From zero to four-dimensional after-treatment models: needs and challenges

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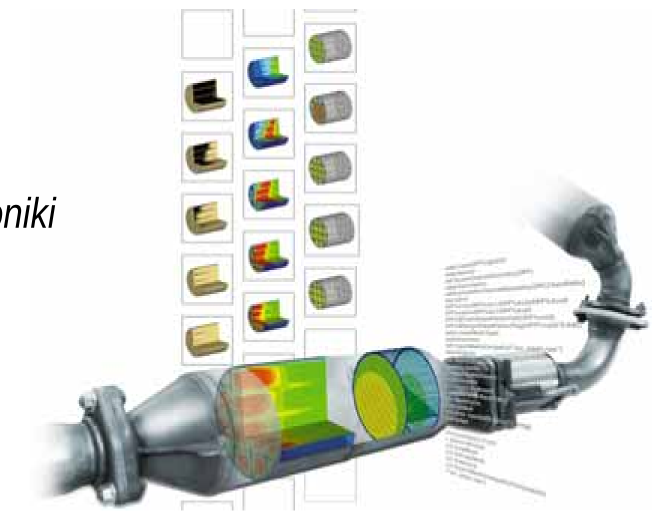

Contents

- *How many dimensions we need for after-treatment modeling?*
- Definitions – fundamentals
- DPF modeling
  - Significance intra-layer modeling
  - Channel and filter scale
  - “3-dimensional” effects
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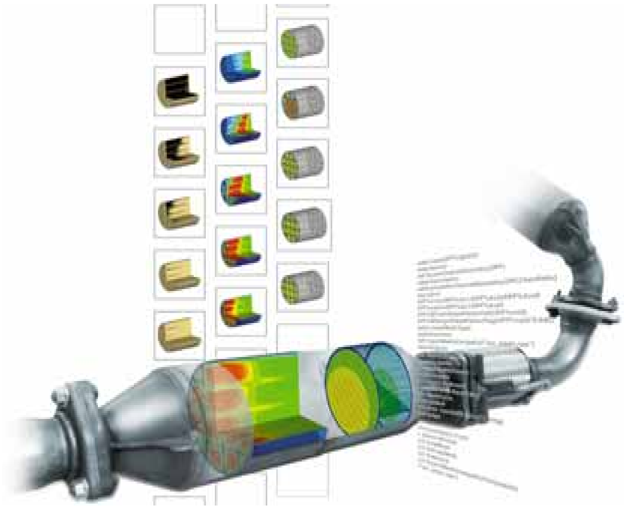
- Flow-through catalyst modeling
  - Flow maldistribution
  - Reductant maldistribution
- Integrated 1d/3d exhaust system modeling
  - Components in series
  - Components in parallel

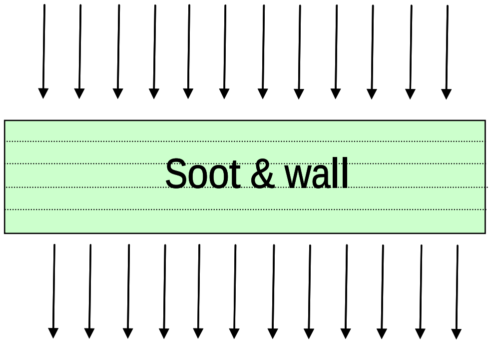
Fundamentals

Definitions and modeling scales
in the case of wall-flow DPF modeling



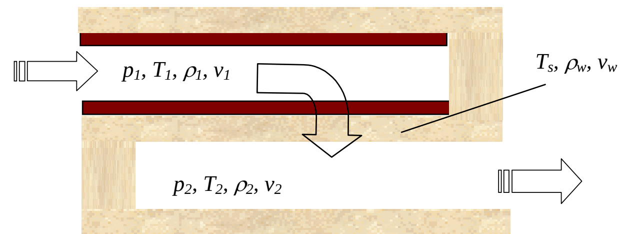
Definitions

0-d

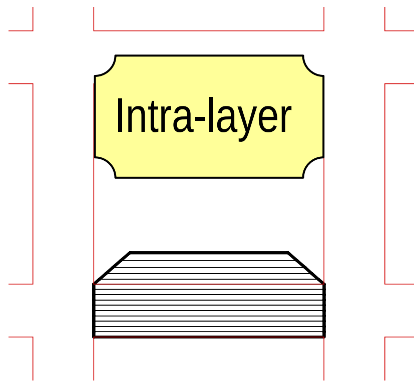


Representative channel
& axial uniformity

1-d

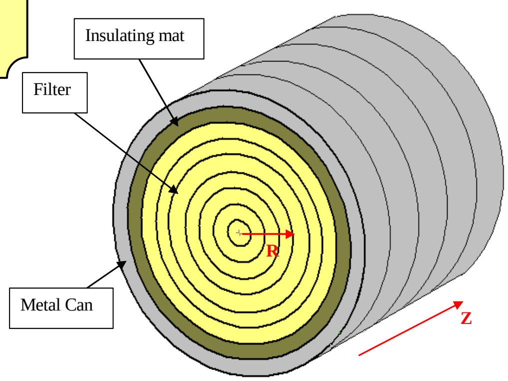


Representative channel
(adiabatic, uniform inlet flow)



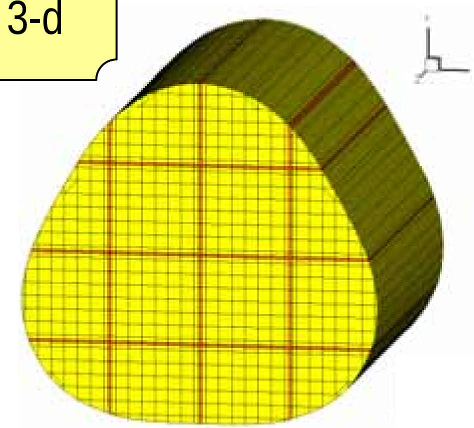
Catalyst effects
soot layer properties

2-d



Axi-symmetric, non-segmented filter
(circular shape, symmetric flow distribution)

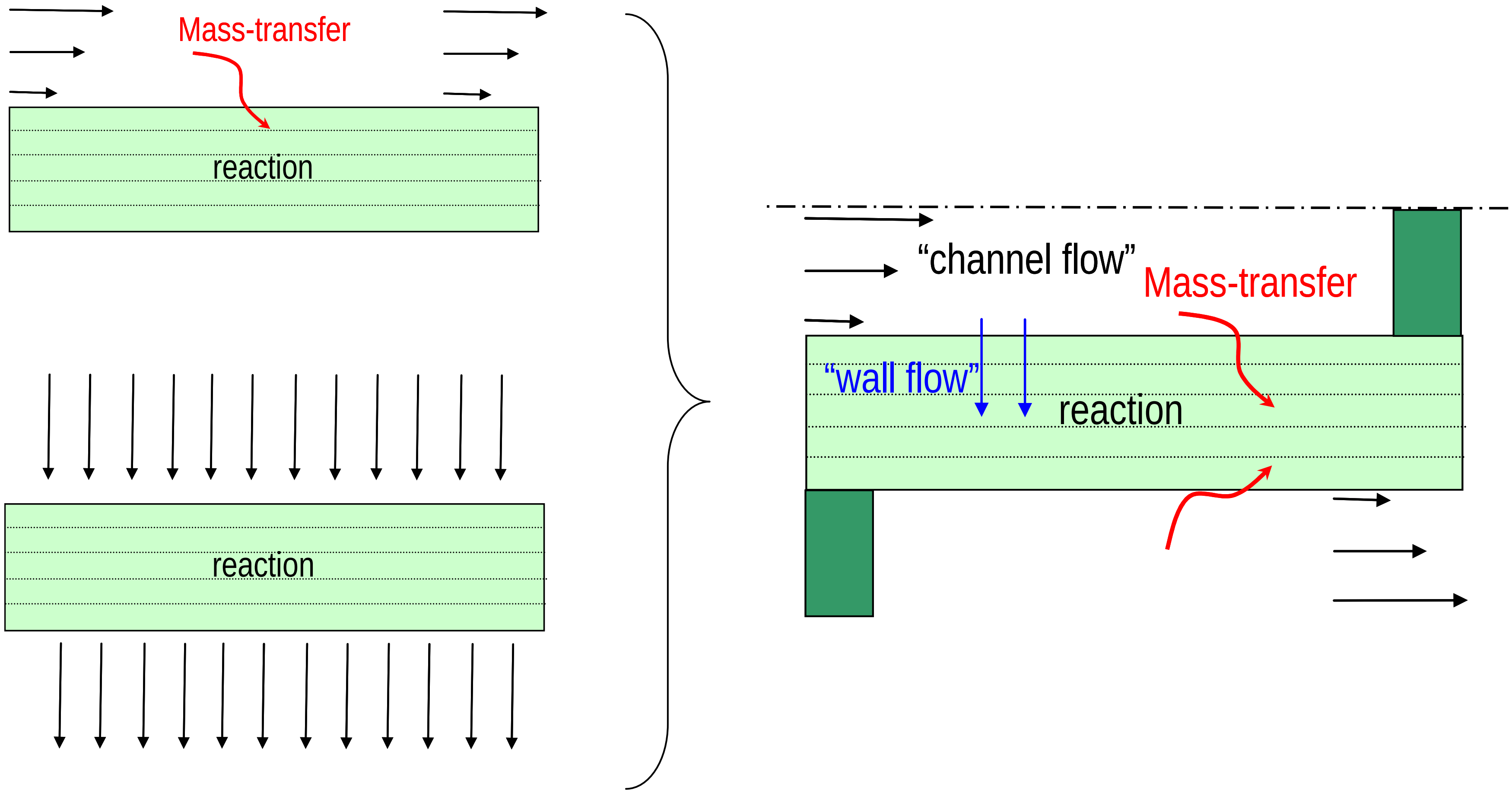
3-d



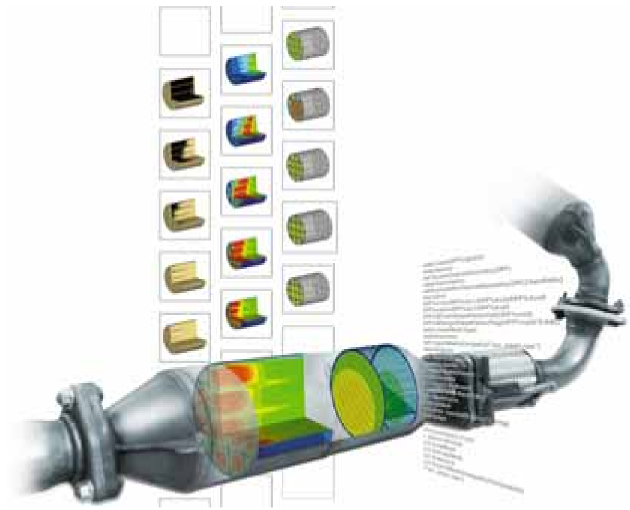
Random shape, segmentation
any flow distribution

The challenge of catalyzed DPF modeling
Mixed reactor

Exothermia



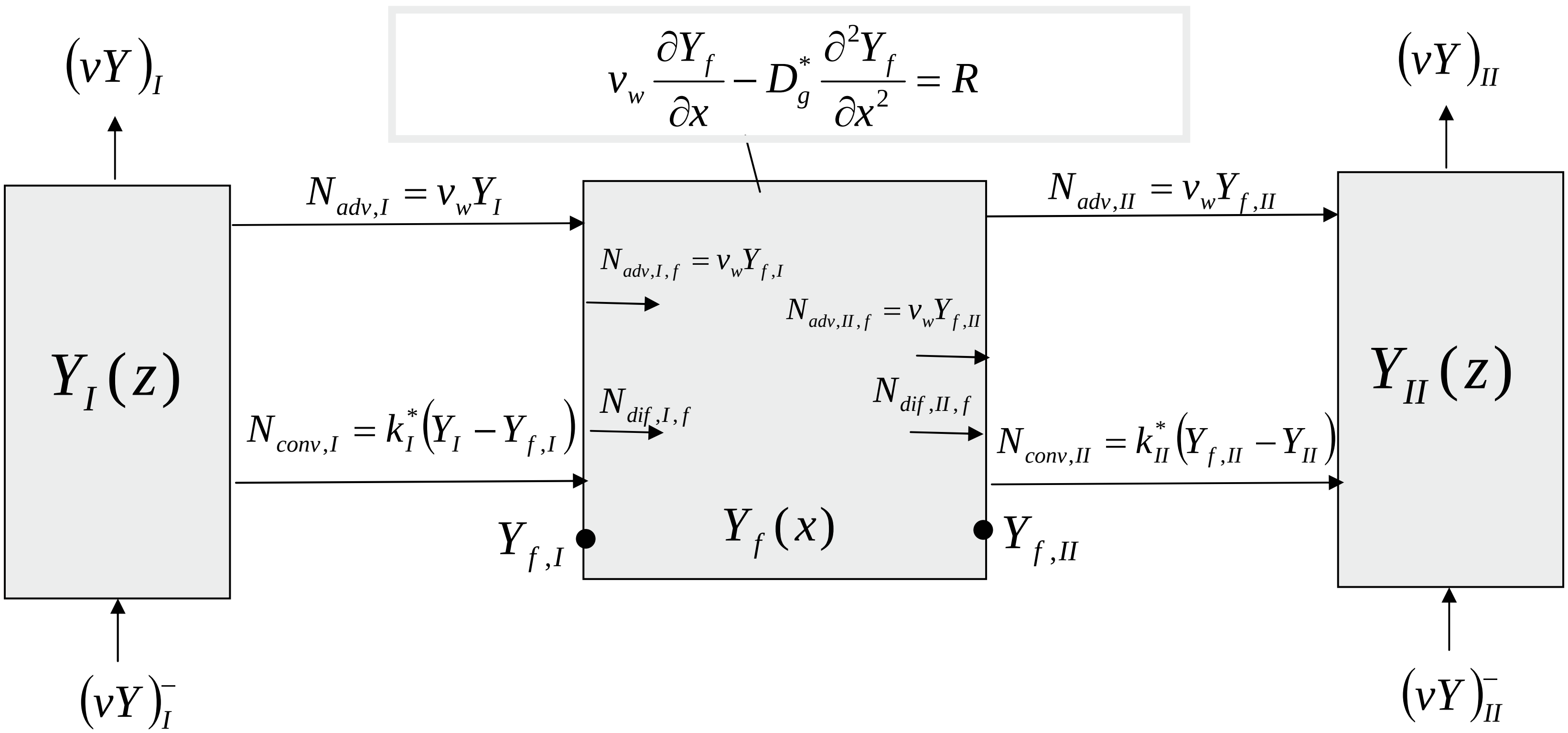
Species balance



Species equations
quasi-steady, k_w=*infinite* ($Y_w=Y_f$)

$$v_w Y_I + k_I\left(Y_I - Y_w\right) = v_w Y_{f,I} - D_g^* \frac{\partial Y_f}{\partial x}$$

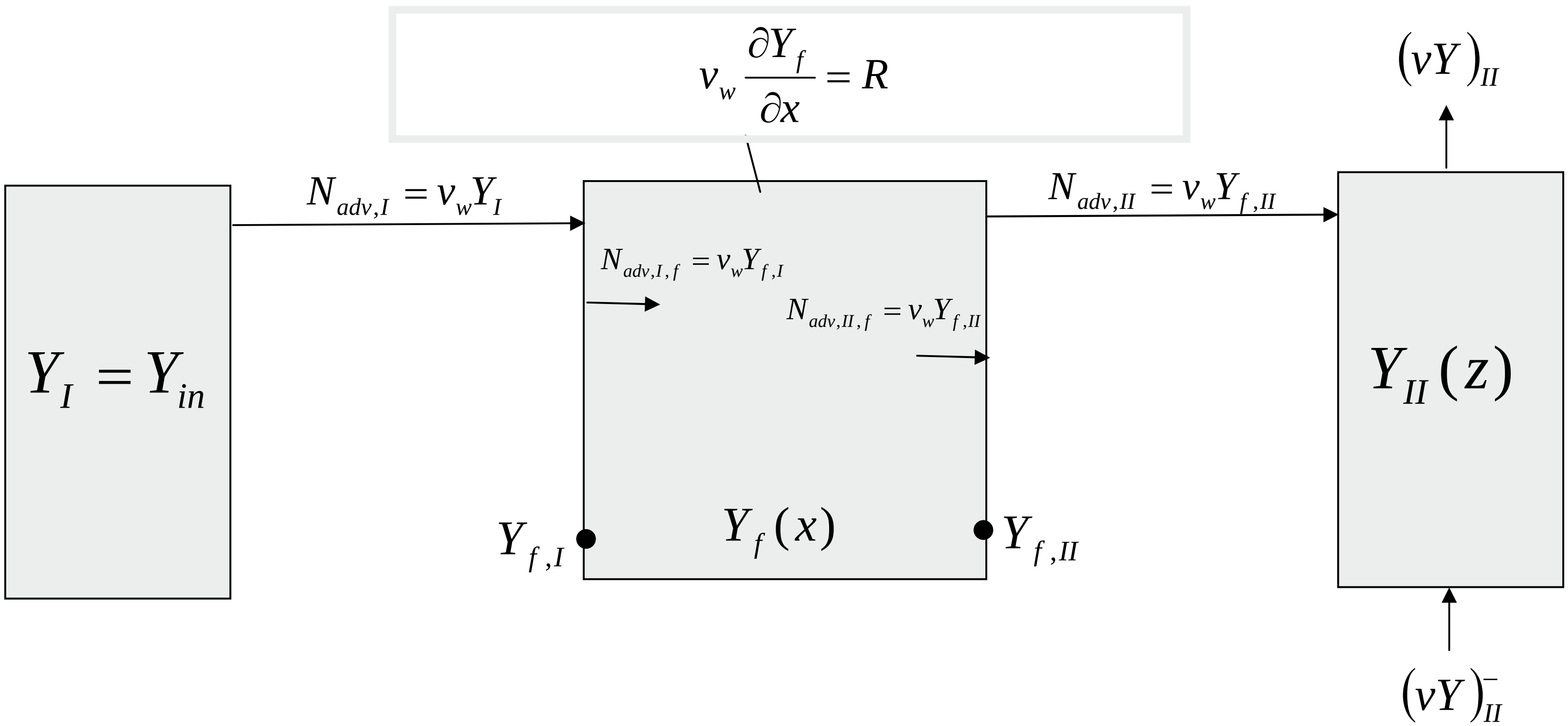
$$-D_g^* \frac{\partial Y_f}{\partial x} = k_{II}\left(Y_{f,II} - Y_{II}\right)$$



Haralampous O. A., Koltsakis G. C.: Industrial & Engineering Chemistry Research, Vol.43, Issue 4, p. 875-883, 2004.

Species equations
quasi-steady, k_w=infinite, k_I=k_{II}=0, D_g^*=0

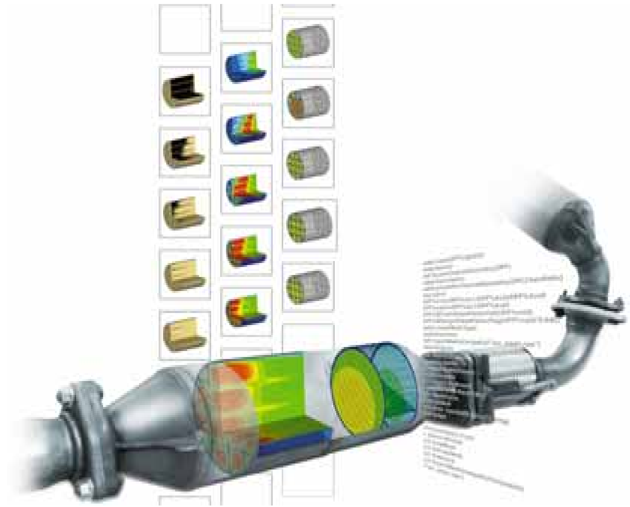
$$Y_I = Y_{f,I}$$



Bissett E. J., *Chemical Engineering Science* Vol. 39, Nos 7/8, pp. 1233-1244 (1984). “1-d model”

Bissett E. J., Shadman F., *AIChE Journal* (Vol31, No5), p. 753, May 1985. ”0-d model”

Energy balance



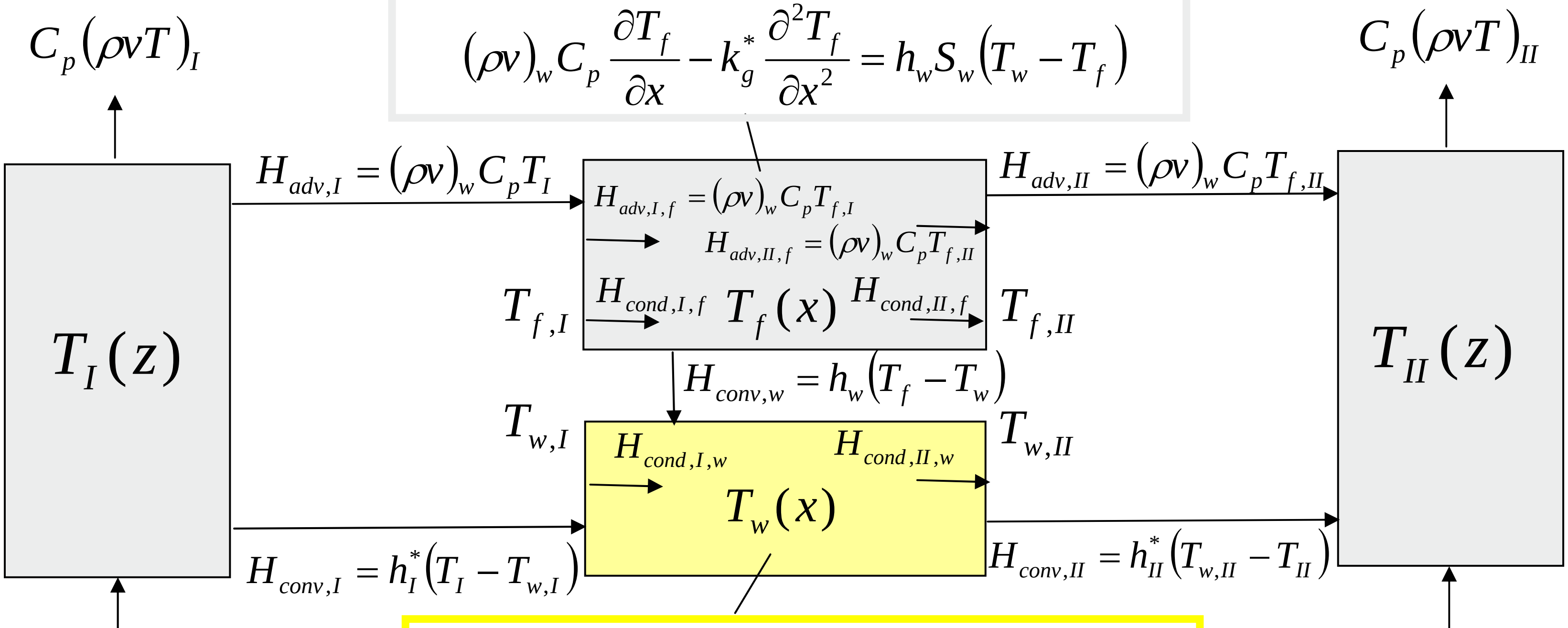
Energy equations

Exothermia

$$(\rho v)_w C_p T_I = (\rho v)_w C_p T_{f,I} - k_g^* \frac{\partial T_f}{\partial x}$$

$$-k_g^* \frac{\partial T_f}{\partial x} = 0$$

$$(\rho v)_w C_p \frac{\partial T_f}{\partial x} - k_g^* \frac{\partial^2 T_f}{\partial x^2} = h_w S_w (T_w - T_f)$$



$$(\rho C_p)_w \frac{\partial T_w}{\partial t} = h_w S (T_f - T_w) + k_w \frac{\partial^2 T_w}{\partial x^2} + H_{react}$$

$$h_I^* (T_I - T_{w,I}) = -k_w \left.\frac{\partial T_w}{\partial x}\right|_{x=0}$$

$$h_{II}^* (T_{w,II} - T_{II}) = -k_w \left.\frac{\partial T_w}{\partial x}\right|_{x=w}$$

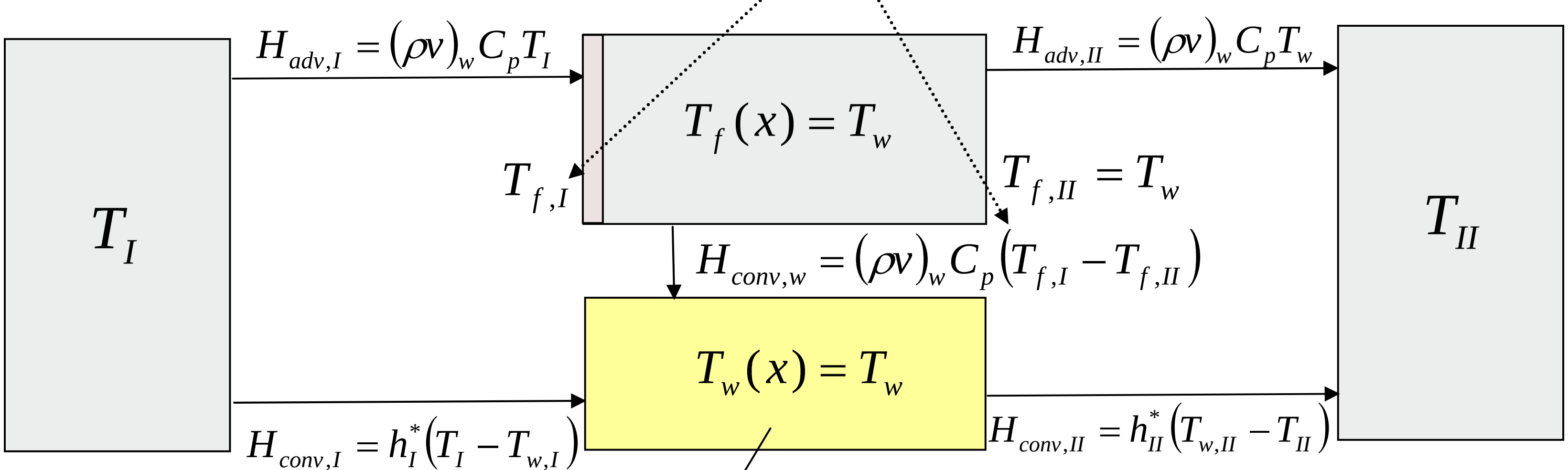
LAT

Energy equations simplification, h_w *infinite*, T_f=T_w *after dx*

$$T_I = T_{f,I}$$

$$T_{f,II} = T_w$$

In Bissett's 1984 model: $T_{f,I} = T_w$



$$(\rho C_p)_w \frac{\partial T_w}{\partial t} = H_{conv,w} + H_{react} + H_{conv,I} + H_{conv,II}$$

