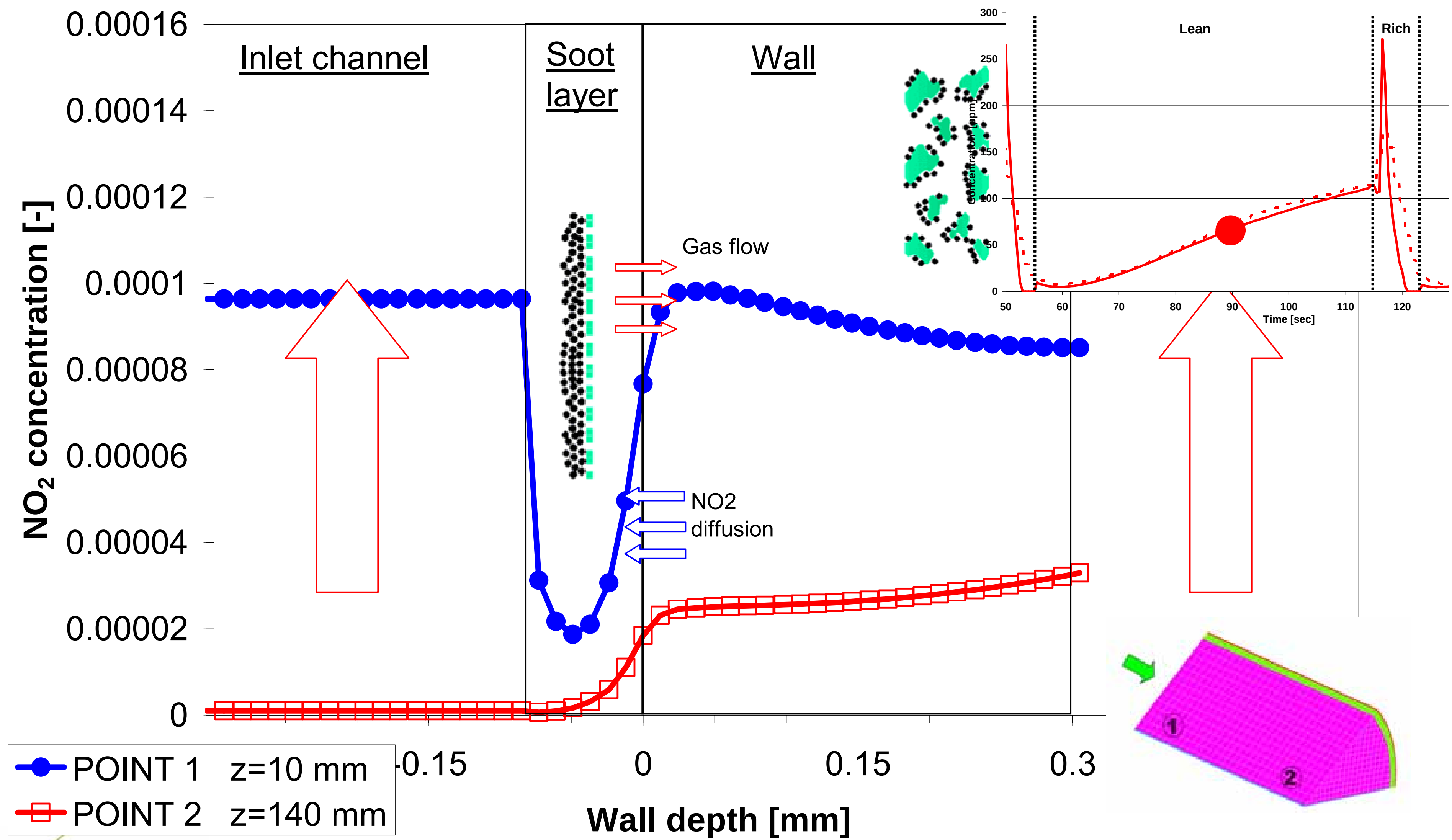
Intra-layer NO_2 profiles
t=90 s



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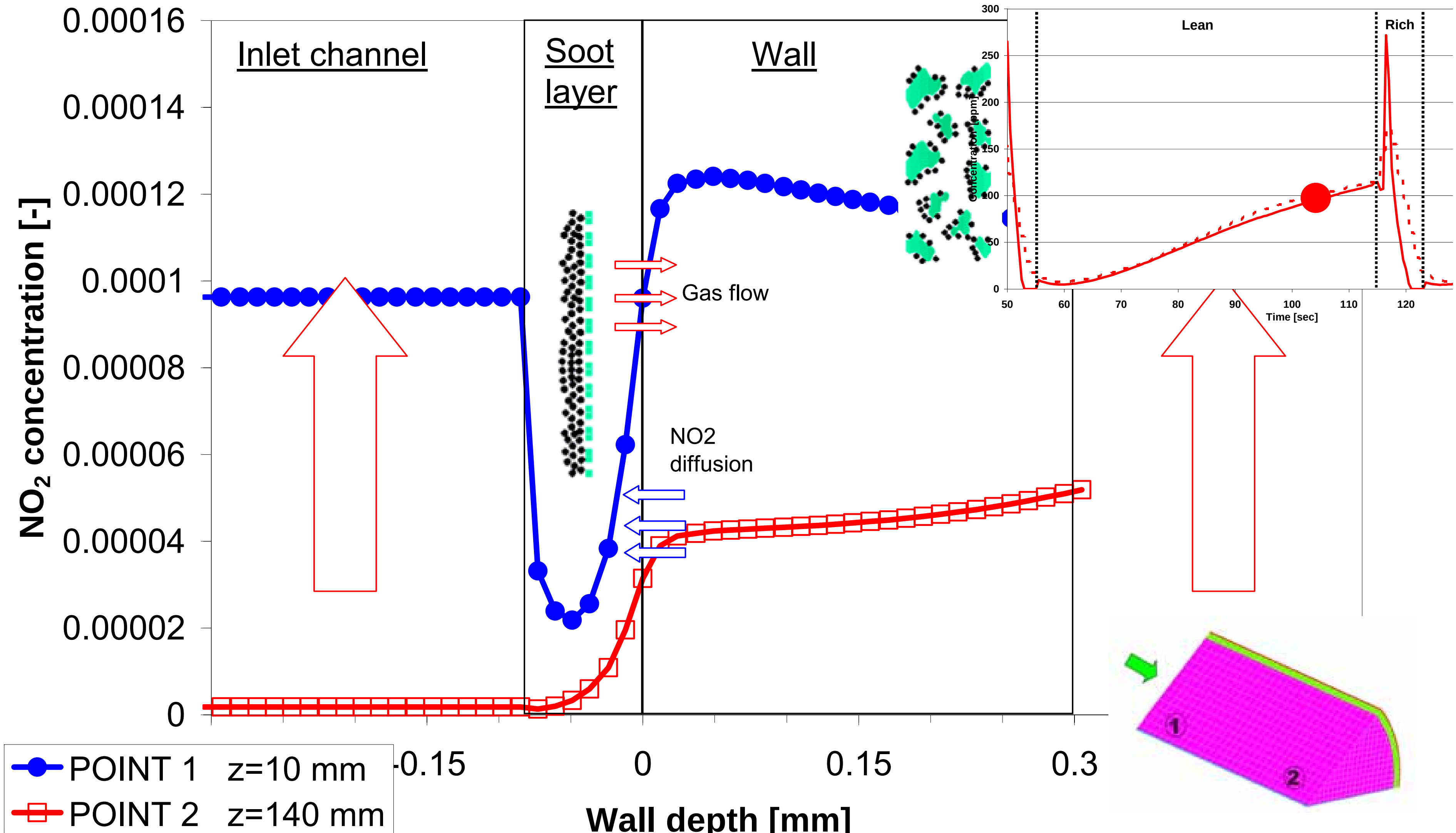
Intra-layer NO_2 profiles
t=105 s



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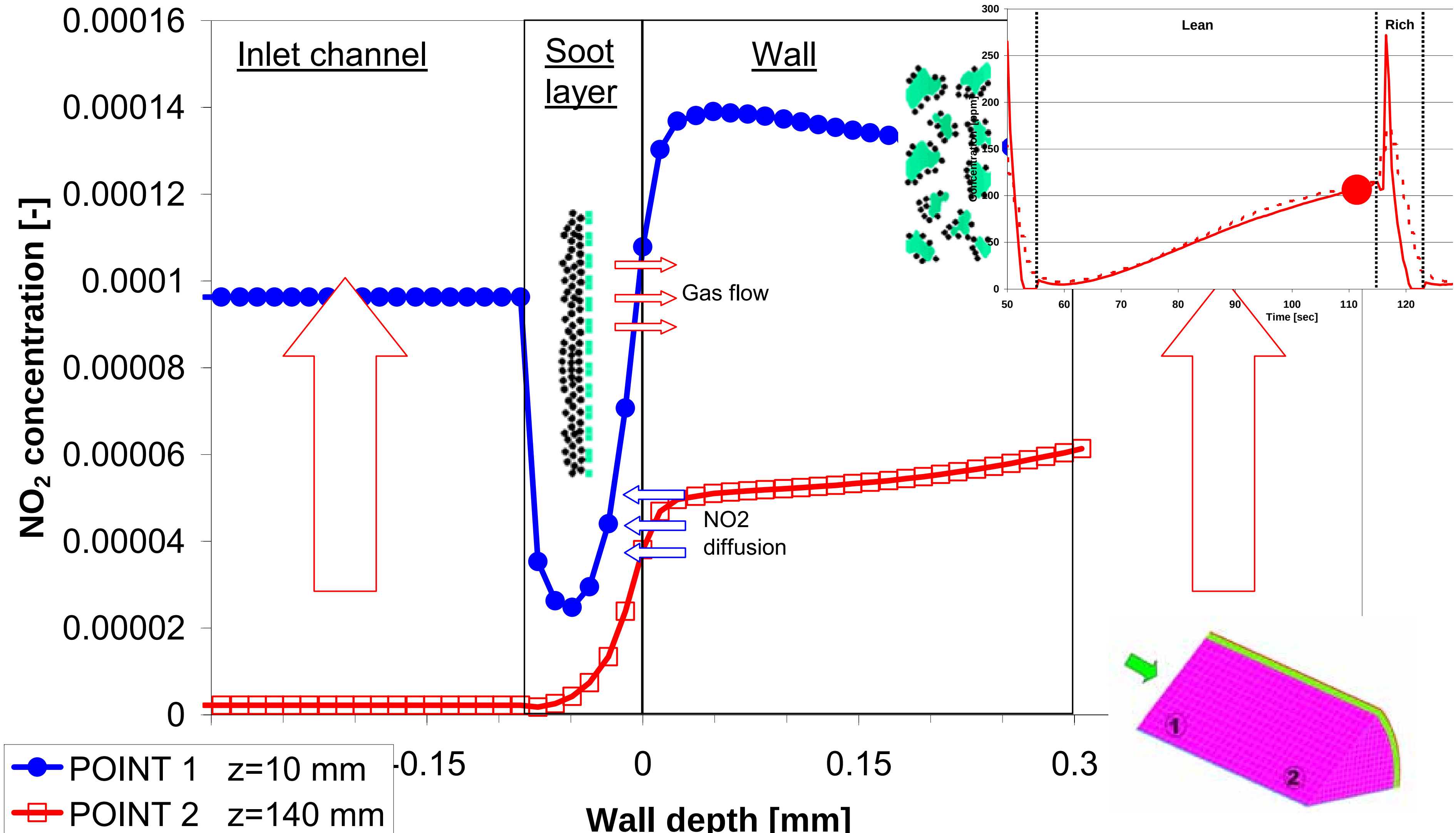
Intra-layer NO_2 profiles
t=114 s



