PÖYRY ADVANCED MODELLING & SIMULATION

REACTIVE FLOWS

July 2019

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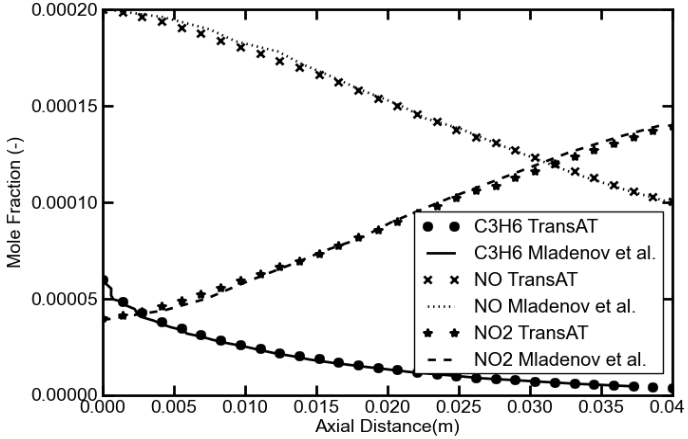
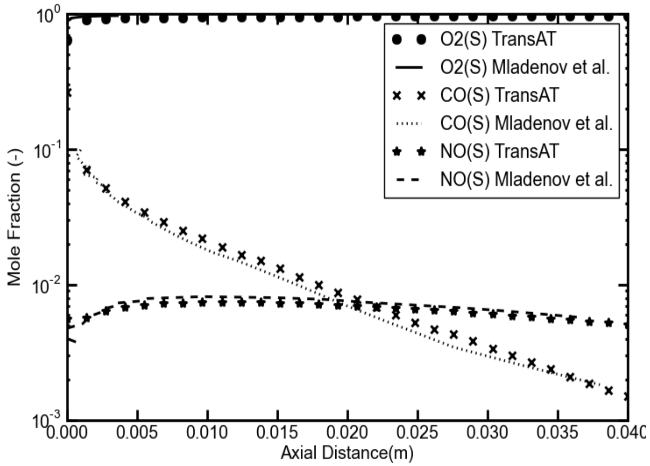
Catalytic Wall Reaction →

EXAMPLE 1: FINITE RATE SURFACE REACTION IN TUBE (MLADENOV ET AL., 2000)



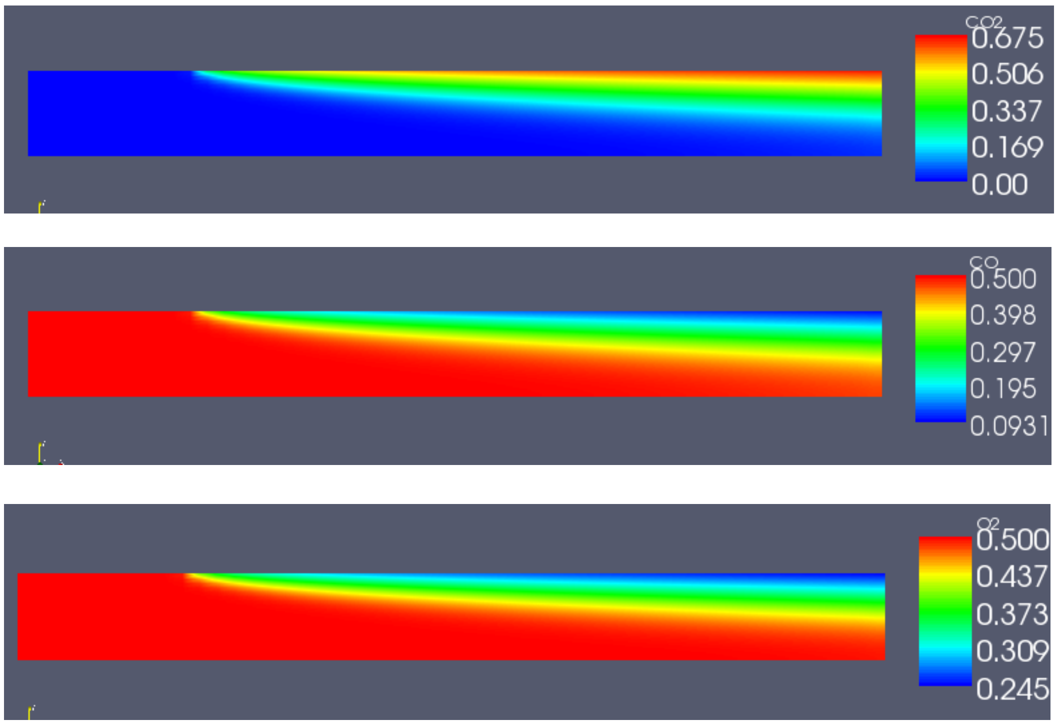
Mass flow averaged gas phase species in a channel. Comparison to the reference results of Mladenov et al.



Surface absorbed species in a channel. Comparison to the reference case of Mladenov et al.

- Flow in a tube Re = 201
- Fixed wall temperature 523 K
- Inlet: Typical exhaust gas of an engine
  - N2, O2, CO2 & H2O
  - Traces of C3H6
  - CO, NO, NO2
- Reactions on the tube surface
- Main pathways:
  - C3H6 oxidation
  - CO oxidation
  - Reactions involving NO and NO2

EXAMPLE 2: CATALYTIC WALL REACTION IN A CHANNEL
(RAJA ET AL., 2000)



Mass fraction of major species

- 2D channel (0.2cm; 10cm) Methane-Air mixture wall-reacting (heterogeneous) flow
- Re=200 (1 bar) & 2000 (10 bar); compressible flow
- U = 5m/s; T = 600K; Tw=600-1290K : x < 0.1cm;
- 8 gas-phase species & 11 surfaces species
- Use Cantera library to extract material properties

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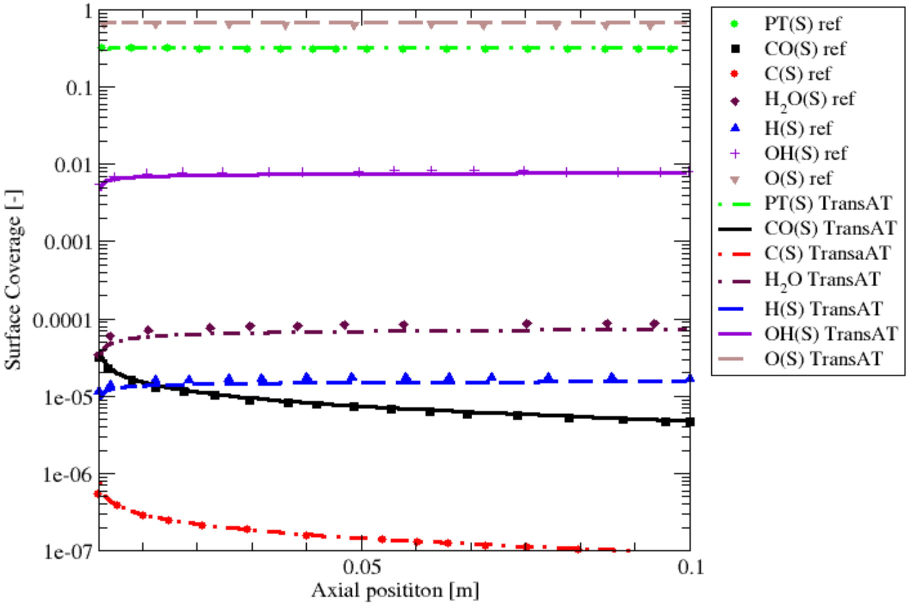
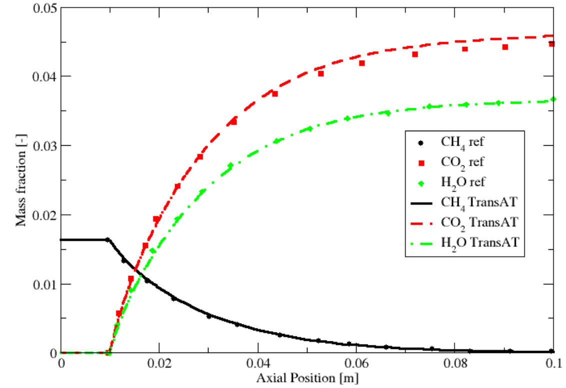
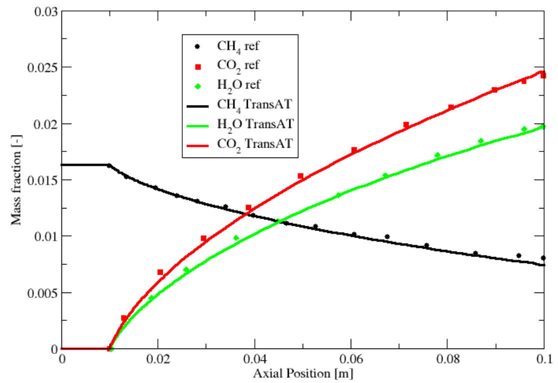
(RAJA ET AL., 2000)



