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Particle depletion in simplified geometries

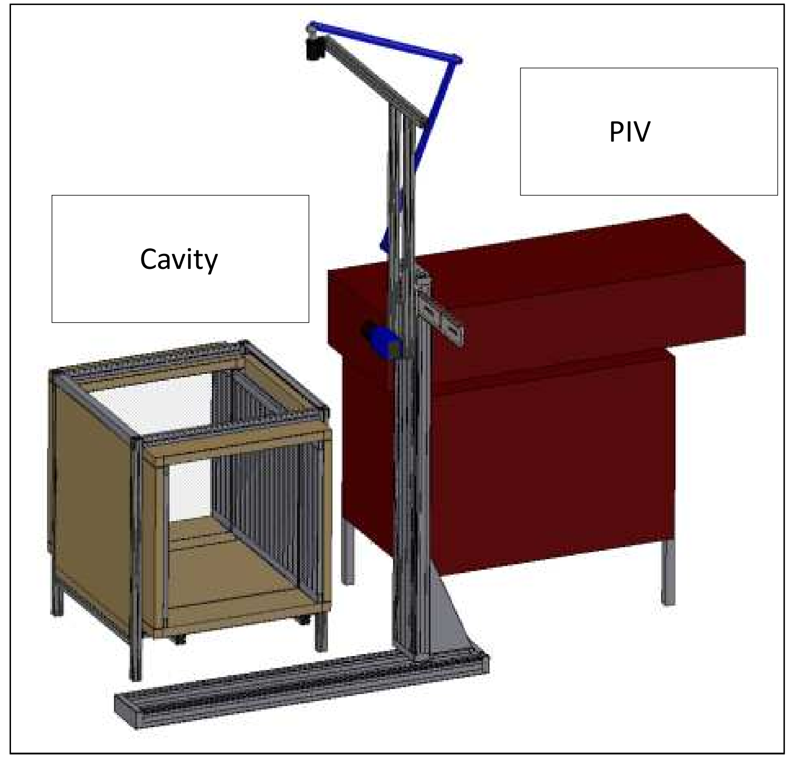
8th Meeting of the “European MELCOR User Group”, Imperial College, London, April 6-7, 2016

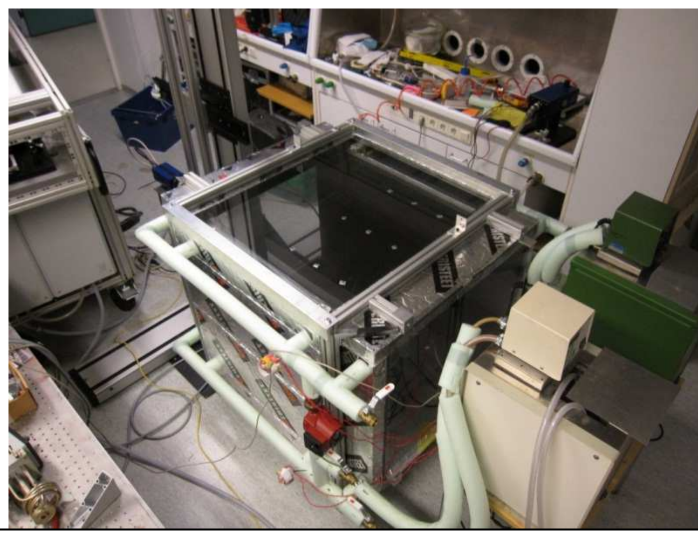
Introduction

- Aerosol behaviour in a containment building of a NPP during an accident scenario has an importance on the fission product release and mitigation.
- Large scale severe accident experiments (e.g. Phebus FPT2-3) observed relatively large deposition to vertical containment walls
  - Possible effects of turbulent natural convective flow to the particle wall deposition?
- Particle retention in a Differentially Heated Cavity (DHC) was investigated experimentally and computationally using CFD large eddy simulation and Lagrangian particle tracking simulations.
- Additionally, MELCOR was used to simulate particle retention in a differentially heated cavity with turbulent natural convection and the results were compare with CFD and measurements.

Measurement facility - DIANA

- **DI**fferentially heated cavity with **A**erosol in turbulent **NA**tural convection (**DIANA**) facility.
- The facility has two vertical isothermal aluminium walls and four adiabatic glass walls.
- The facility must allow optical access for laser-based measurement devices used to determine the flow properties as well as particle deposition rates
- In order for the Boussinesq approximation, used in the CFD simulation work to be valid the heat difference between the walls must remain below 50 K.
- Fluid: air, ΔT = 57 C -18 C = 39 C, Rayleigh number Ra ~ 10^9. Turbulent flow.



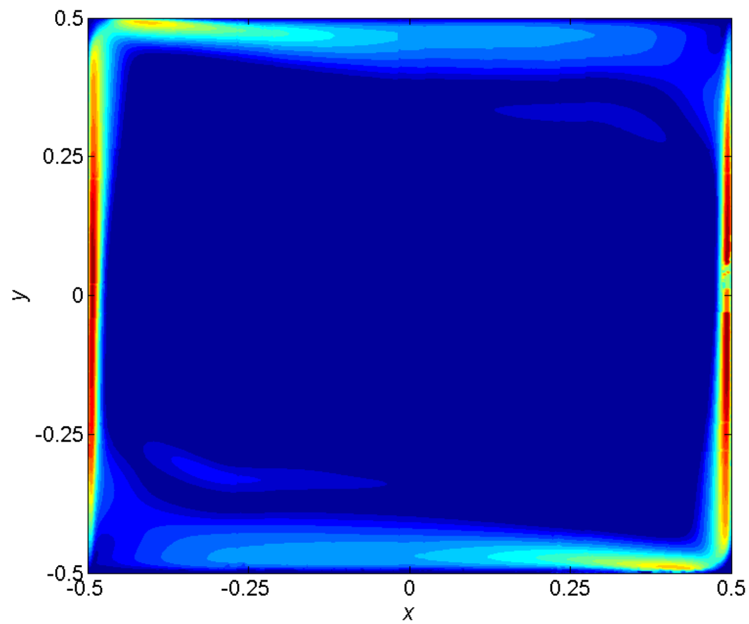


Experimental study and CFD simulations

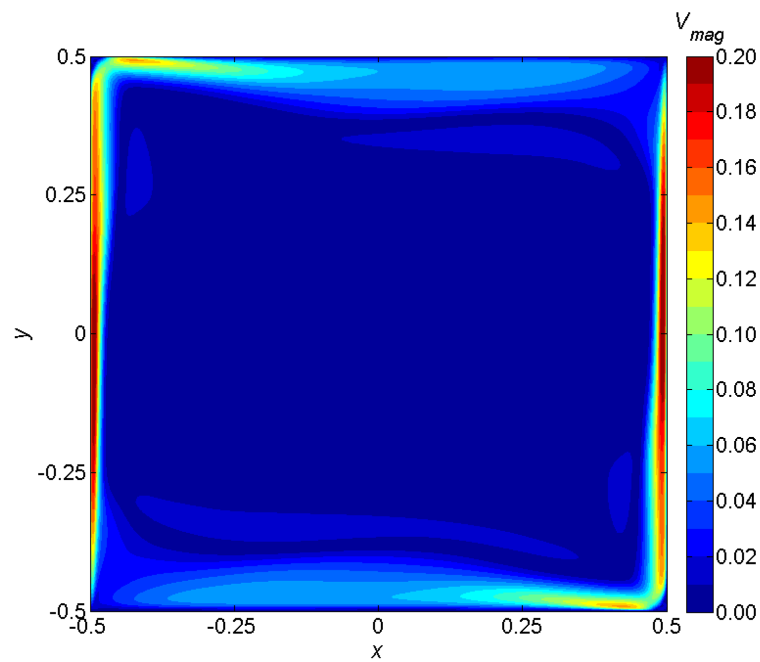
- Experimental investigation:
  - Measurement of flow field and gas temperature in the DIANA cavity.
  - Measurement of particle deposition rates using monodisperse SiO_2 particles with diameters 1 µm and 2.5 µm.
- Large Eddy Simulation (LES) and particle tracking:
  - Validation of the LES using experimental temperature boundary conditions.
  - Comparison of measurement to Lagrangian particle tracking data obtained using the validated LES.