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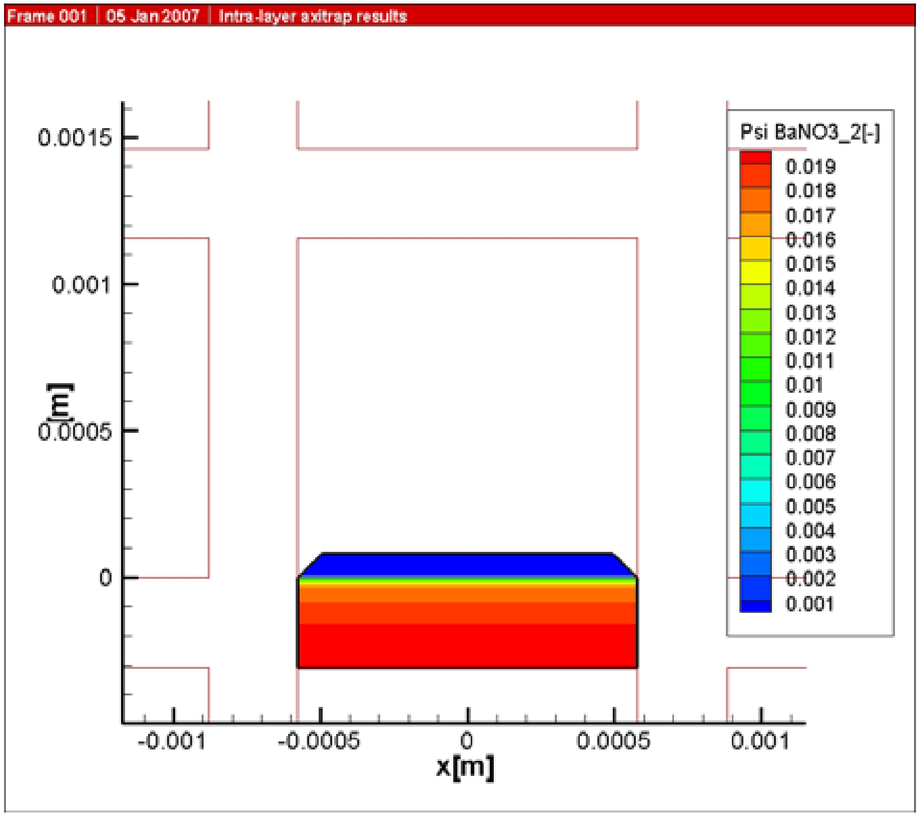
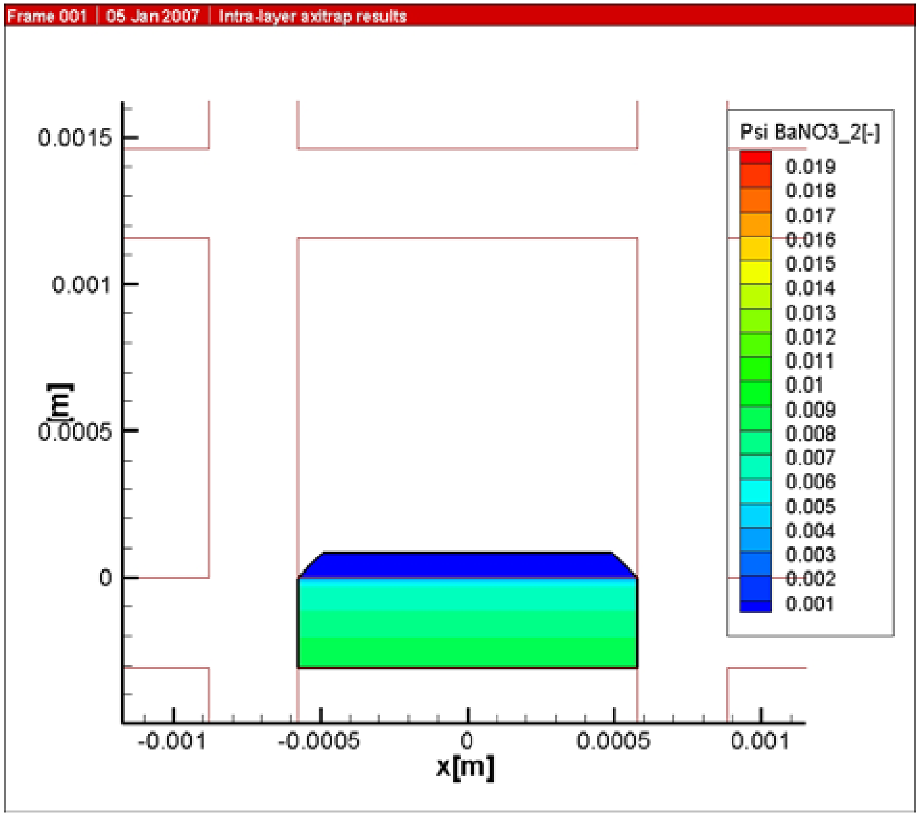
DPNR simulation example
Saturation profiles at the end of storage phase

Near filter entrance



Near filter exit



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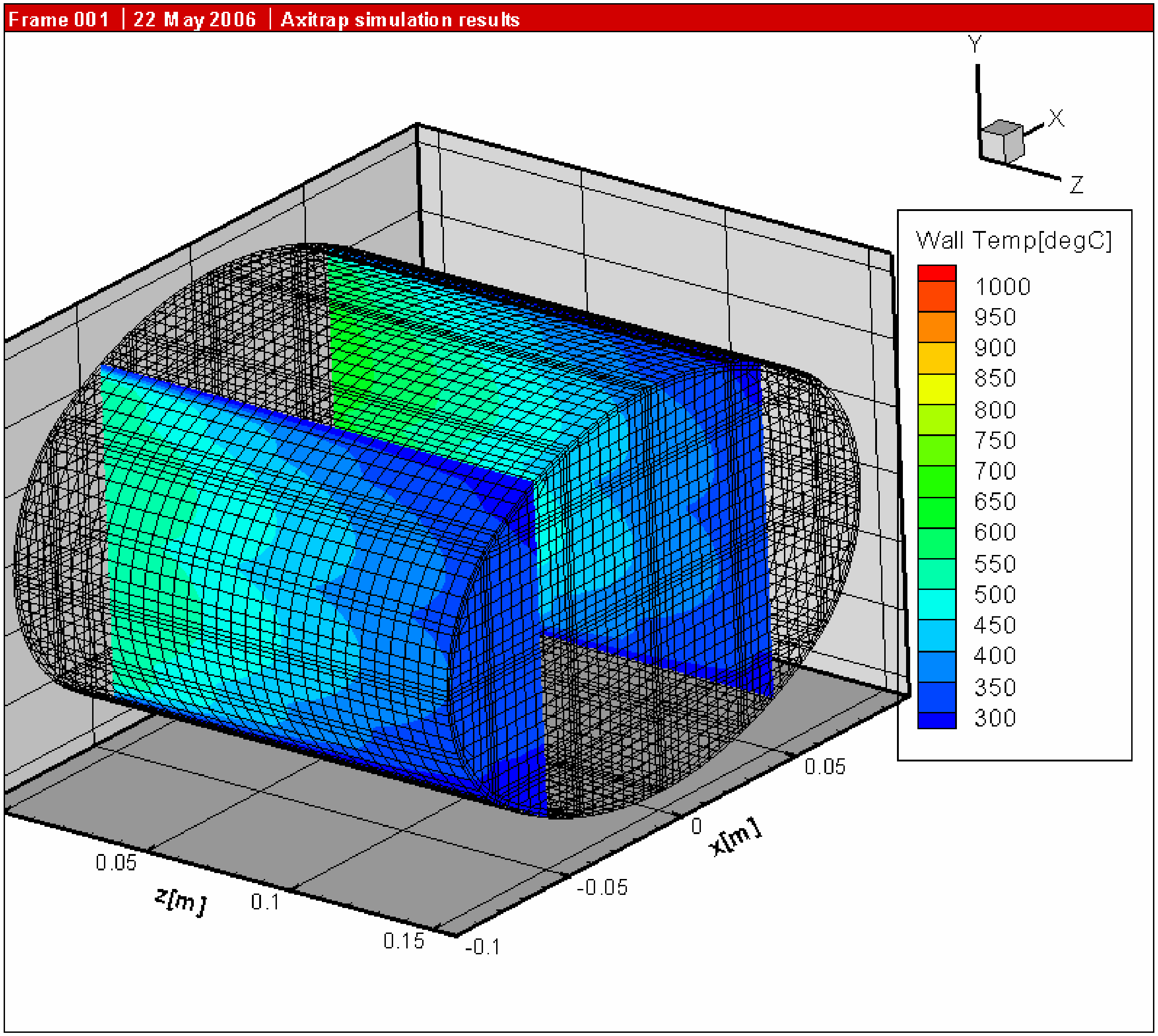
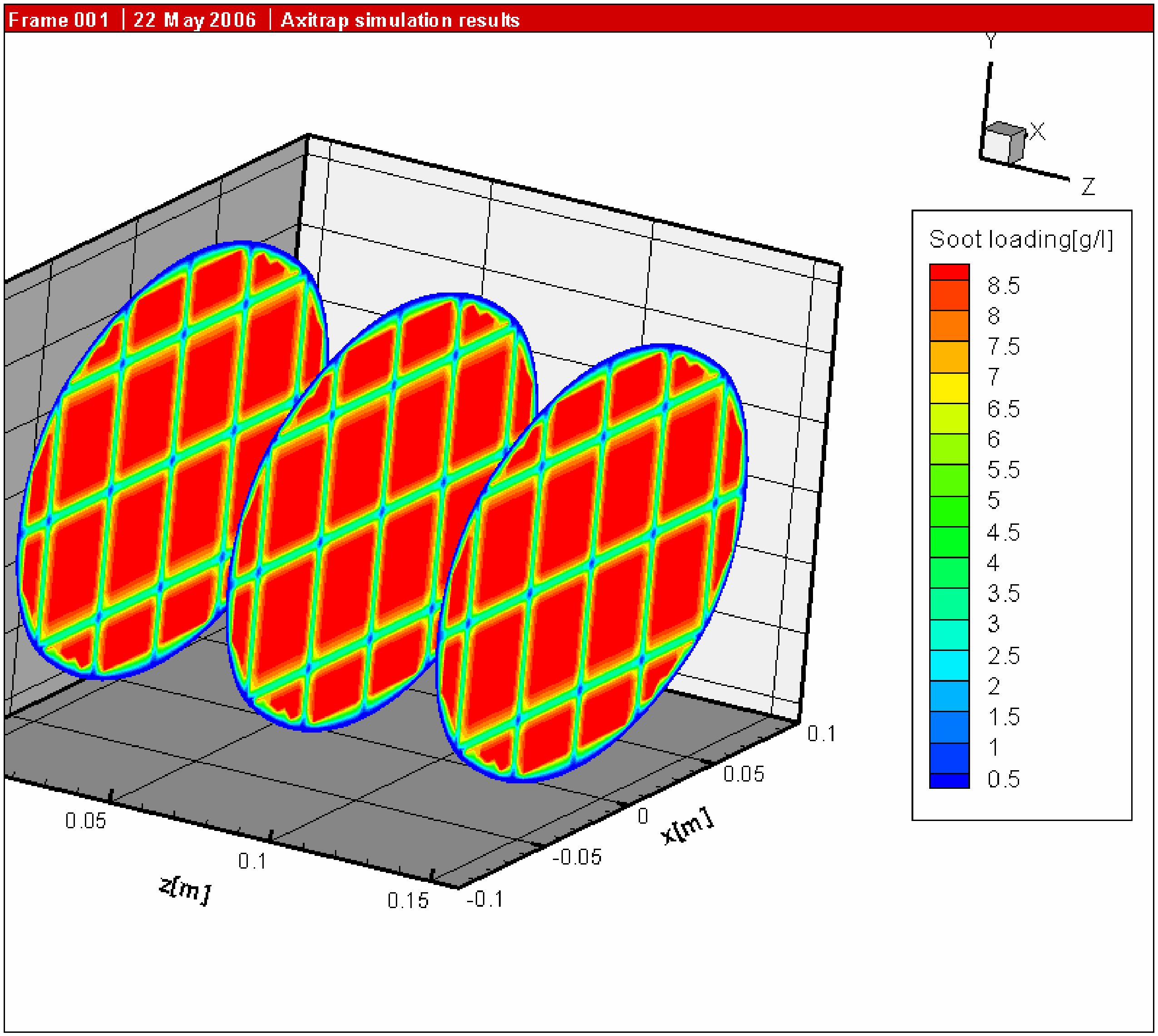
Catalytic DPF regeneration