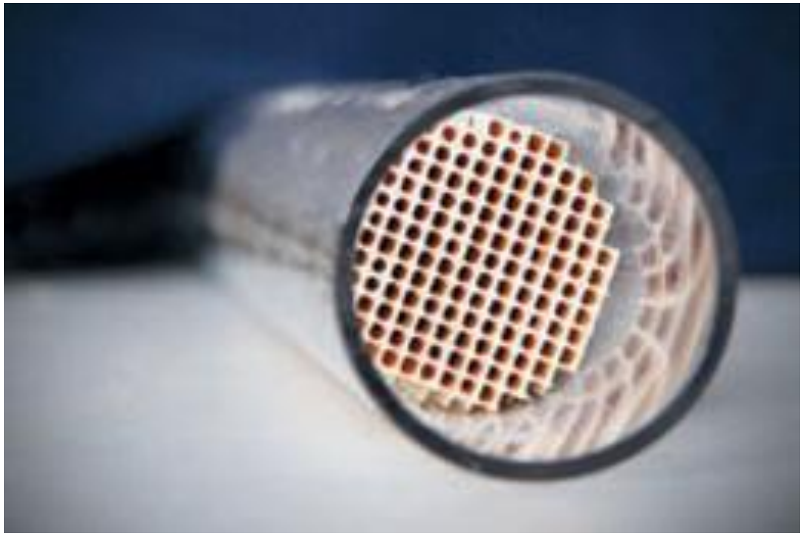




Surface coverage and surface species mass fractions

EXAMPLE 3: CATALYTIC WALL REACTION IN A DUCT (GHERMAY ET AL., 2010)

- A square duct (section: 0.7cm; 30cm) with Hydrogen-Air mixture wall-reaction
- Using Benzene reaction chemistry
- Walls coated with platinum
- U = 9.6m/s; T = 572K; Tw=1150 K : x < 0.1cm
- 7 gas-phase species & 5 surfaces species
- Use Cantera library to extract material properties



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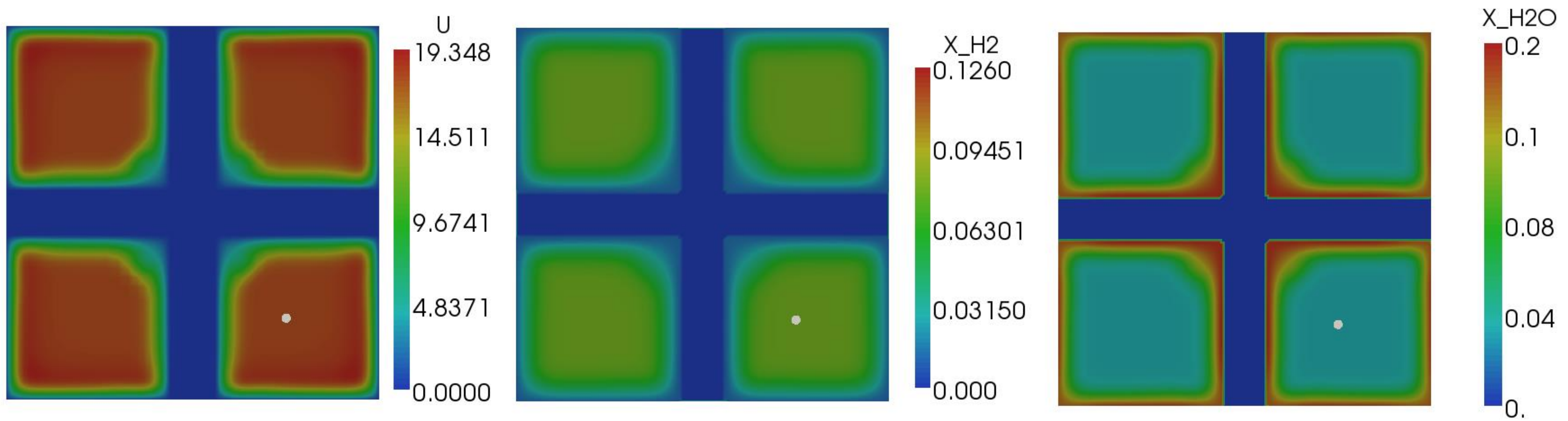
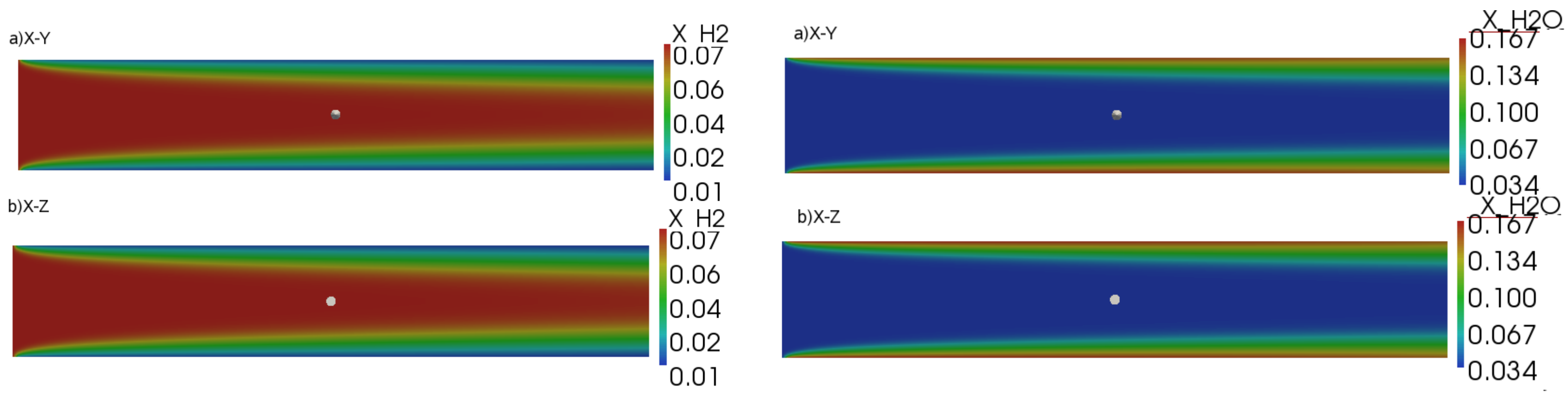
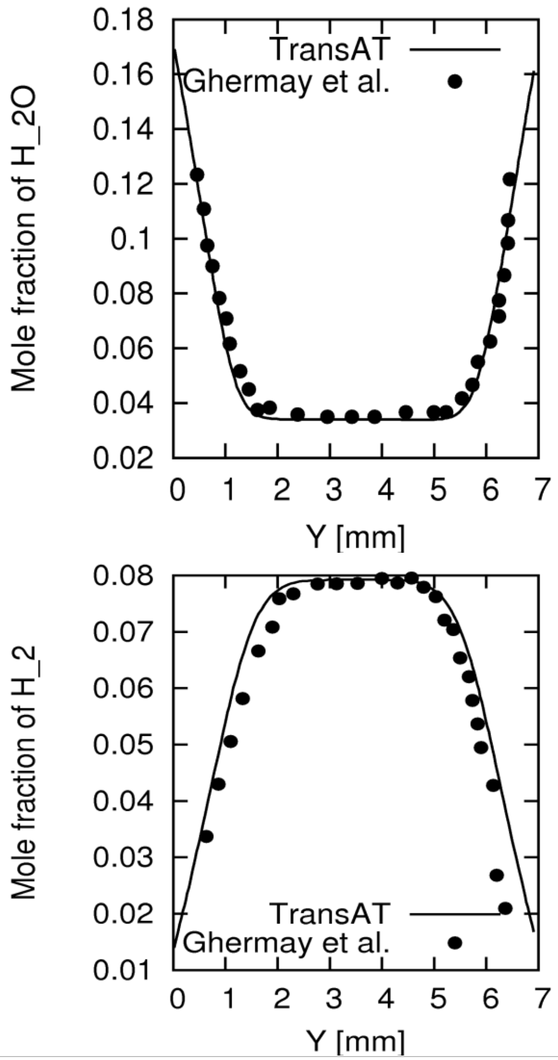
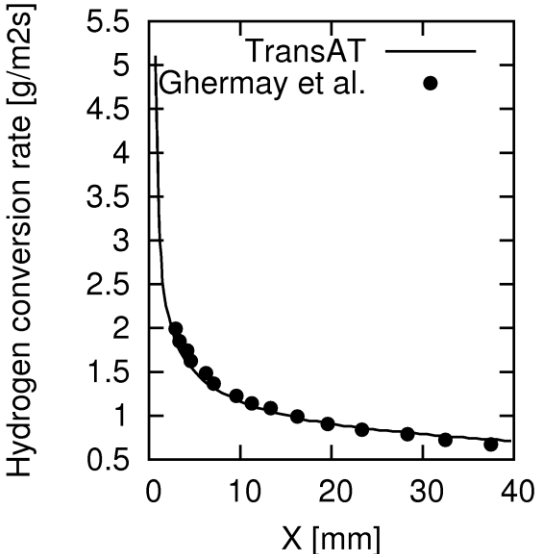