LES of DIANA cavity

- In the LES-WT simulation, the thermal boundary conditions for isothermal and horizontal walls were obtained from the wall temperature measurement data.
- The LES-WT validated using the measurement data.



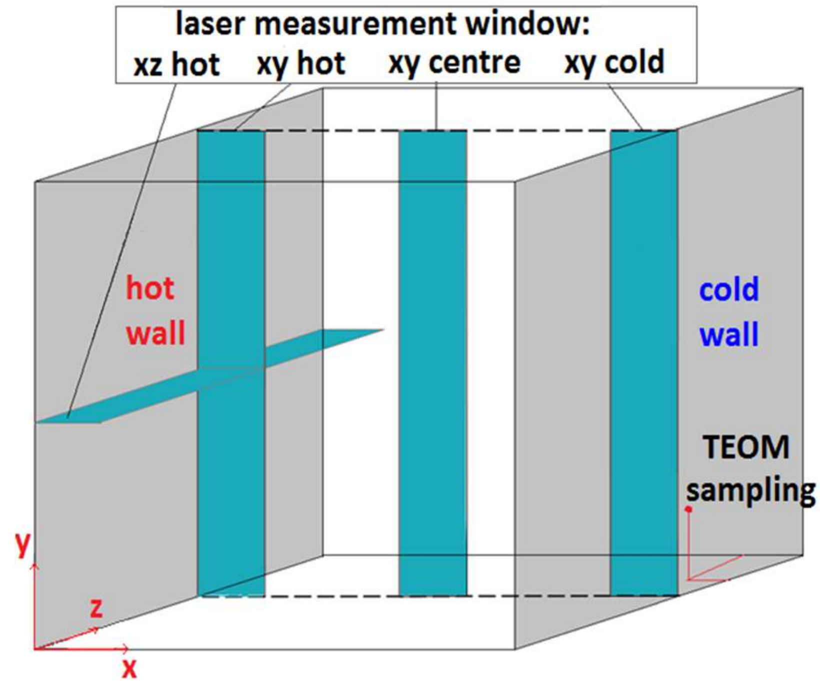
Velocity magnitudes from the experiments.



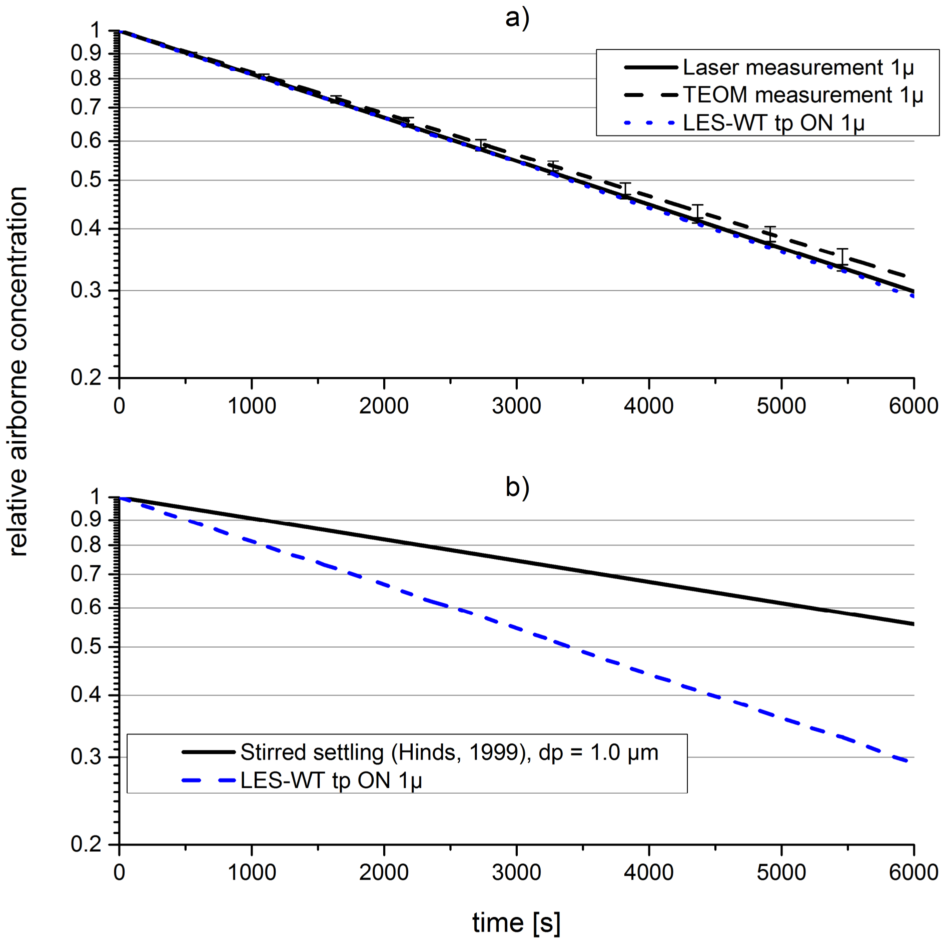
Velocity magnitudes from the LES-WT.

Deposition measurements with DIANA

- Monodisperse SiO_2 (diameters 1 and 2.5 μm) particles seeded from the bottom of the cavity.
- The change of airborne particle concentration was investigated by a laser sheet and reflected light from the particles.
- Tapered Element Oscillating Microbalance (TEOM) was used in addition to laser intensity measurements.
- Particles were approximately uniformly distributed to the cavity at the lateral direction.
- The results indicated uniform deposition rates throughout the cavity atmosphere.



Particle deposition – comparison of exp. and simulations



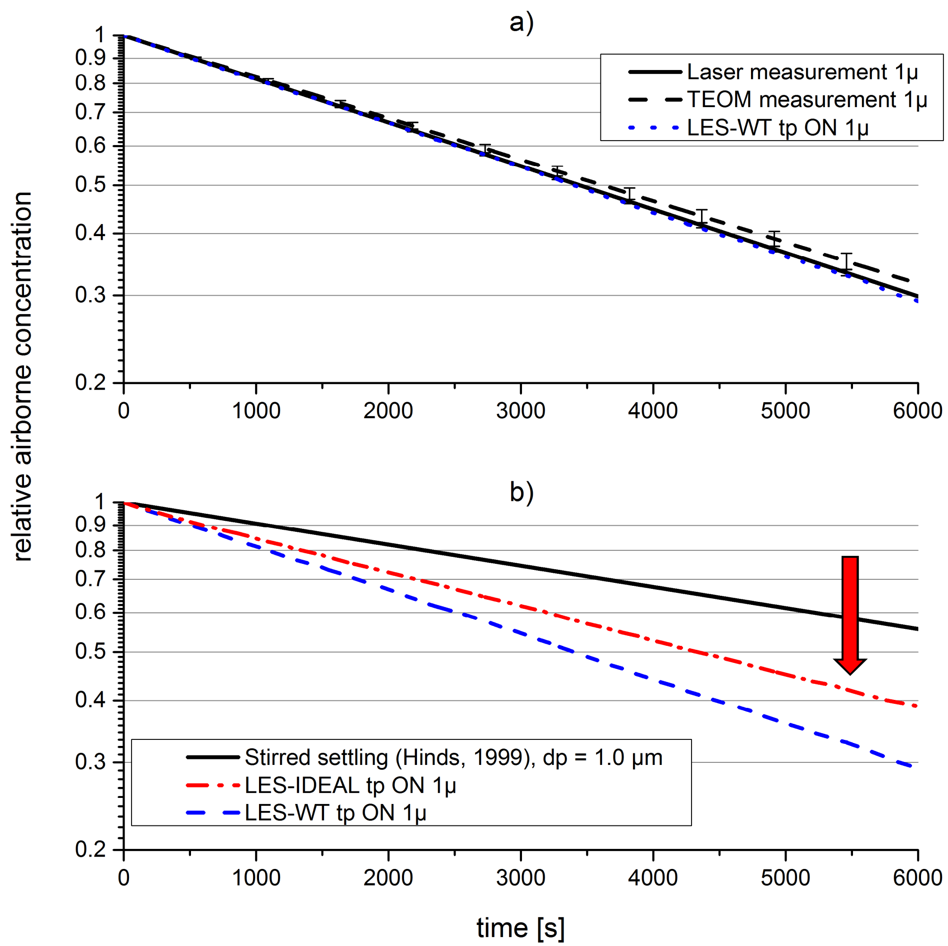
Comparison of particle decay from the cavity atmosphere with d_p = 1 µm particles. Good agreement with CFD and experimental results.