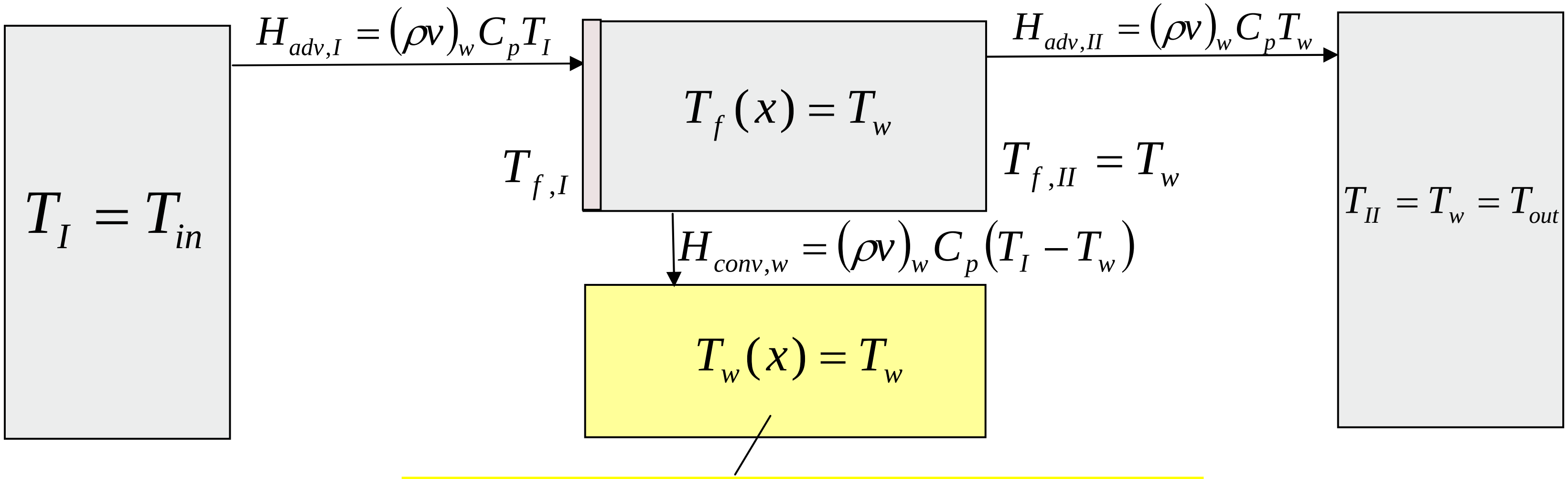
Bissett E. J., *Chemical Engineering Science* Vol. 39, Nos 7/8, pp. 1233-1244 (1984). "1-d model"

Koltsakis G. C., Stamatelos A. M., *Ind. Eng. Chem. Res.*, 1997 Vol. 36 p. 4155-4165. "catalytic 1-d model, modified energy balance"

Energy equations simplification, $h_I^*=0$, $h_{II}^*=0$

$$T_I = T_{f,I}$$

$$T_{f,II} = T_w$$



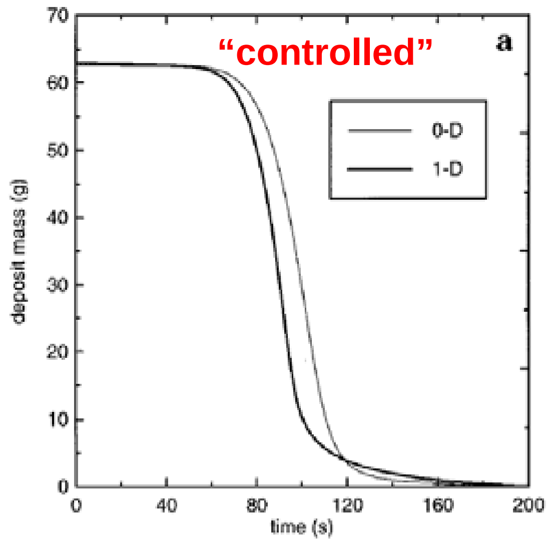
$$(\rho C_p)_w \frac{\partial T_w}{\partial t} = H_{conv,w} + H_{react}$$

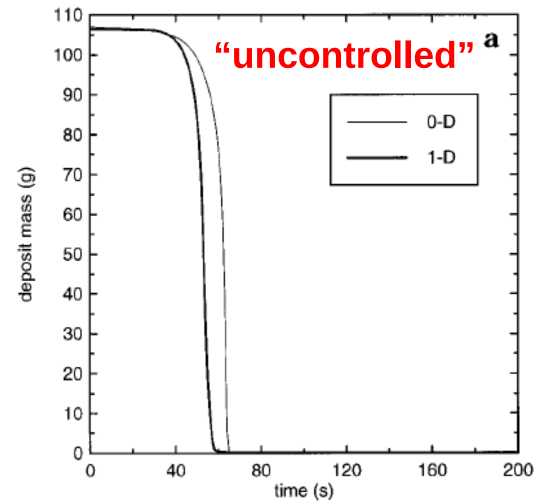
Bissett E. J., Shadman F., *AIChE Journal* (Vol31, No5), p. 753, May 1985. "0-d model"

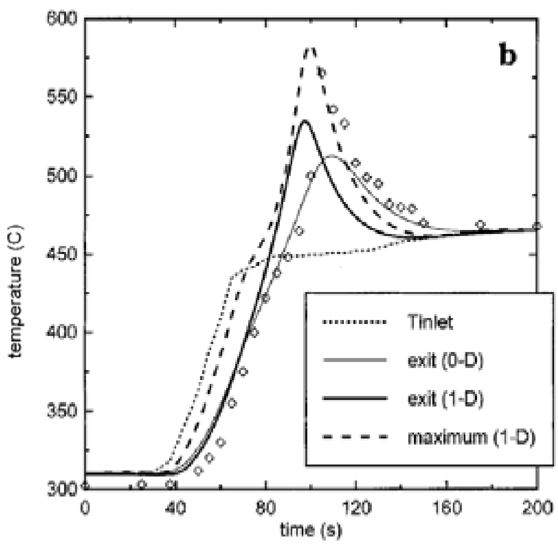
Koltsakis G. C., Stamatelos A. M., *Ind. Eng. Chem. Res.,* 1996, 35, 2-13 "catalytic 0-d model"

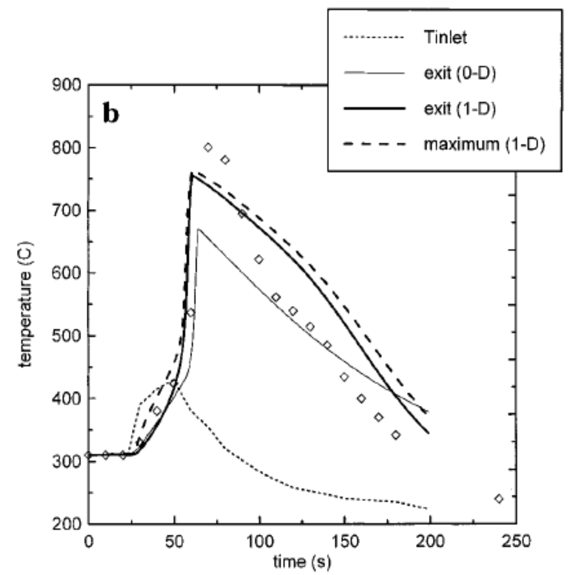
0-d vs 1-d modeling results

Exothermia





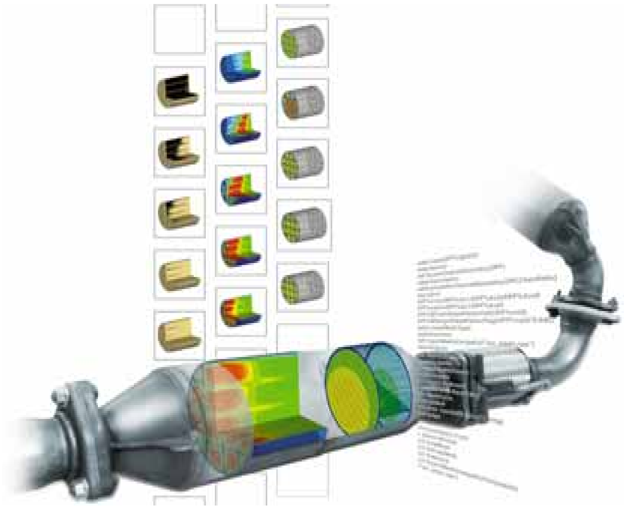




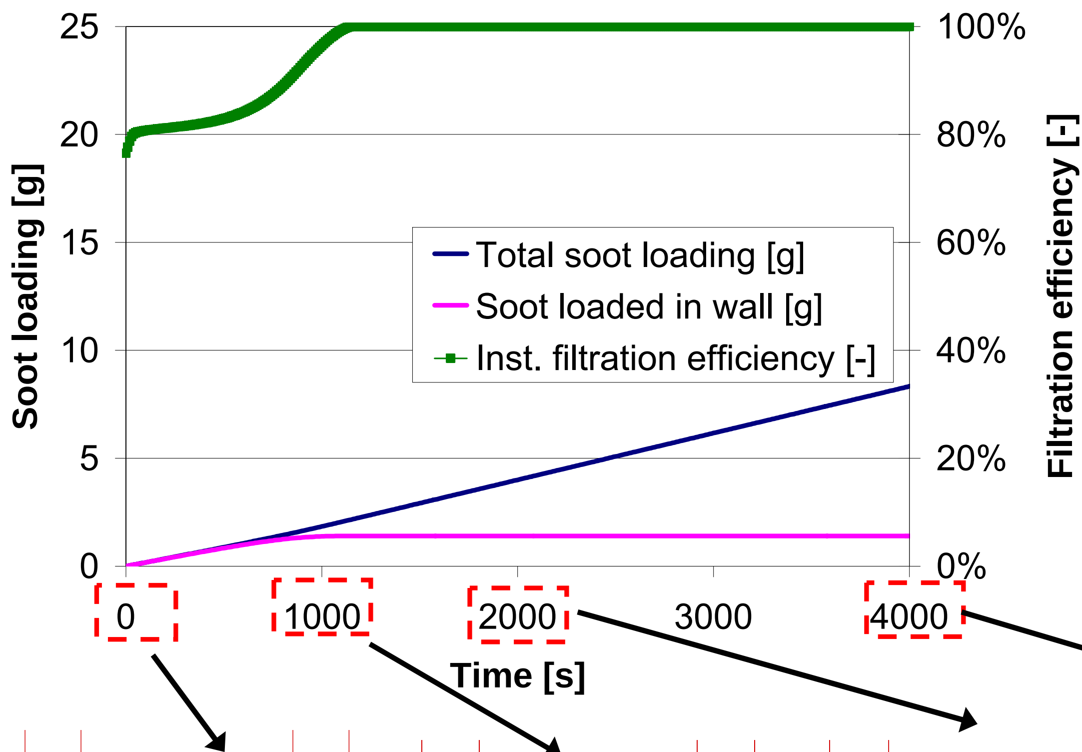
Koltsakis G. C., Stamatelos A. M., *Ind. Eng. Chem. Res.*, 1997, Vol. 36 p. 4155-4165.

Intra-layer dimension in DPF modeling

Soot filtration and pressure drop effects



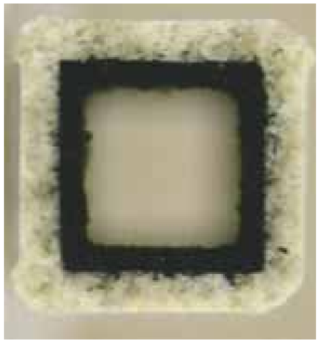
Intra-layer dimension
Filtration efficiency and soot accumulation

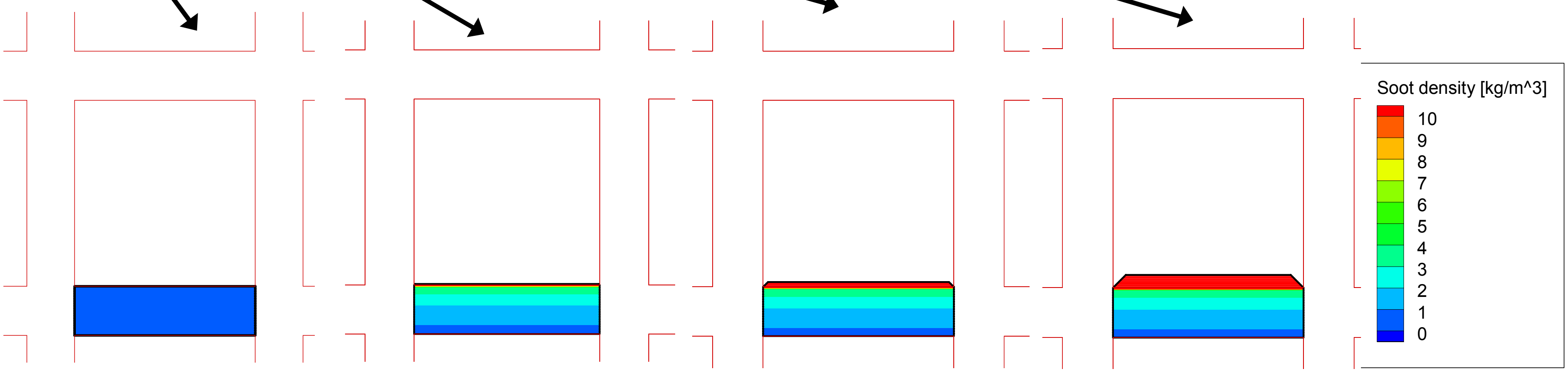


Transition from wall to cake filtration

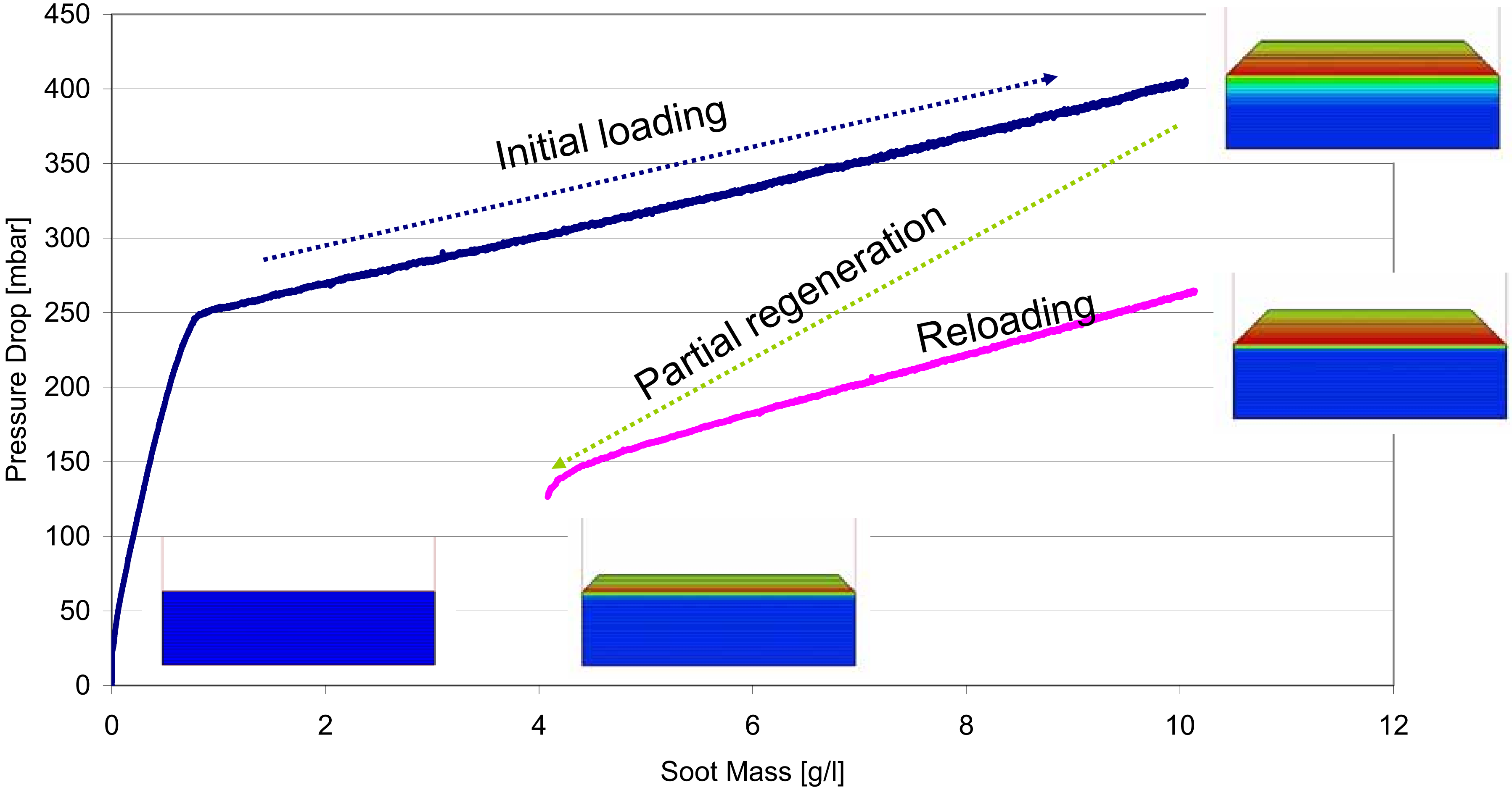
Calculation of soot distribution within the wall

Model calibration with in-house single-channel studies



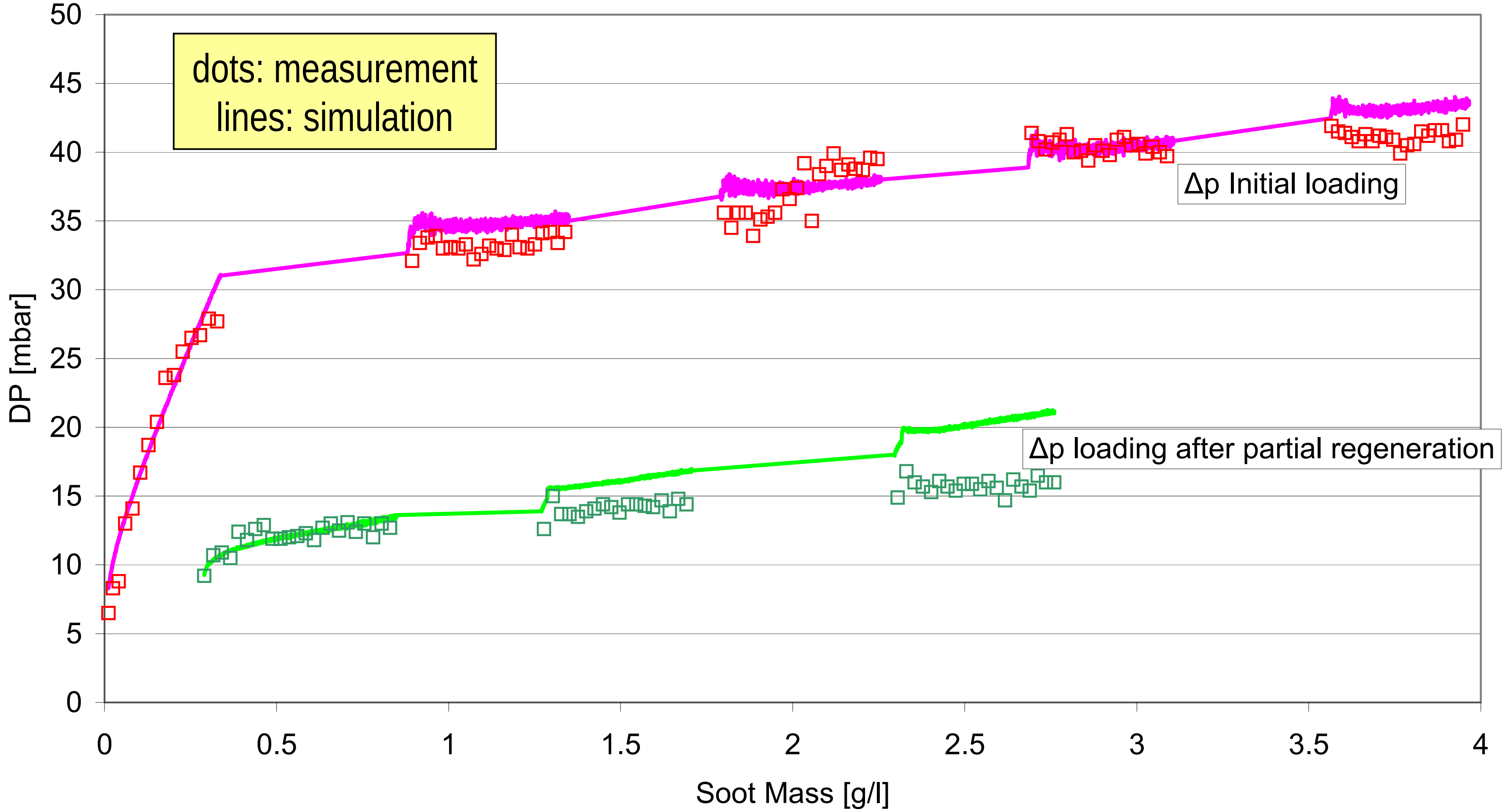


Pressure drop "hysteresis"
Wall-scale effects



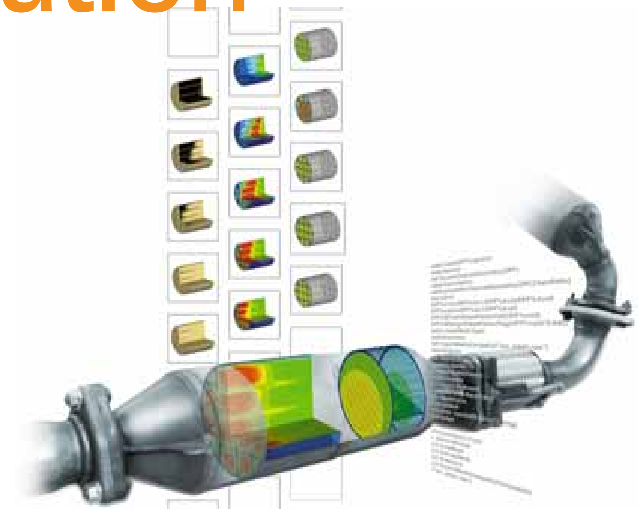
Incoming soot does not re-penetrate the wall. The correlation of pressure drop vs soot loading is depends on partial regeneration history.

Pressure drop hysteresis effect



Following an incomplete regeneration, the cake soot does not allow the incoming soot to-penetrate the wall. The pressure drop correlation with soot loading changes dramatically.

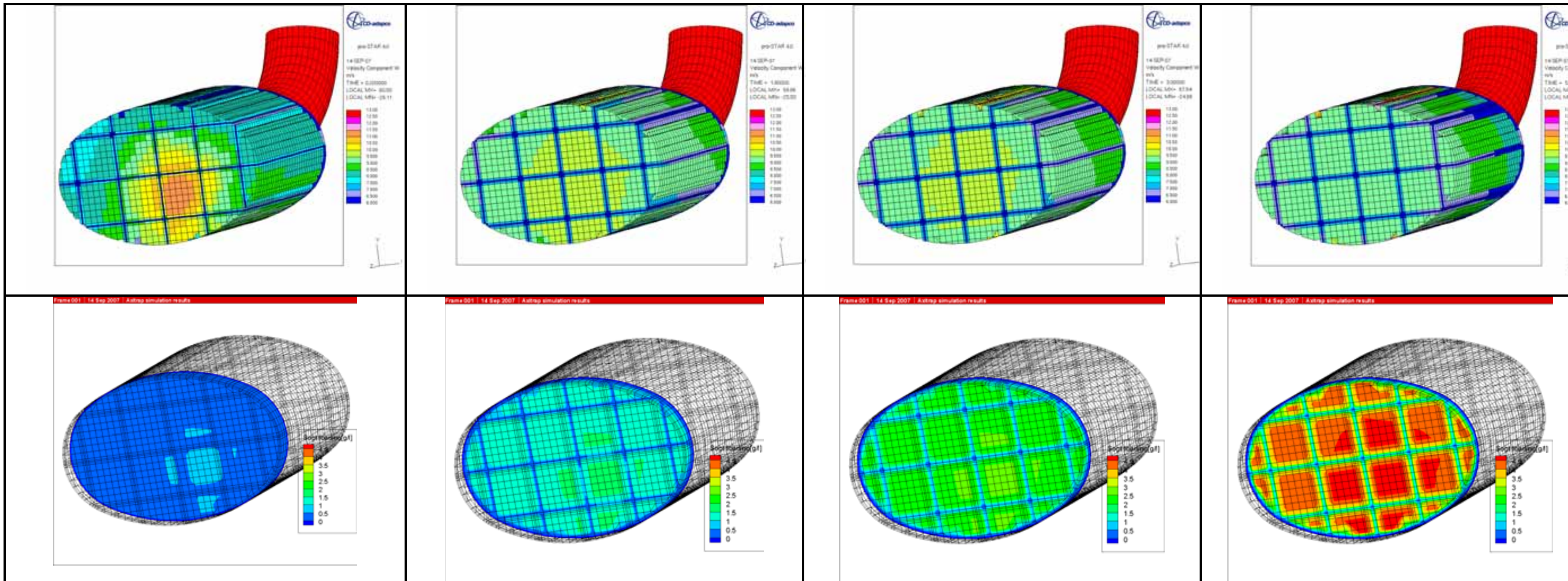
Channel and filter scale effects on flow & soot distribution



Soot accumulation
Filter scale

<u>Example : Coupling of *axitrap*™ with Adapco Star-CD</u>

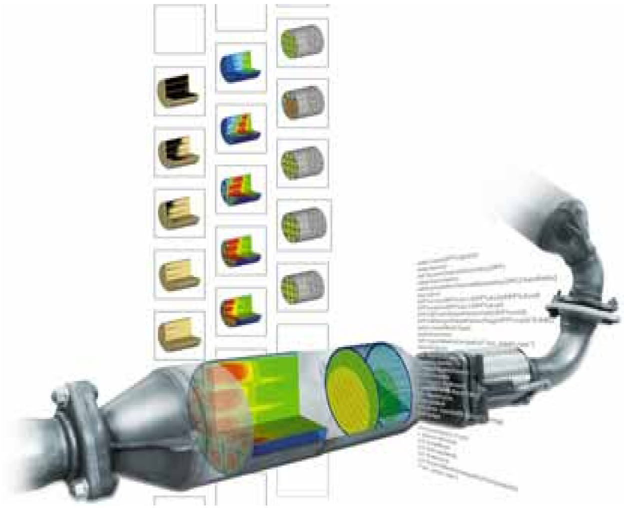
Transient soot accumulation (bottom) and flow redistribution (top) in an asymmetric DPF geometry