EXAMPLE 3: CATALYTIC WALL REACTION IN A DUCT
(GHERMAY ET AL., 2010): 2D RESULTS





EXAMPLE 3: CATALYTIC WALL REACTION IN A DUCT
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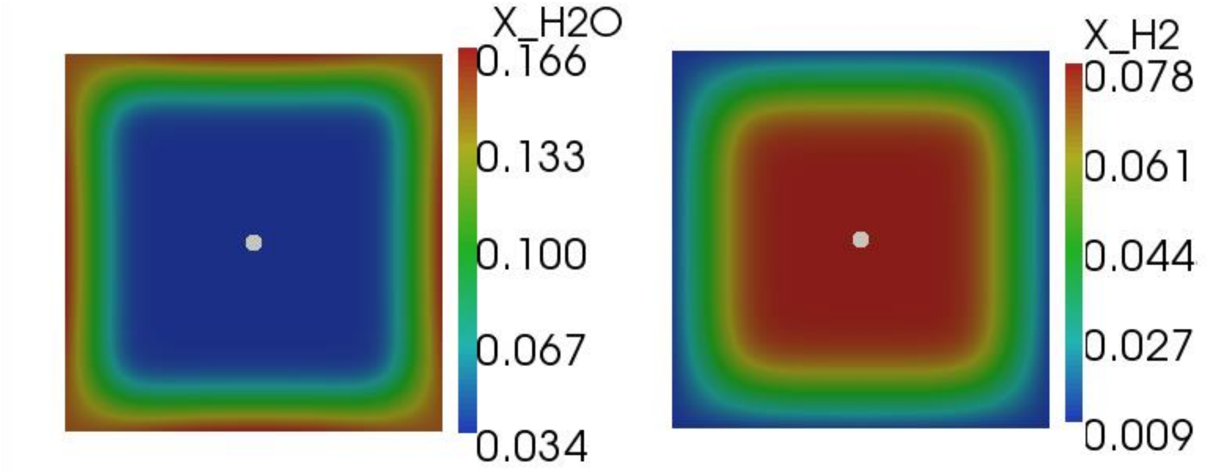