Regeneration simulation example
Filter temperature calculation



Regeneration simulation example
Soot distribution calculation



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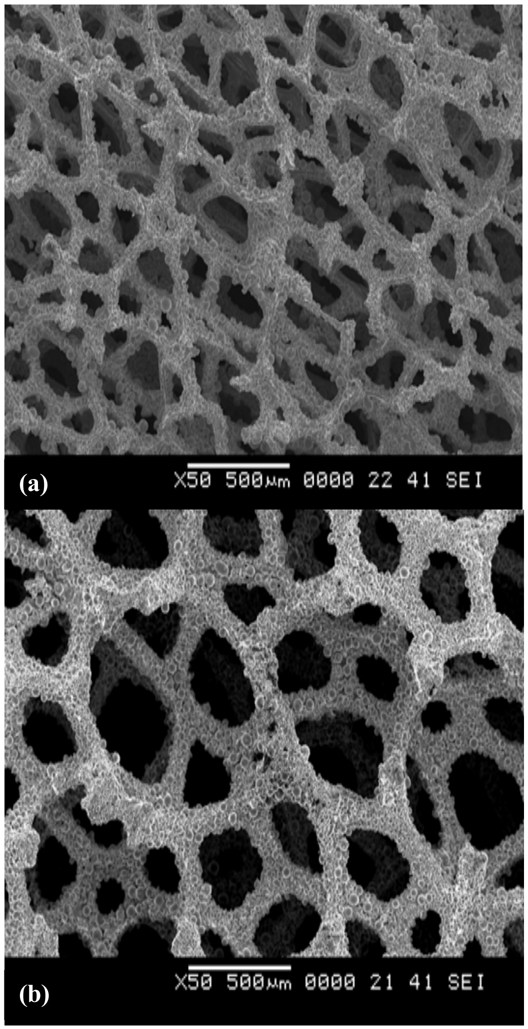
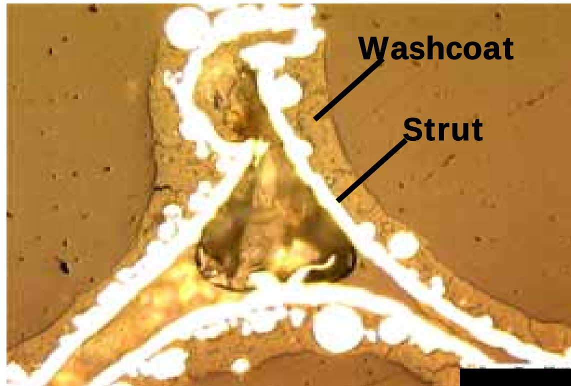
De-NO_x Modeling on Foam Substrates

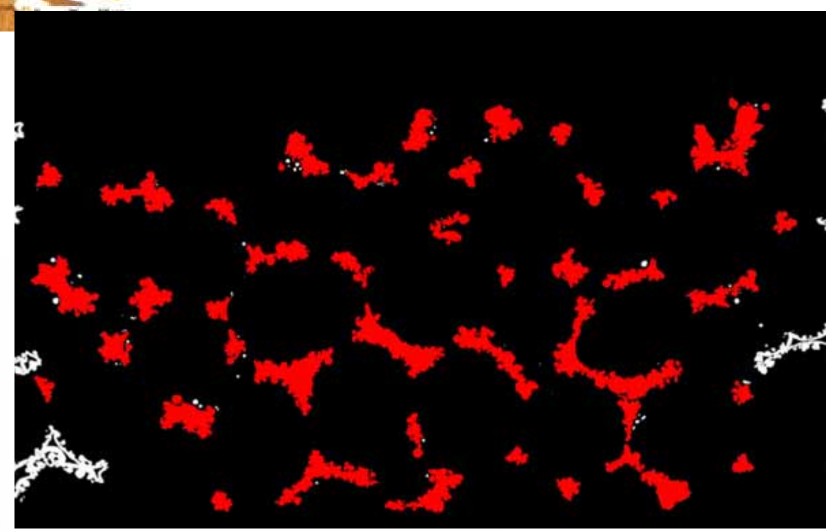
Foam morphology characterization
(example with INCOFOAM®HighTemp)

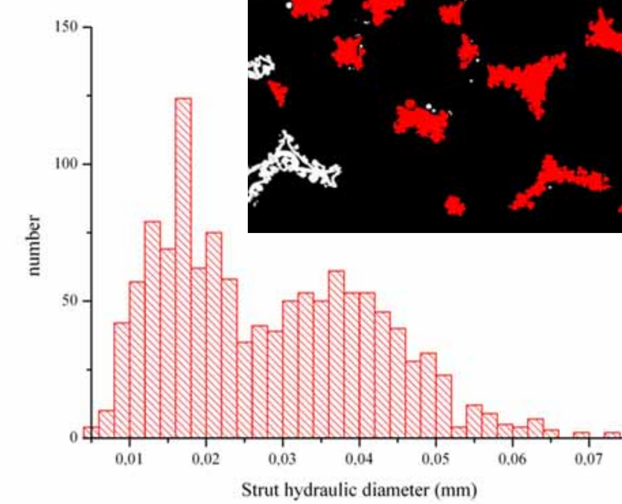


Uncoated metal foams



Coated foam cross-section





Optical characterization of microstructure

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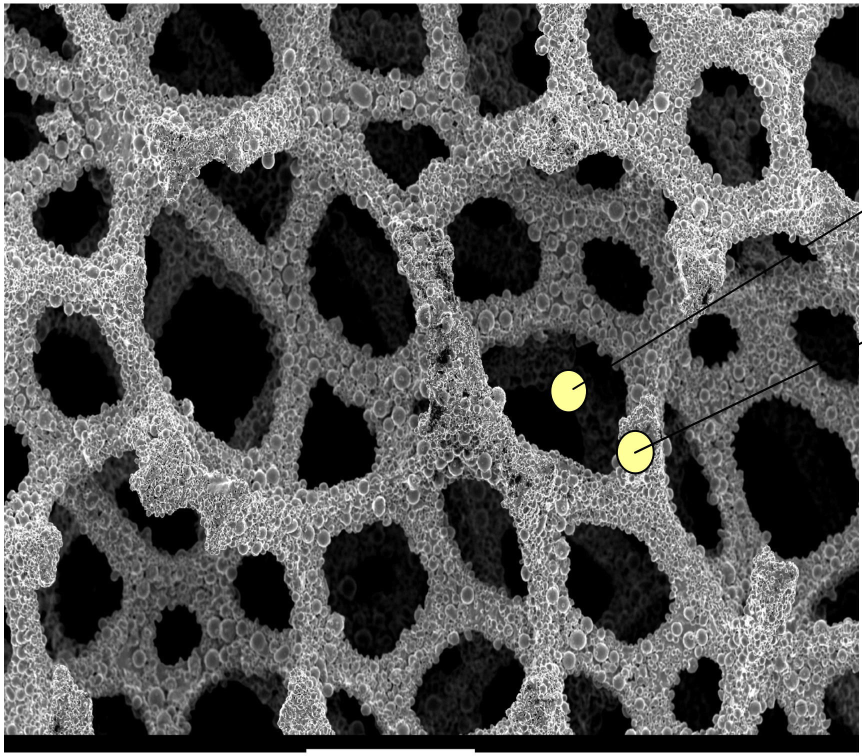
Definitions



Gas phase concentration: c_g

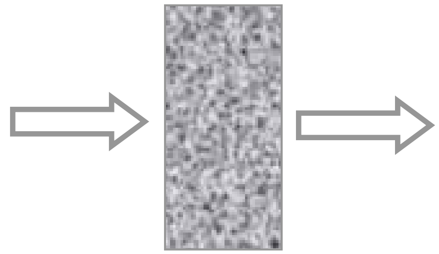
Surface concentration: c_s

The catalytic reaction rates are functions of c_s

$$R_1 = \frac{A_1 \cdot e^{-E_1/RT} \cdot c_{CO} \cdot c_{O_2}}{G_2}$$

Inhibition term depending on surface species concentrations

1-d modeling: Transport / Reaction
Axial flow concept



Gas energy balance

$$\rho_g v_g \frac{\partial T_g}{\partial x} = -h \cdot \left(\frac{S}{\varepsilon}\right) \cdot \left(T_g - T_s\right)$$

Gas species balance

$$\frac{\partial \left(v_g c_g\right)}{\partial x} = -k_j \cdot \left(\frac{S}{\varepsilon}\right) \cdot \left(c_{g,j} - c_{s,j}\right)$$

Transient energy balance

$$\underbrace{\rho_s C_{p,s} \frac{\partial T_s}{\partial t}}_{\text{Solid heat capacity}} = \underbrace{\lambda_s \frac{\partial^2 T_s}{\partial x^2}}_{\text{Conduction}} + \underbrace{h\left(\frac{S}{1-\varepsilon}\right)\left(T_g - T_s\right)}_{\text{Convection}} - \underbrace{\frac{1}{1-\varepsilon}\sum_{k=1}^{n_k} \Delta H_k R_k}_{\text{Reaction heat}}$$

$$\frac{\rho_g}{M_g} k_j \left(\frac{S}{\varepsilon}\right)\left(c_{g,j} - c_{s,j}\right) = R_j$$

Mass-transfer rate = reaction rate

Heat / mass transfer coefficients

Heat transfer coefficient

$$h = \frac{Nu \cdot k_g}{d_s}$$

$$Re = \frac{\rho_{gas} \cdot \upsilon_f \cdot d_s}{\eta_{gas}}$$

$$Nu = A \cdot Re^{0.43} \cdot Pr^{1/3}$$

$$Pr = \frac{\eta_g C_{p,g}}{k_g}$$

Mass transfer coefficient

$$k_j = \frac{Sh \cdot D_j}{d_s}$$

$$Sh_i = A \cdot Re^{0.43} \cdot Sc_i^{1/3}$$

$$Sc_i = \frac{\eta_g}{\rho_g \cdot D_i}$$

Parameter to be calibrated from experiments (A)

D_j	Species diffusivity
ρ_{gas}	Gas density
υ_f	Face velocity
d_s	Mean strut diameter
η_{gas}	Dynamic gas viscosity