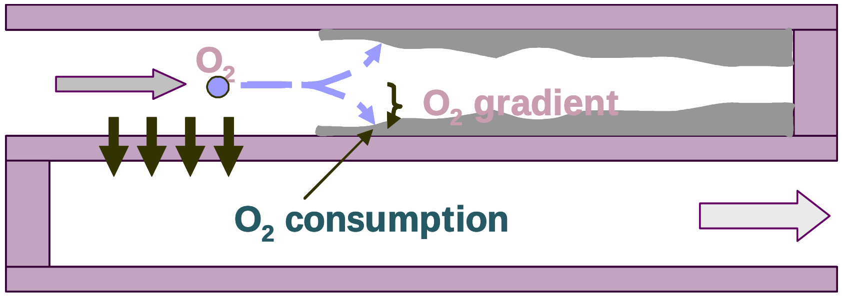
t=0	t= 2 h	t= 3 h	t= 5 h

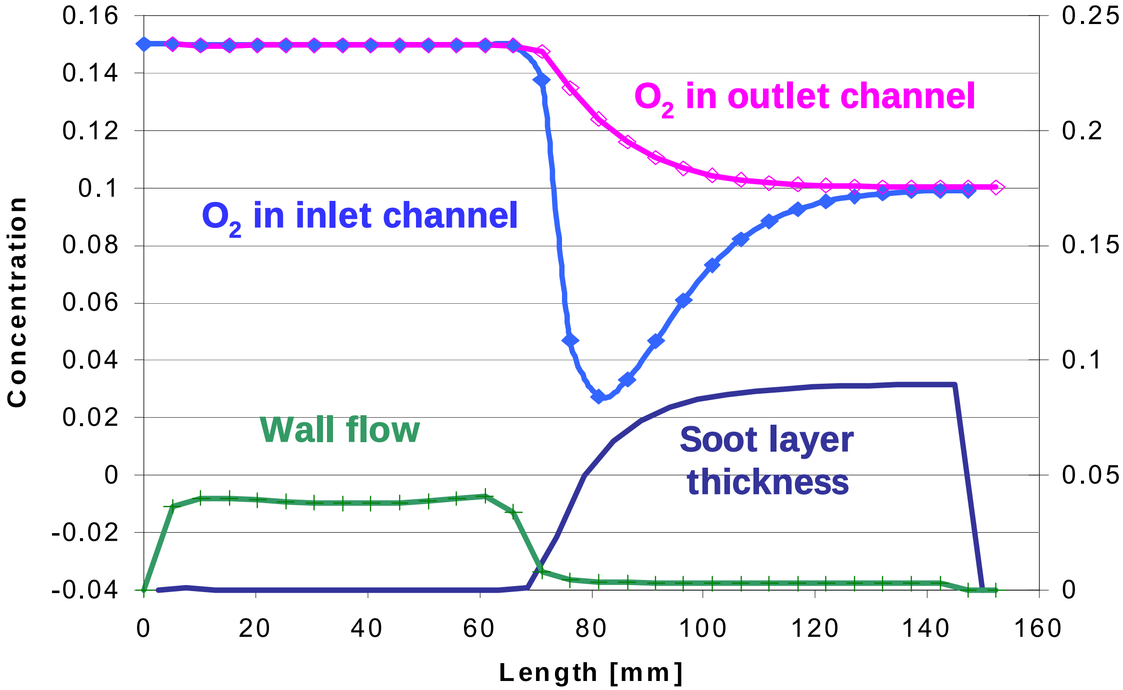
Knowledge of soot accumulation is important for pressure drop and regeneration predictions

O_2 transfer effects on soot limit calculation



O_2 transfer from channel gas to soot surface

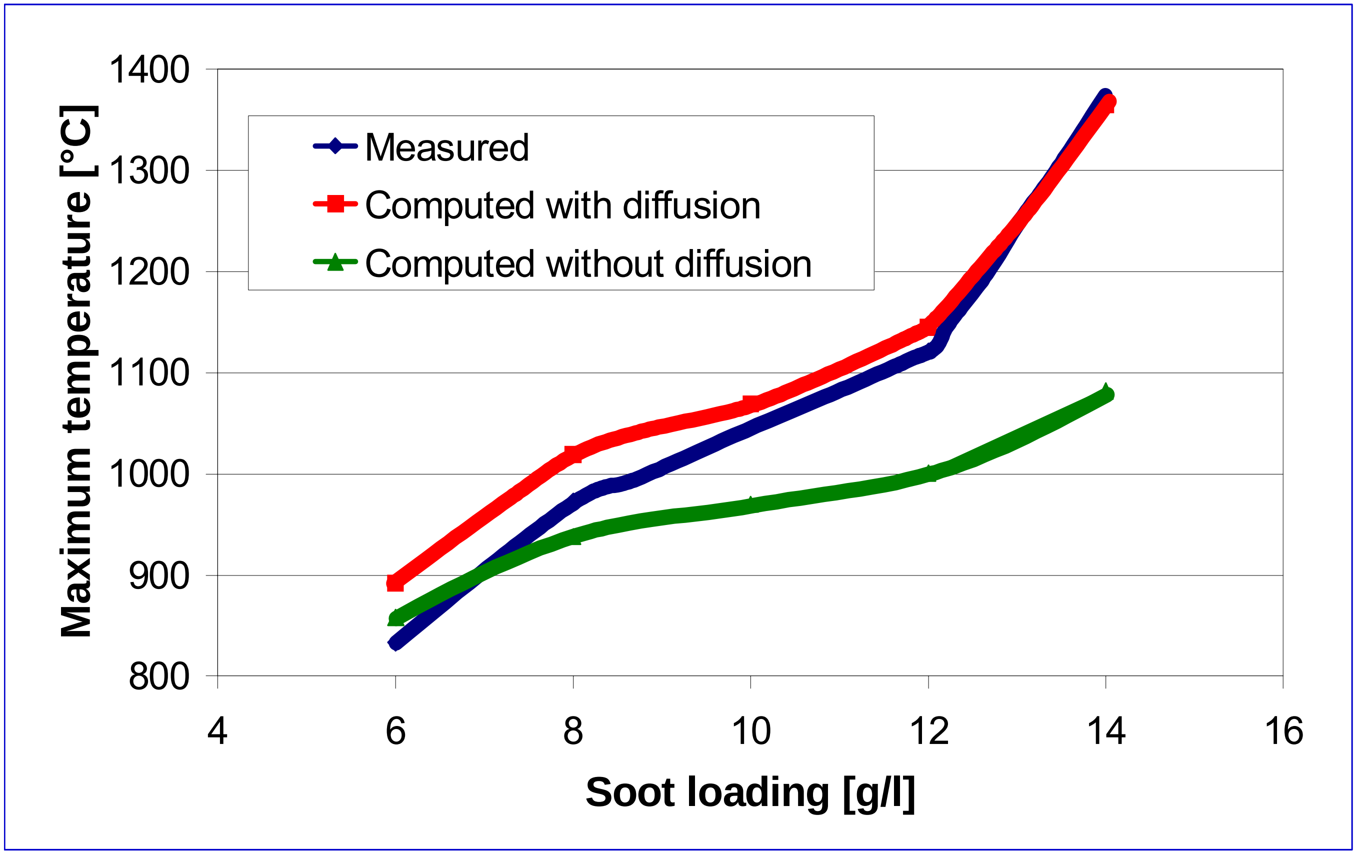




Due to concentration gradient, O_2 is transferred from the axial flow to the soot layer and increases availability and reaction rates

Importance of O_2 transfer for the prediction of filter temperature

Exothermia



Test conditions: Gas burner, cordierite filter, T_{in}=600°C

Ignoring O_2 mass-transfer effects (diffusive-convective) leads to serious under-prediction of peak temperatures

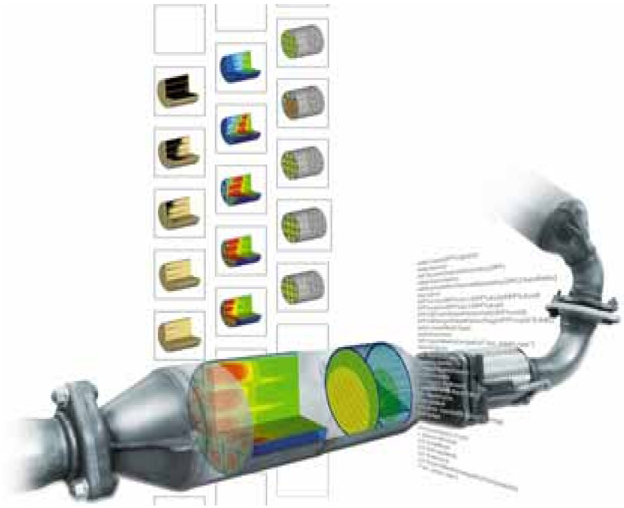
NO_2 transfer effects on CDPF modeling

Back-diffusion

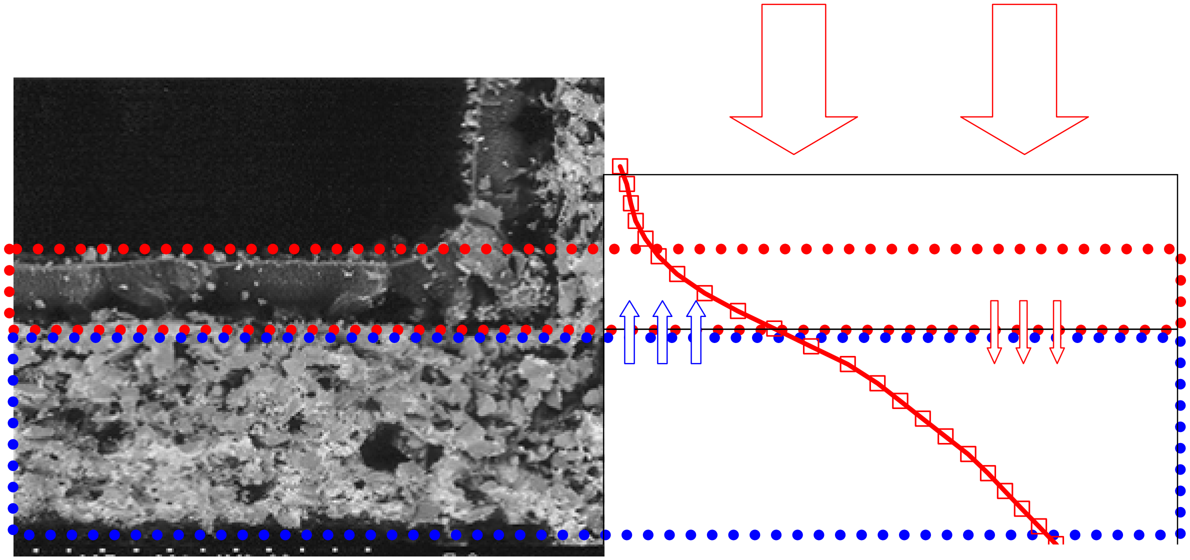
NO_2 “recycling”

WLNT modeling

WSCR modeling

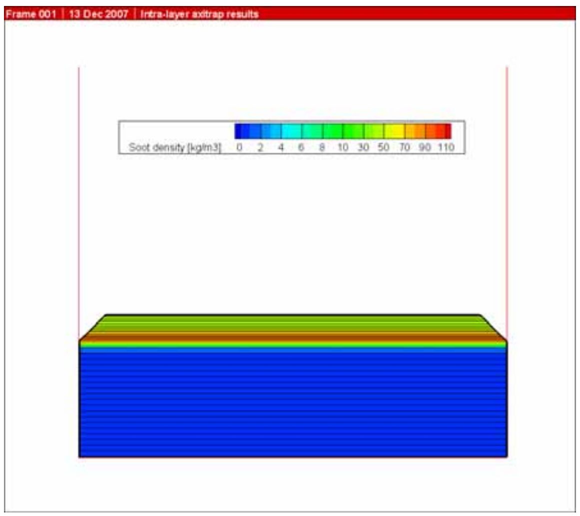


“Passive” regeneration via NO_2 in catalyzed filters

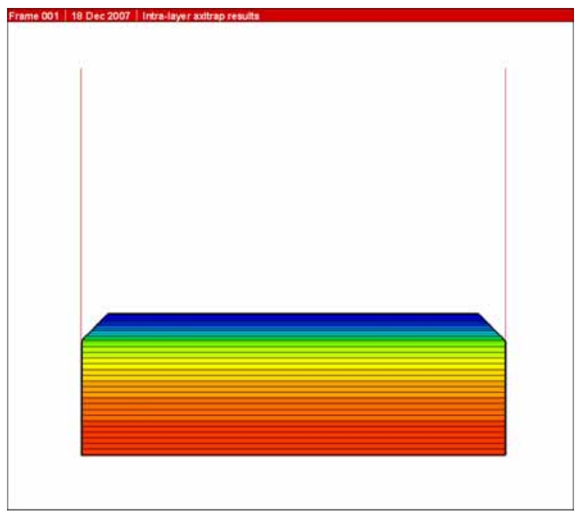


- Soot is consumed in NO_2-rich regions
- NO_2 diffuses back to the soot layer
- NO_2 is produced in the catalyzed wall

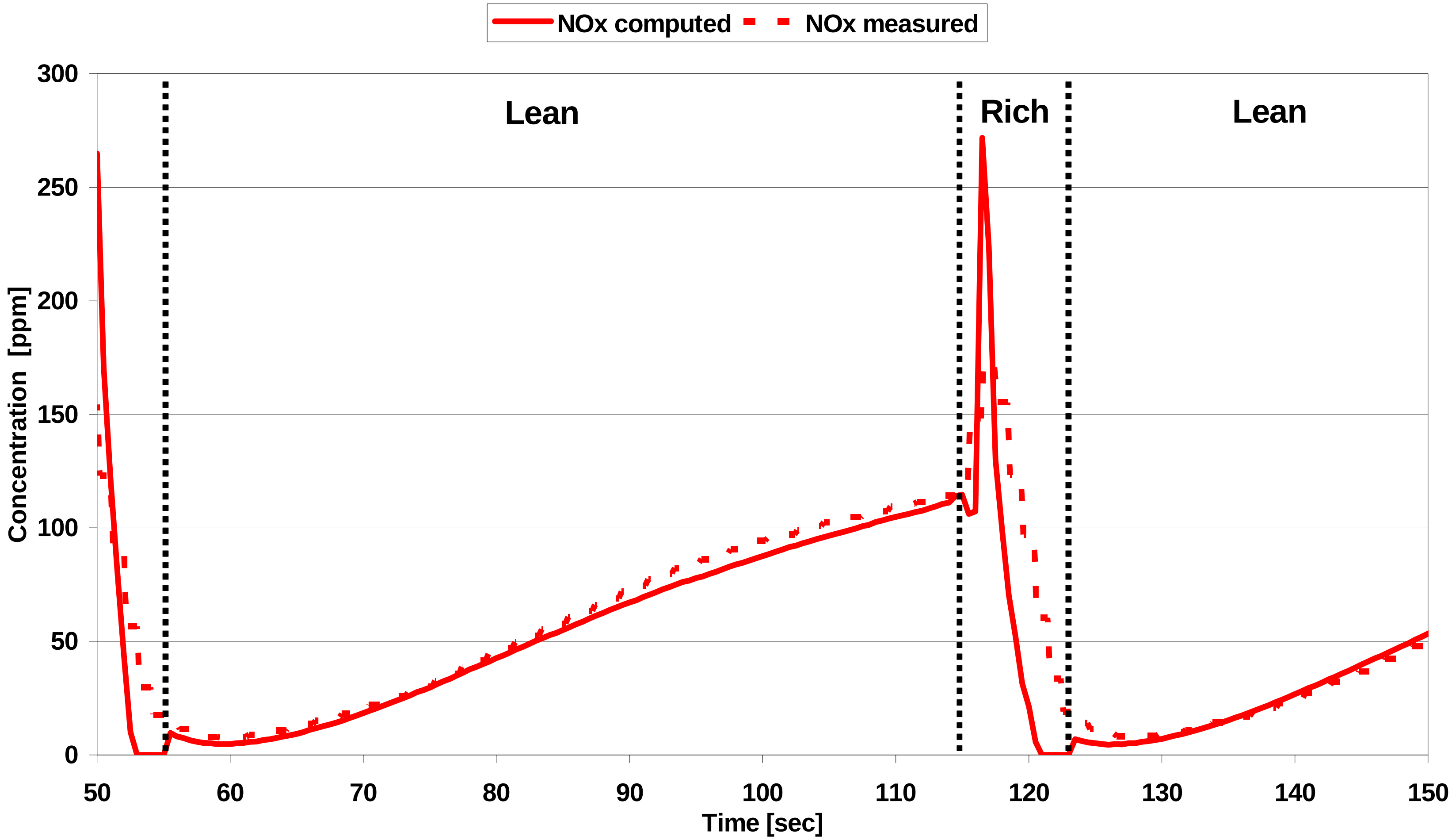
Soot density



NO_2 concentration



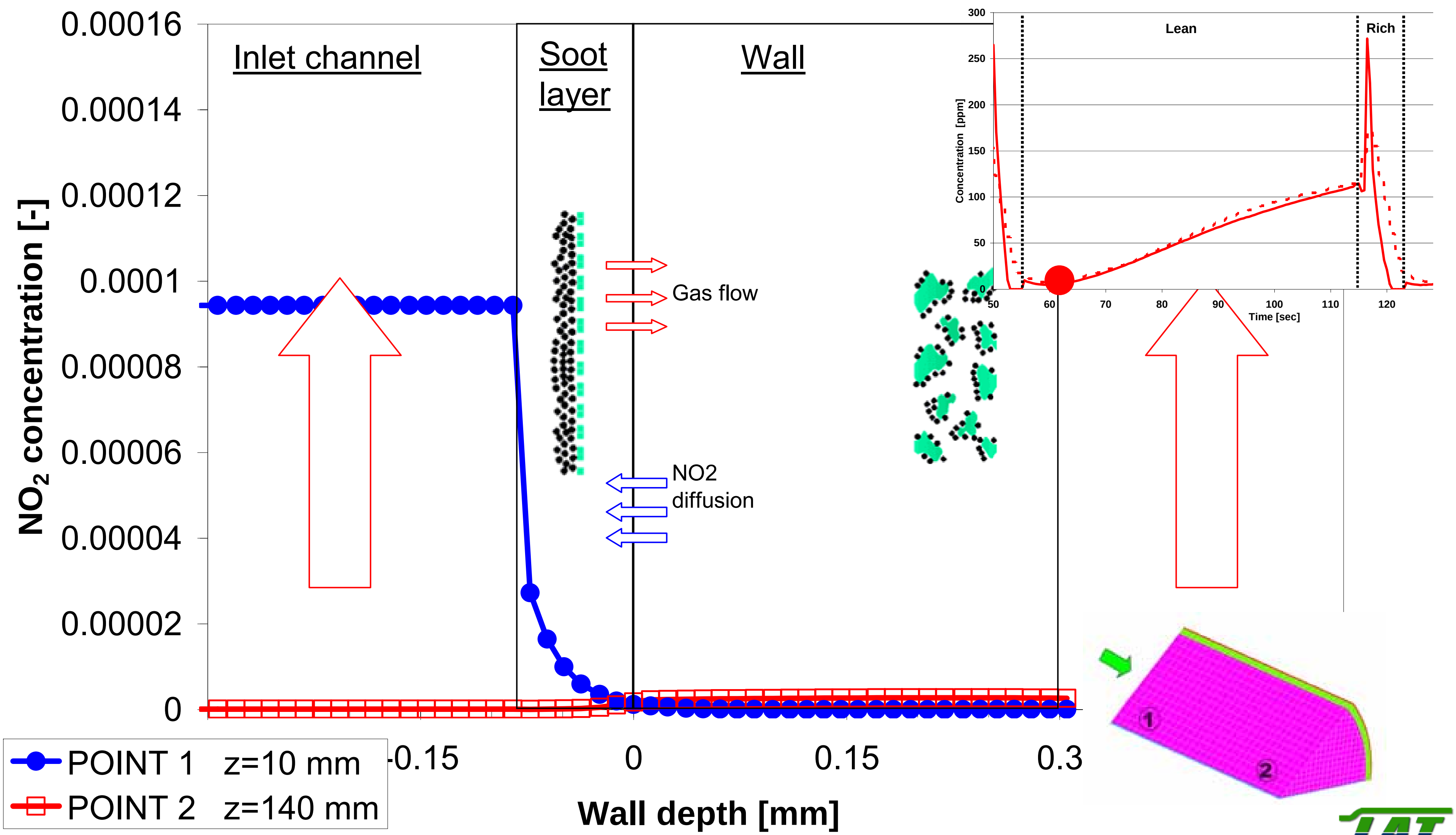
WLNT (DPNR) simulation example
Lean-rich cycle at 350°C



Experimental data from engine testing at IAV GmbH

Intra-layer NO_2 profiles t=60 s

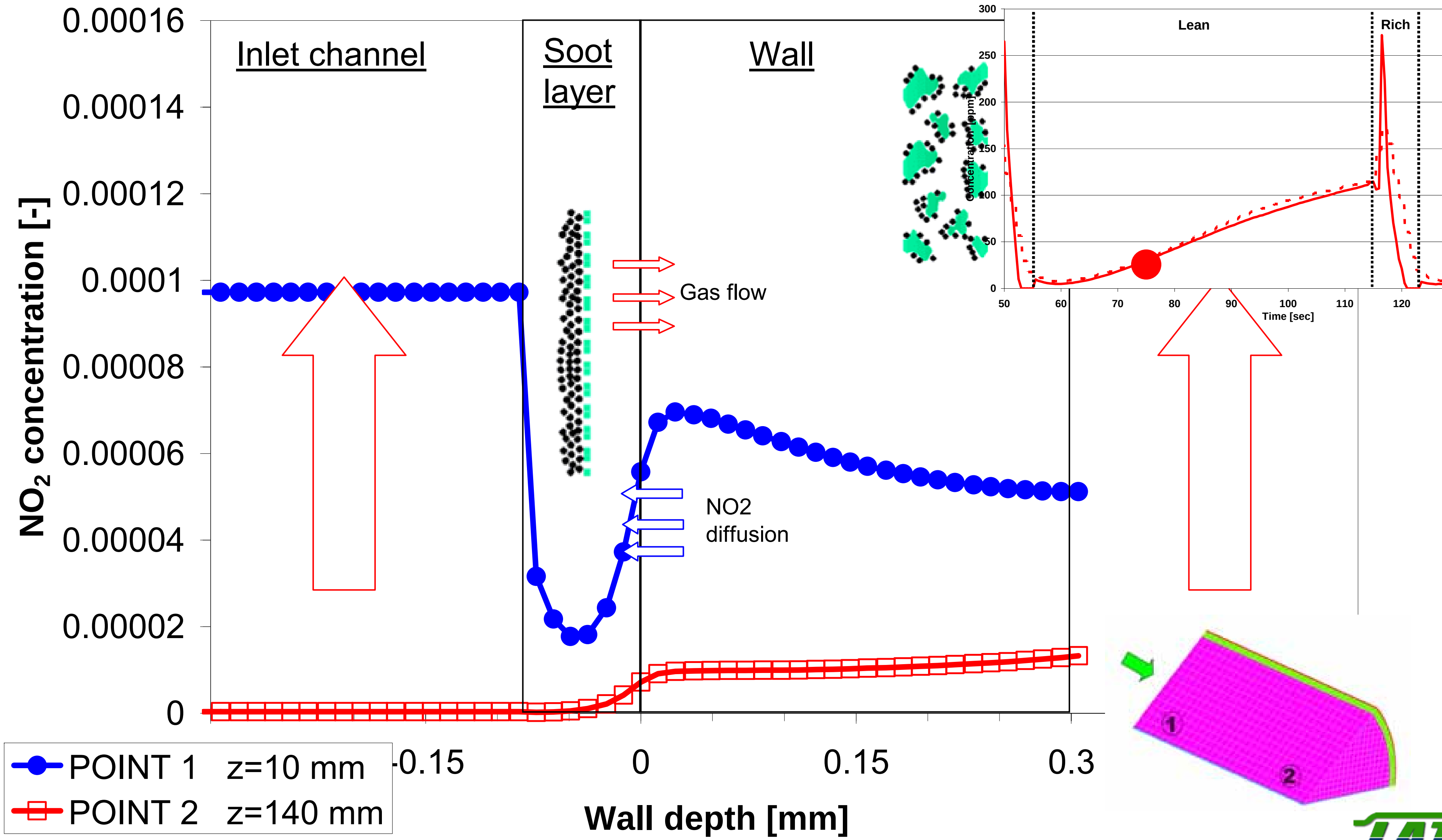
Exothermia



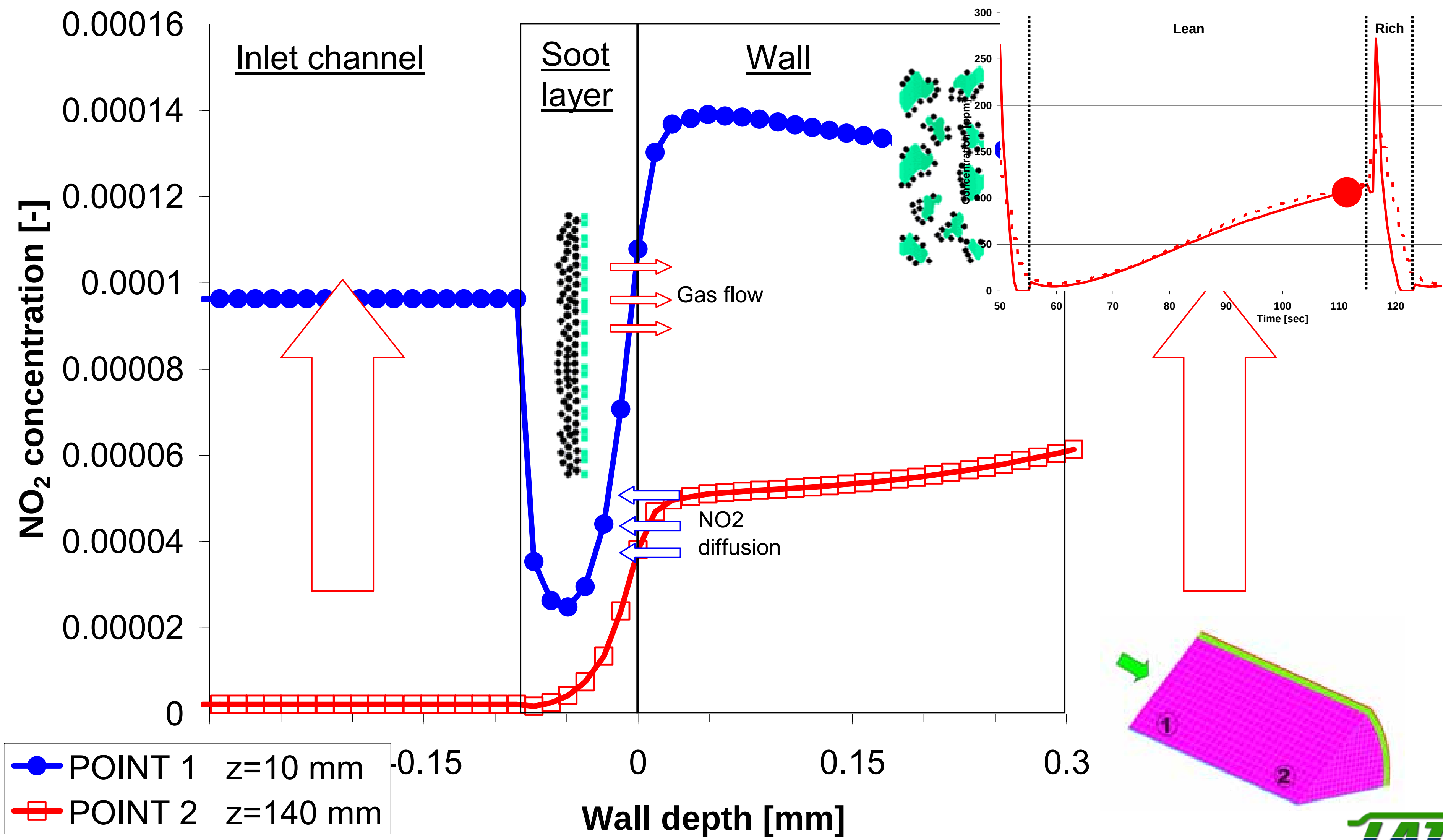
LAT

Intra-layer NO_2 profiles t=75 s

Exothermia



Intra-layer NO_2 profiles
t=114 s

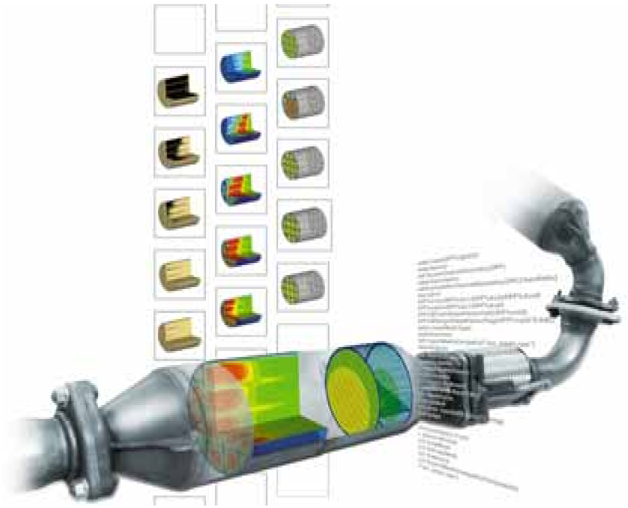


DOC functionality

CO, HC oxidation

DOC replacement

Catalyst zoning



Catalyzed DPF simulation
Catalyst zoning (Precious Metal saving concept)