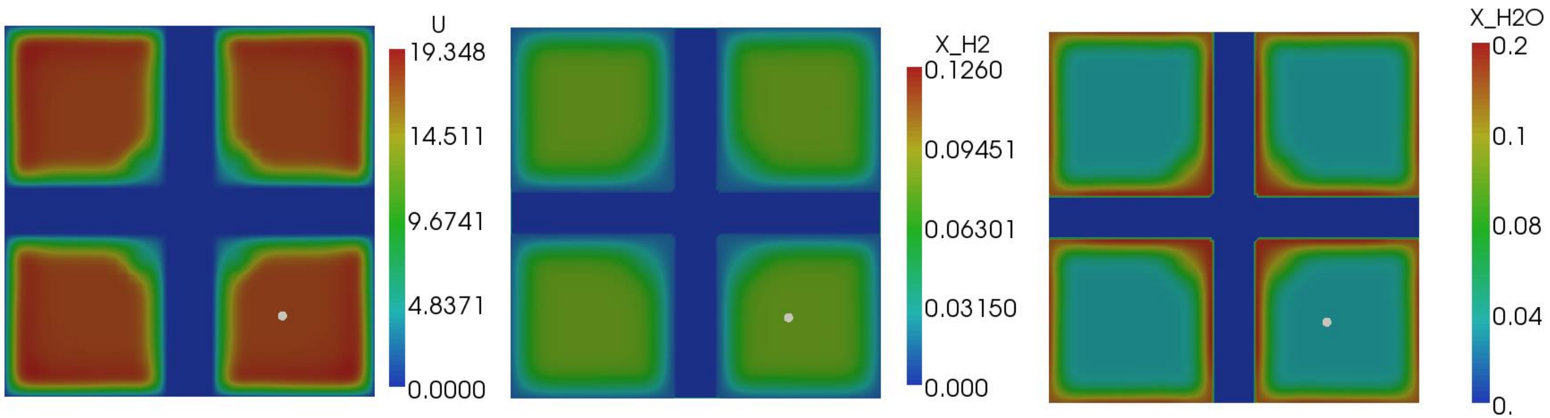

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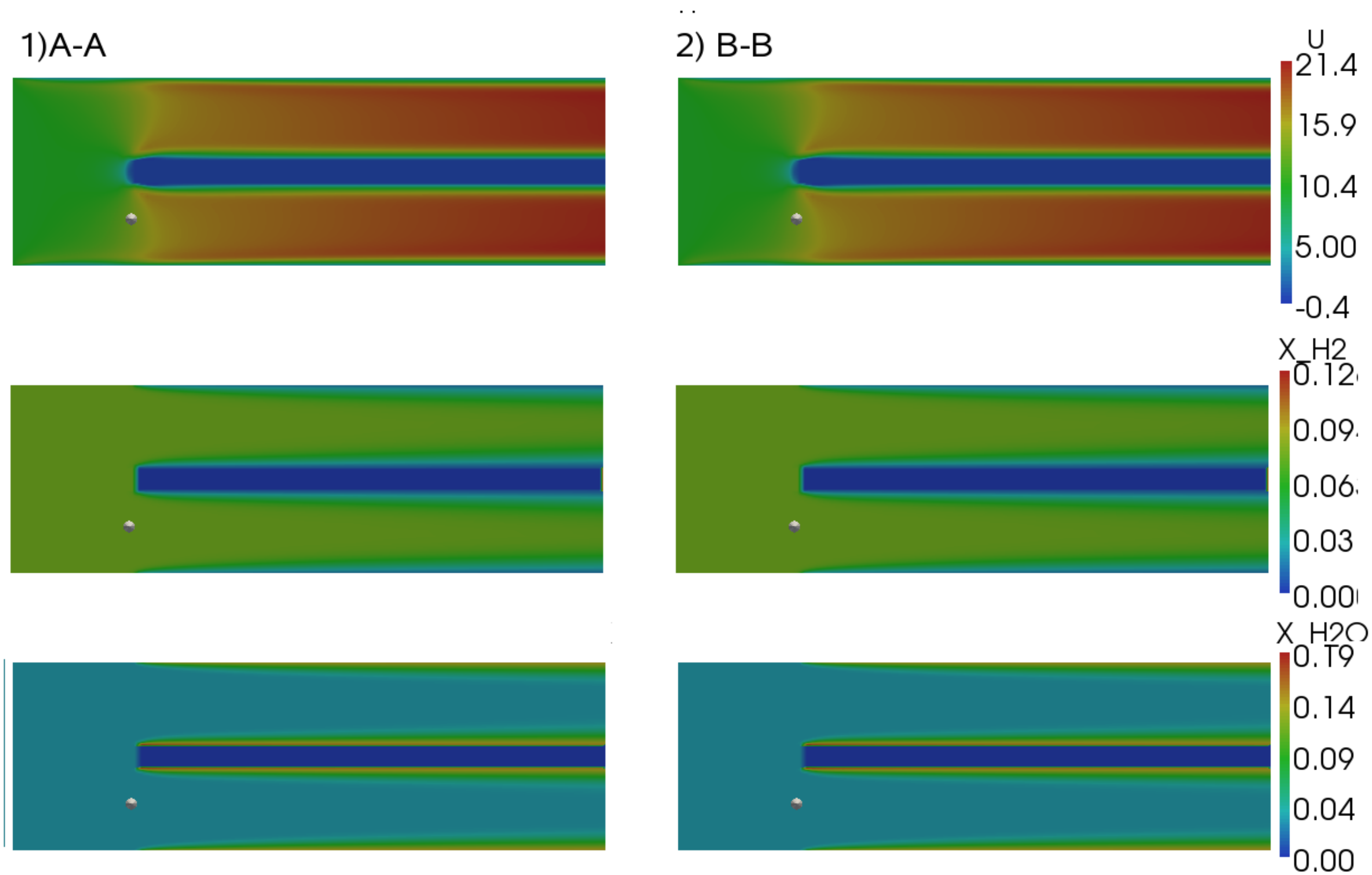
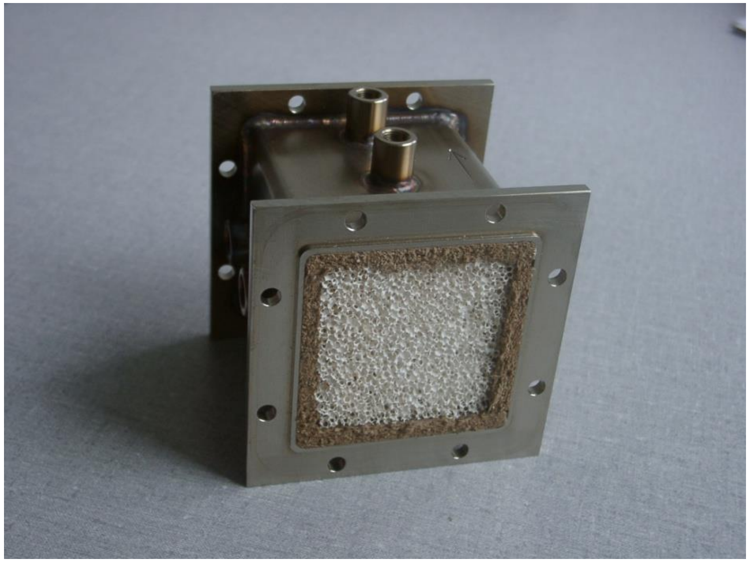


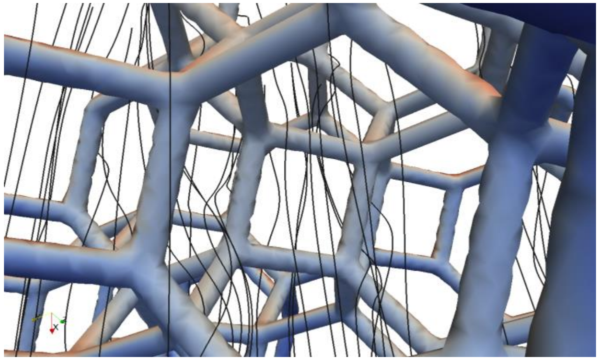
3D SIMULATIONS OF FLOW/CATALYTIC REACTION IN COMPLEX KELVIN-CELLS STRUCTURES

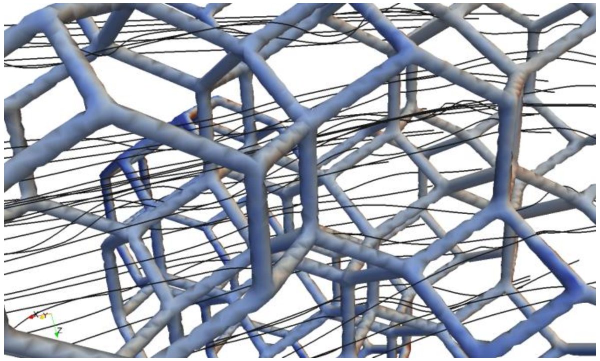
- A Kelvin cell with Hydrocarbons-Air-CO mixture wall-reaction
- Walls coated with platinum
- U = 10 m/s; T = 1000K
- Infinite fast reaction
- Heat release (exothermal reaction combined with conjugate heat transfer)

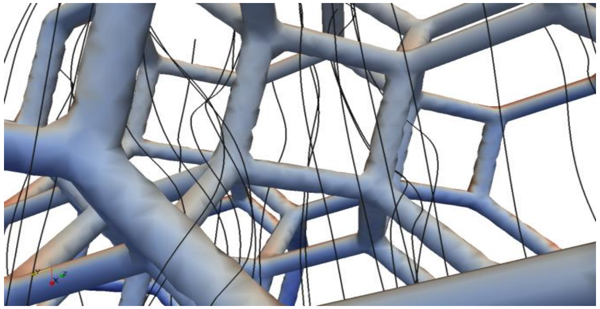


(catalytic Reactors for gas exhaust in cars: EMPA, Switzerland)