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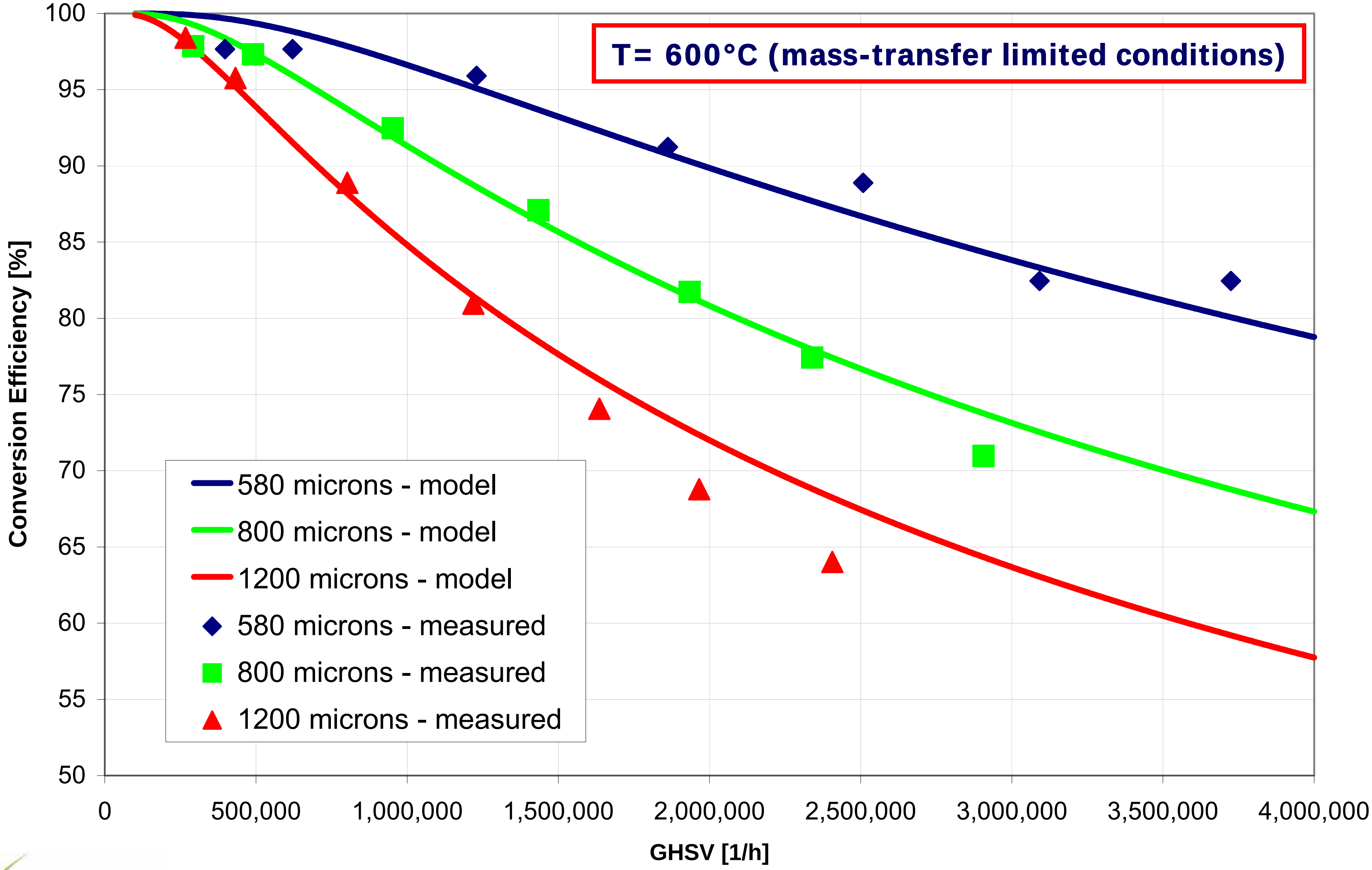
Foam model calibration



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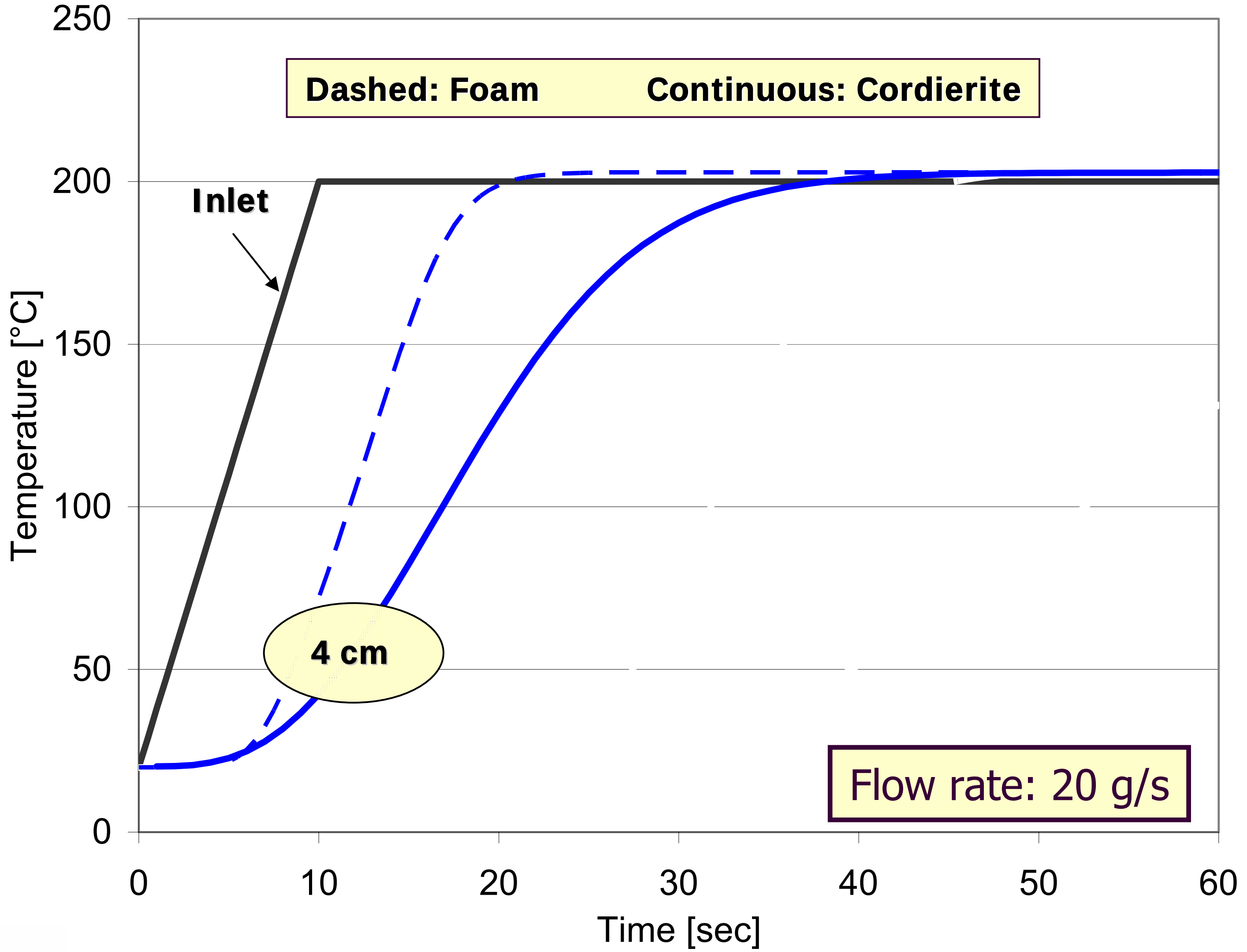
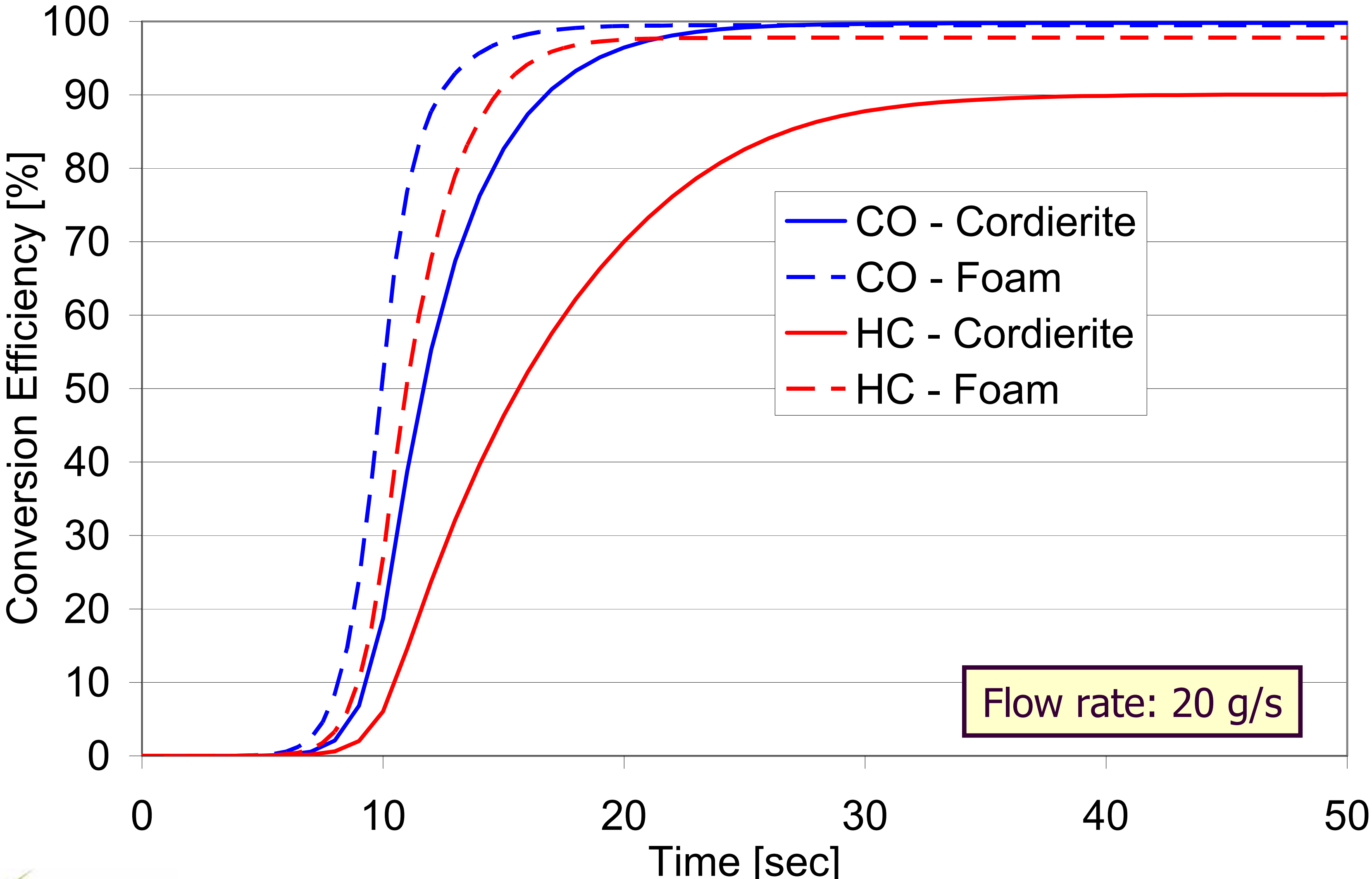
Temperature response modeling study
Foam 1200 microns vs Cordierite 400 cpsi



CO, HC conversion efficiency vs time
Length: 4 cm



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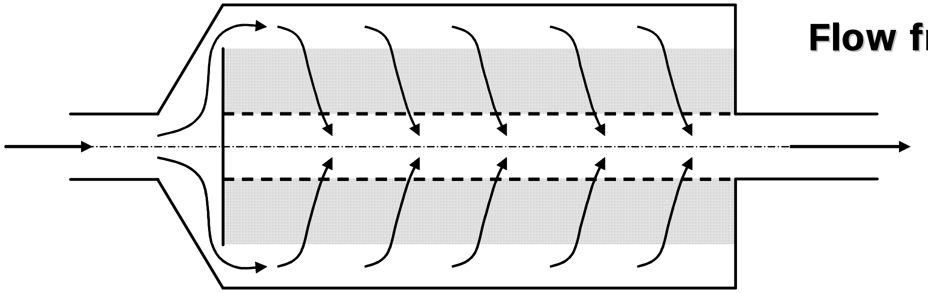
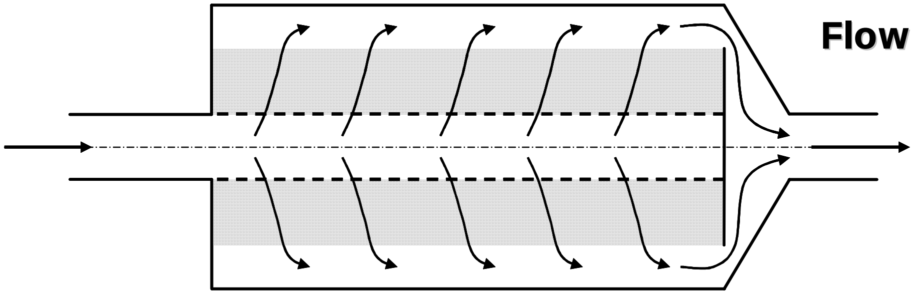
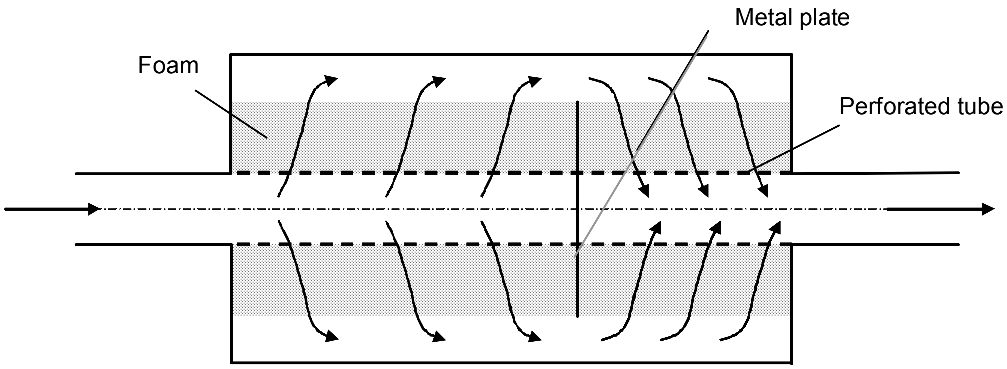
2-d modeling
"Radial flow", "Cross flow" designs