- Uncoated DPF

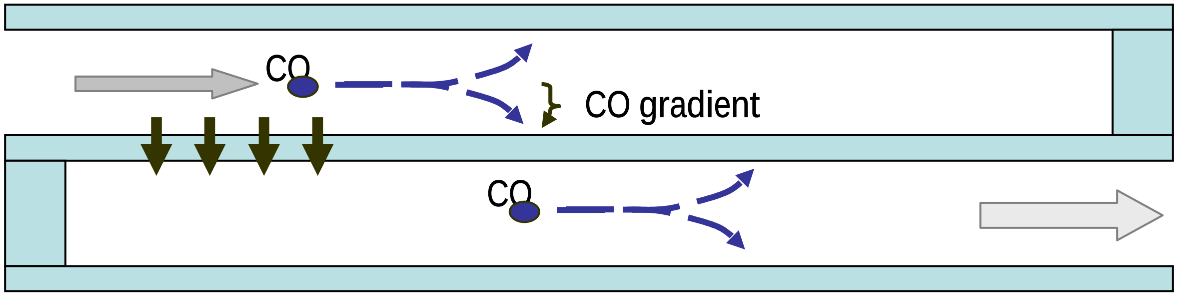
- "Axial" zoning
  - More PGM in front part
  - Better cold-start performance

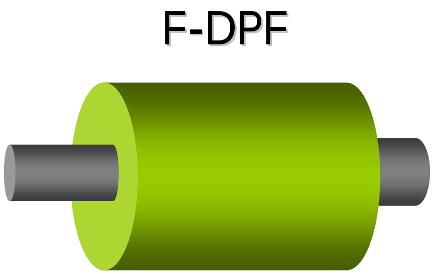
- "Intra-wall" zoning
  - More catalyst close to soot layer
  - Better passive regeneration performance

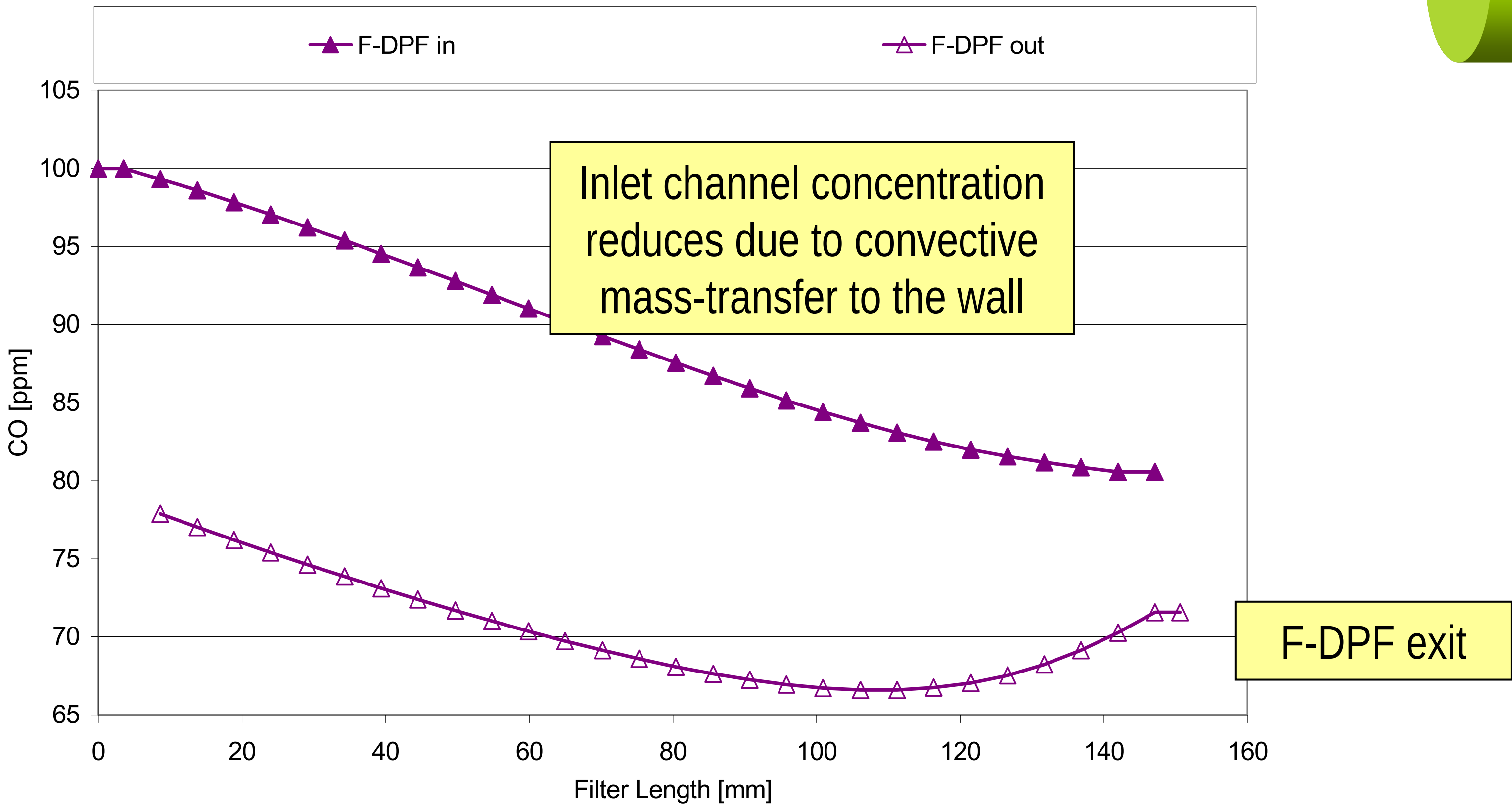
Transport/reaction coupling necessary to account for catalyst zoning

Uncatalyzed wall
Catalyzed with high PGM
Catalyzed with low PGM
Soot layer

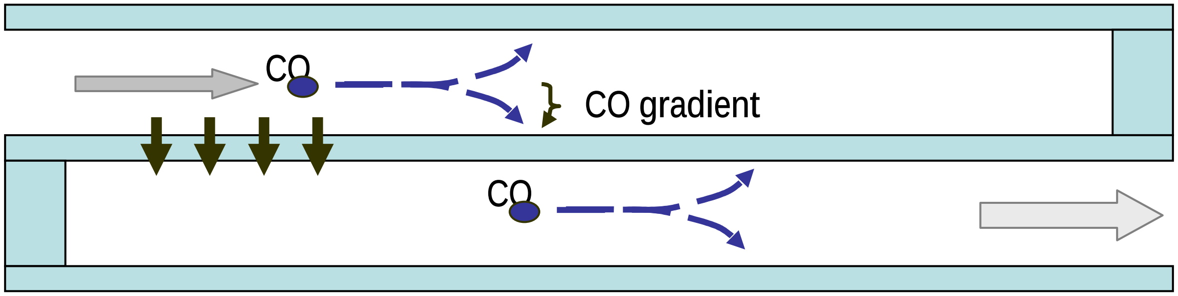
Computed concentration profiles in catalyzed filters @ T=150°C

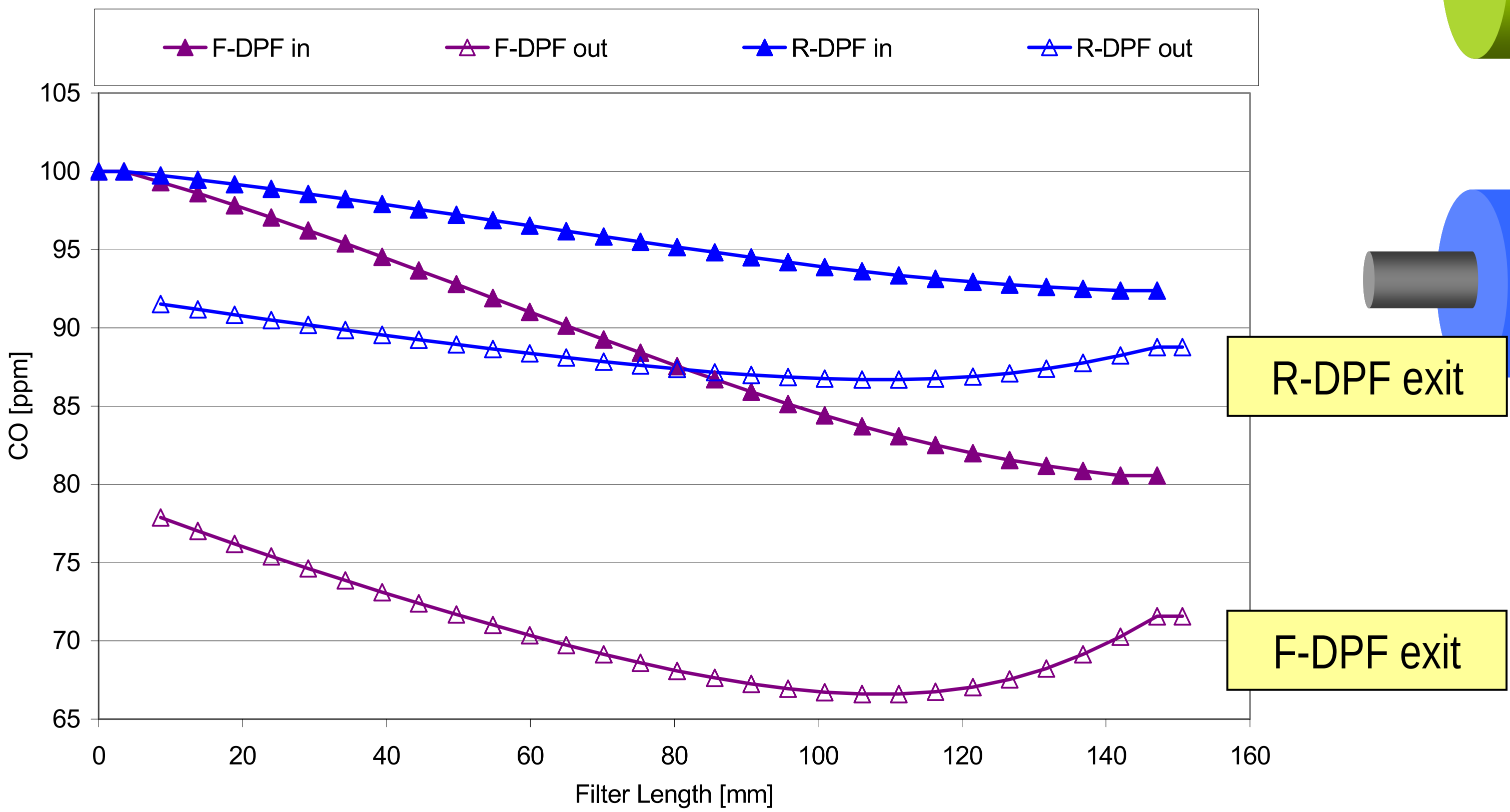


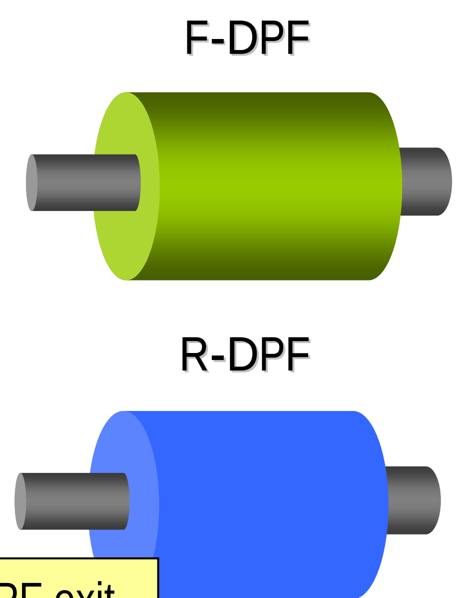




Computed concentration profiles in catalyzed filters @ T=150°C

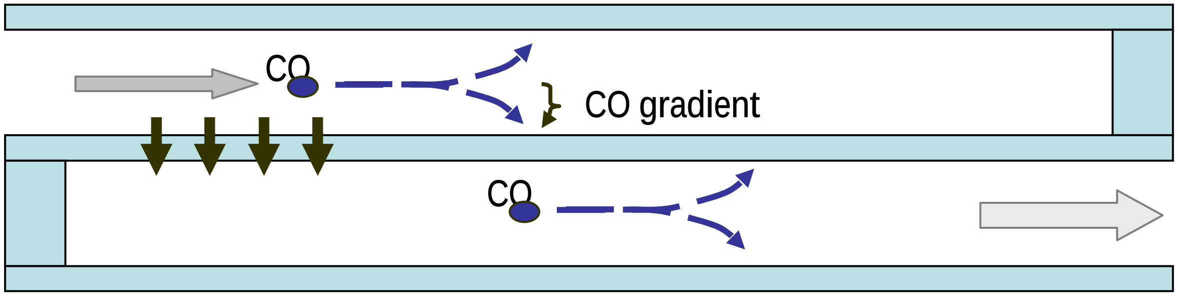


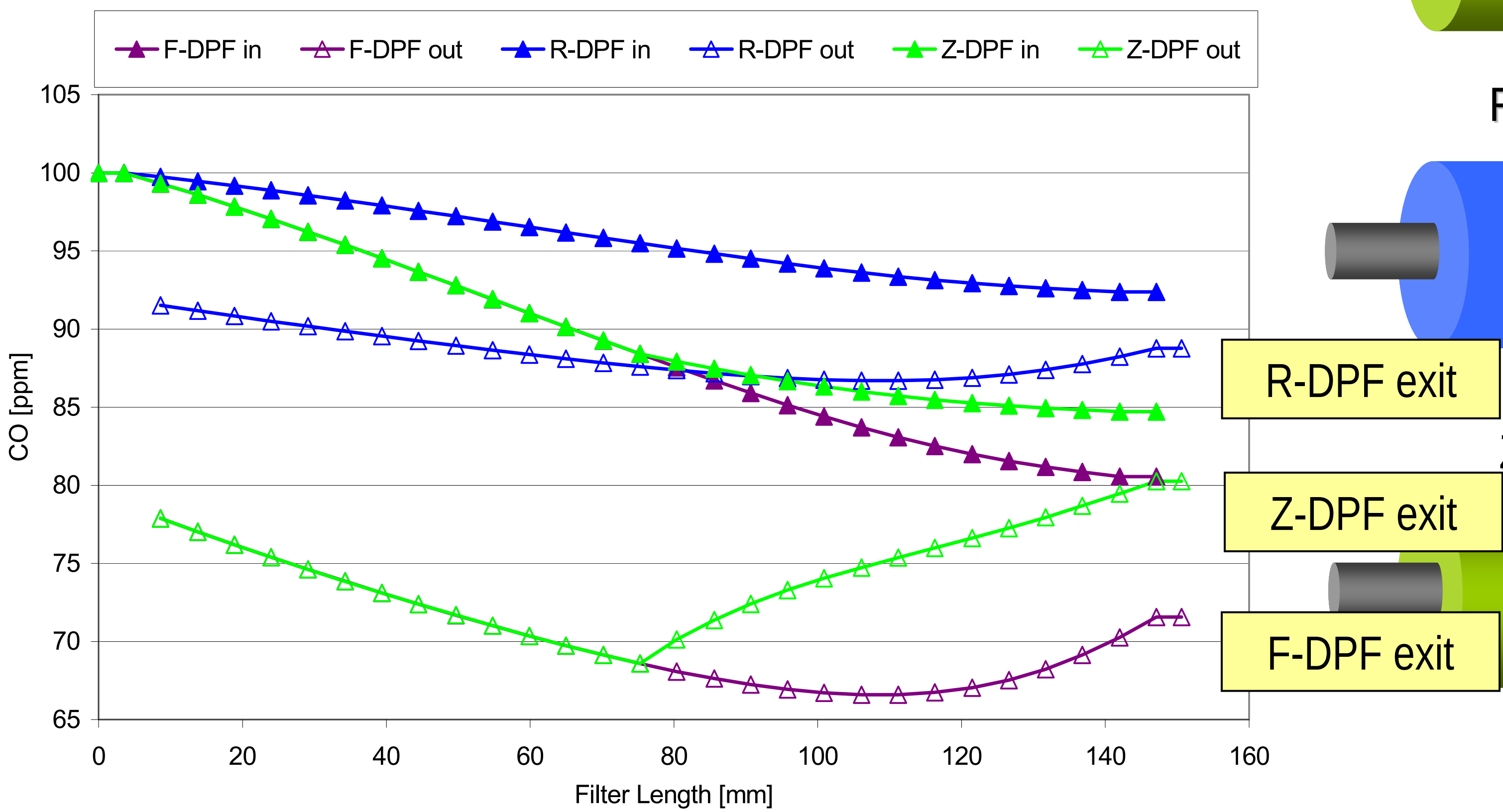


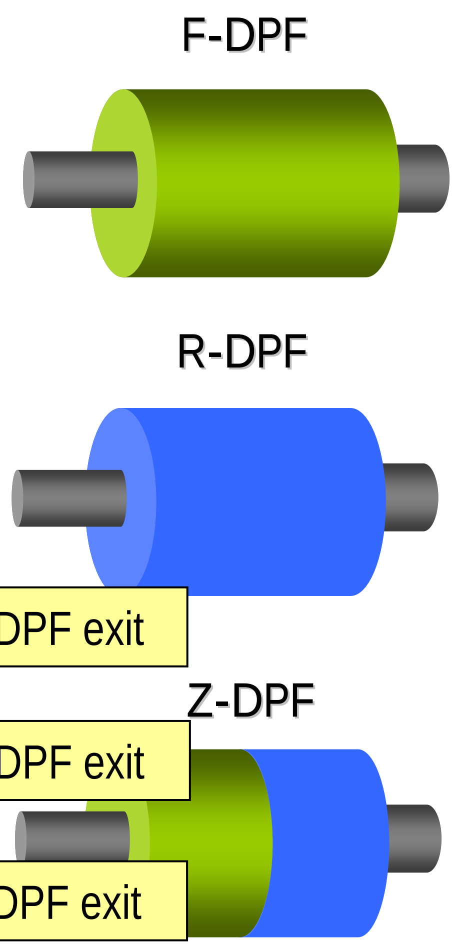


Computed concentration profiles in catalyzed filters @ T=150°C

Exothermia





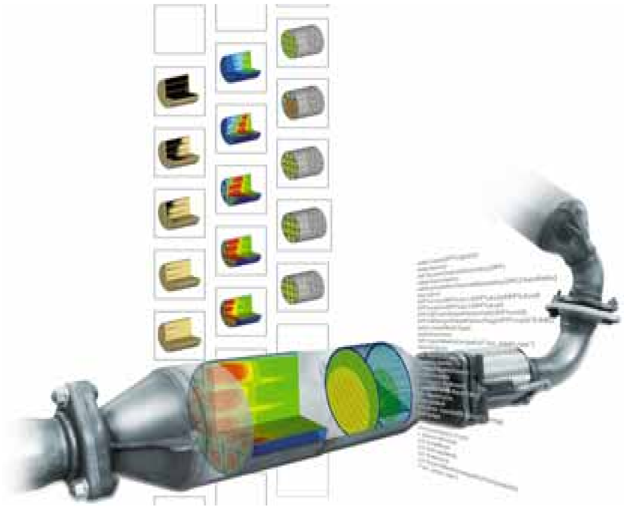


3-d effects

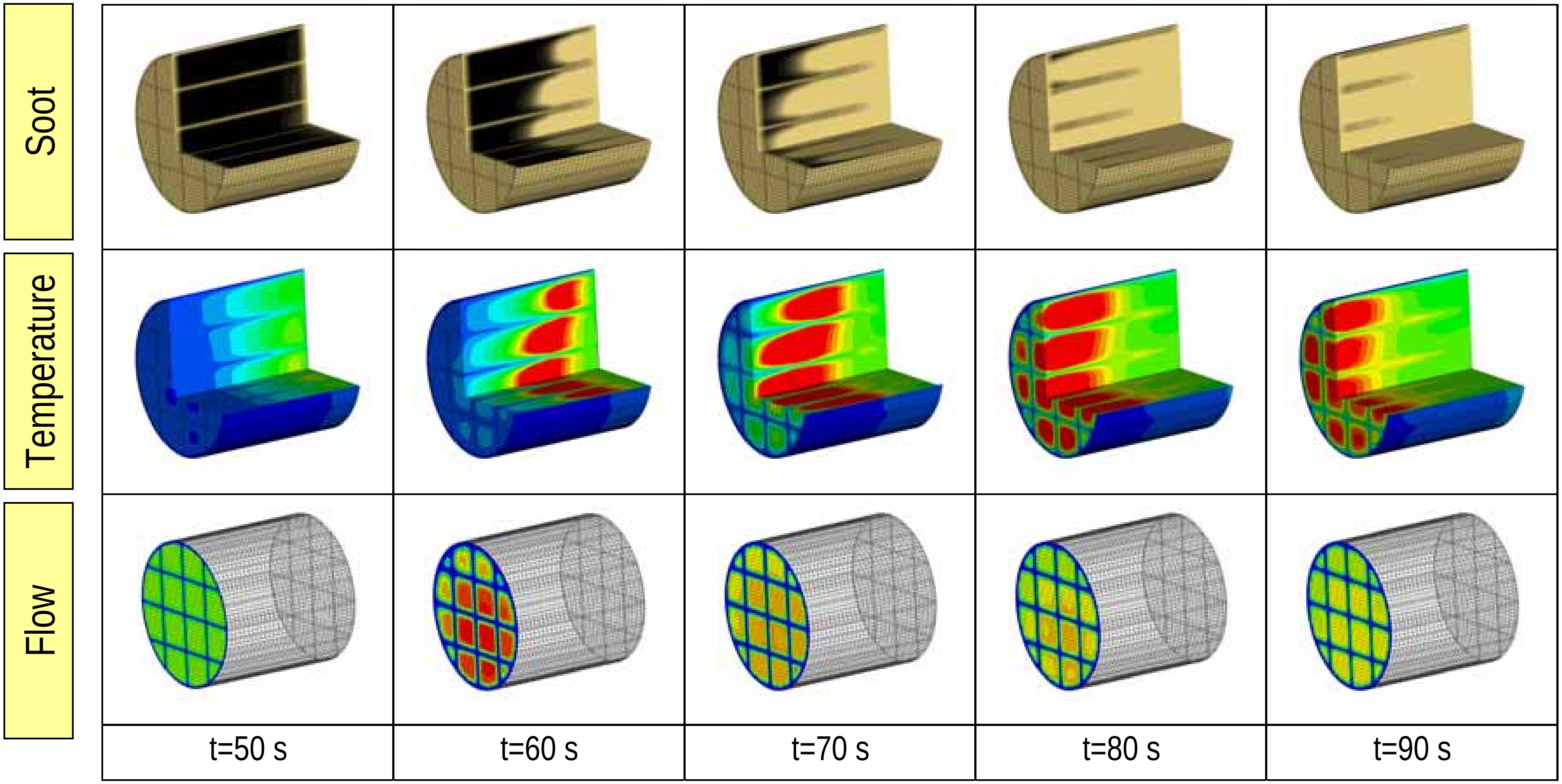
Heat transfer

Flow

Stress analysis



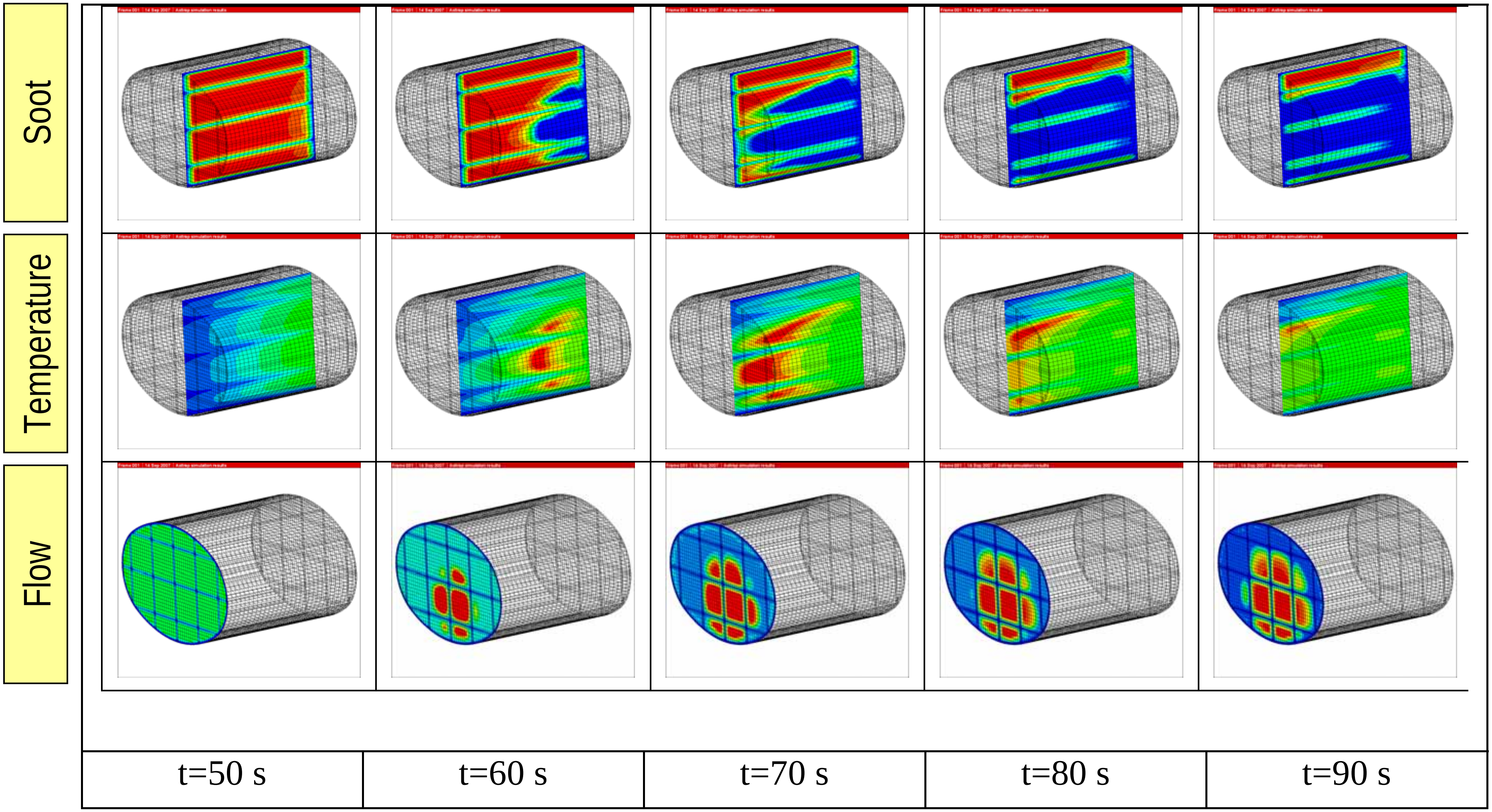
3-d DPF regeneration simulation
Sources of "3-dimensionality"