- The inclusion of thermophoretic force to the simulation has only relatively small effect on the deposition speed. Small increase of deposits on the cold surface slightly altered the surface deposition distribution.
- In the stirred settling case, particles are kept uniformly distributed in a cubic volume with side length *L*, and are deposited only through gravitational settling to the enclosure floor (Hinds, 1999).
  - ➢ Deposition in DHC not depicted accurately by stirred settling.

Average decay time constants from the laser intensity and mass concentration measurements, particle tracking simulations and from the stirred settling calculation.

	d_p = 1 µm	d_p = 2.5 µm
Average τ, TEOM [s]	5220 ± 190 s	1700 ± 90 s
Average τ, laser intensity [s]	4970 ± 60 s	1800 ± 80 s
LES-WT tp ON	4890 s	1510 s
LES-WT tp OFF	5060 s	1520 s
Theoretical Stirred Settling (Hinds, 1999)	10210 s	1780 s

Particle deposition – comparison of exp. and simulations



Comparison of particle decay from the cavity atmosphere with d_p = 1 µm particles. Good agreement with CFD and experimental results.

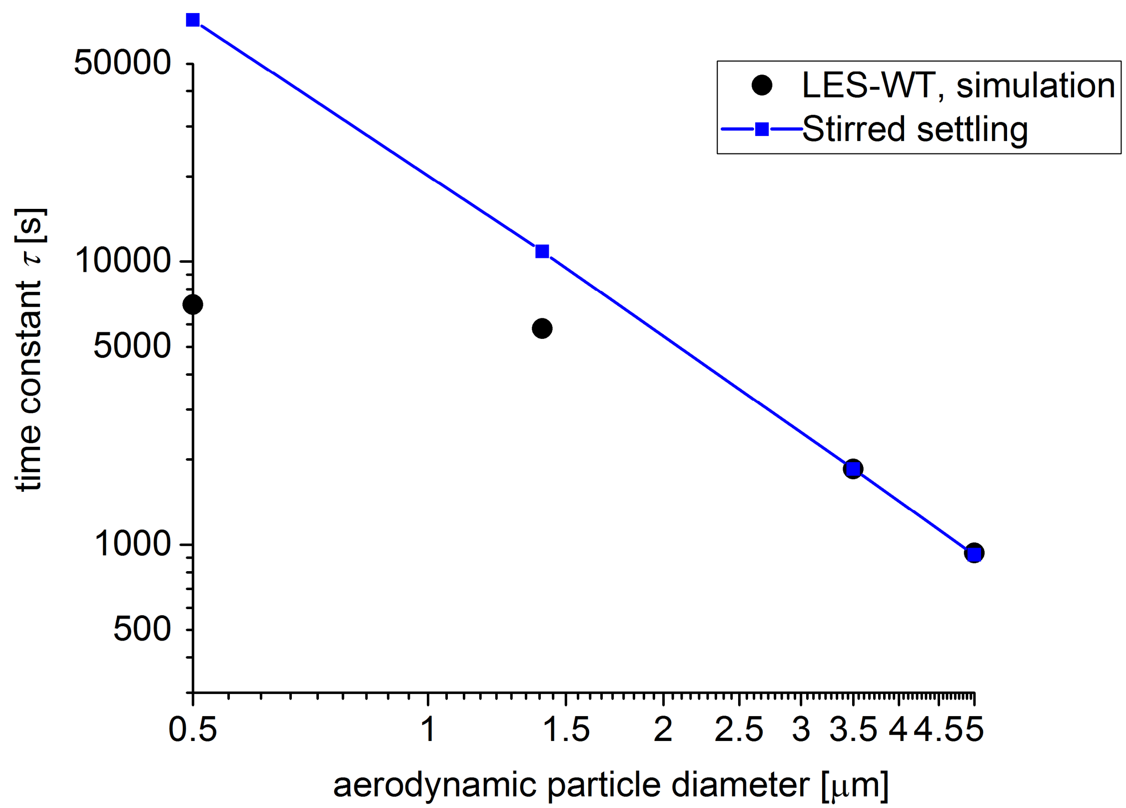
- Additional simulations using idealized adiabatic boundary conditions on horizontal walls (LES-IDEAL), was validated against the DNS data by Puragliesi (PhD thesis, EPFL, 2010) with similar conditions.
- Flow and temp. field differed with LES-IDEAL – Flow geometry different, less turbulent.
  - Particle depletion slower from the cavity atmosphere.
  - The LES-IDEAL simulations indicate that the turbulence has significant effect on the deposition rate of 1 micron particles in the cavity.

Average decay time constants from the laser intensity and mass concentration measurements, particle tracking simulations and from the stirred settling calculation.

	d_p = 1 µm	d_p = 2.5 µm
Average τ, TEOM [s]	5220 ± 190 s	1700 ± 90 s
Average τ, laser intensity [s]	4970 ± 60 s	1800 ± 80 s
LES-WT tp ON	4890 s	1510 s
LES-WT tp OFF	5060 s	1520 s
LES-IDEAL tp ON	6360 s	1860 s
LES-IDEAL tp OFF	6920 s	1840 s
Theoretical Stirred Settling (Hinds, 1999)	10210 s	1780 s

Comparison of CFD and stirred settling with 4 particle sizes

- Additional particle tracking simulations were performed using the realistic boundary conditions at the cavity surfaces in LES with four different particle sizes.
- Stirred settling unable to predict the deposition behaviour with small, d_p = 0.5 µm and 1.4 µm particles.



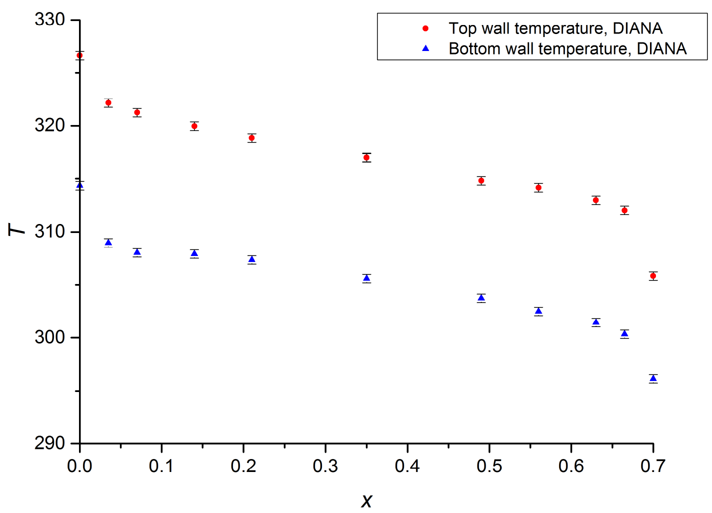
Deposition time constant as a function of particle diameter