3D SIMULATIONS OF FLOW/CATALYTIC REACTION IN COMPLEX KELVIN-CELLS STRUCTURES







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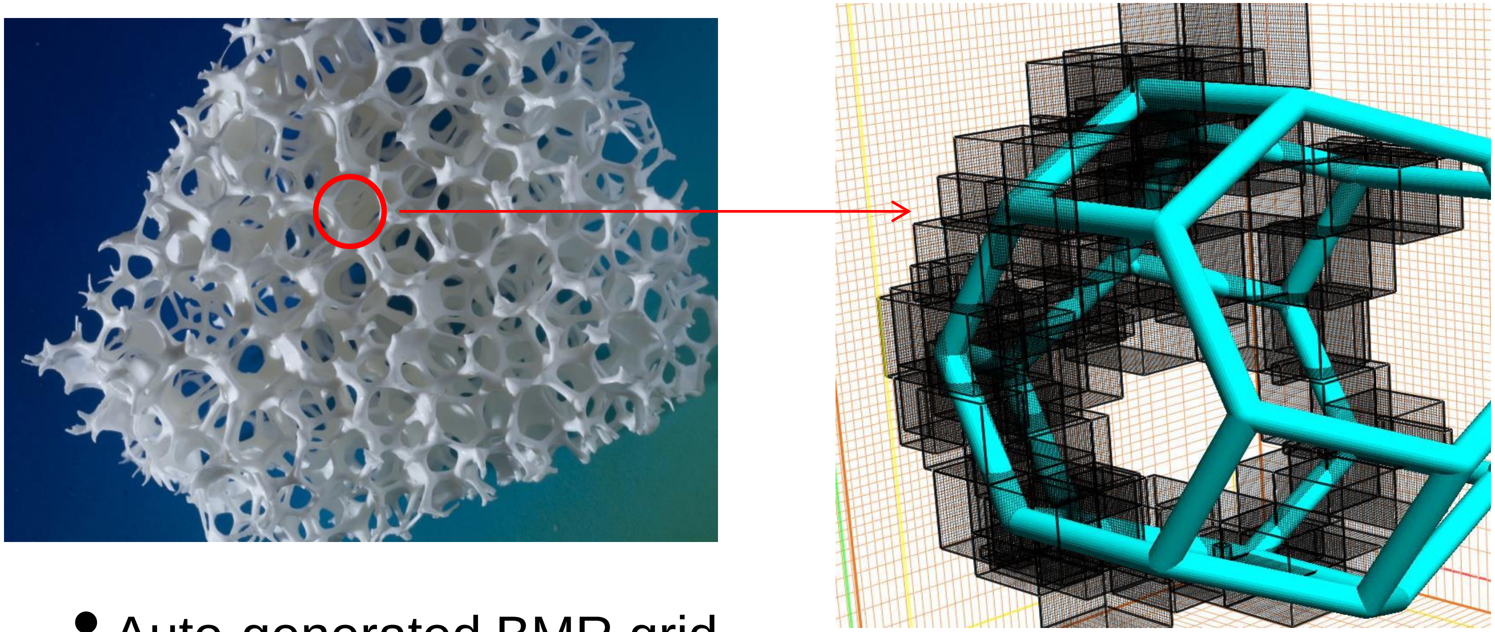
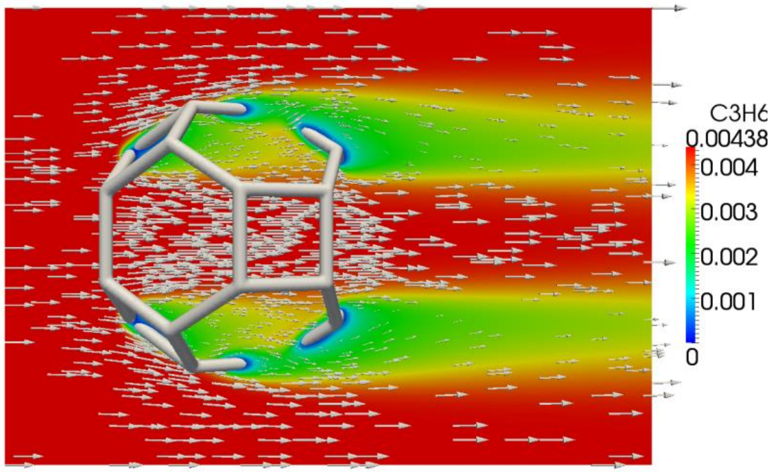
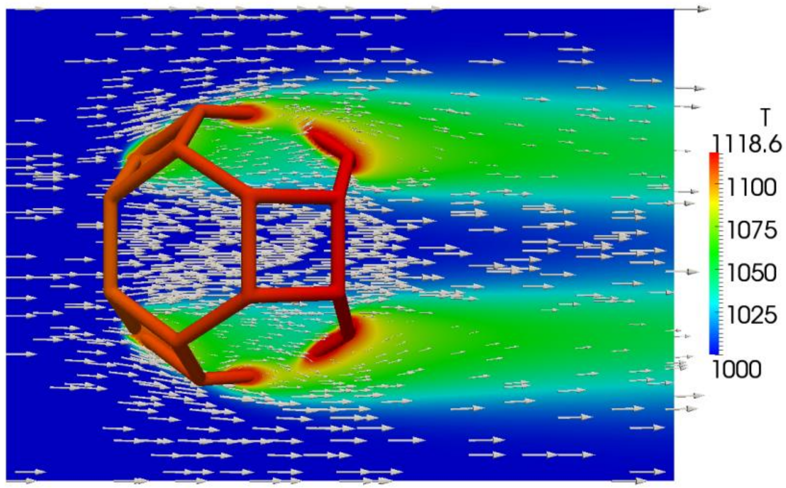


- Auto-generated BMR grid
- Pollutant conversion
- Multi-step reaction mechanism
- Conjugate heat transfer
- Heat release due to the reaction

3D SIMULATIONS OF FLOW/CATALYTIC REACTION IN COMPLEX KELVIN-CELLS STRUCTURES

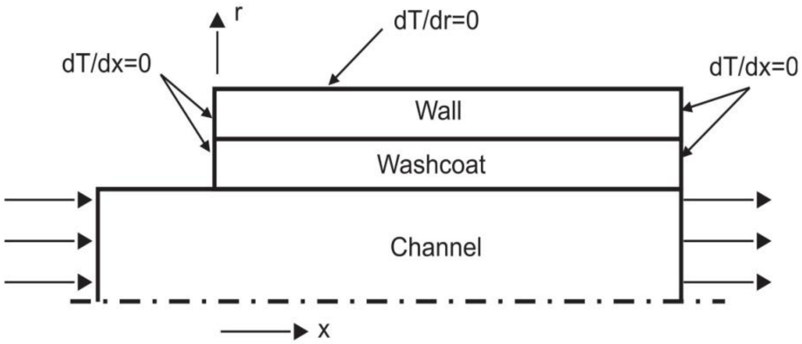


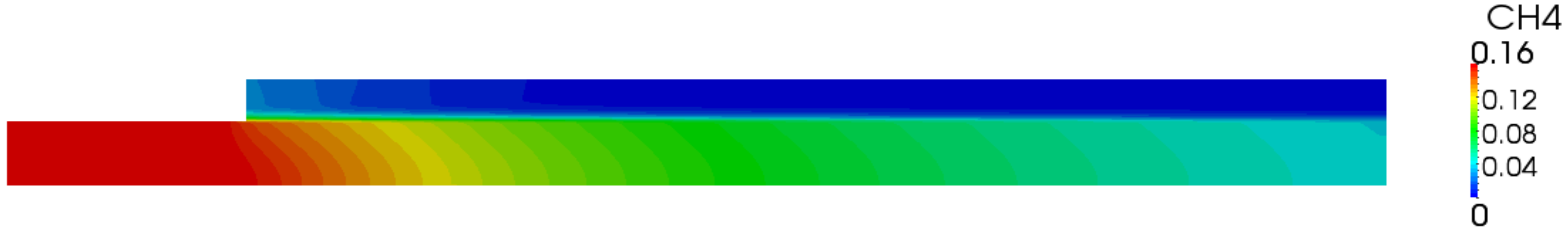


- catalytic reaction on the kelvin-cell walls, with conjugate heat transfer.
- Use is the made of the IST to mesh the cells, on a Cartesian grid

2D SIMULATIONS OF FLOW/CATALYTIC REACTION IN A CHANNEL WITH WASHCOAT

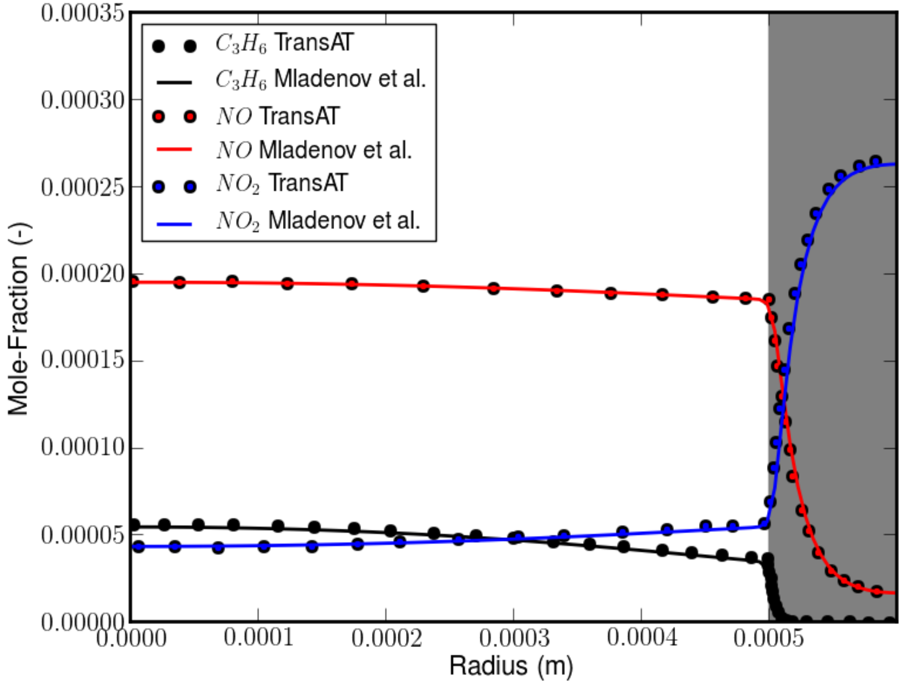
- Catalytic combustion of Methane in a thermally isolated channel
- Multi-step reaction mechanism
- Species diffusion and reaction in the washcoat
- Conduction in the washcoat
- Conjugate heat transfer





2D SIMULATIONS OF FLOW/CATALYTIC REACTION IN A CHANNEL WITH WASHCOAT

- Channel case of Mladenov et al. with washcoat model
- Multistep reaction mechanism (~ 80 reactions)