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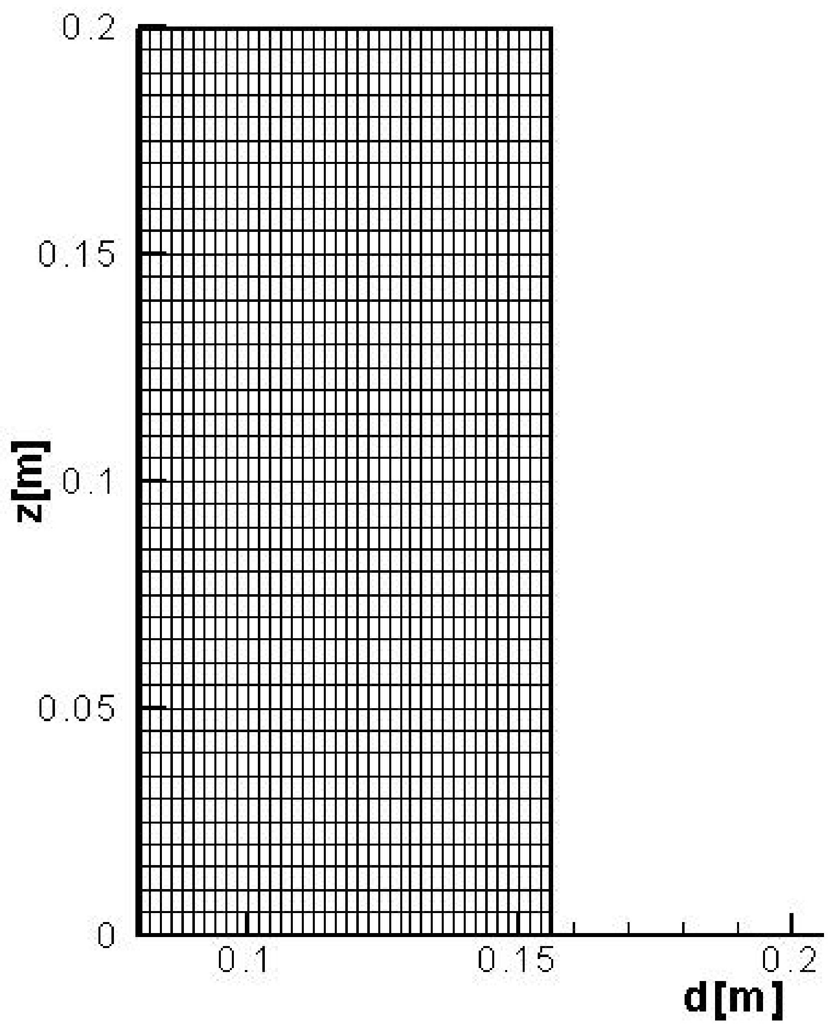
2-d modeling for “radial-flow” or “cross-flow” designs

- Solution of
  - Mass balance
  - Momentum balance
  - Energy balance
  - Species balance
- The filtration equations are also applied in each node
- The equations are solved in the gas channels and the foam phase



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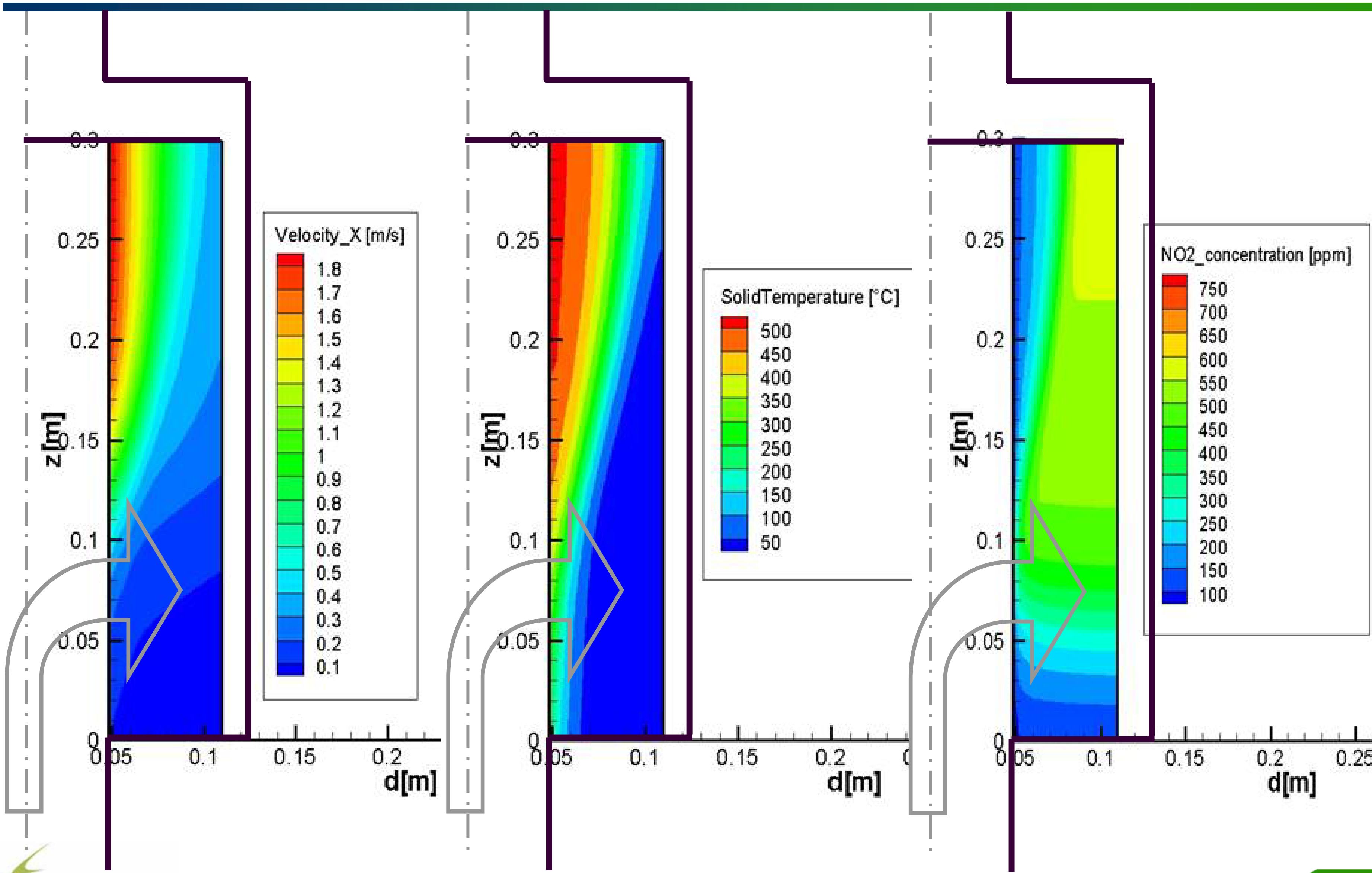
Transient 2-d simulation of foam catalyst warm-up
Time = 5 s



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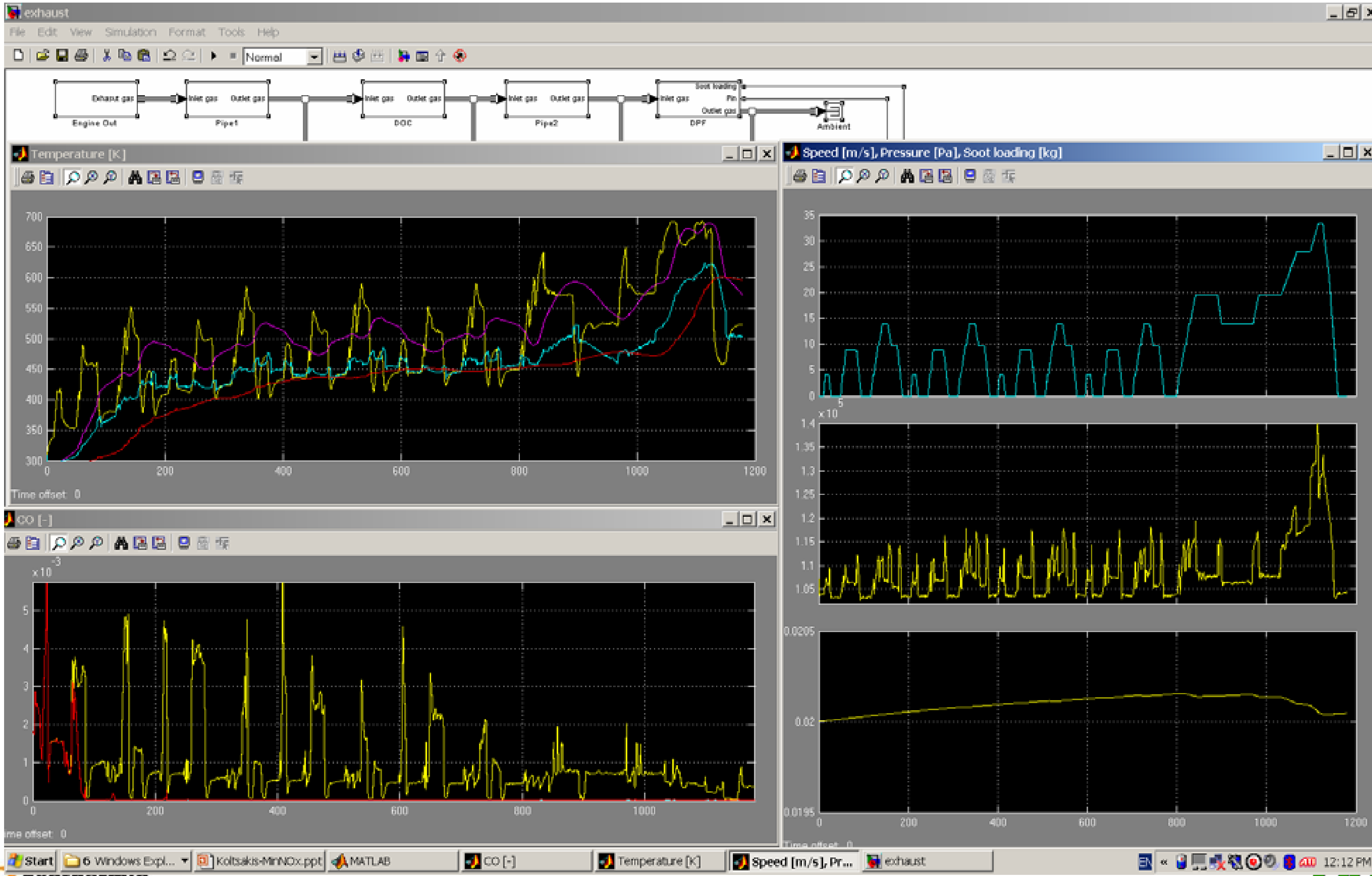
Integrated exhaust line simulation