Time constants from the simulations, from stirred settling and the relative difference of the two

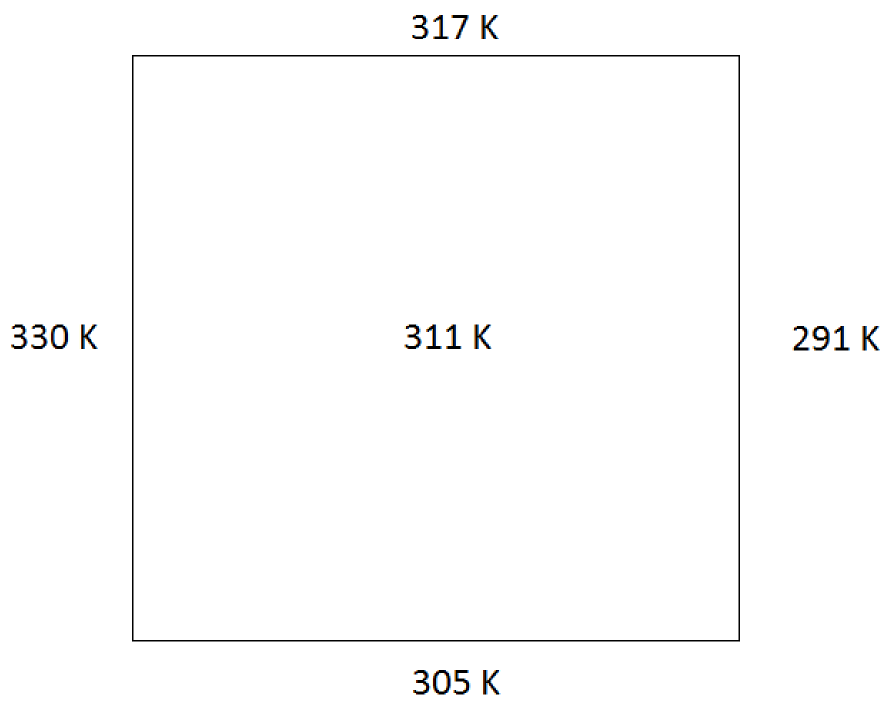
particle size d_p [µm]	Realistic BC simulation (LES) τ_{WT} [s]	Stirred settling τ_{theor} [s]	$\frac{\tau_{theor}}{\tau_{WT}}$
0.5	6975	71427	10.2
1.4	5764	10848	1.9
3.5	1706	1853	1.1
5.0	937	921	1.0

MELCOR simulation

- One control volume, 0.7 x 0.7 m, volume 0.343 m^3.
- Constant temperatures at boundaries determined from the measurement data (average).
- Control volume temperature constant after 500 s.



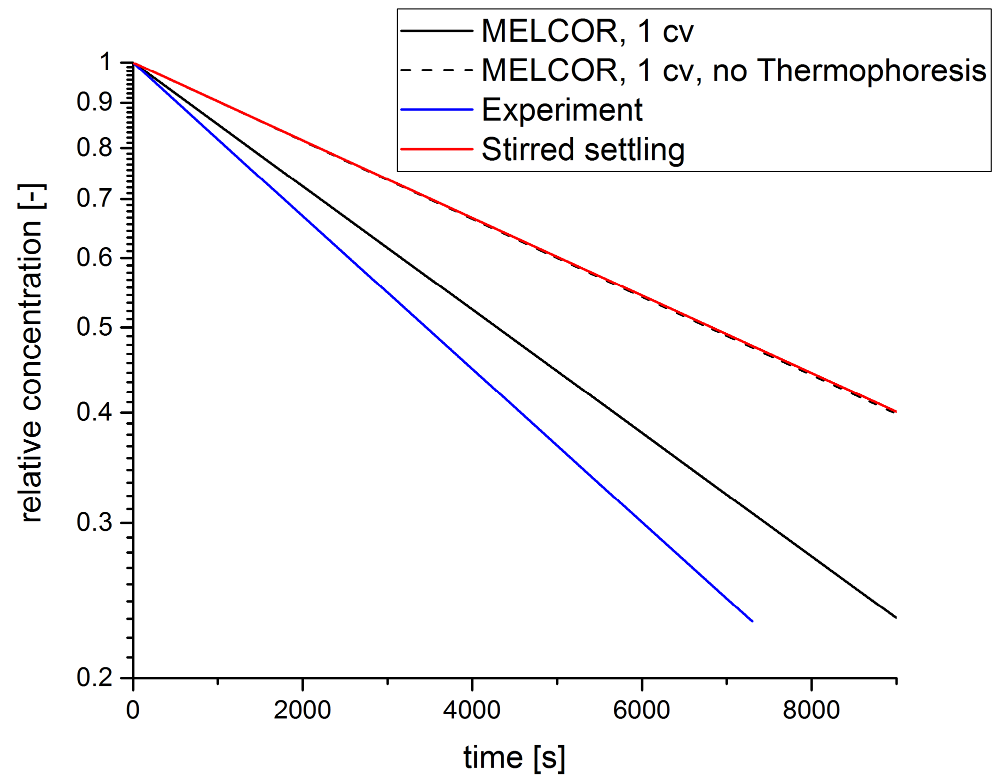
Measured temperature profiles at top and bottom wall center lines.



Temperatures in the MELCOR simulation.

MELCOR simulation

- Aerosol calculation using one section in MELCOR (monodisperse particles with diameter 1 µm). Density 2000 kg/m^3.
- Initial concentration approx. 16E-10 kg (less than 5 particles / cc, agglomeration negligible).
- Concentration change after steady state (constant temperature) was achieved (500 s).
- Deposition mechanisms effecting the particles: gravitational settling, thermophoresis, Brownian diffusion.
  - Diffusion boundary layer thickness estimated for 1 µm particles $\Delta \approx 1.25 \cdot 10^{-3}$.
- The effect of thermophoresis investigated by discarding it from the simulation
  - k_{gas}/k_p and c_t set to 0.



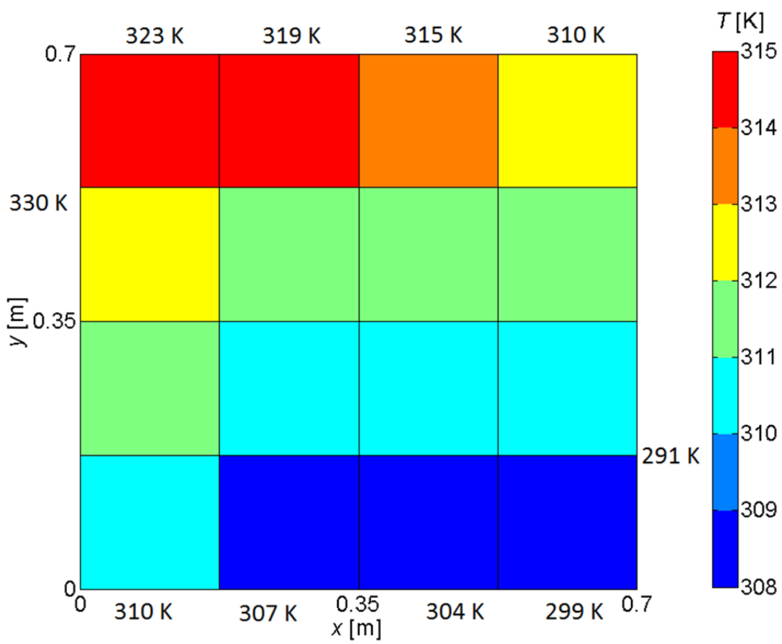
Particle depletion, $d_p = 1\ \mu m$, 1 control volume.