"3-d effects"

Heat losses, segmentation, asymmetric inlet temperature/flow, oval DPF geometry

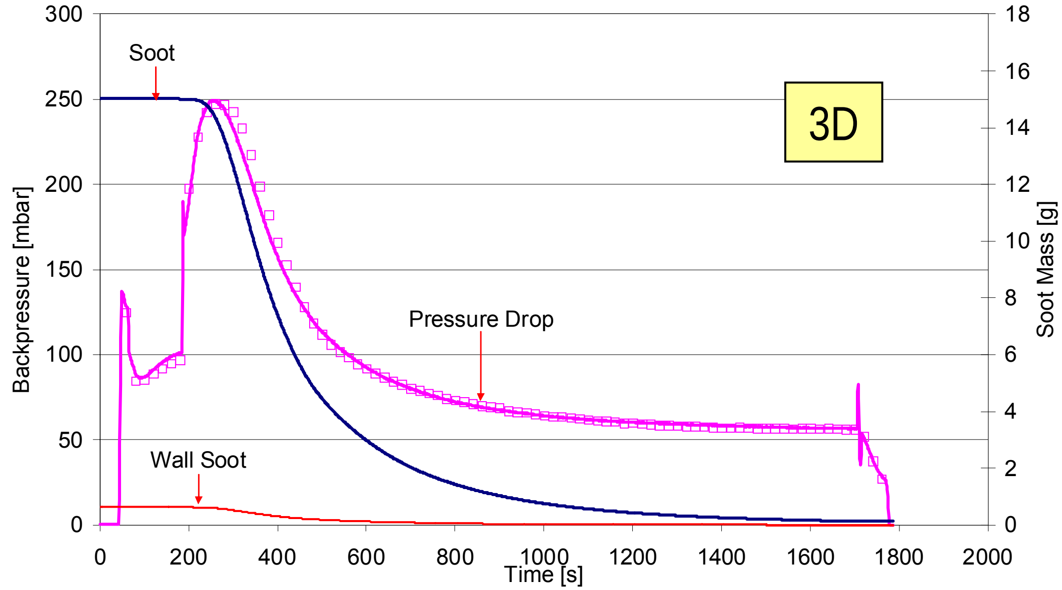
Oval geometries

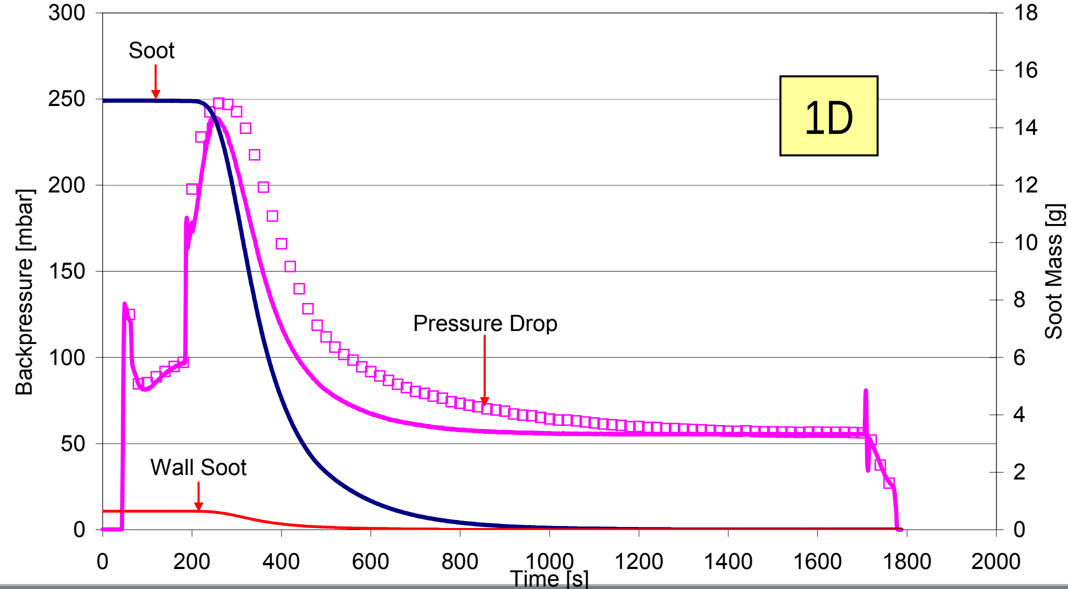


Regeneration simulations of oval filters with asymmetric flow profiles are completed with minimum CPU cost without CFD coupling

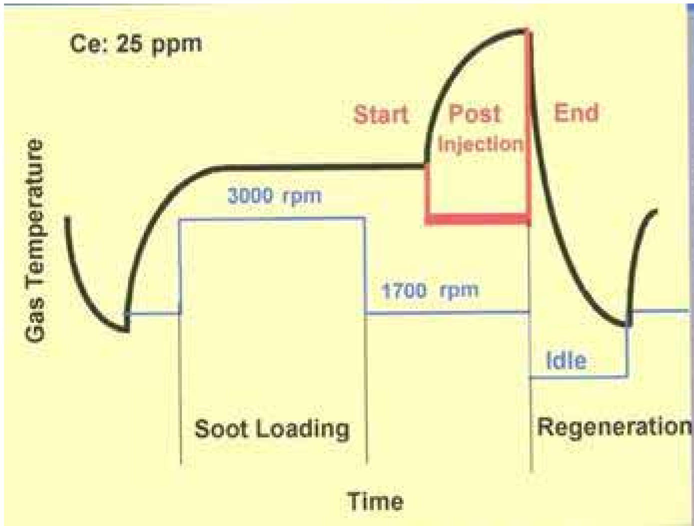
Forced regeneration
3-d vs 1-d simulation results

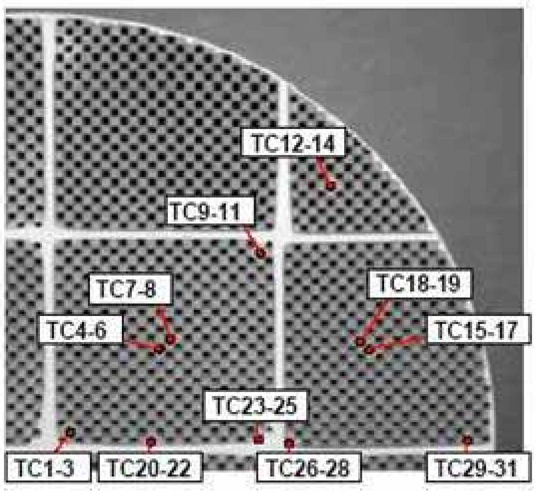
dots: measurement
lines: simulation

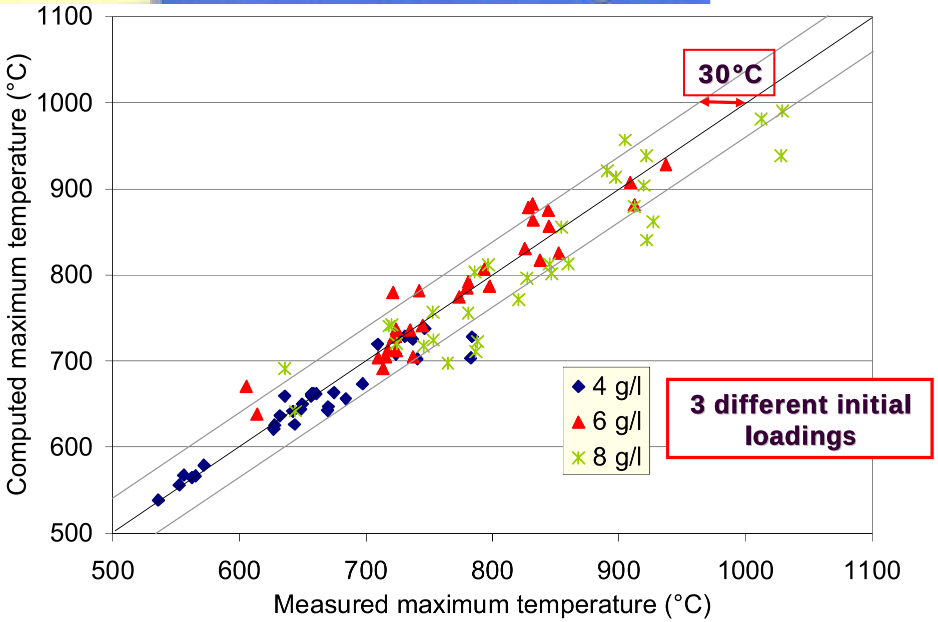




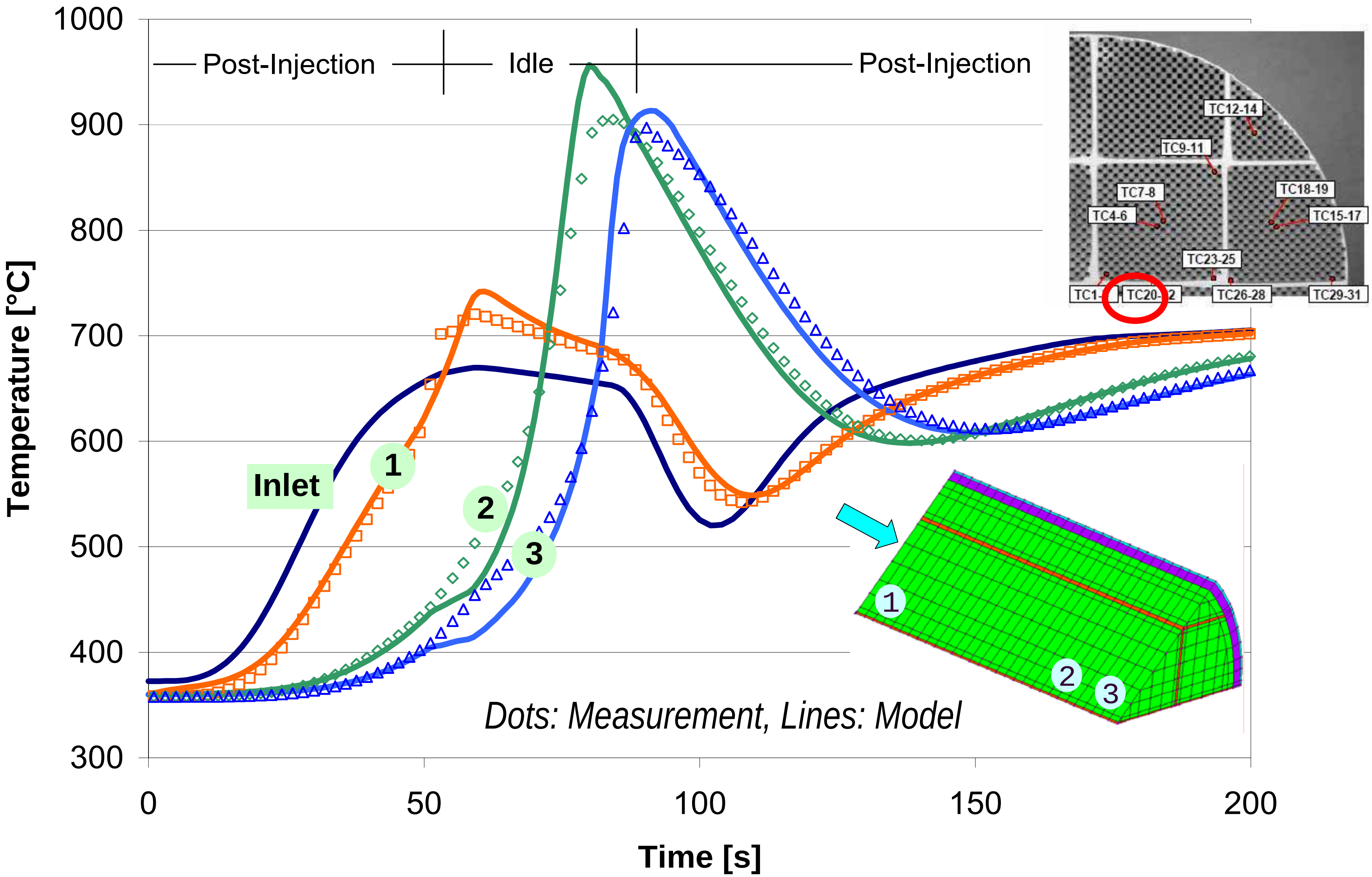
Model validation vs experimental data (LAT & NGK: SAE 2005-01-0953)



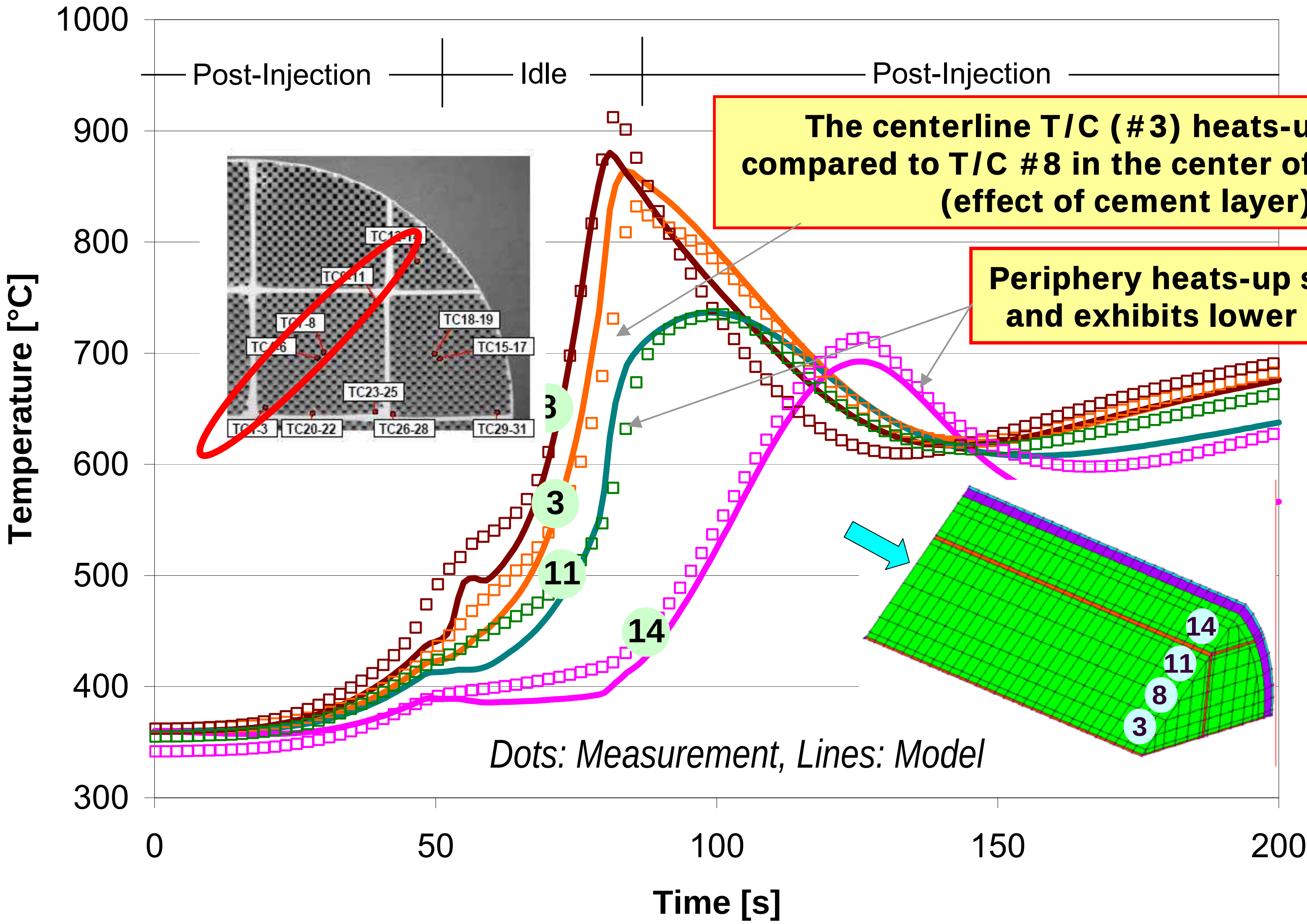




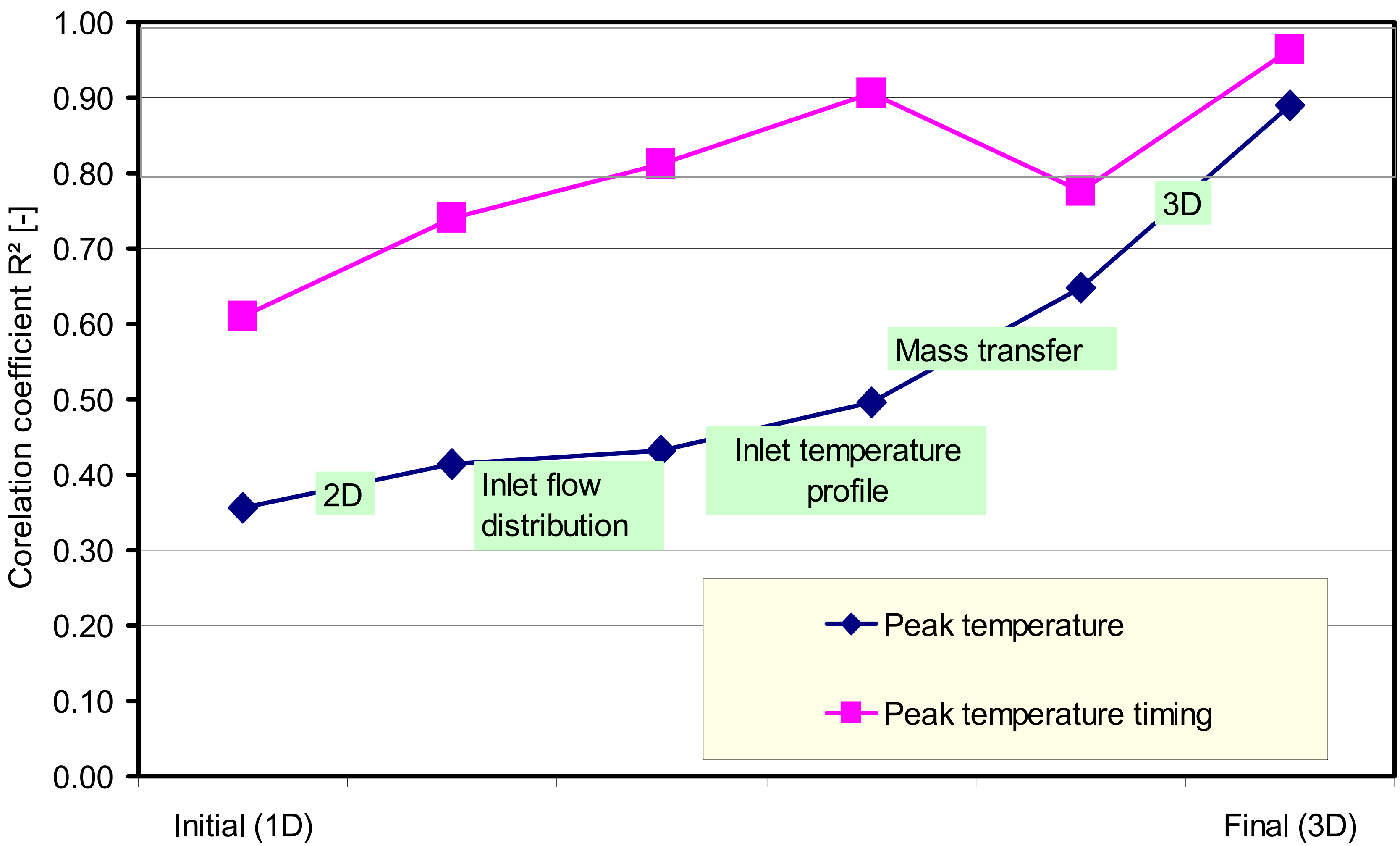
Model validation – centerline channel
Initial soot loading: 8 g/l



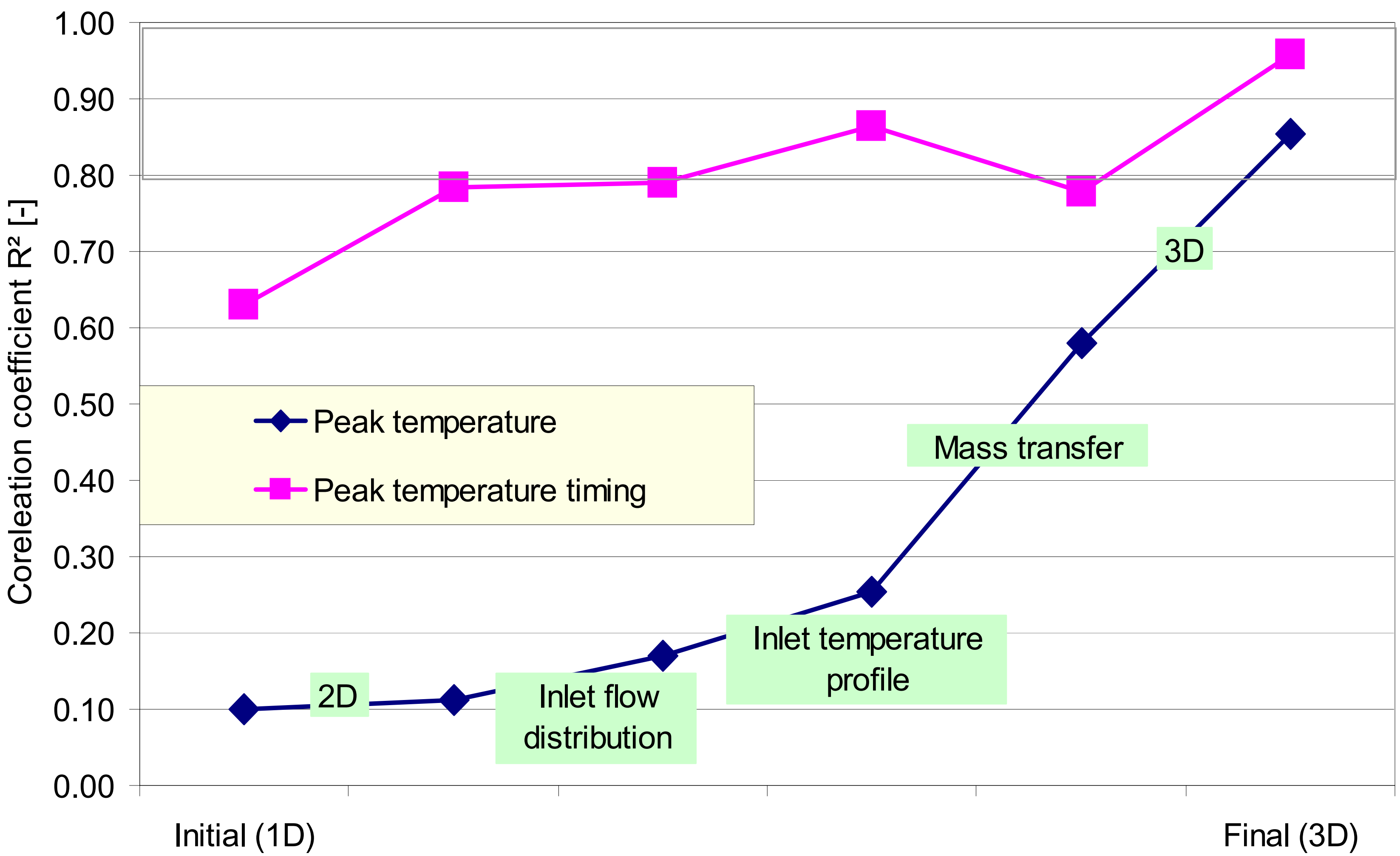
Model validation – 8 g/l
Filter exit – 45° plane