System simulation
in MATLAB/SIMULINK environment



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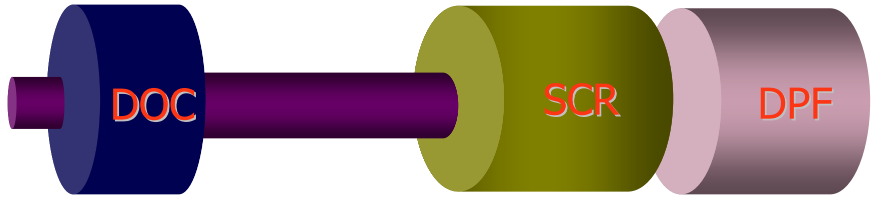
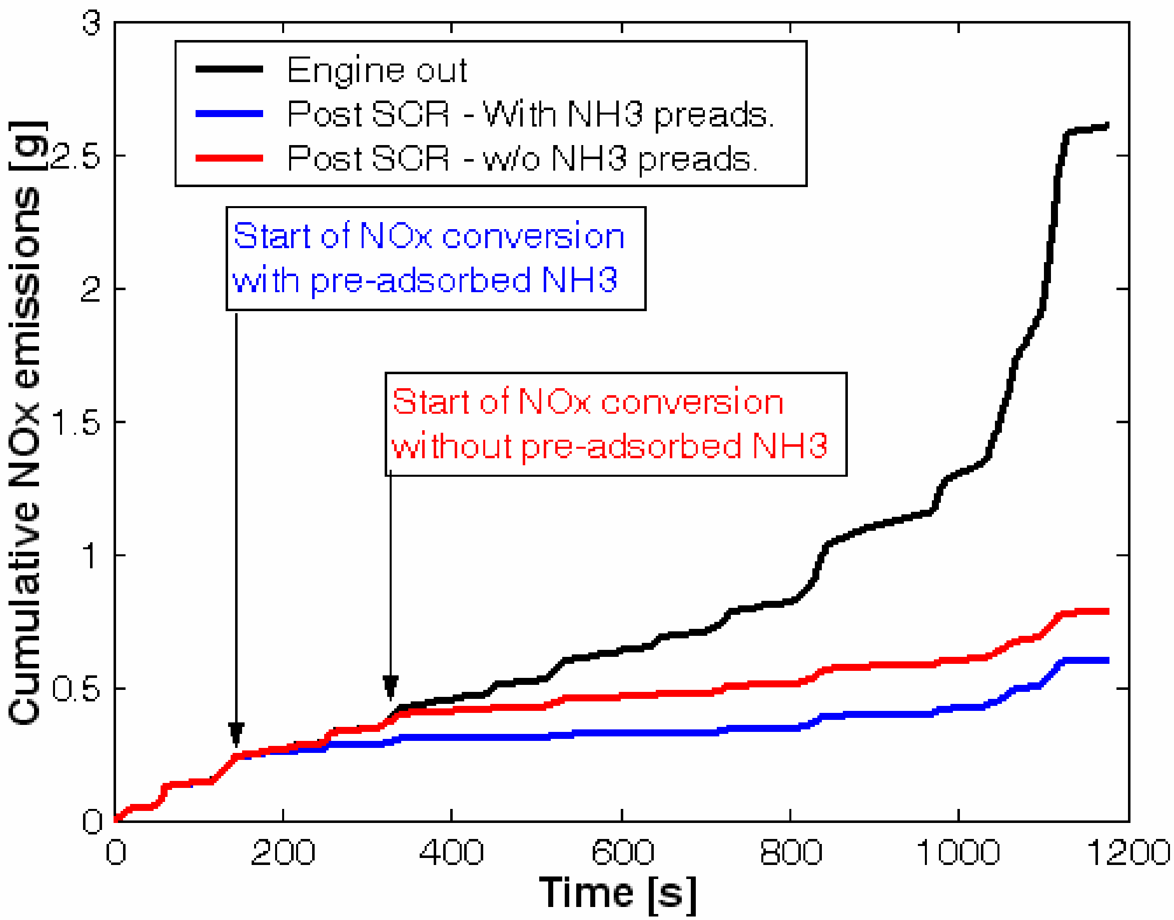
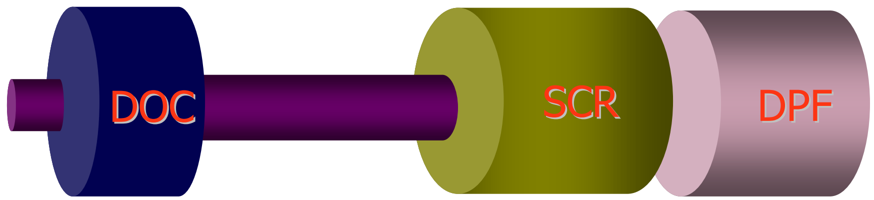
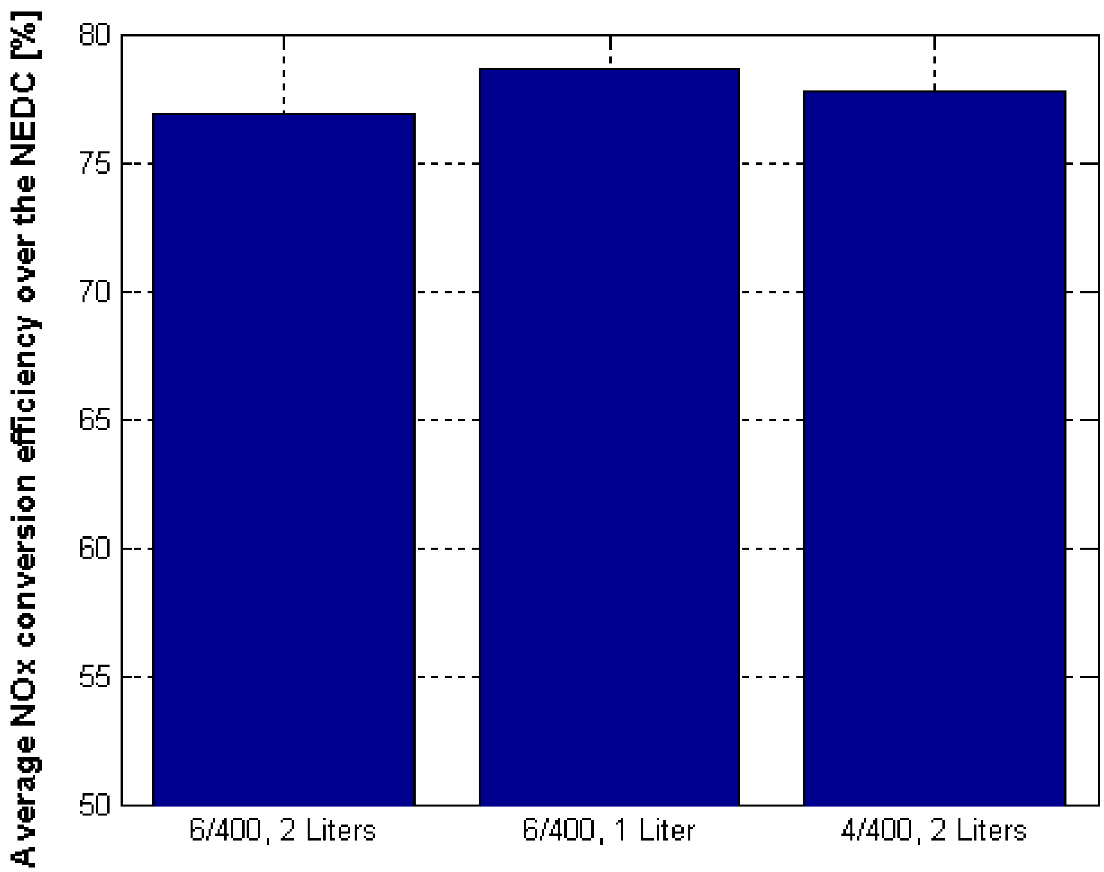
Reactors in series
Effect of NH_3 pre-adsorption





Reactors in series
Effect of DOC geometry





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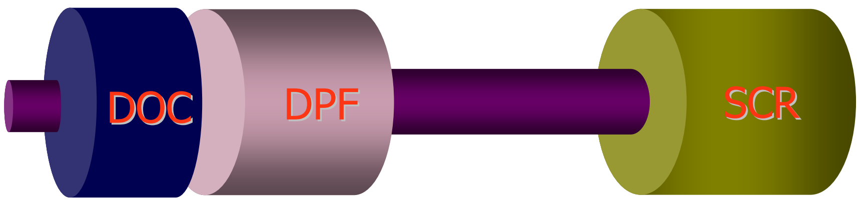
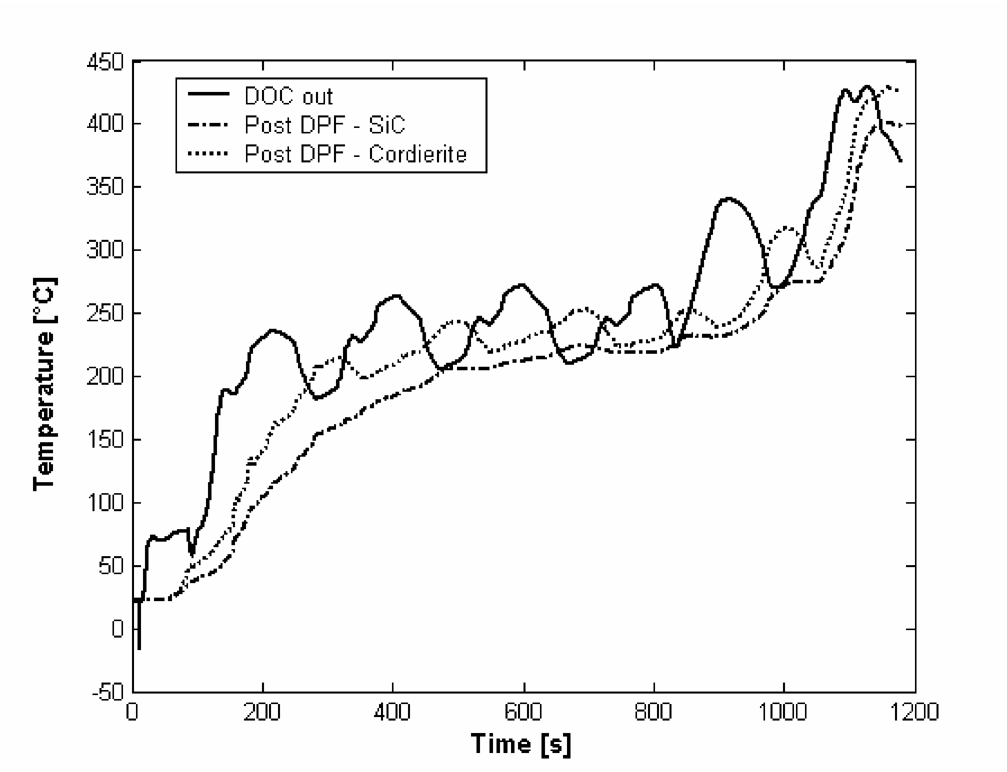
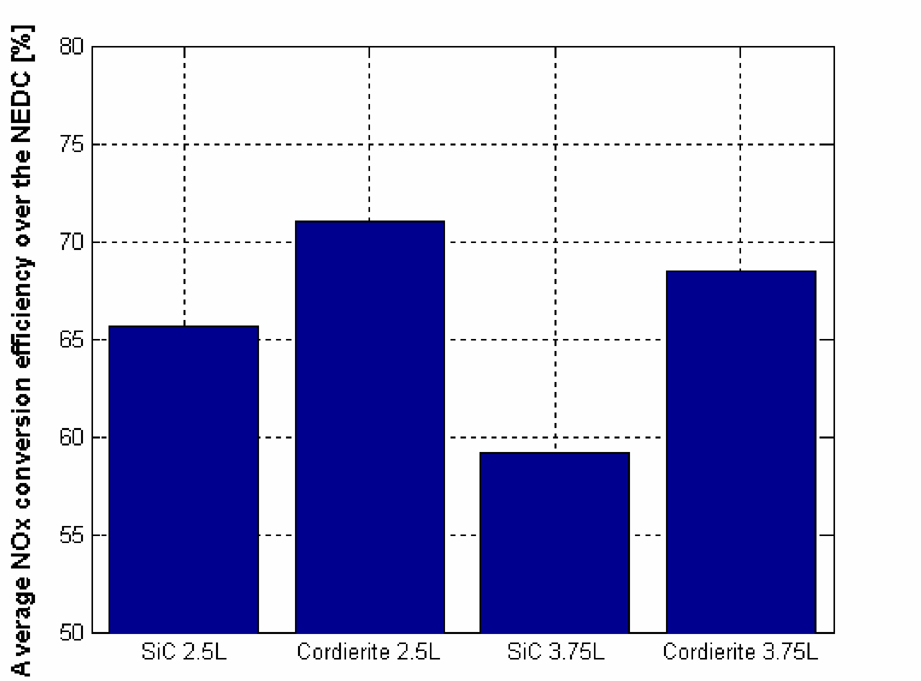
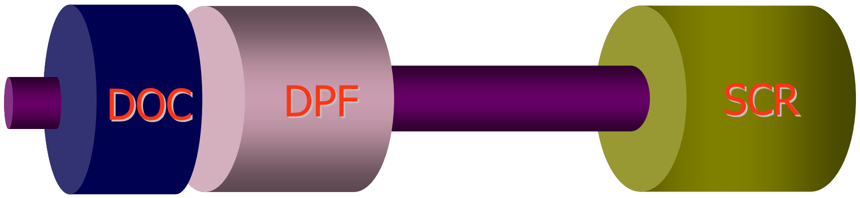
Reactors in series
Effect of DPF size, material