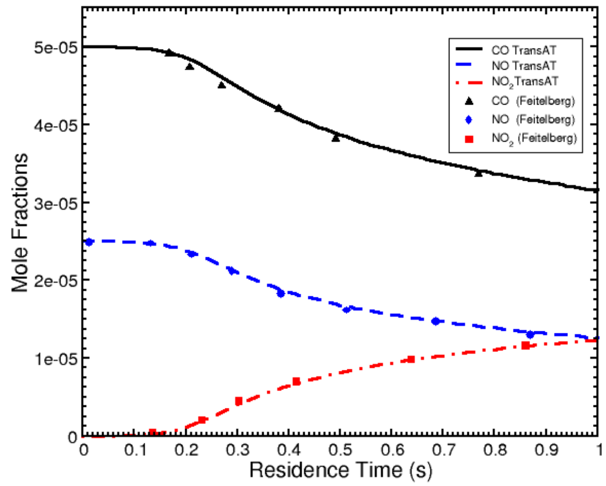
Homogeneous Combustion→

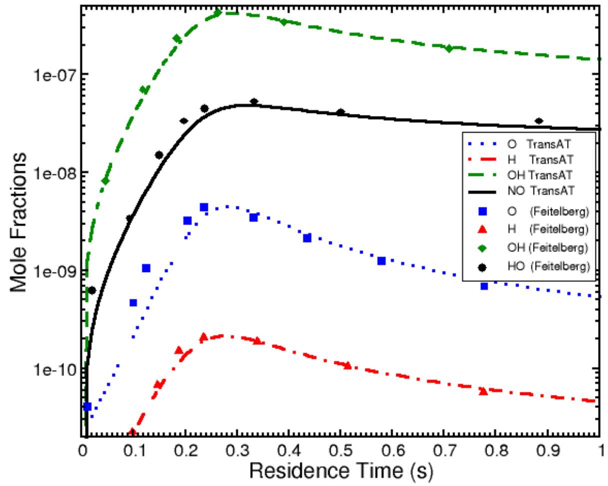
EXAMPLE 1: NO2 FORMATION (ARHENIUS APPROACH)
(FEITELBERG & COREA, 2000)

- Exhaust gas from gas turbine
- Create a plug flow reactor (1D)
- Apply NO2 formation mechanism
- Use Arrhenius model
- Use Cantera library

	REACTION	Forward rate parameters A	b	E
1.	$CO + O + M = CO_2 + M$	6.17×10^{14}	0.00	3000.
2.	$CO + OH = CO_2 + H$	1.51×10^{07}	1.30	–758.
3.	$CO + O_2 = CO_2 + O$	1.60×10^{13}	0.00	41000.
4.	$HO_2 + CO = CO_2 + OH$	5.80×10^{13}	0.00	22934.
5.	$H_2 + O_2 = 2\,OH$	1.70×10^{13}	0.00	47780.
6.	$H + H_2 = H_2O + H$	1.17×10^{09}	1.30	3626.
7.	$O + OH = O_2 + H$	4.00×10^{14}	–0.50	0.
8.	$O + H_2 = OH + H$	5.06×10^{04}	2.67	6290.
9.	$H + O_2 + M = HO_2 + M$	3.61×10^{17}	–0.72	0.
	Enhanced third-body efficiencies: $H_2O = 18.6$, $CO_2 = 4.2$, $H_2 = 2.9$, $CO = 2.1$, $N_2 = 1.3$			
10.	$OH + HO_2 = H_2O + O_2$	7.50×10^{12}	0.00	0.
11.	$H + HO_2 = 2\,OH$	1.40×10^{14}	0.00	1073.
12.	$O + HO_2 = O_2 + OH$	1.40×10^{13}	0.00	1073.
13.	$2\,OH = O + H_2O$	6.00×10^{08}	1.30	0.
14.	$H + H + M = H_2 + M$	1.00×10^{18}	–1.00	0.
	Enhanced third-body efficiencies: $H_2 = 0.0$, $H_2O = 0.0$, $CO_2 = 0.0$			
15.	$H + OH + M = H_2O + M$	1.60×10^{22}	–2.00	0.
	Enhanced third-body efficiencies: $H_2O = 5.0$			
16.	$O + O + M = O_2 + M$	1.89×10^{13}	0.00	–1788.
17.	$H + HO_2 = H_2 + O_2$	1.25×10^{13}	0.00	0.
18.	$2\,HO_2 = H_2O_2 + O_2$	2.00×10^{12}	0.00	0.
19.	$H_2O_2 + M = 2\,OH + M$	1.30×10^{17}	0.00	45500.
20.	$H_2O_2 + H = HO_2 + H_2$	1.60×10^{12}	0.00	3800.
21.	$H_2O_2 + OH = H_2O + H$	1.00×10^{13}	0.00	1800.
22.	$CO_2 + N = NO + CO$	1.90×10^{11}	0.00	3400.
23.	$HO_2 + NO = NO_2 + OH$	2.11×10^{12}	0.00	–479.
24.	$NO_2 + H = NO + OH$	3.50×10^{14}	0.00	1500.
25.	$NO_2 + O = NO + O_2$	1.00×10^{13}	0.00	600.
26.	$NO_2 + M = NO + O + M$	1.10×10^{16}	0.00	66000.
27.	$N_2O + H = N_2 + OH$	7.60×10^{13}	0.00	15200.
28.	$N_2O + M = N_2 + O + M$	1.60×10^{14}	0.00	51600.
29.	$N_2O + O = N_2 + O$	1.00×10^{14}	0.00	28200.
30.	$N_2O + O = 2\,NO$	1.00×10^{14}	0.00	28200.
31.	$N + NO = N_2 + O$	3.27×10^{12}	0.30	0.
32.	$N + O_2 = NO + O$	6.40×10^{09}	1.00	6280.
33.	$N + OH = NO + H$	3.80×10^{13}	0.00	0.

Note: forward rate coefficients (k_f) are of the form $k_f = A\,T^b \exp(-E/_{RT})$, where the dimensions of A are mole-cm-sec-K, the units of E are cal/mole, T is absolute temperature, and R is the ideal gas constant.





EXAMPLE 2: H2 NON-PREMIXED TURBULENT FLAME
(ARHENIUS APPROACH; OBIEGLO, GASS & POULIKAKOS, 2000)

- Axisymmetric H2-Air reacting flame flow
- Axisymmetric, Re=10‘000; K-e model
- Comparisons with LDA Lab. data
- Standard EDC model
- Cantera library for material properties

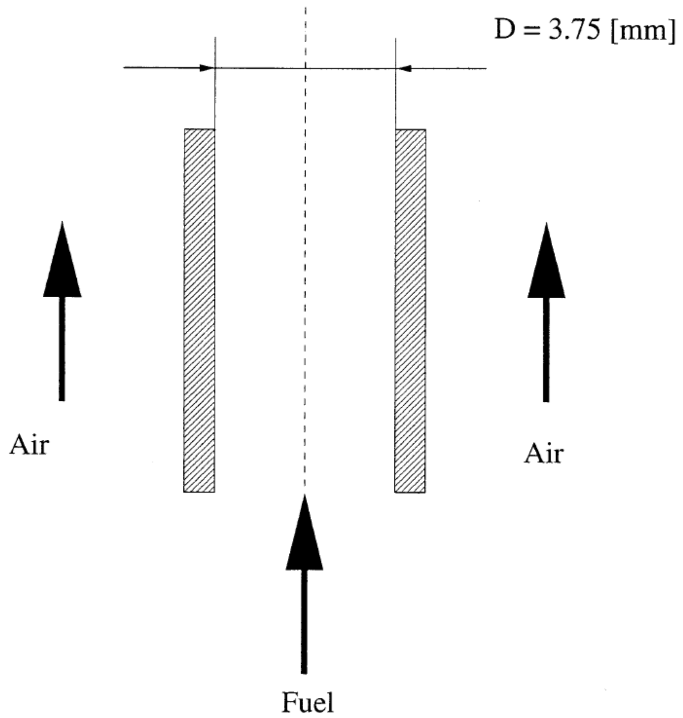


Fig. 1. Scheme of the nozzle for the jet flame. The inner diameter is $D = 3.75$ mm.