$$V_{diff} = \frac{\sigma\, T\, C_m}{3\pi\, \mu\, \chi\, d_p \Delta}$$

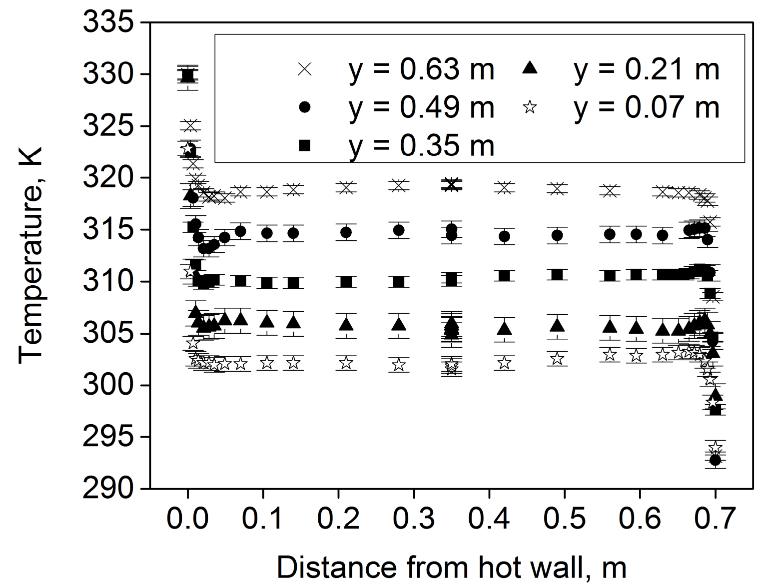
$$V_{therm} = \frac{3\, \mu\, C_m \left(c_t\, Kn + k_{gas}/k_p\right)}{2\ \chi\ \rho_{gas}\, T \left(1 + 3\, F_{slip} Kn\right)\left(1 + 2\, c_t\ Kn + k_{gas}/k_p\right)} \nabla T$$

MELCOR simulation

- Improved model with 16 control volumes.
- Steady temperatures in control volumes reached after 500s.
- Signs of temperature stratification evident. Typical for differentially heated cavities.



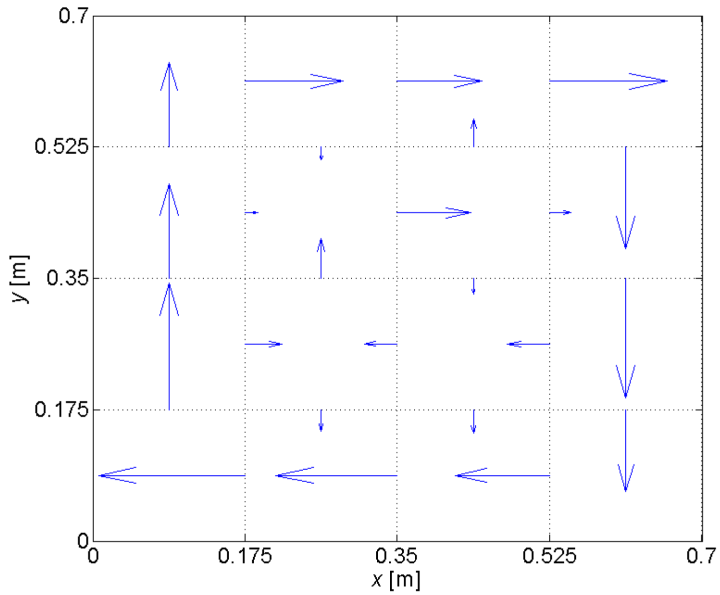
Temperatures (t = 500 s) in MELCOR control volumes.



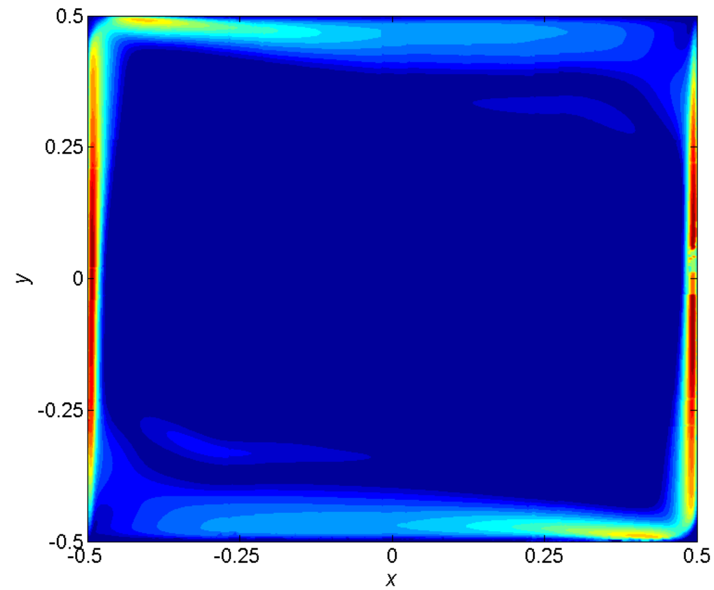
Measured temperature profiles.

MELCOR simulation

- MELCOR simulation induced a circling flow near the isothermal vertical and horizontal walls.
- Typical feature of a differentially heated cavity.
- Discrepancies do exist:
  - ➢ Smaller velocities, location of maximum velocity…



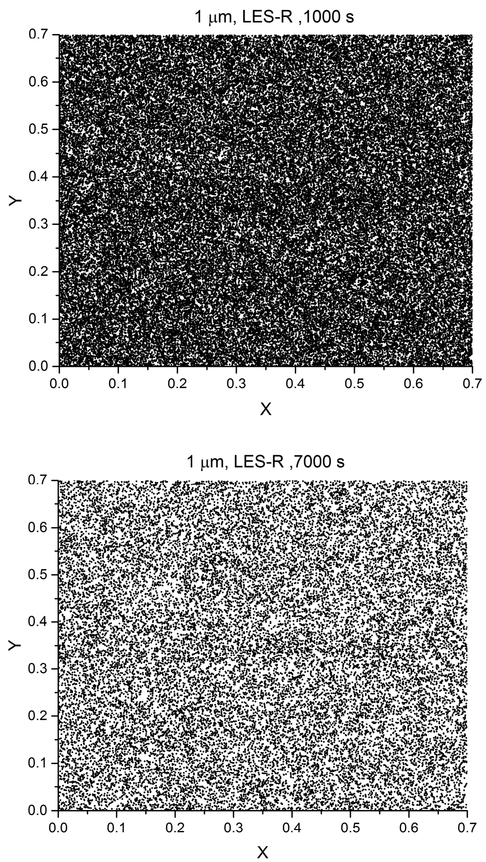
Flow velocities in MELCOR. Max. velocity approx. 0.08 m/s (bottom wall).