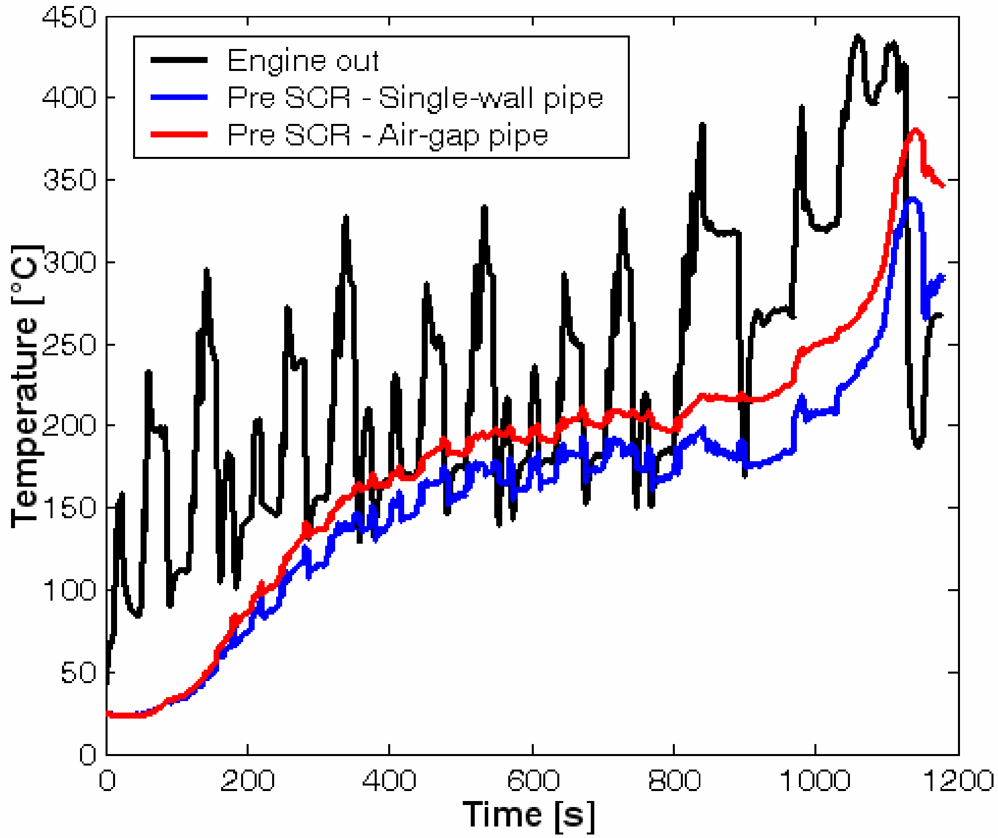


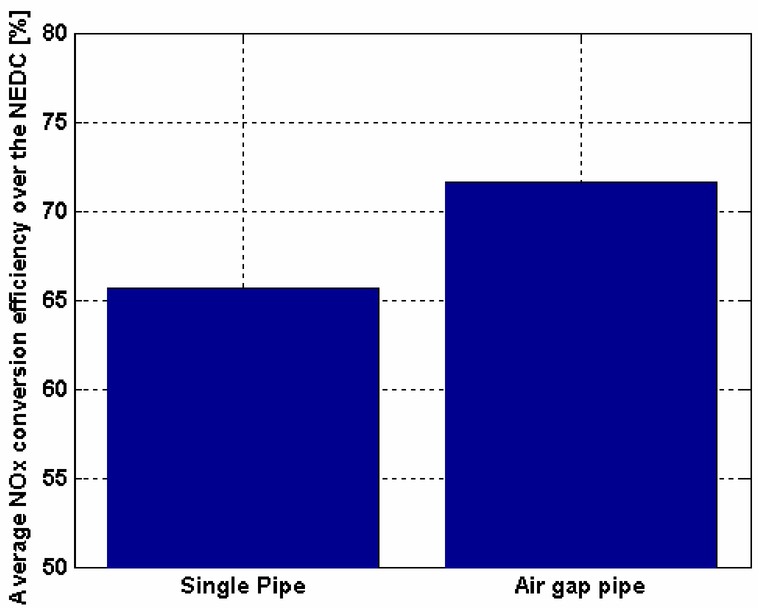




Effect of pipe insulation







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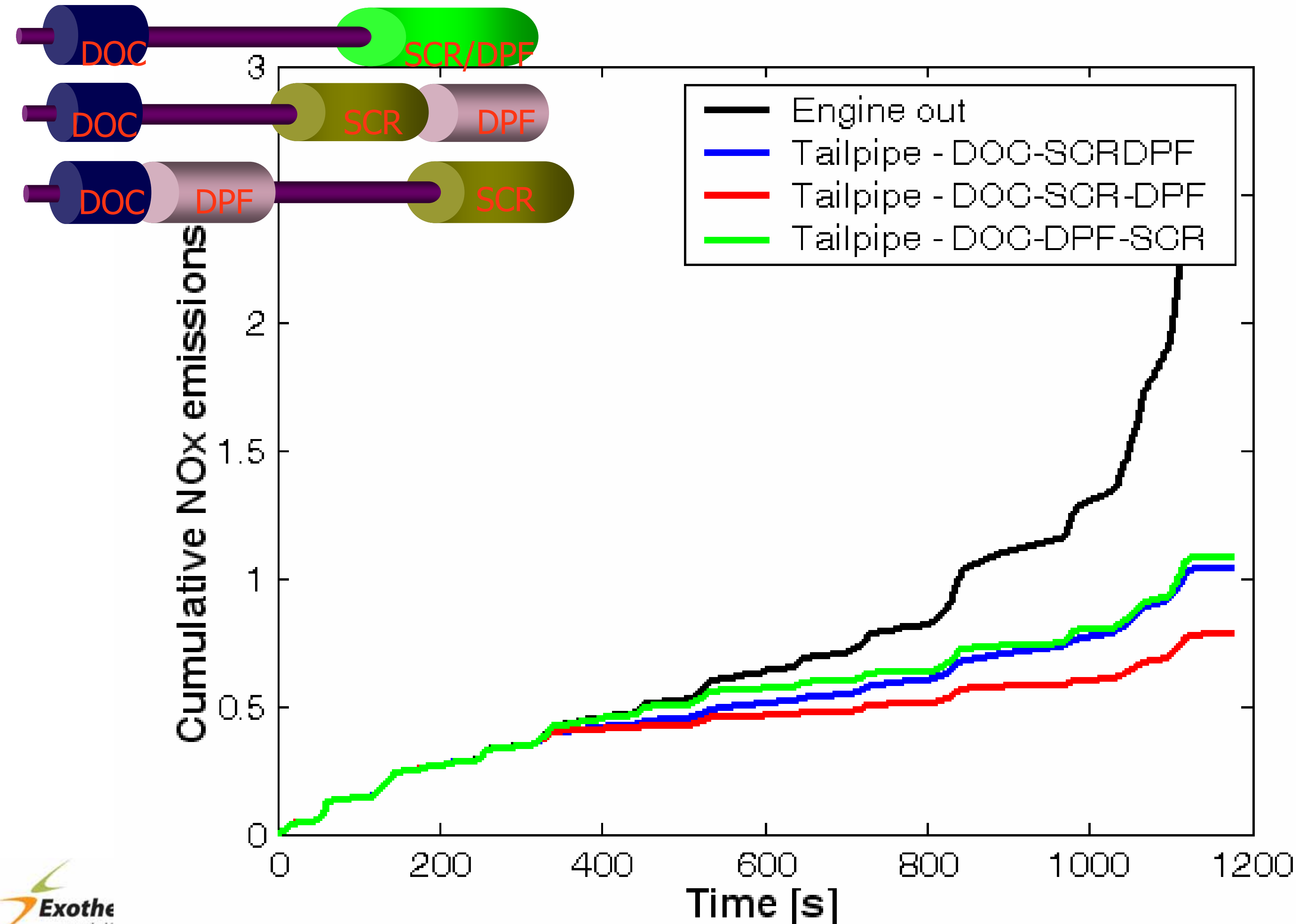
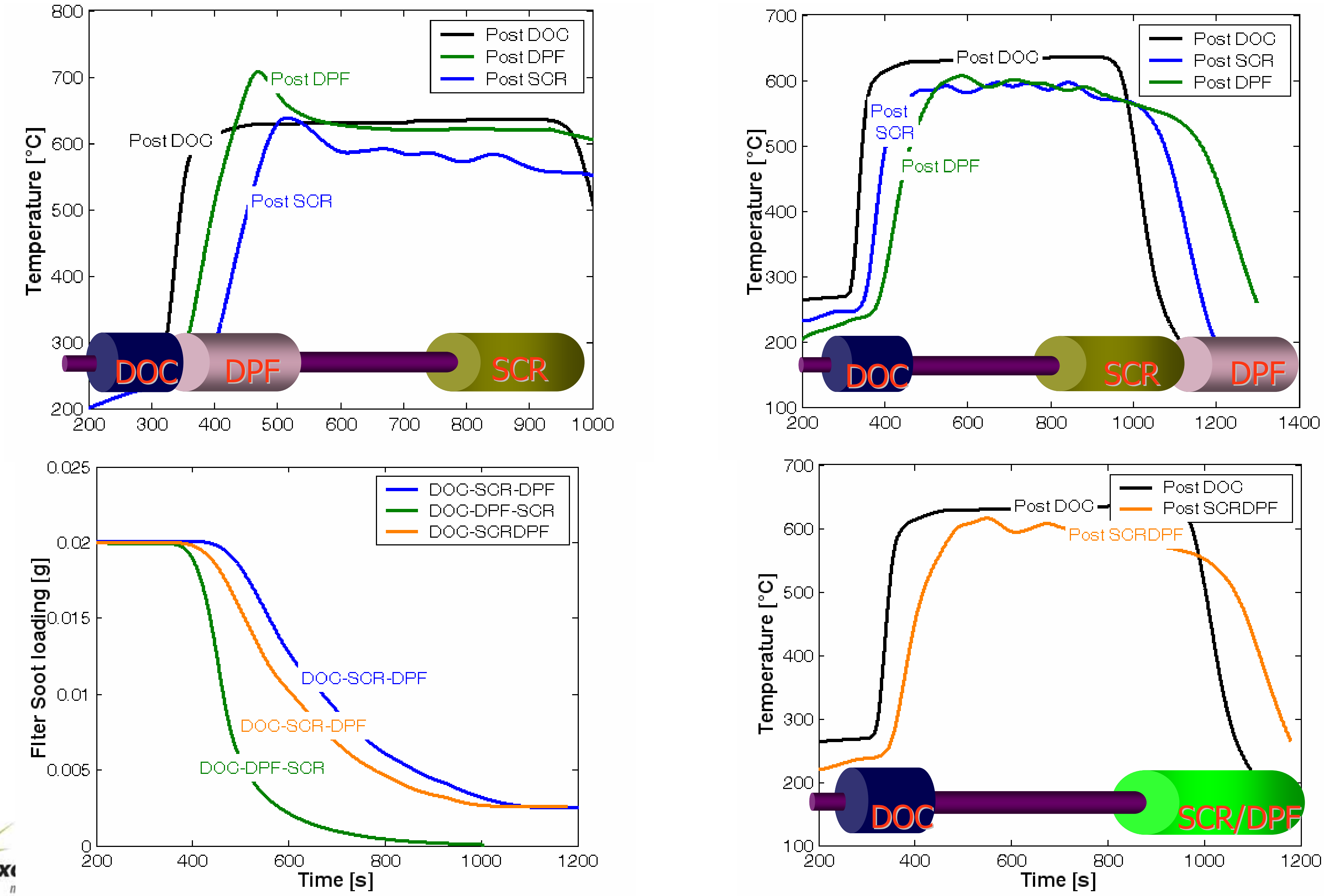
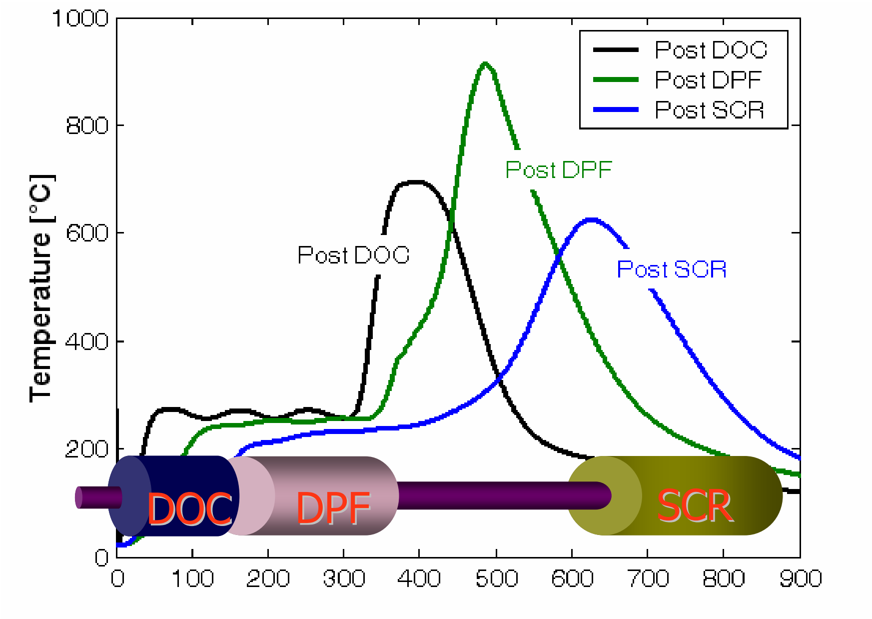
Comparison of various positioning strategies, including "wall-flow" SCR