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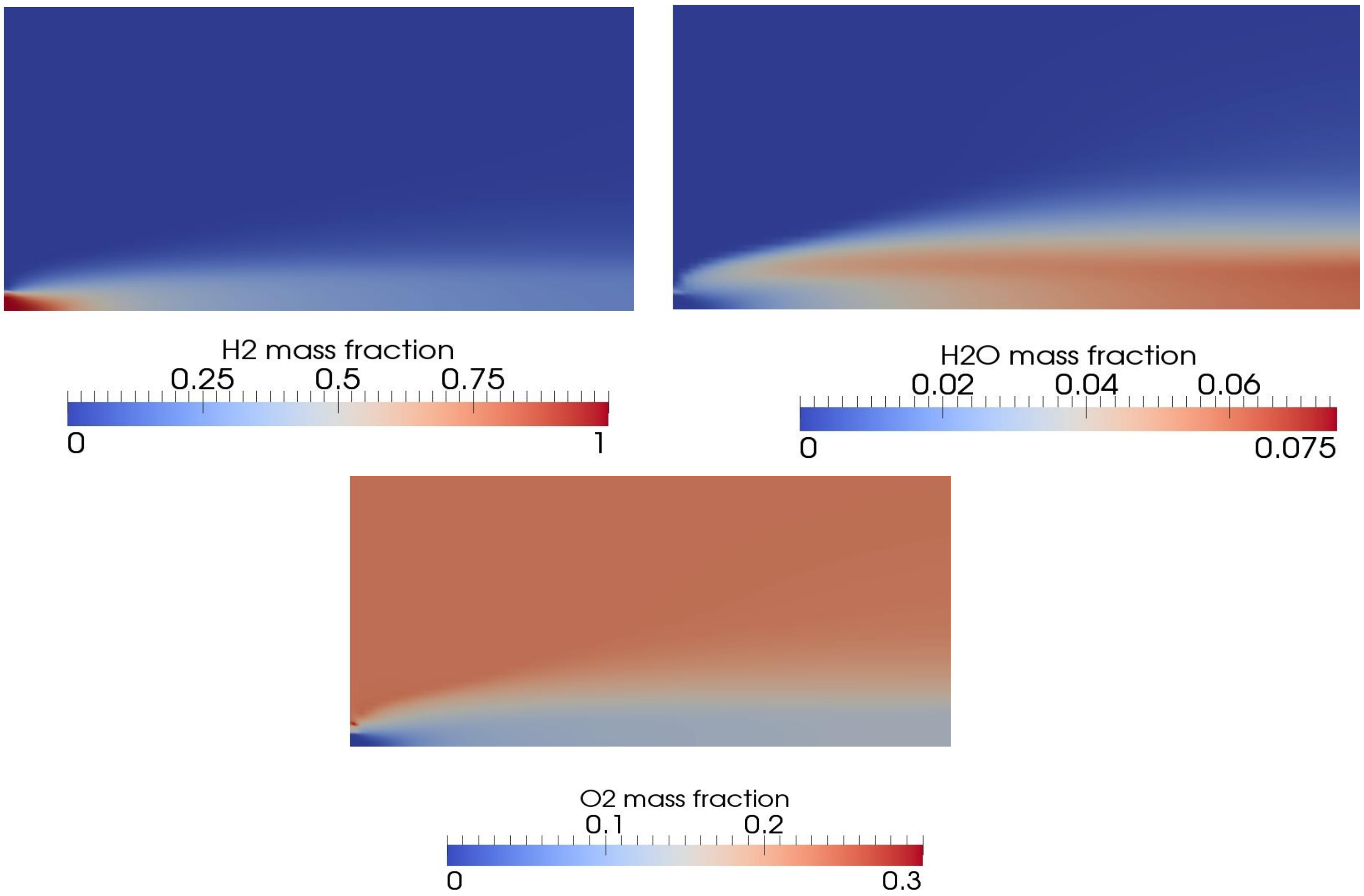
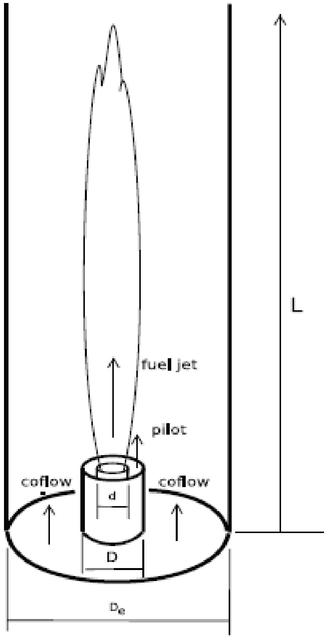
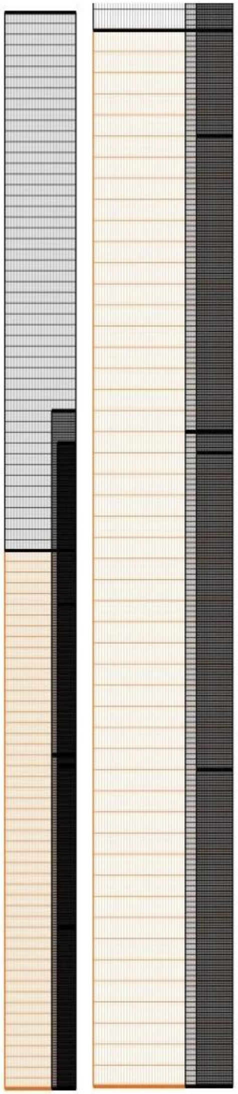


EXAMPLE 3: PARTIALLY PREMIXED COMBUSTION
(EDC CLOSURE)

Sandia Flame D, Setup

- 2D axisymm.
- BMR (multiblock Grid)
- 55.292 cells; 3 blocks

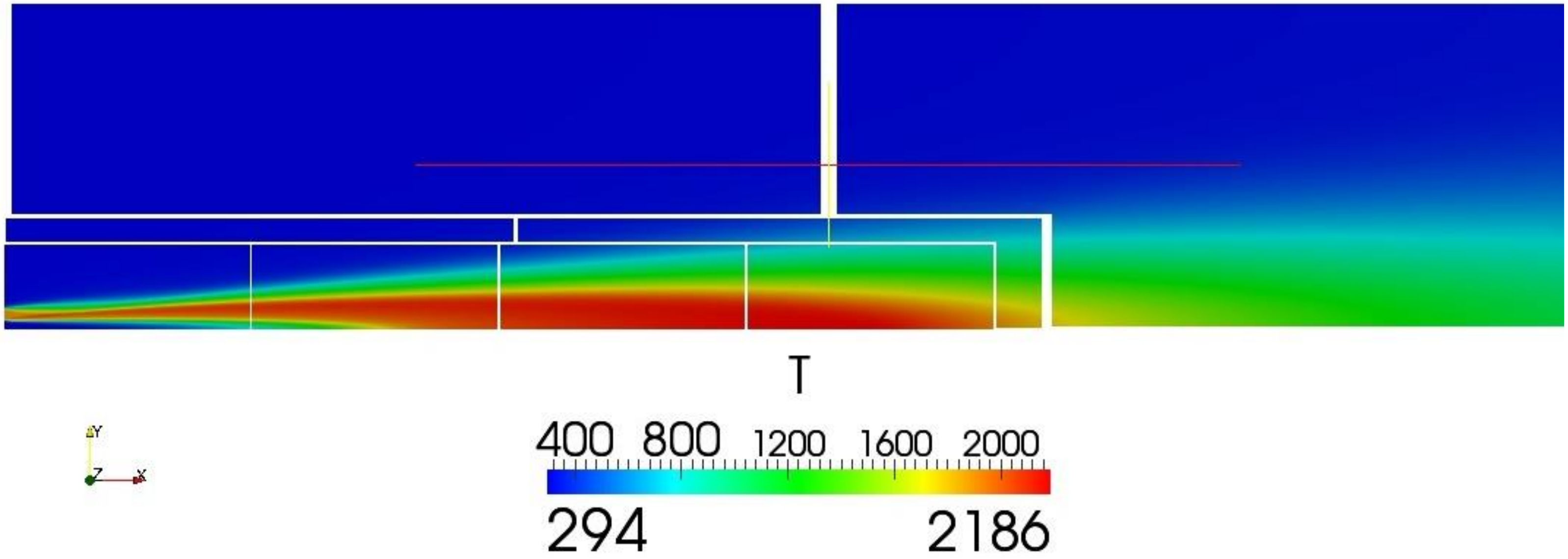




EXAMPLE 3: PARTIALLY PREMIXED COMBUSTION
(EDC CLOSURE)