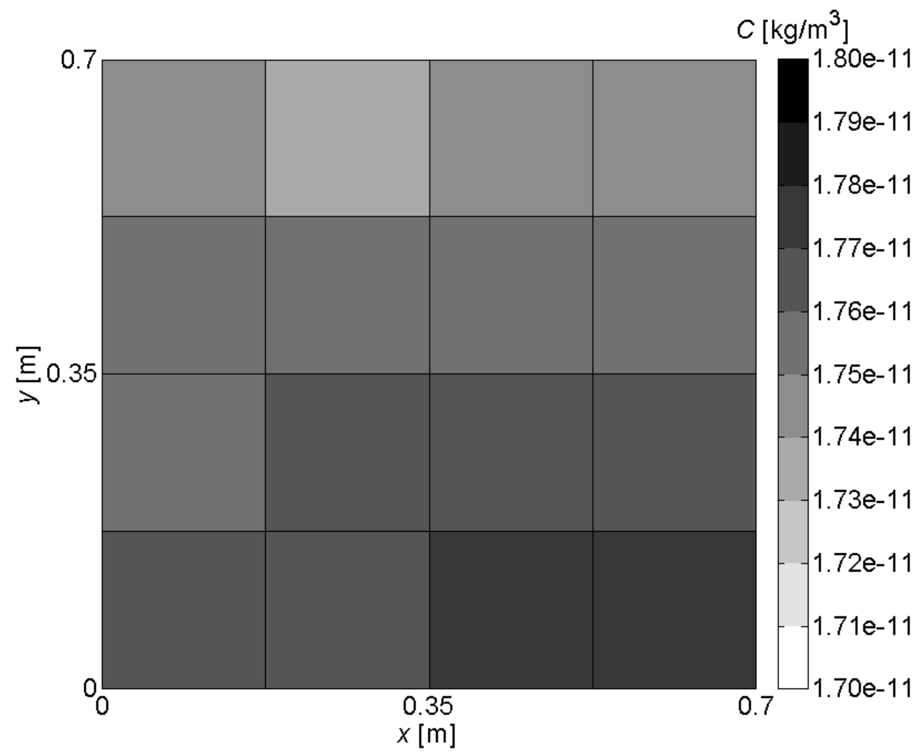
Measured velocity profiles from DIANA. Max. velocity approx. 0.23 m/s (hot wall).

MELCOR simulation – d_p = 1 μm

- Particle concentration almost uniformly distributed throughout the volumes at the end of the simulation.
- Consistent with the measurement and CFD simulations.



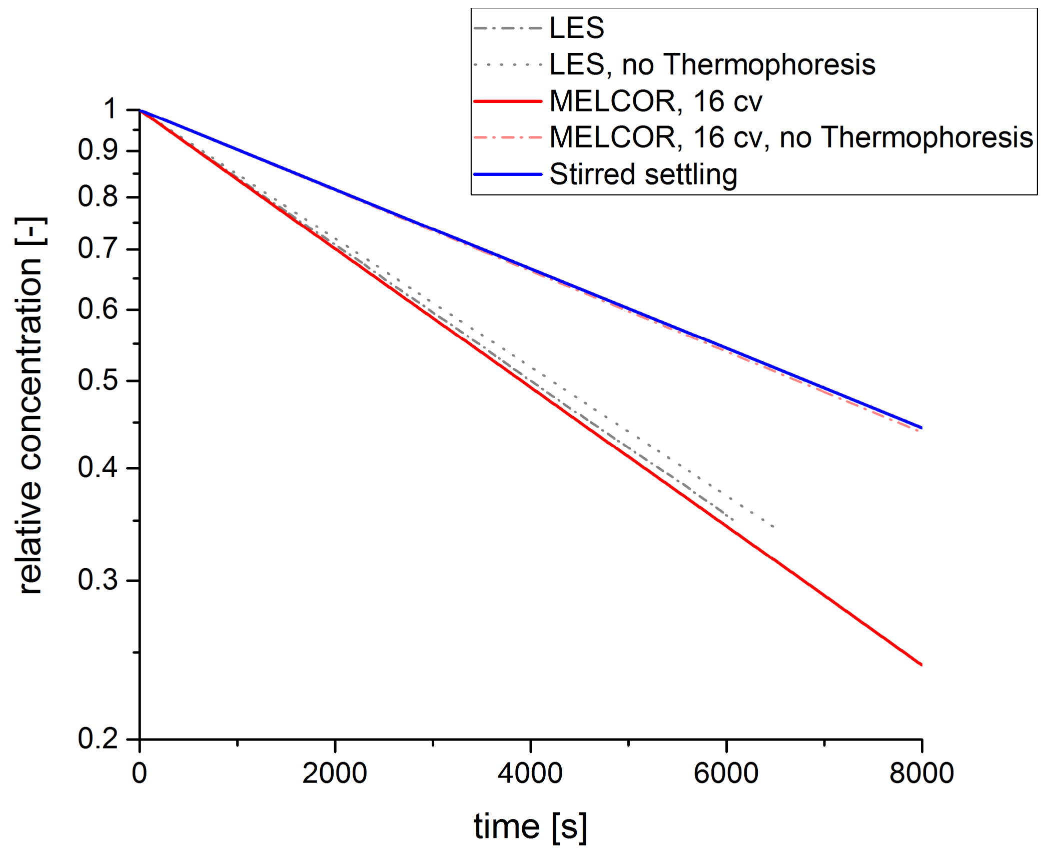
LES particle placement



MELCOR: mass concentration at t = 9500 s

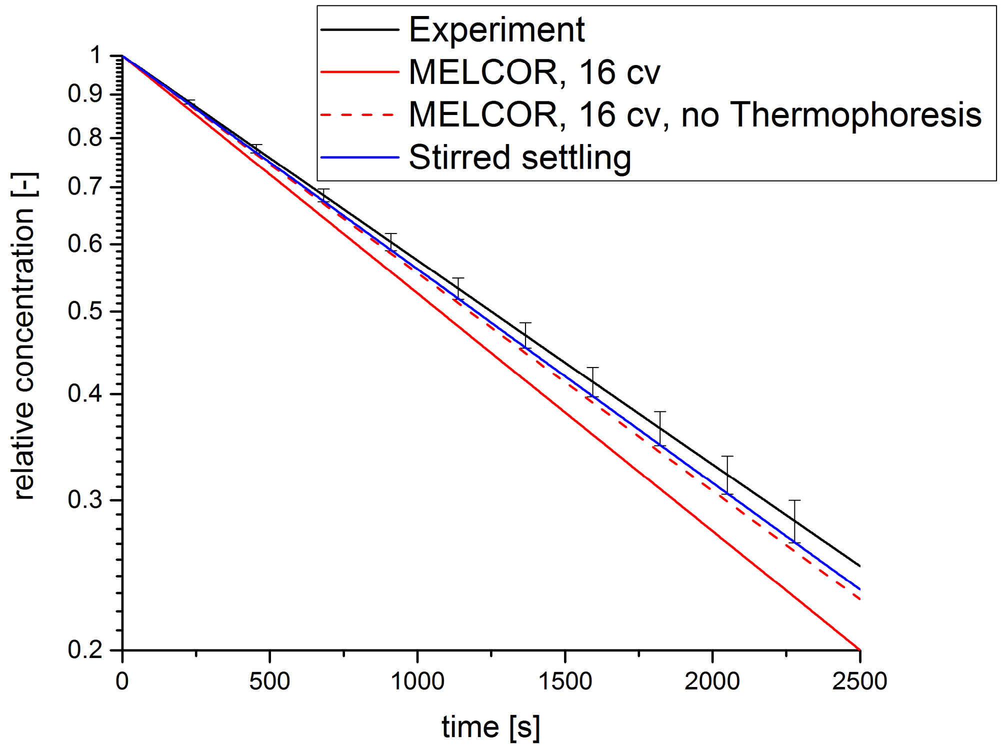
MELCOR simulation – d_p = 1 µm

- Particle depletion of 1 µm particles: similar result in MELCOR simulations using 16 control volumes than with the single volume.
- Depletion rate relatively close to measurement and LES + Lagrangian particle tracking results.
- With CFD, the exclusion of thermophoresis has only minimal effect on depletion rate.
- On MELCOR the effect is substantial.
  - Further investigation shows that MELCOR substantially overestimates the thermophoresis velocity, especially near the cold wall (1-6 times larger than in the LES data).