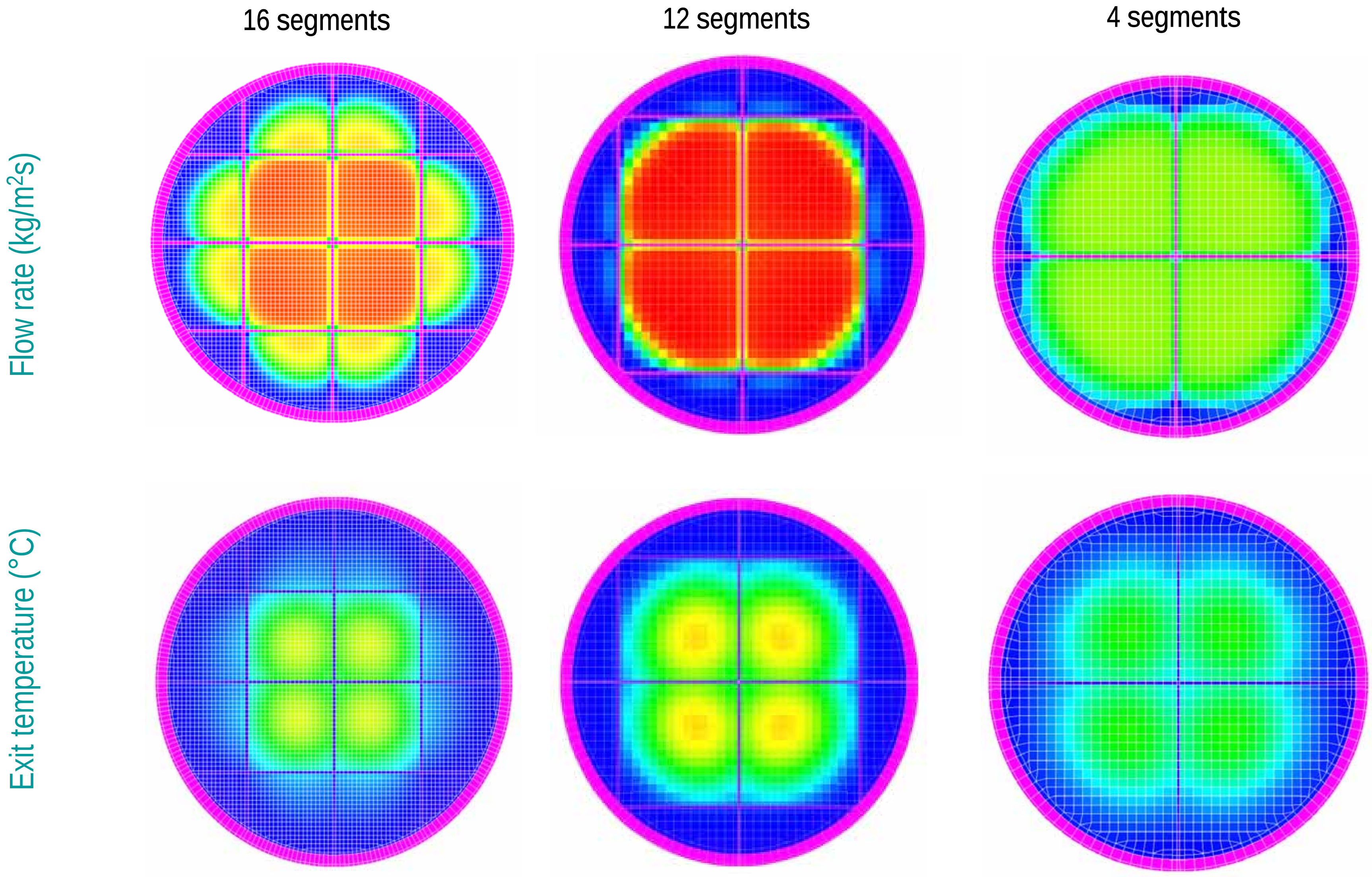
Accuracy assessment
FBC system - Initial soot loading: 6 g/l



Accuracy assessment
FBC system - Initial soot loading: 8 g/l



Segmentation effects
Simulation results with same protocol, time=80 s

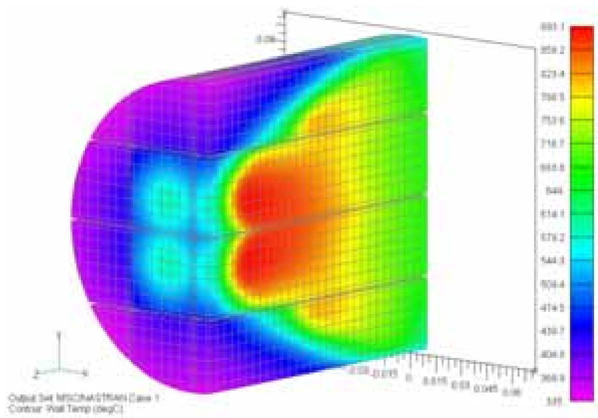


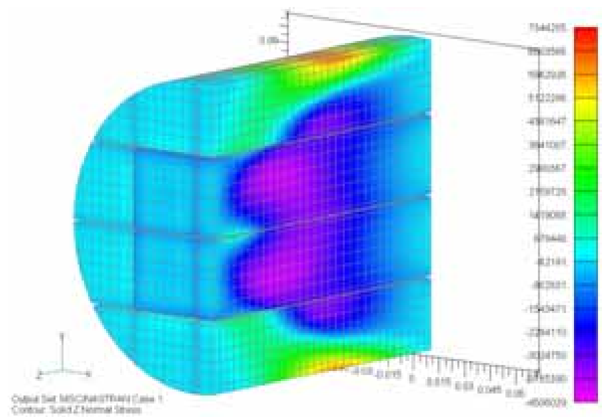
Stress analysis

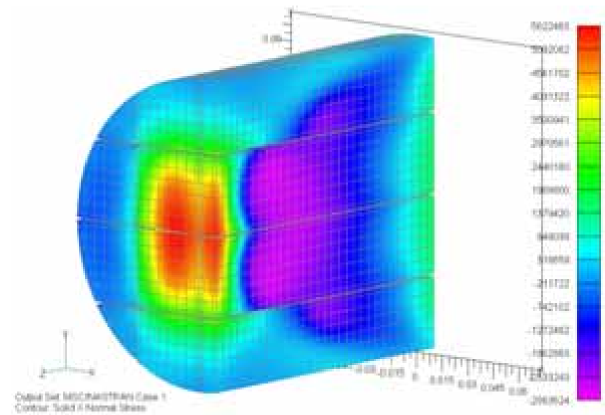
Exothermia

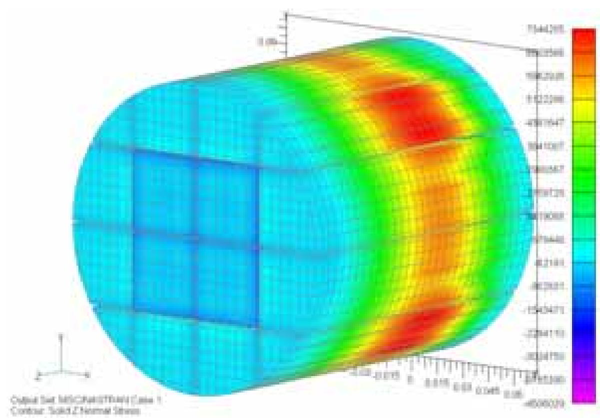
Axitrap™ → Nastran™

Temperature	σ_Z	σ_X

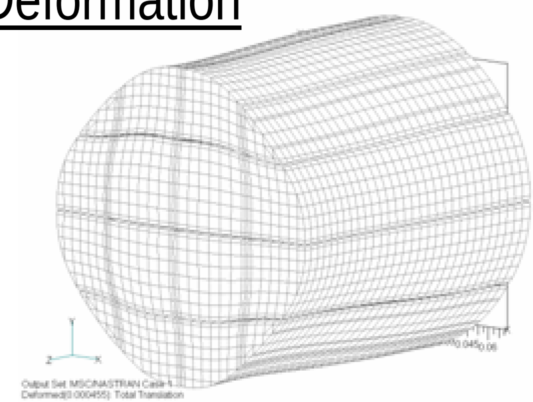








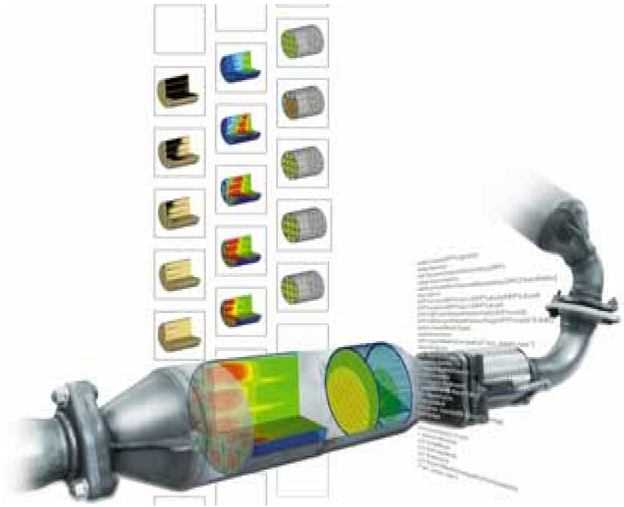
Deformation



Exothermia
modeling efficiency

DOC modeling

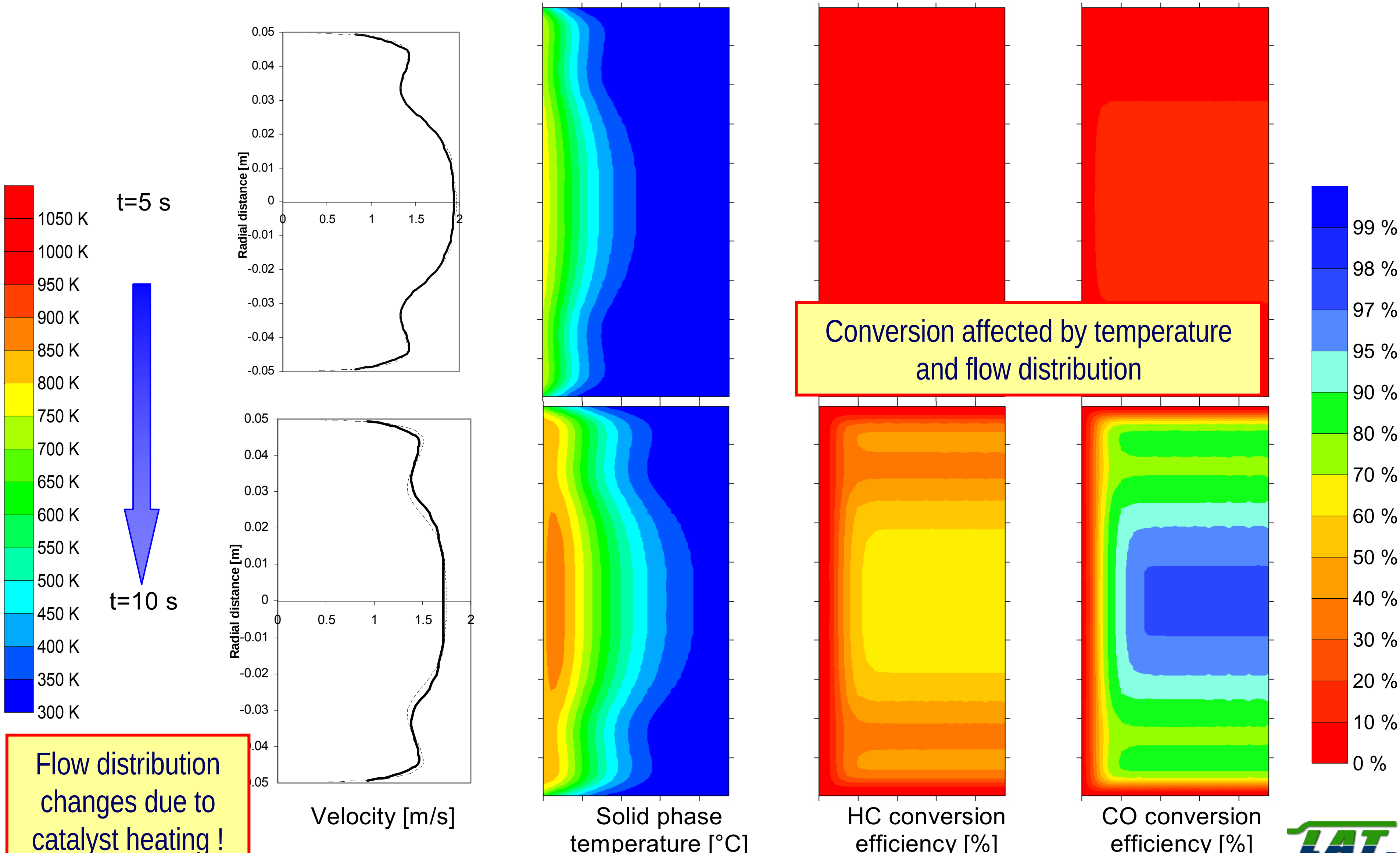
Multi-dimensional effects for the case of driving cycle performance prediction



LAT

2-d effects
Flow distribution effects during catalyst warm-up

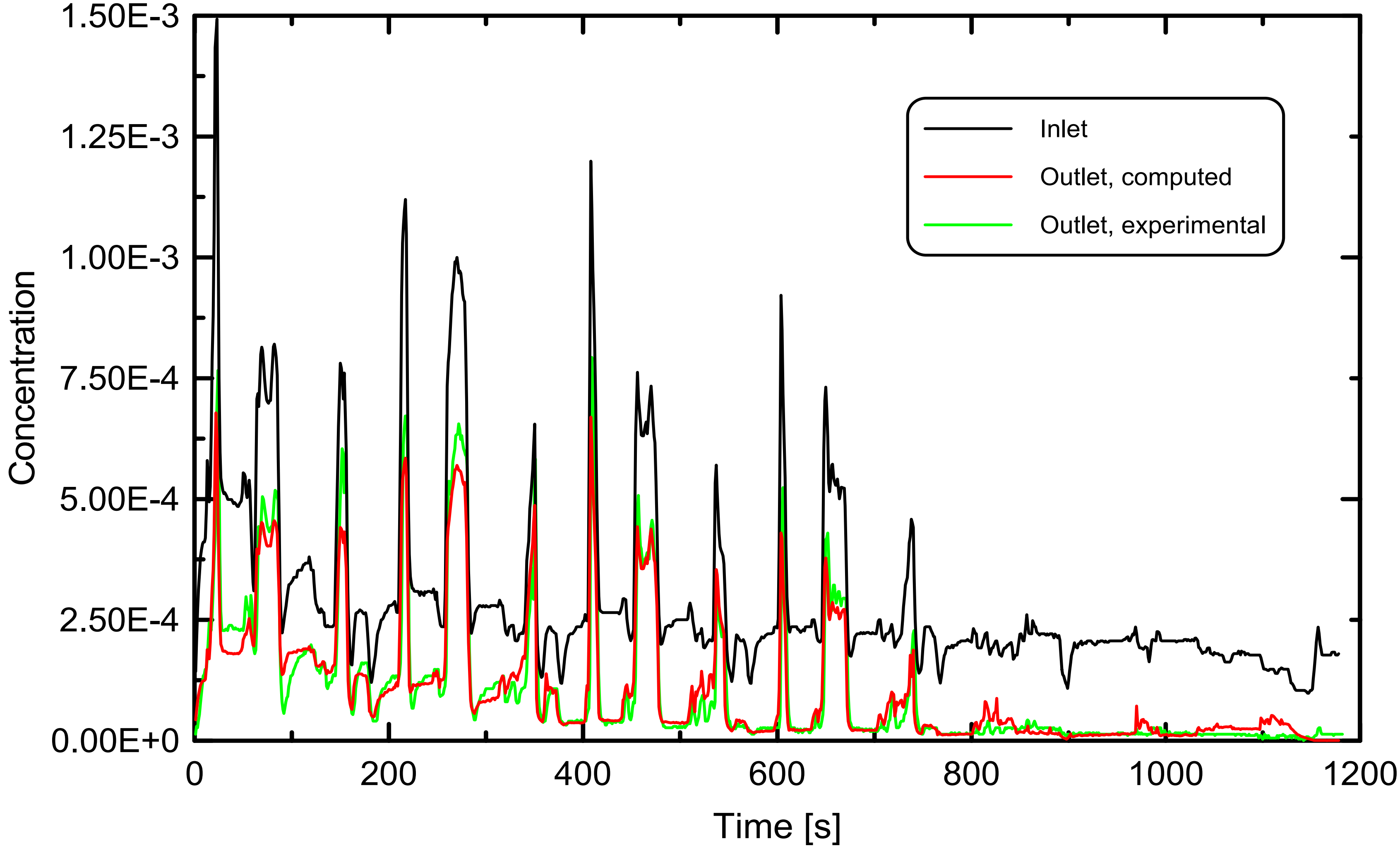
Exothermia



Flow distribution changes due to catalyst heating !

LAT

HC prediction instantaneous emissions



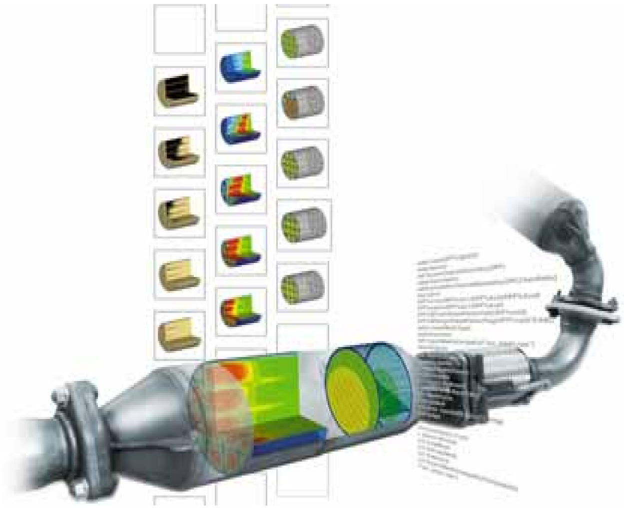
Pontikakis G. N., Koltsakis G. C., Stamatelos A. M., Noirot R., Agliany Y., Colas H., Versaevel Ph., Bourgeois C.: Experimental and Modeling Study on Zeolite Catalysts for Diesel Engines, Topics in Catalysis, 6/17, Nos. 1-4, September 2001, pp. 329-335.

DOC model sensitivity

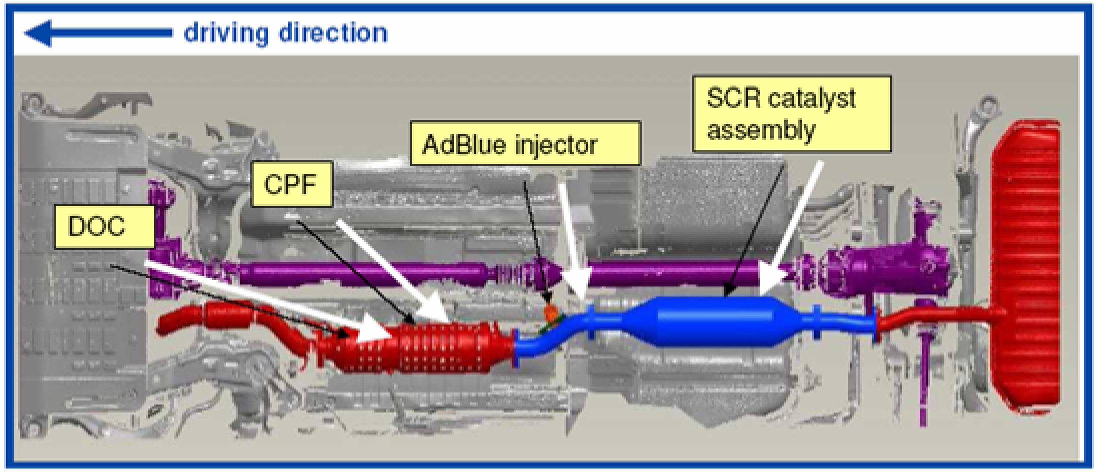
	CO (efficiency [%])				HC (efficiency [%])			
	I	**II**	**III**	**total**	**I**	**II**	**III**	**total**
Measurement	*11.4*	*32.1*	*99.1*	*42.1*	*45.3*	*55.1*	*91.8*	*62.5*
Model results	*2.5*	*32.5*	*99.6*	*40.3*	*46.6*	*56.7*	*86.9*	*62.3*
Assumptions								
Uniform flow distribution	2.7	38.2	100	**43.4**	46.9	64.6	93.0	**68.1**
HC adsorption neglected	2.4	31.5	99.5	39.7	**3.8**	34.4	87.1	**41.3**
2 HC species (propene/propane)	2.4	32.2	99.6	40.1	**7.3**	50.6	83.7	**49.6**
H_2O adsorption neglected	2.9	35.5	99.5	41.9	46.8	59.0	87.1	63.6

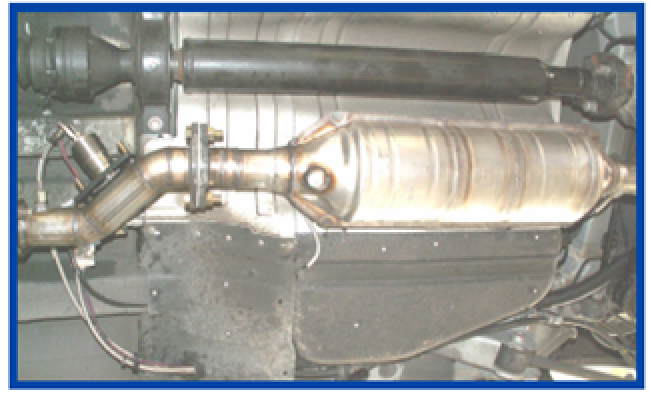
Pontikakis G. N., Koltsakis G. C., Stamatelos A. M., Noirot R., Agliany Y., Colas H., Versaevel Ph., Bourgeois C.: Experimental and Modeling Study on Zeolite Catalysts for Diesel Engines, Topics in Catalysis, 6/17, Nos. 1-4, September 2001, pp. 329-335.

SCR modeling

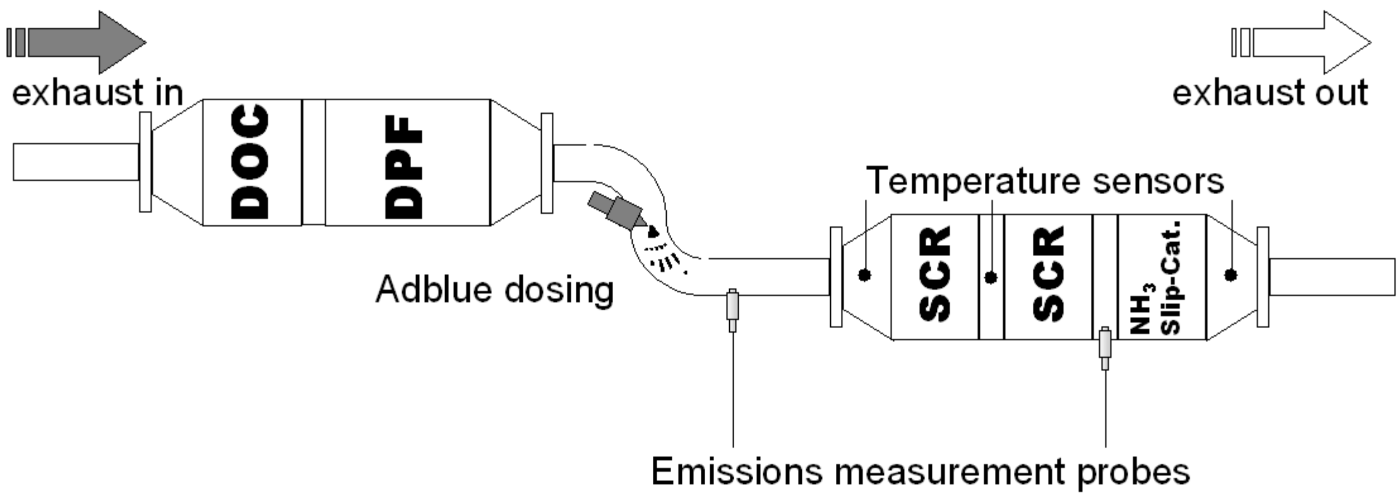


Exhaust system layout

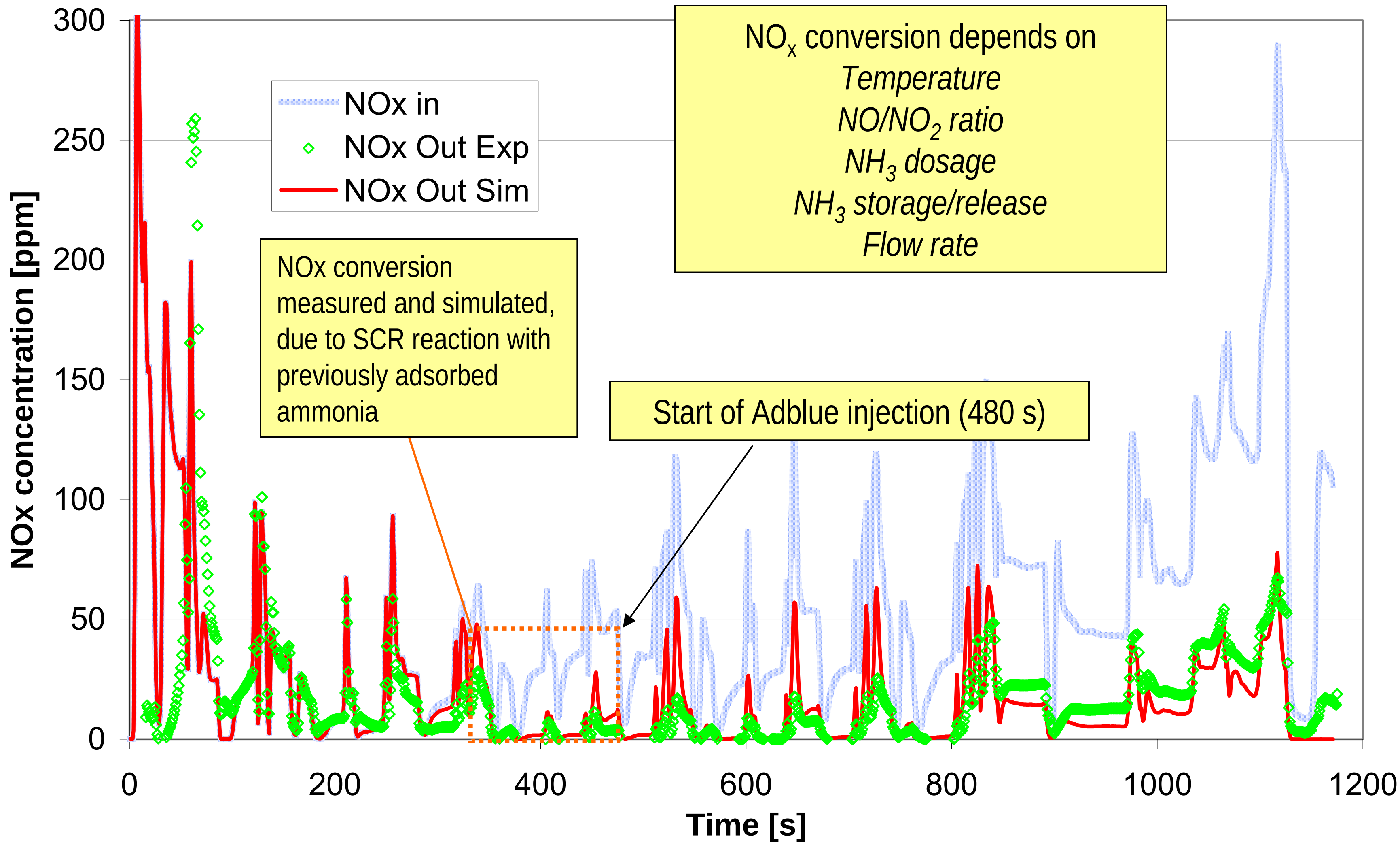




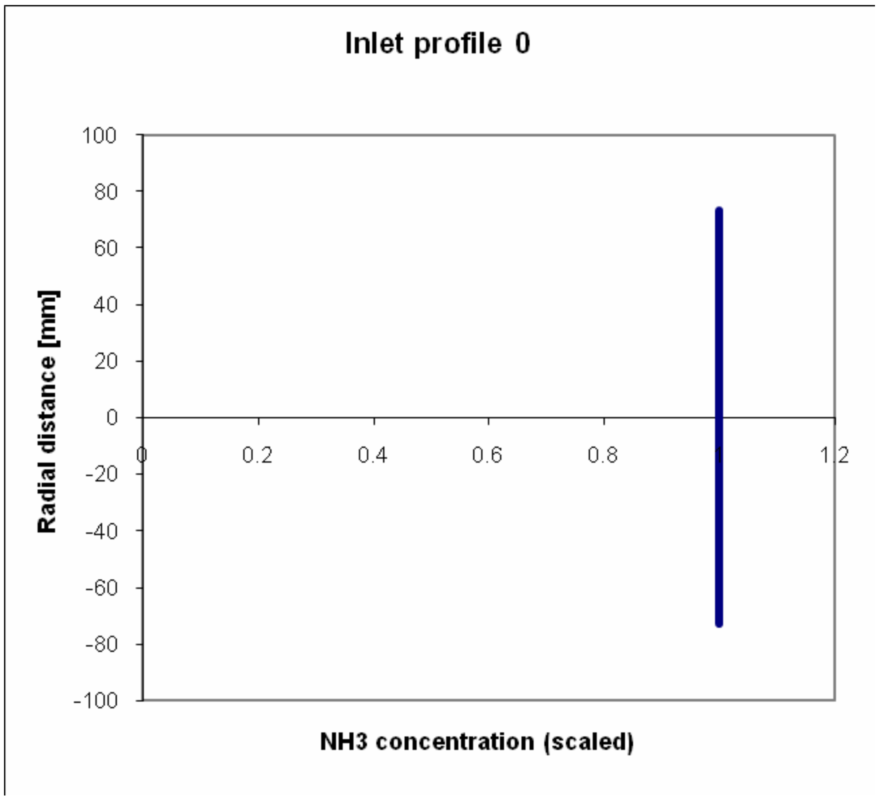
3-D Scan of Vehicle underbody & boot by IAV; SCR catalyst designed to fit in existing Vehicle Package