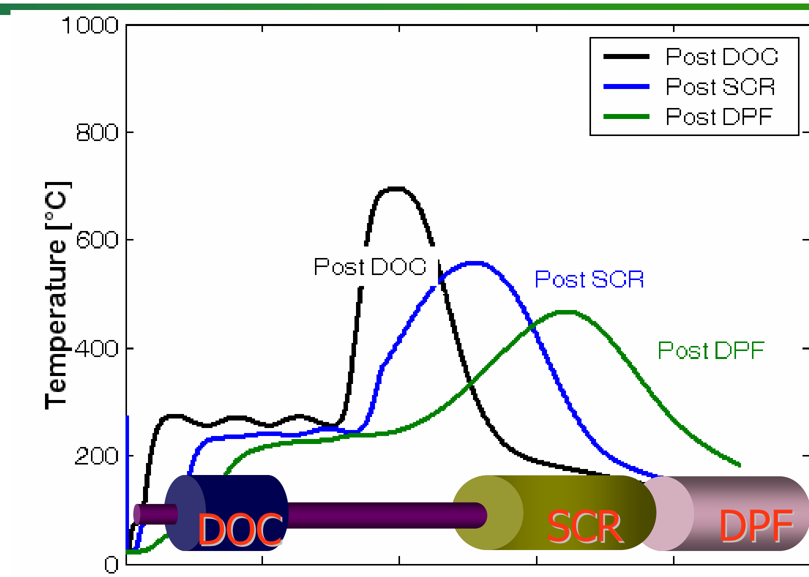


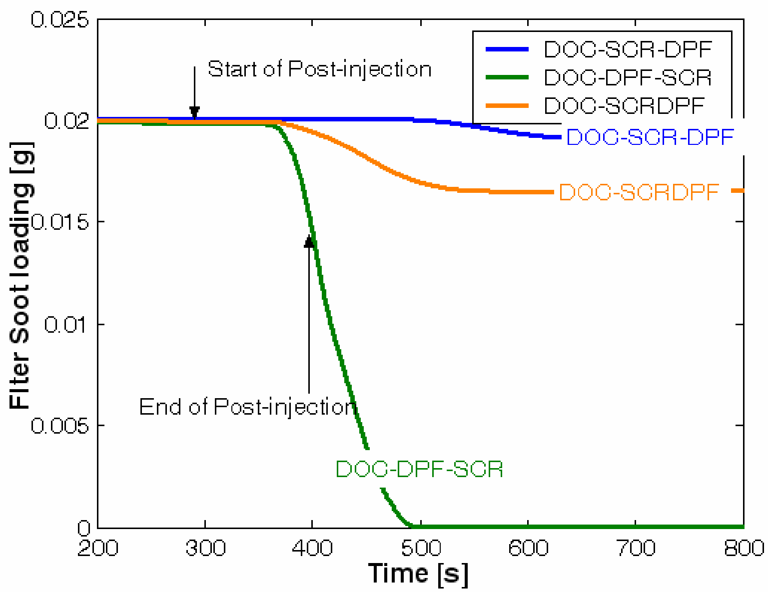
Controlled regeneration

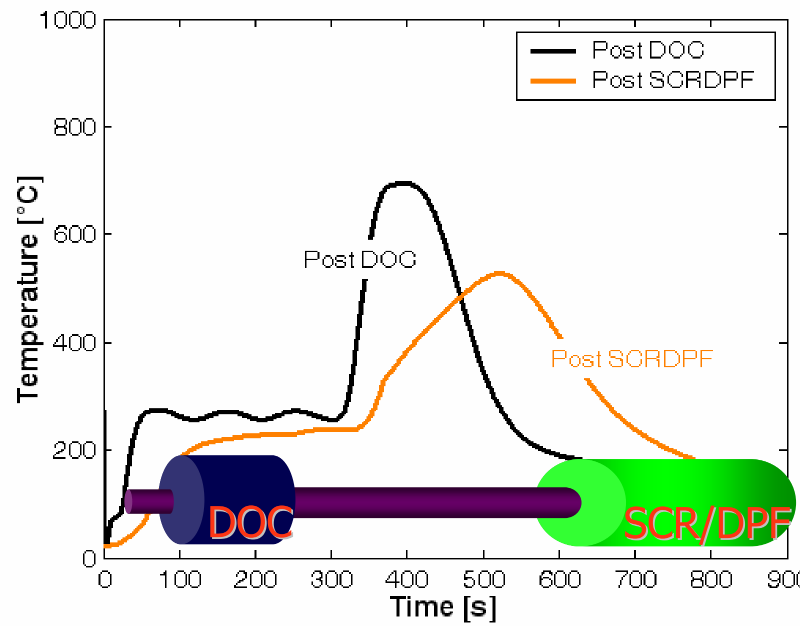


Uncontrolled regeneration

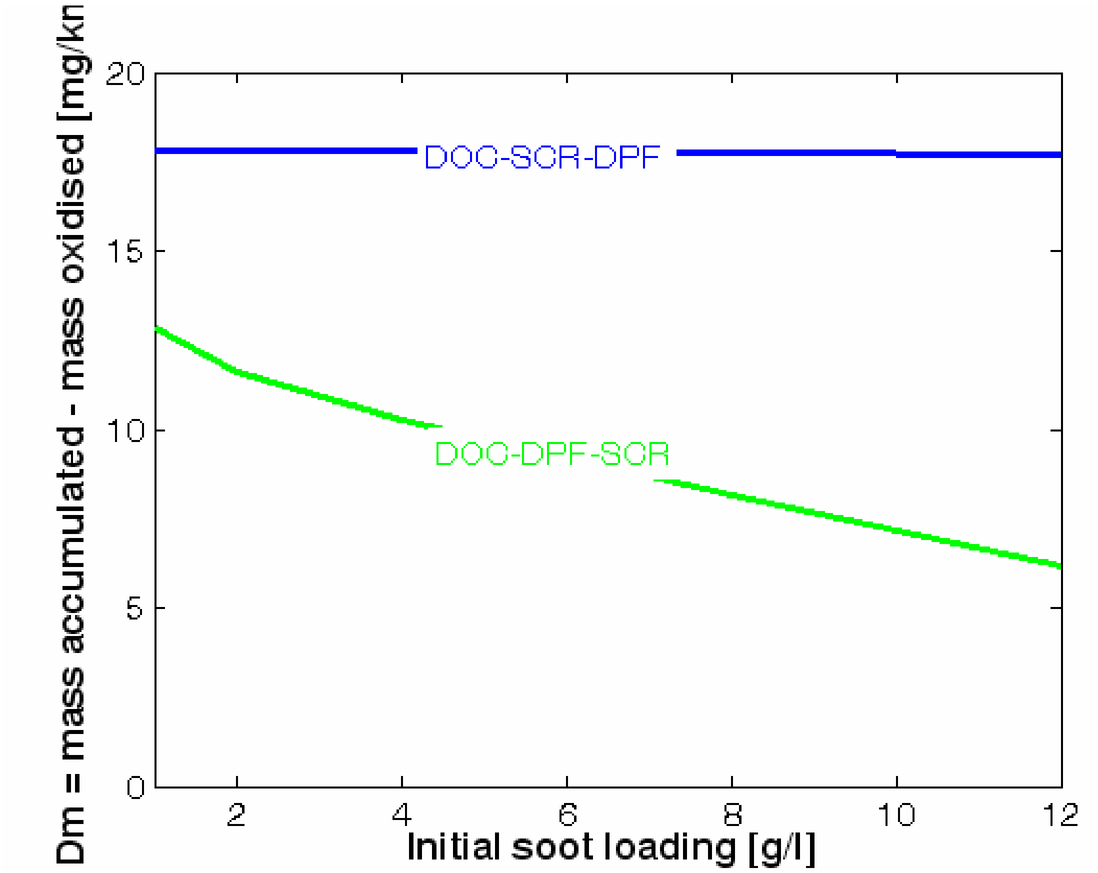








Effect of passive regeneration
Soot accumulation rate in successive European Driving Cycles



Summary
Flow-through reactors

- DOC modeling
  - HC adsorption
  - Radial effects
- LNT modeling
  - T dependence of effective NOx storage capacity
  - Effect of OSC during regeneration
  - Sulfation/desulfation
- SCR modeling
  - NO/NO_2 ratio
  - NH_3 adsorption/desorption

Summary
4-way reactors

- CDPF modeling
  - Transport-reaction modeling
  - Catalyst zoning (axially/intra-wall)
  - 3-d regeneration modeling
- Wall-flow de-NO_x modeling (NSC, SCR)
  - Axial, intra-wall variations
- Foam de-NO_x modeling
  - Filtration/Flow/Heat transfer interactions
- System simulation
  - Emission cycle predictions
  - Passive/active regeneration predictions