Sandia Flame D, modelling & Results

- Methane-air jet flames
- Partialy premixed
- Eddy dissipation concept



EXAMPLE 3: PARTIALLY PREMIXED COMBUSTION
(EDC CLOSURE)

EDC WITH TRANSAT

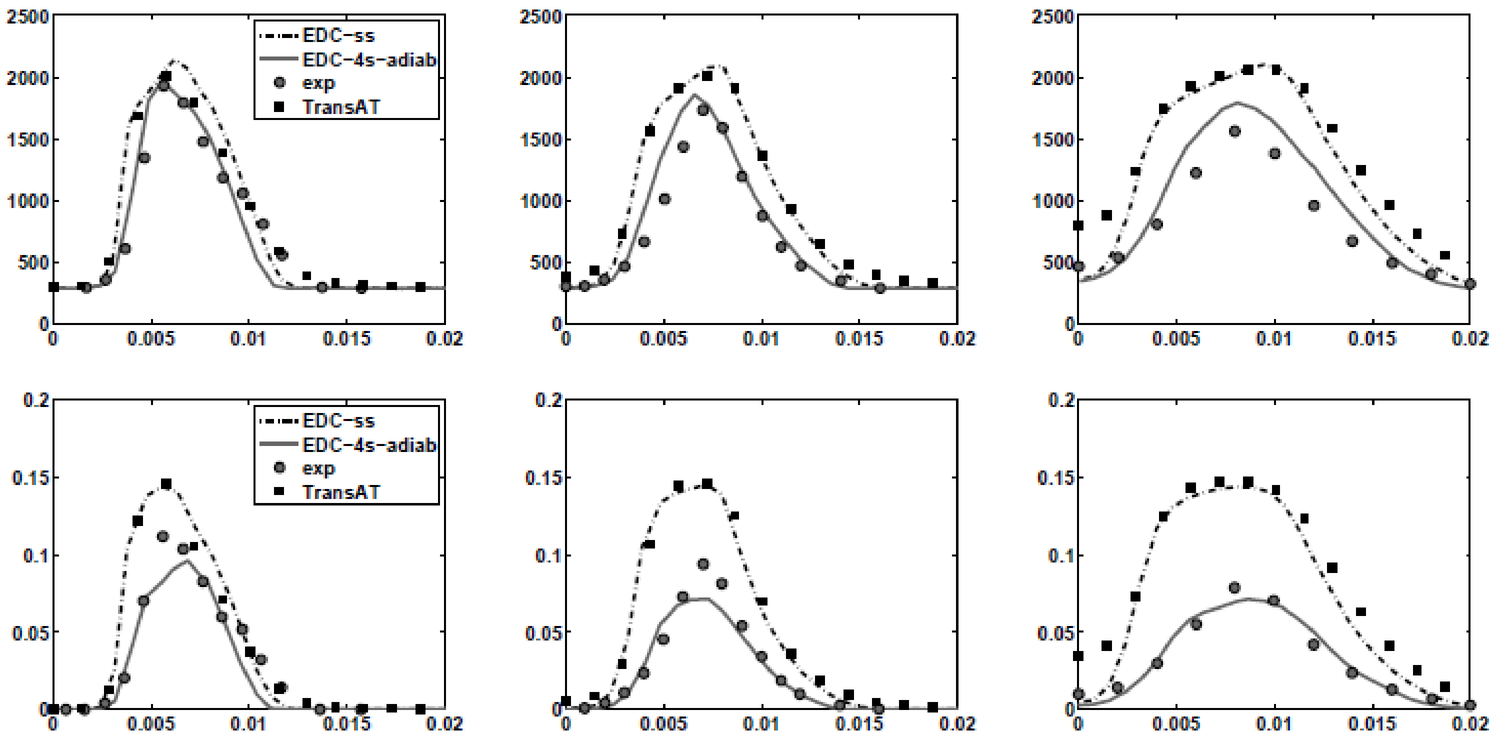


Figure: Radial profiles of Flame–D. EDC simulations at $z/d = 3$, $z/d = 7.5$, $z/d = 15$. (Top: Temperatures, Bottom: CO_2 mass fractions

EXAMPLE 3: PARTIALLY PREMIXED COMBUSTION
(EDC CLOSURE)

EDC WITH TRANSAT

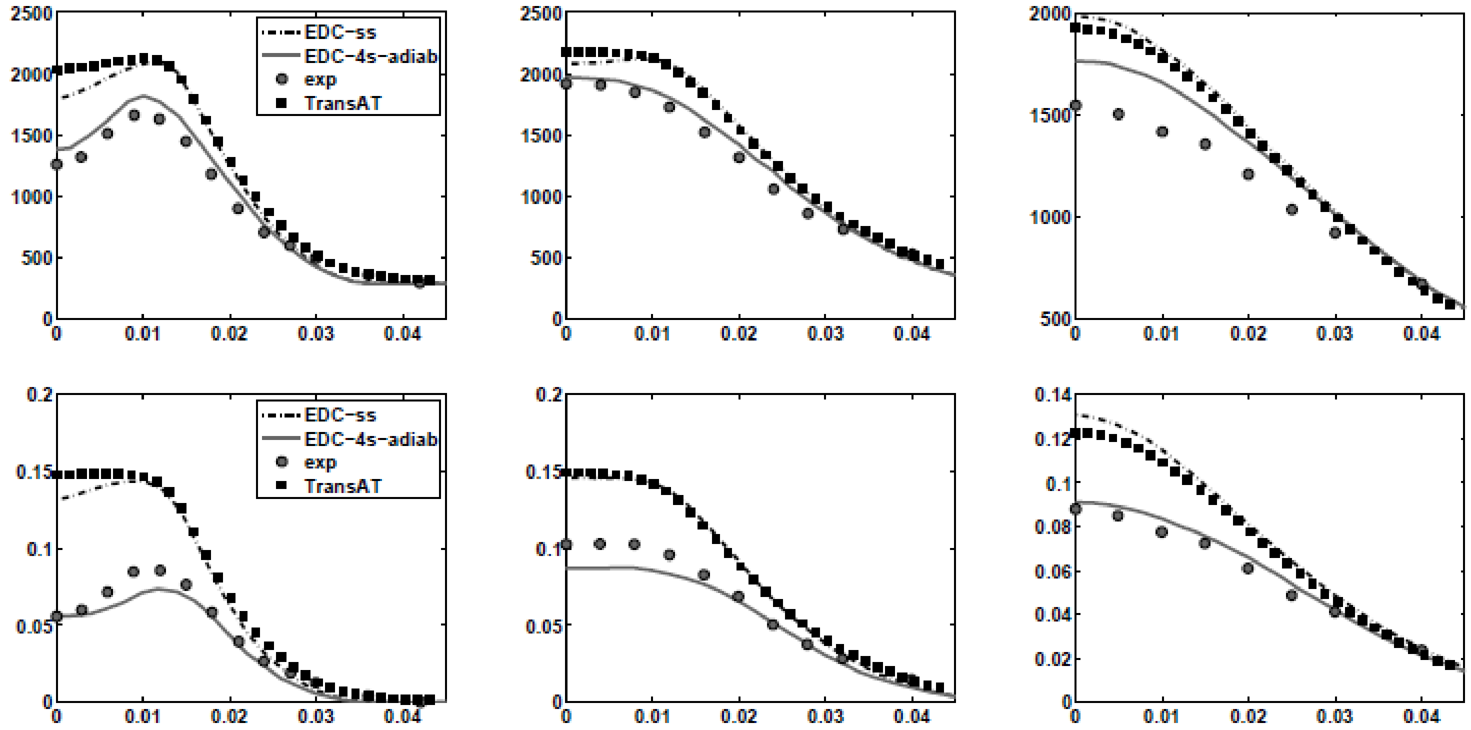


Figure: Radial profiles of Flame–D. EDC simulations at $z/d = 30$, $z/d = 45$, $z/d = 60$. (Top: Temperatures, Bottom: CO_2 mass fractions