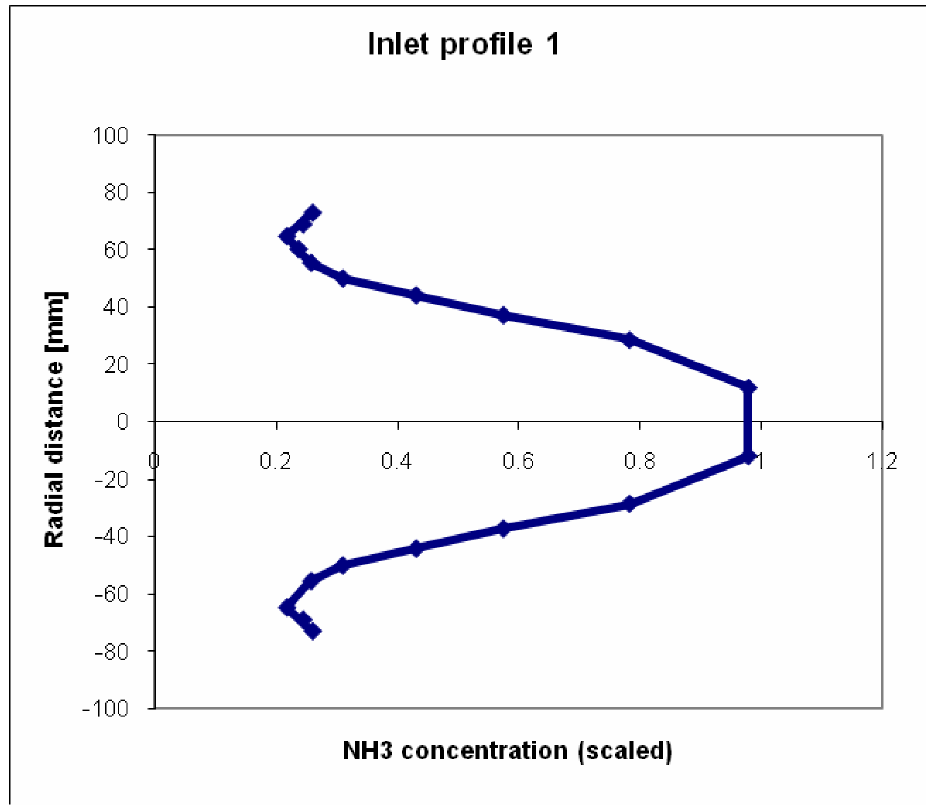


SCR catalyst simulation
NEDC NO_x predictions



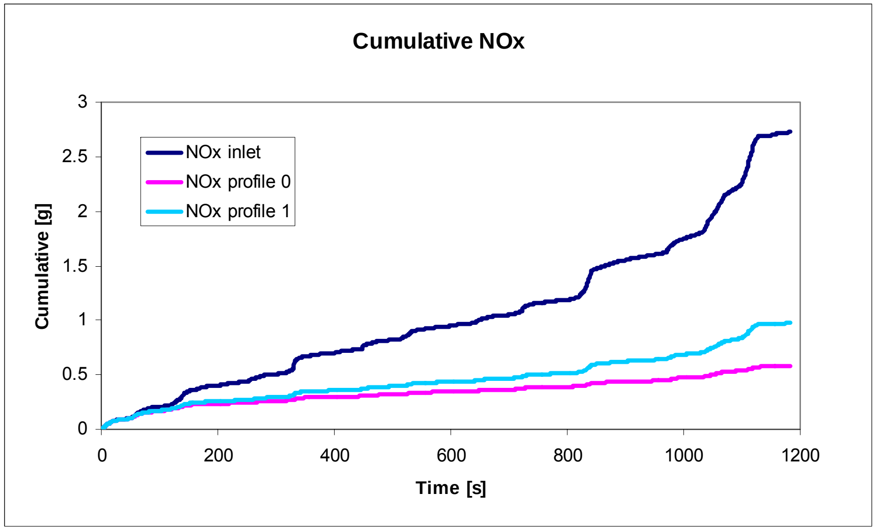
Effect of NH_3 inlet profile
Simulation study



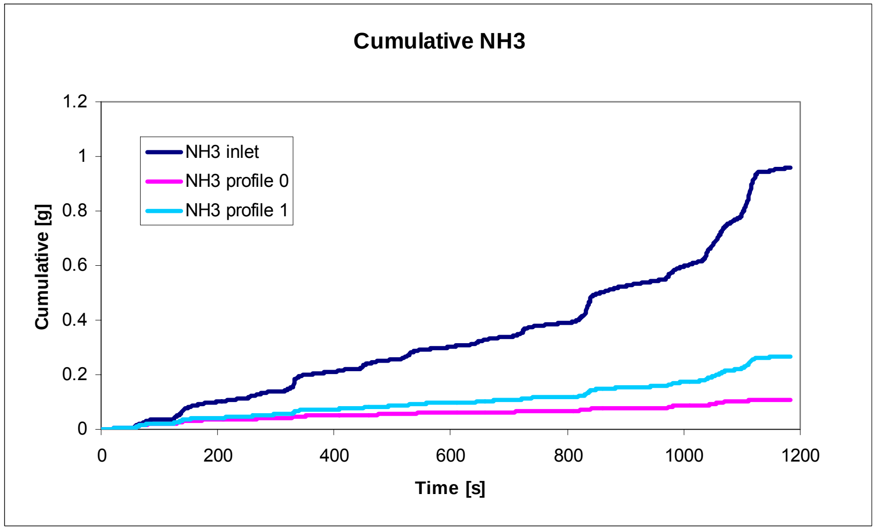


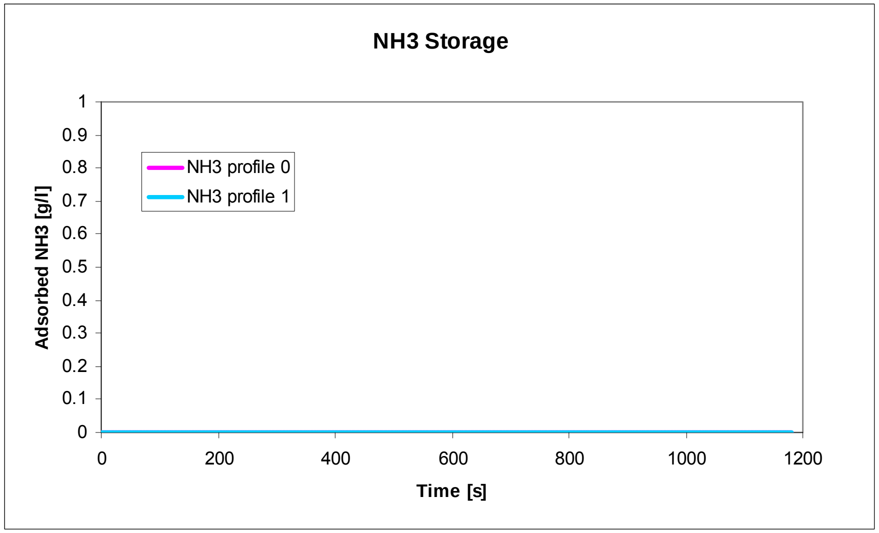
Simplifying assumptions:
NH_3/NO_x=1, only when T_{in}>190 °C
Uniform inlet flow/NO_x distribution

Assumption: zero NH_3 storage capacity

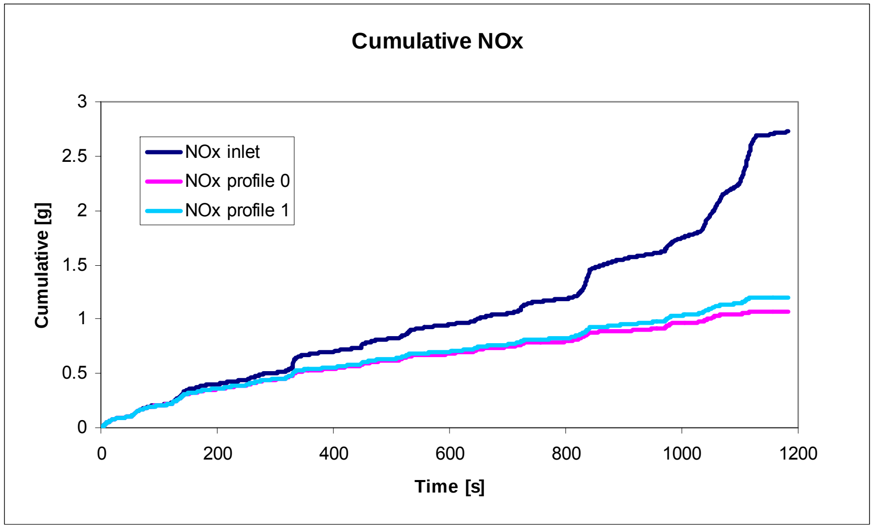


As expected, the non-uniform NH_3 distribution is strongly reflected in the SCR de-NOx performance and NH_3 slip

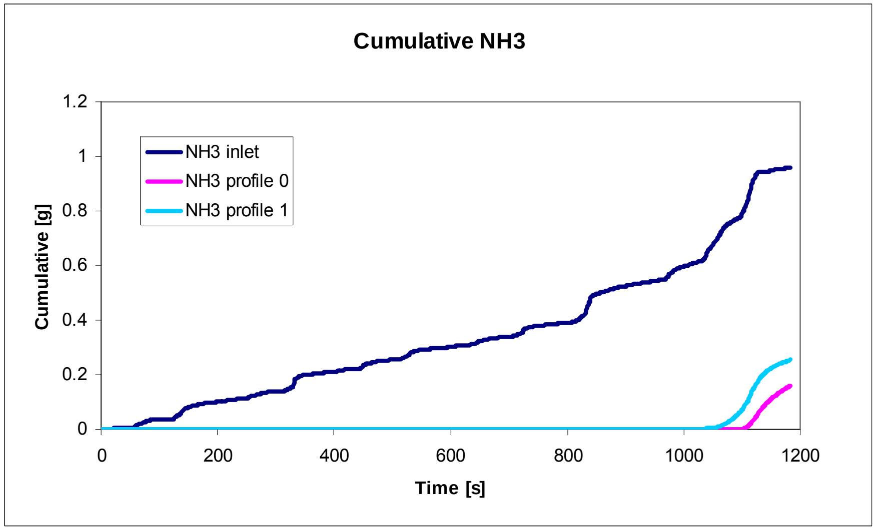


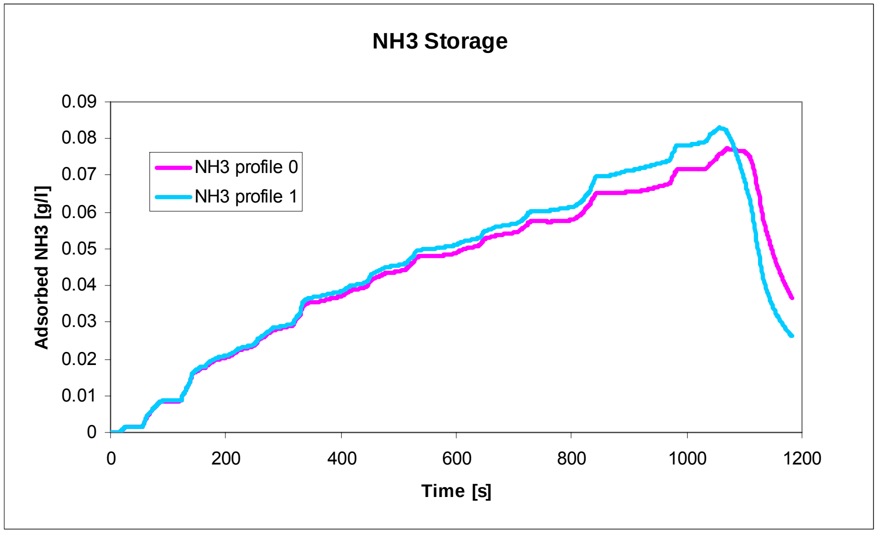


Assumption: zeolite-based with NH_3 storage capacity, *no pre-adsorbed NH_3*



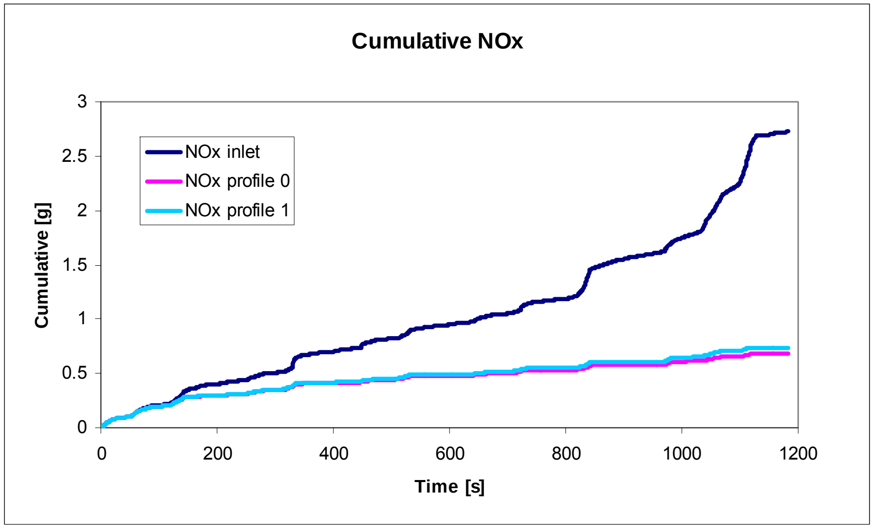
The NH_3 adsorption capacity partially "relieves" the detrimental effects of non-uniform distribution

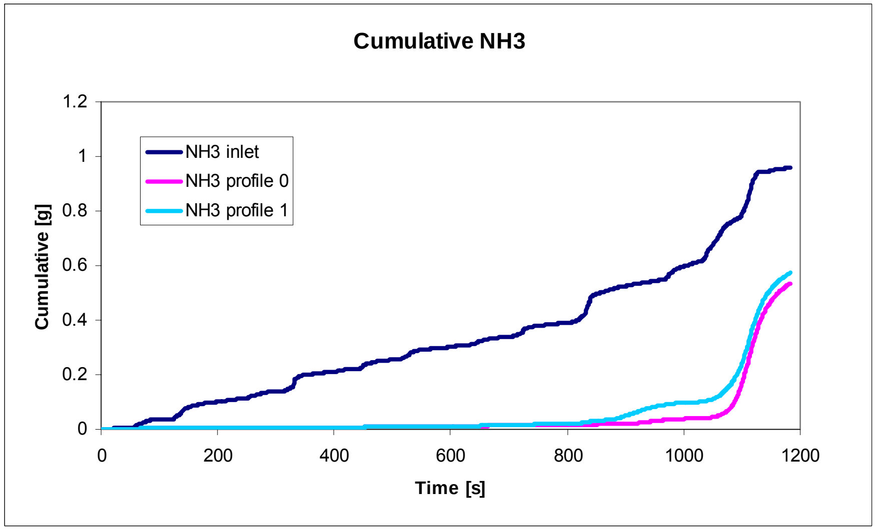


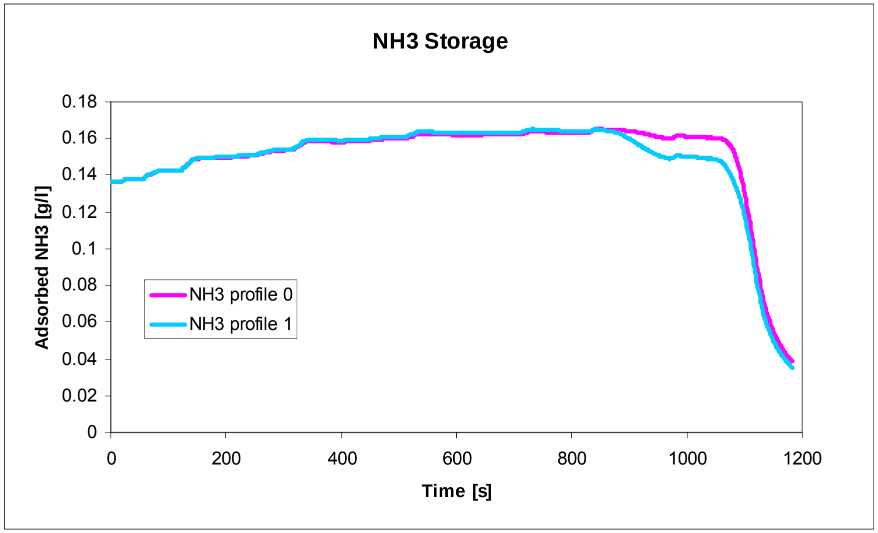


Assumption: zeolite-based with NH_3 storage capacity, *with pre-adsorbed NH_3*

Exothermia

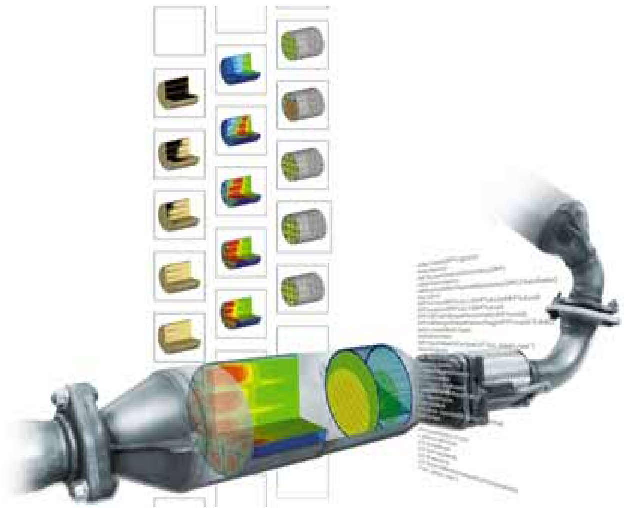






LAT

Complete exhaust line simulation



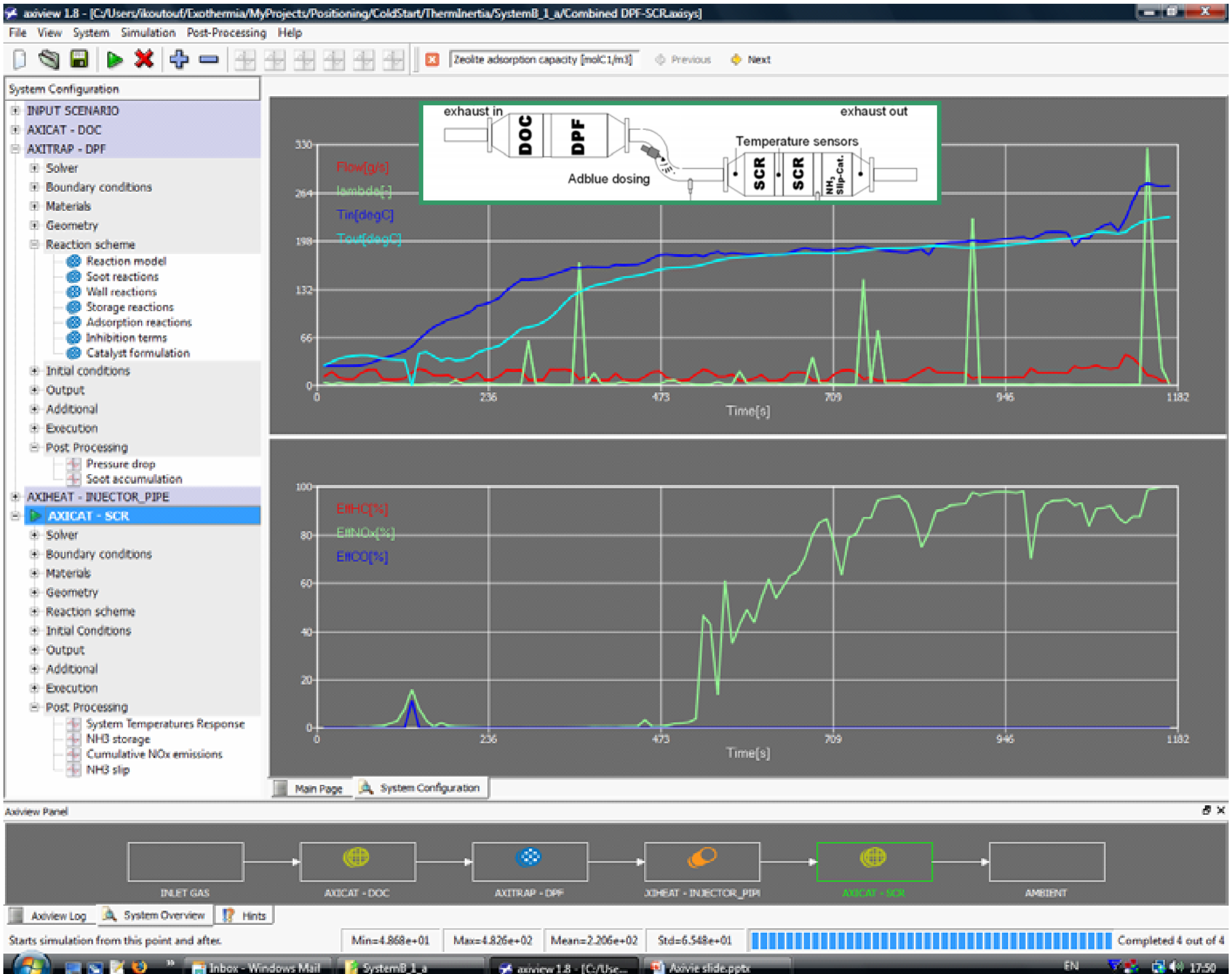
Simulation modules

Exothermia

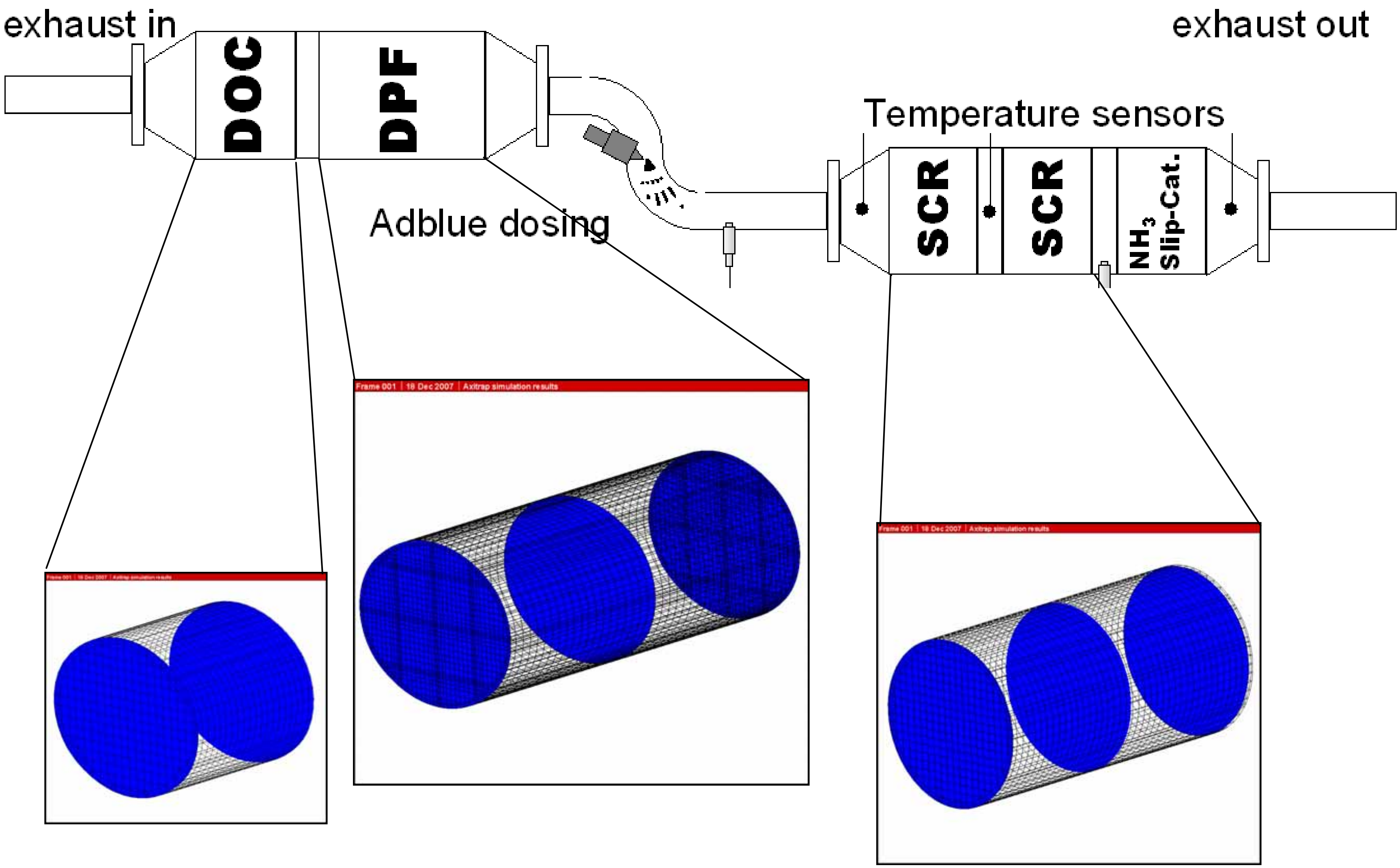
axisuite

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	✓	✓	✓	✓
axifoam	deep-bed	n/a	✓	✓	✓	✓
axiheat	exhaust pipe	single-wall	double-wall	insulating material	flanges	reacting flow