MELCOR simulation – d_p = 2.5 µm

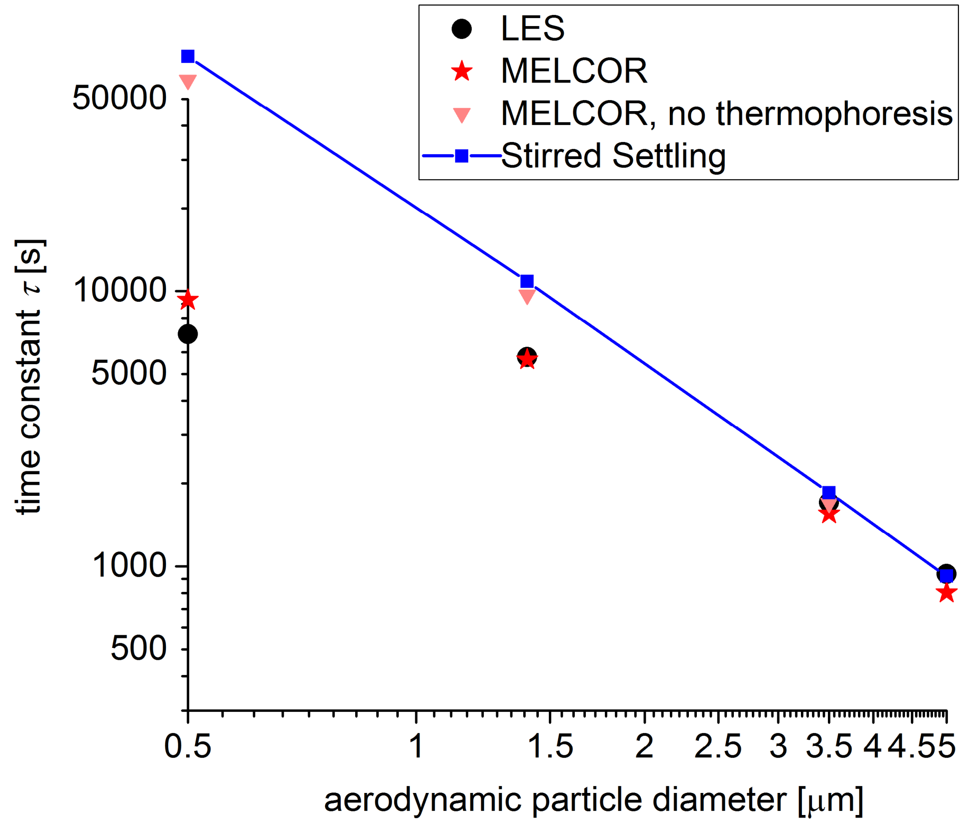
- Similar behavior with 2.5 micron particles.
- However, experimental (+ CFD) and MELCOR simulation results much closer to stirred settling values.



MELCOR, 16 cv, d_p = 2.5 µm particles.

Comparison of CFD and MELCOR with 4 particle sizes

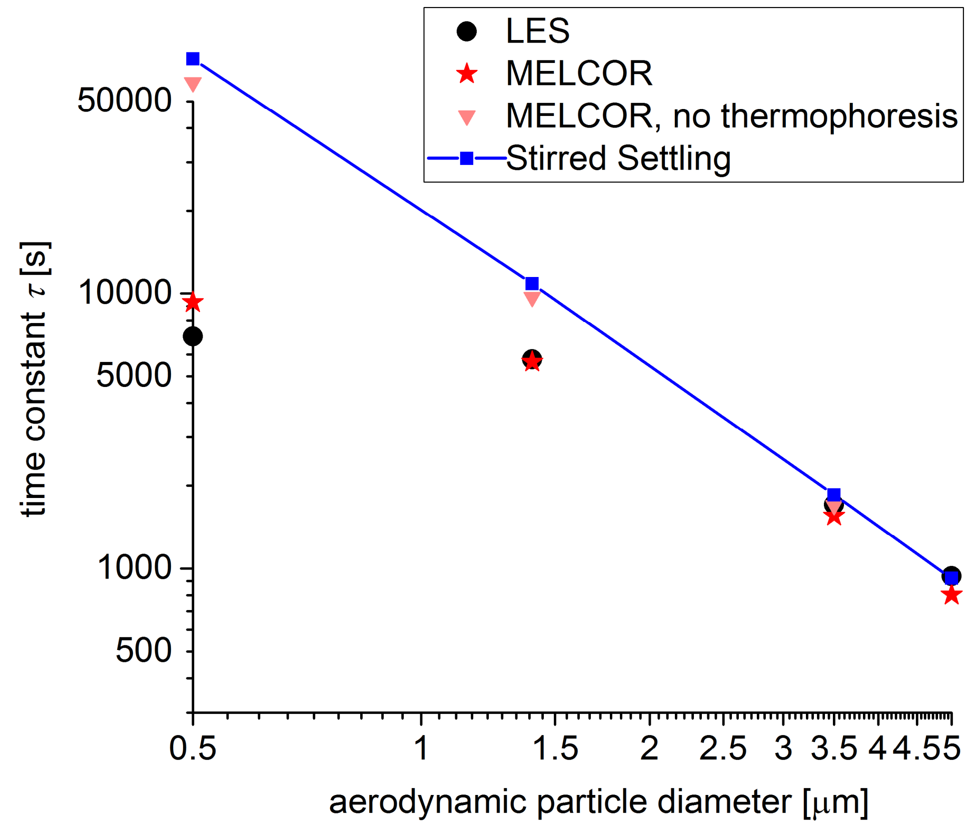
- Comparison between the LES and MELCOR with all 4 particle sizes
  - Good agreement with larger particles where deposition follows stirred settling model
  - With d_p = 0.5 µm and 1.4 µm particles, variations start to occur



Deposition time constant as a function of particle diameter

Comparison of CFD and MELCOR with 4 particle sizes

- Comparison between the LES and MELCOR with all 4 particle sizes
  - Good agreement with larger particles where deposition follows stirred settling model
  - With d_p = 0.5 µm and 1.4 µm particles, variations start to occur
  - For d_p = 1.4 µm the agreement between LES and MELCOR due to overestimation of thermophoretic force in MELCOR. Similar behaviour also observed with d_p = 0.5 µm particles



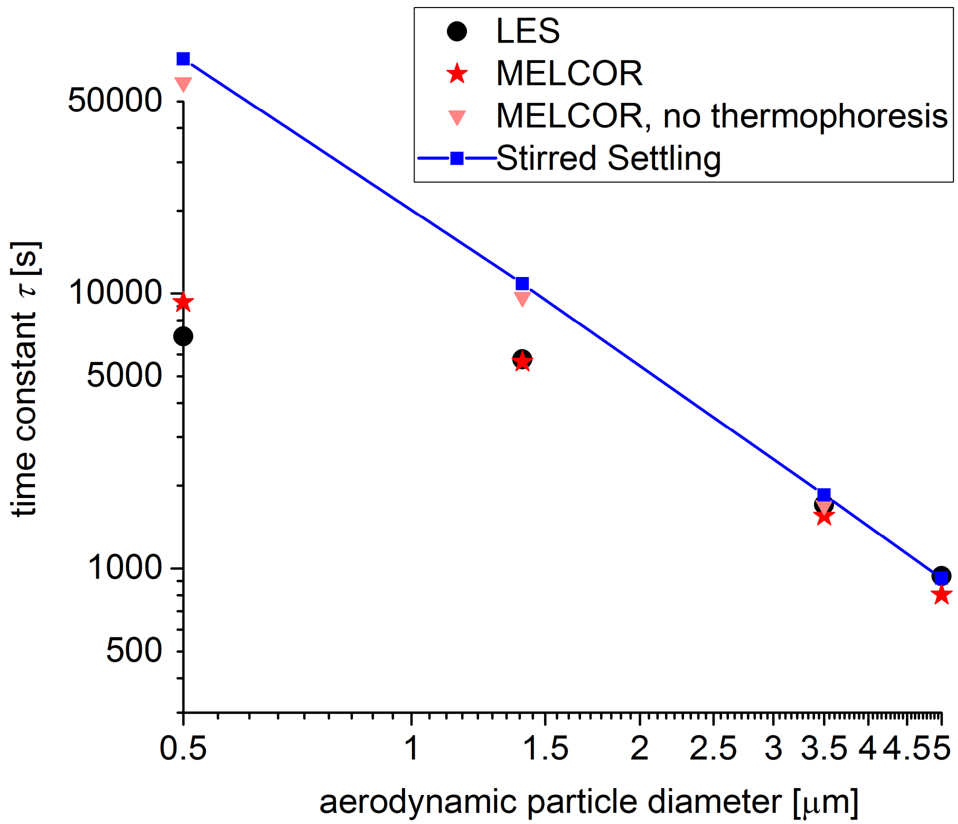
Deposition time constant as a function of particle diameter