System simulation

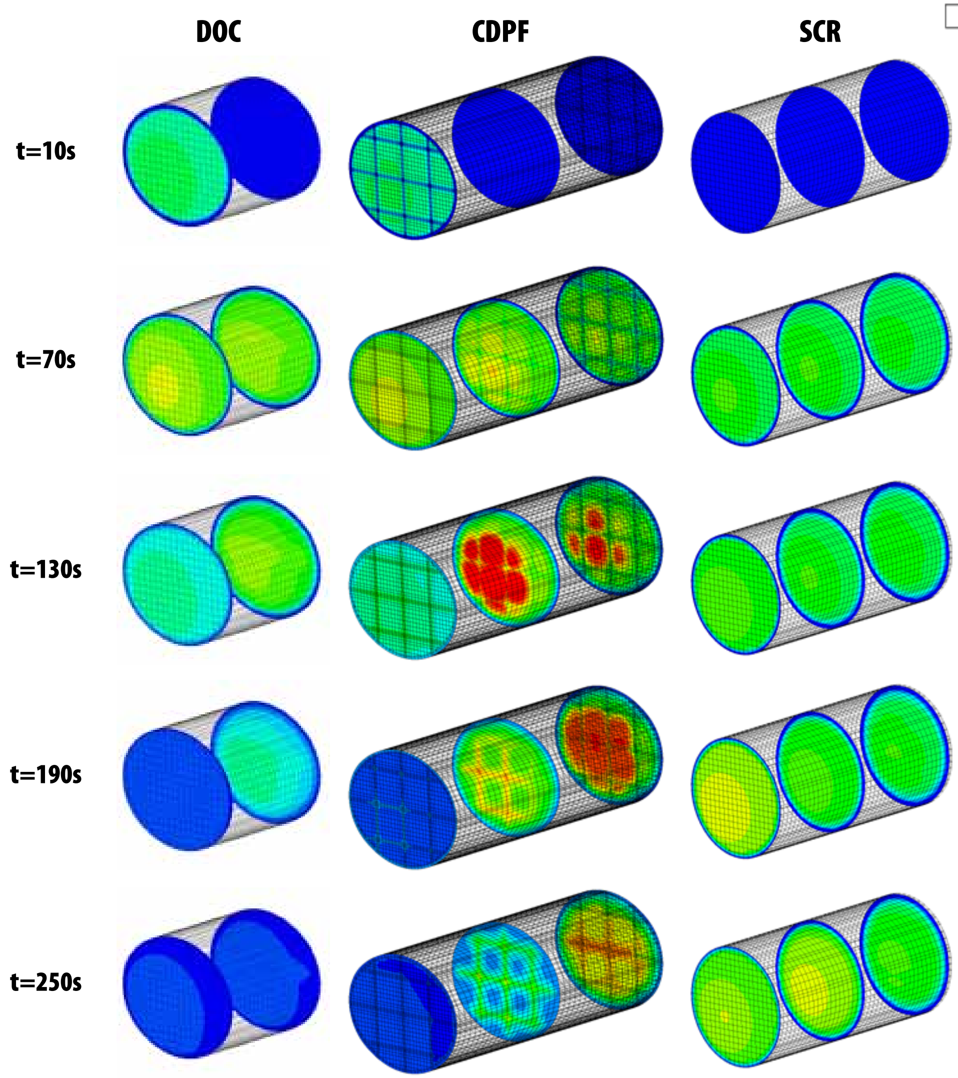


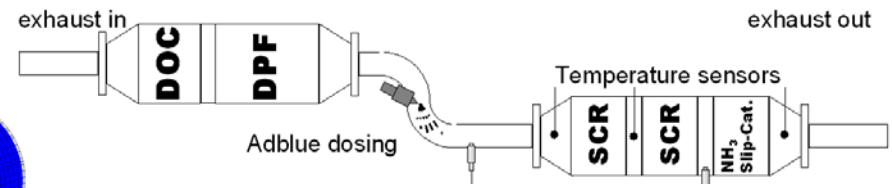
Complete system simulation: Soot limit with respect to SCR thermal loading

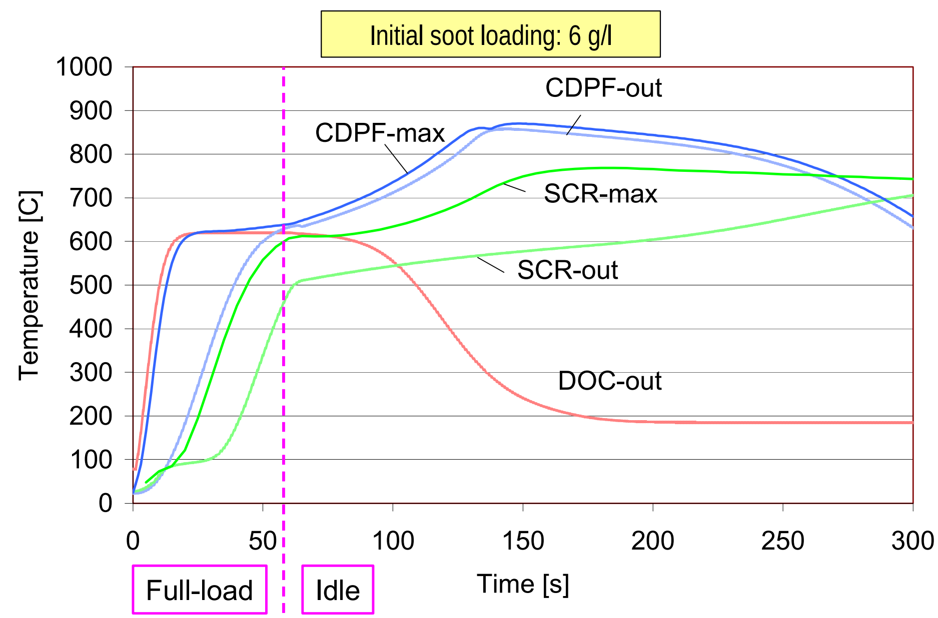


Koltsakis et al., FAD Conference-2007 (LAT-IAV GmbH-Exothermia)

3-d system temperature simulation
"Worst-case" DPF regeneration case



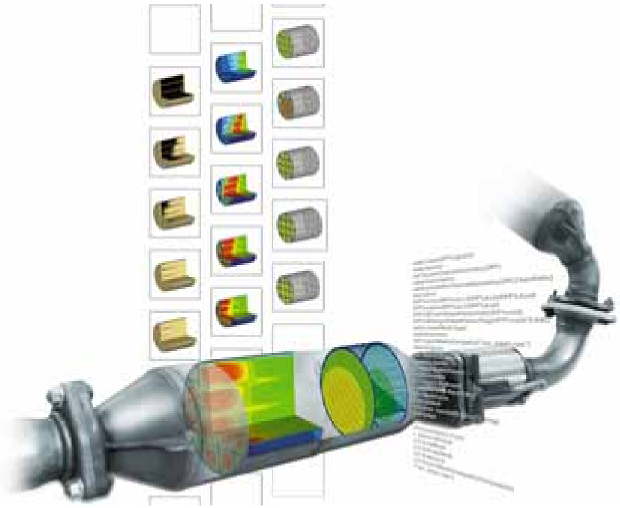




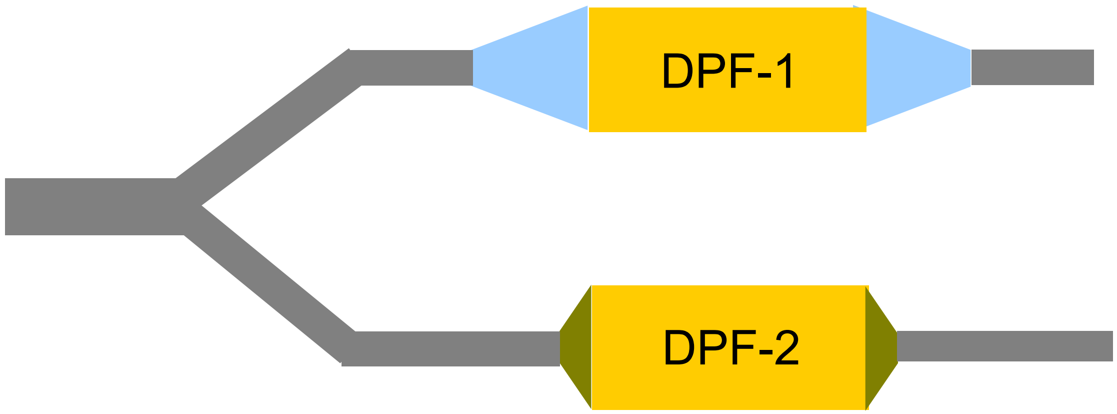
Test data for model input from IAV engine bench (SAE 2007-01-1127)

Koltsakis et al., FAD Conference-2007 (LAT-IAV GmbH-Exothermia)

Parallel DPF systems



Illustrative example: 2 branches
Identical DPFs, different flow conditions

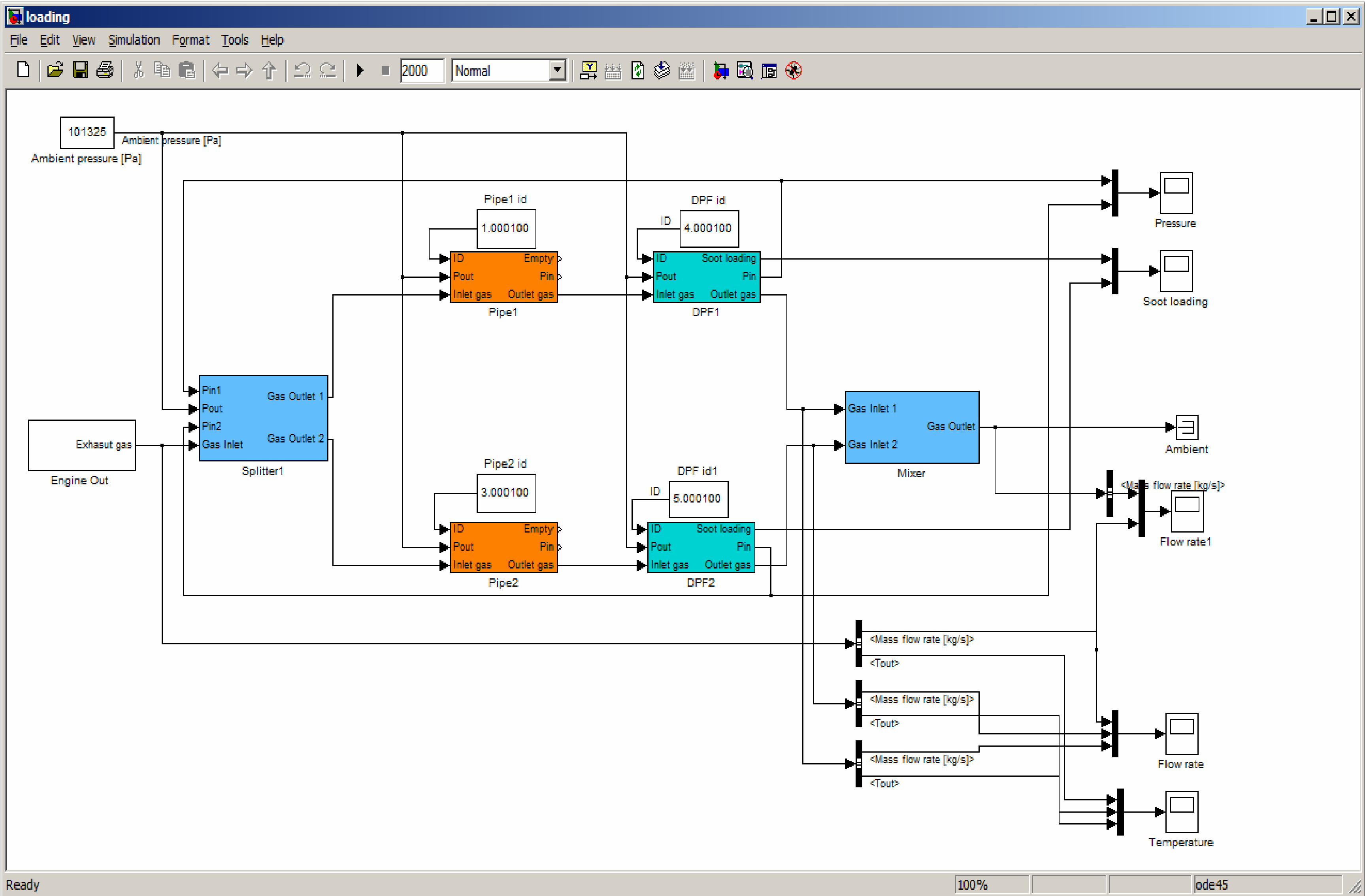


- As a simple illustration case, we consider two DPFs with different cones. DPF-1 cone ensures uniform flow. DPF-2 cones result in significant maldistribution.

- How will the flow and soot be distributed during loading?
- Will there be any differences during regeneration?

Parallel DPFs simulation in MATLAB/Simulink using *axisuite* S-functions

Exothermia



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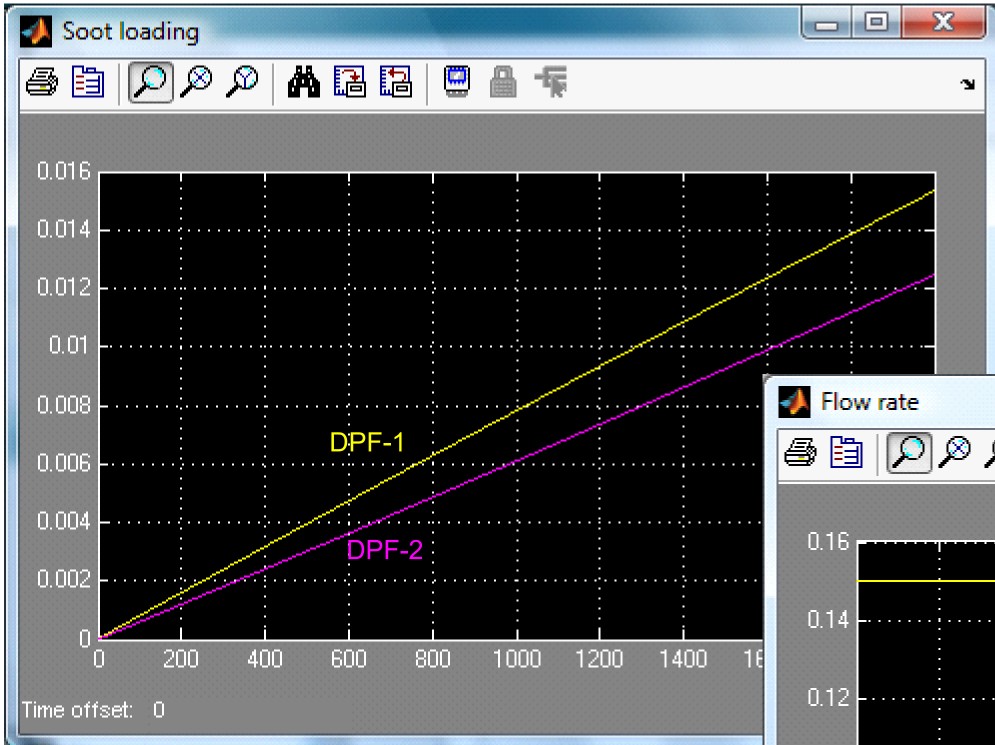
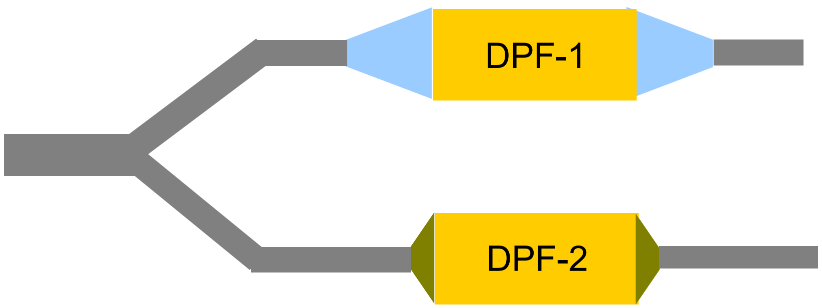
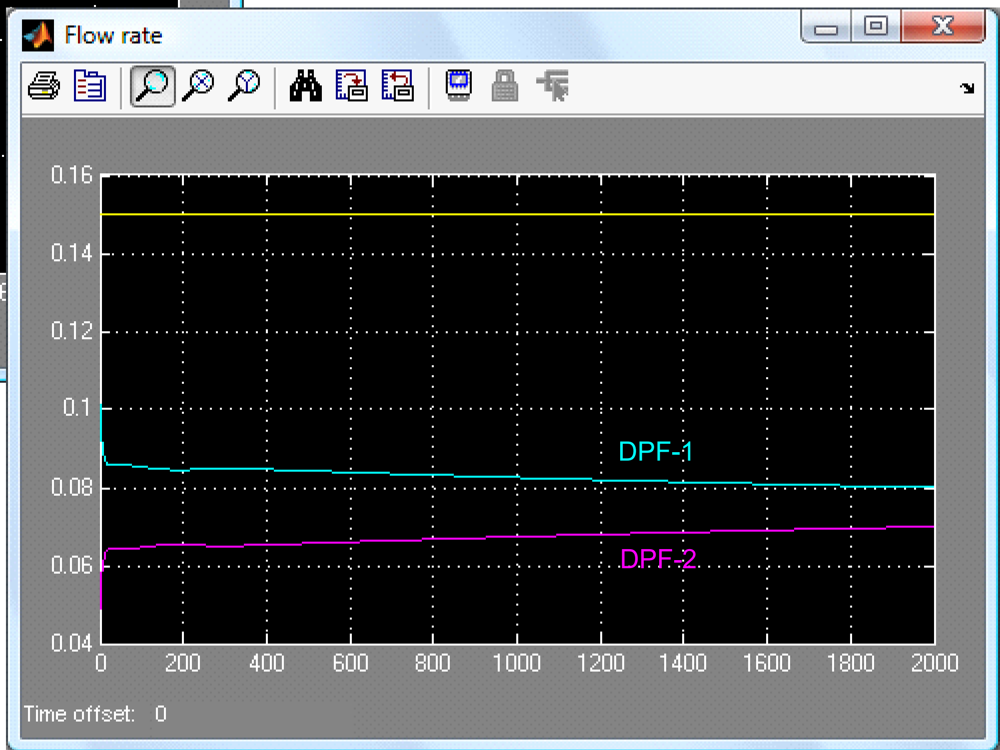
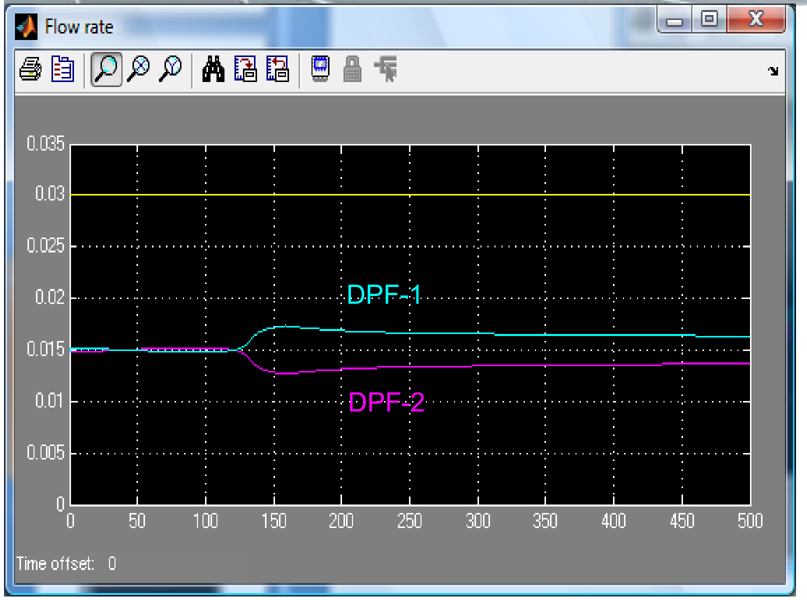
Flow division and soot accumulation during loading mode

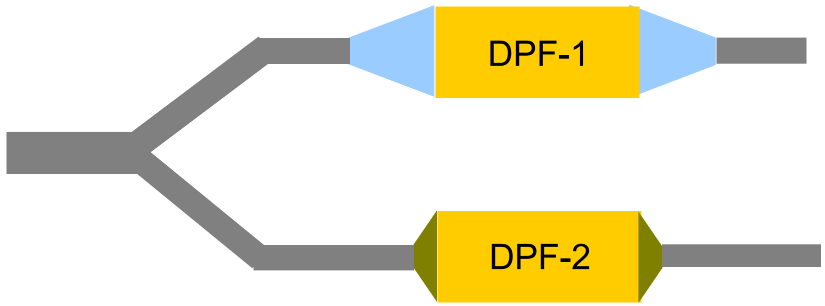


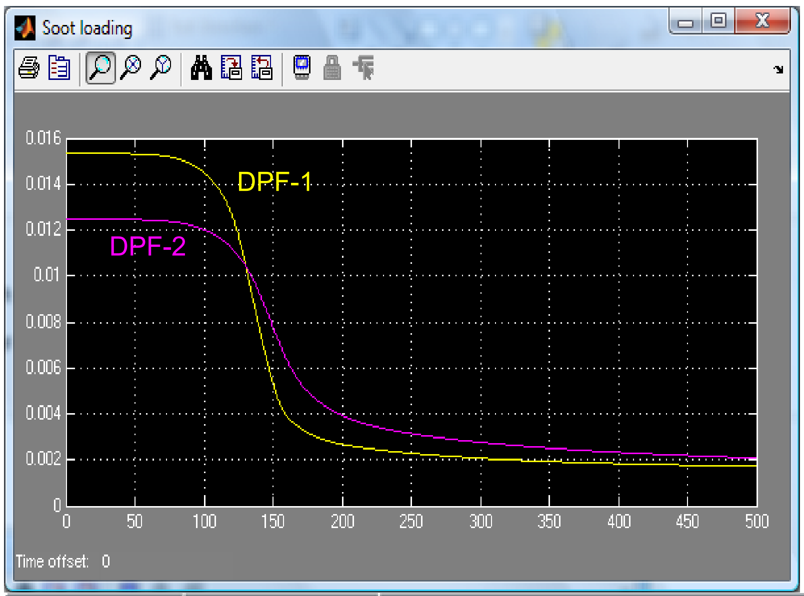


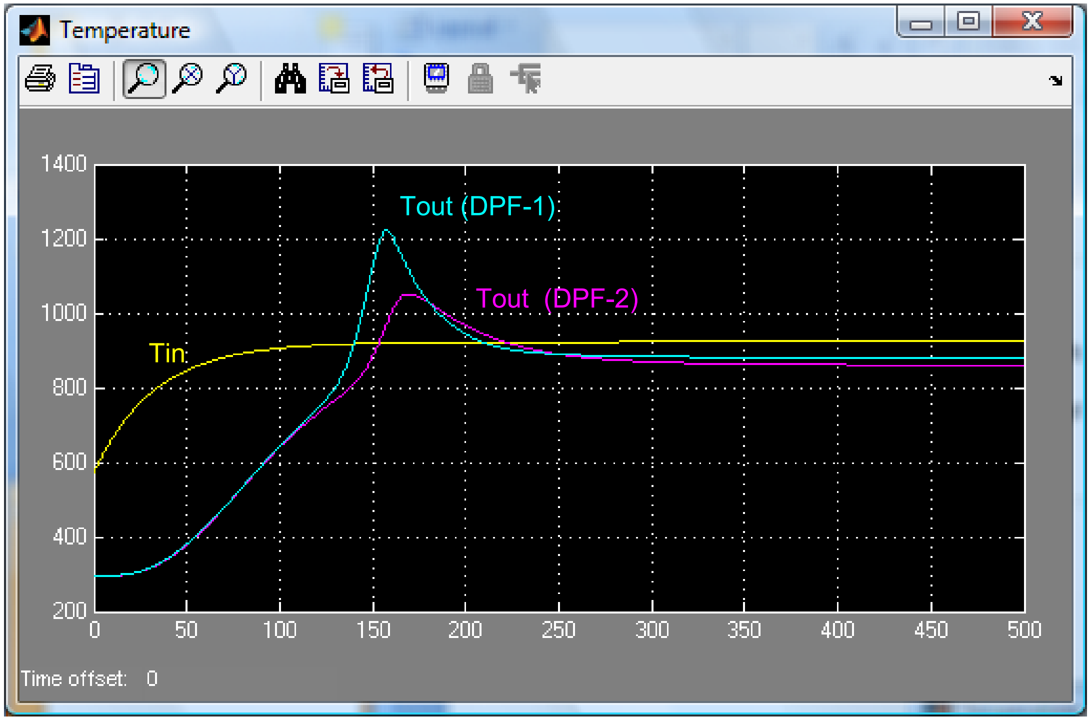


Parallel filters
Regeneration simulation









Conclusions

- Depending on the application the detail of modeling – number of model dimensions has to be correctly identified.
- For the case of DPF modeling
  - intra-wall dimension is important for filtration/pressure drop and catalyzed reactions modeling
  - 2-d and 3-d DPF discretization is necessary for regeneration modeling
- Flow-through catalyst modeling
  - 2-d and 3-d modeling is necessary to account for flow/heat maldistribution
  - For SCR applications, multi-dimensional modeling is crucial for NH_3calculations
- Parallel systems should be modelled concurrently, to account for the interactions.

Thank you very much for your attention!

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http://lat.eng.auth.gr

www.exothermia.com