Time constants from the LES, from MELCOR and the relative difference of the two

particle size d_p [µm]	Realistic BC simulation (LES) τ_{WT}[s]	MELCOR τ_{MELCOR} [s]	$\frac{\tau_{MELCOR}}{\tau_{WT}}$
0.5	6975	9294	1.3
1.4	5764	5641	1.0
3.5	1706	1553	0.9
5.0	937	802	0.9

Comparison of CFD and MELCOR with 4 particle sizes

- To further illustrate effect of thermophoresis in the MELCOR model
  - The temperature gradients were extracted from the LES data and new thermophoretic deposition velocities were calculated at each MELCOR heat structure surface for d_p = 0.5 µm and 1.4 µm particles.



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$$V_{therm} = \frac{3\,\mu\,C_m\left(c_t\,Kn + k_{gas}/k_p\right)}{2\;\chi\;\rho_{gas}\,T\left(1+3\,F_{slip}Kn\right)\left(1+2\,c_t\,Kn + k_{gas}/k_p\right)}\nabla T$$

From the LES

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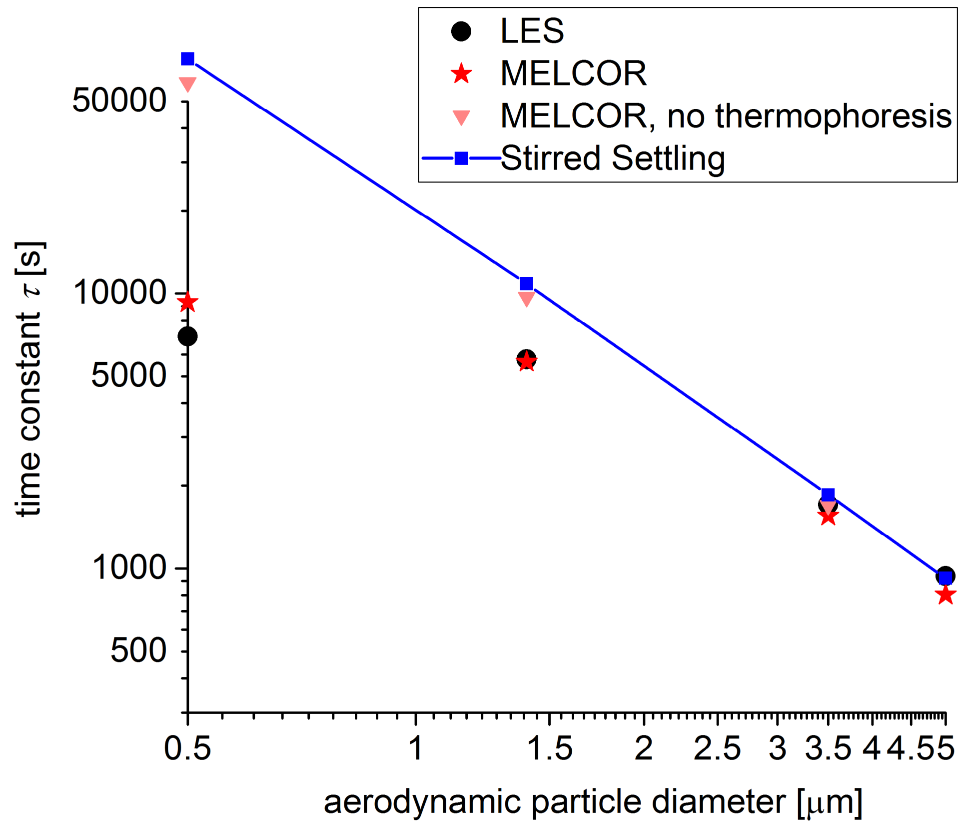
Comparison of CFD and MELCOR with 4 particle sizes

- To further illustrate effect of thermophoresis in the MELCOR model
  - The temperature gradients were extracted from the LES data and new thermophoretic deposition velocities were calculated at each MELCOR heat structure surface.
  - New depletion rates were estimated for the MELCOR model, assuming uniform particle distribution in the cavity.

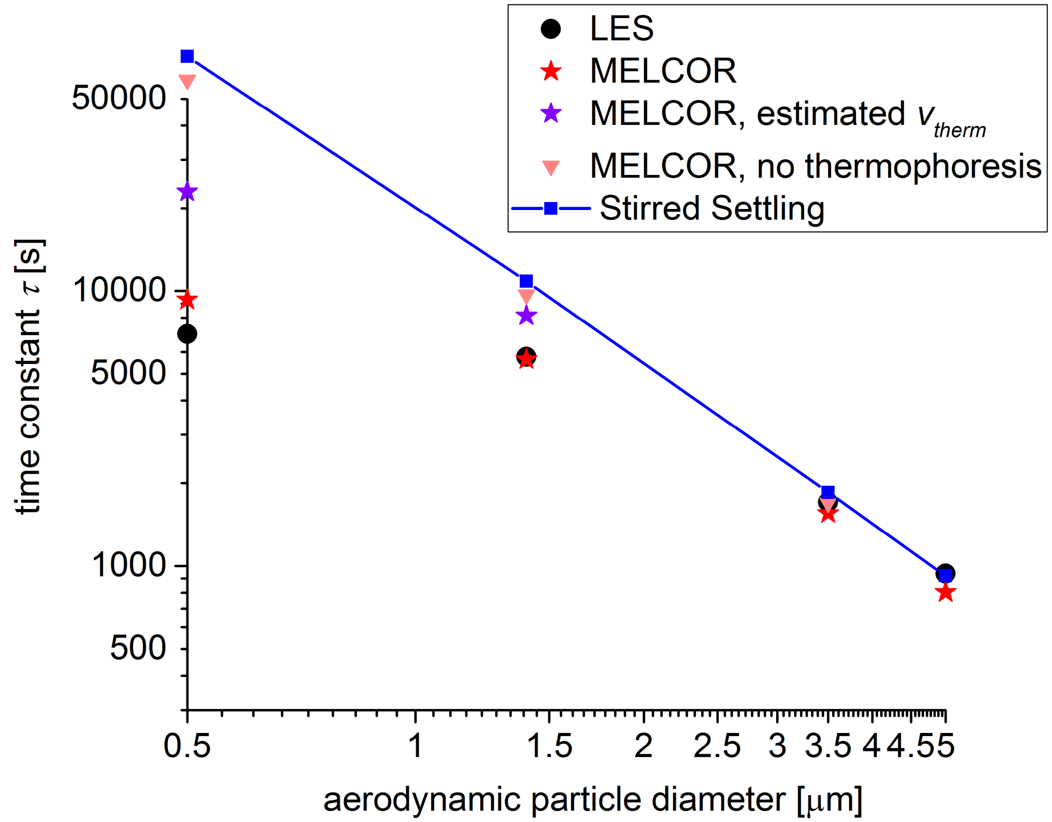


Time constants from the LES, from MELCOR and the relative difference of the two

particle size d_p [μm]	Realistic BC simulation (LES) τ_{WT}[s]	MELCOR τ_{MELCOR} [s]	MELCOR (realistic v_{therm}) τ_{MEL_upg} [s]	$\frac{\tau_{MELCOR}}{\tau_{WT}}$	$\frac{\tau_{MEL\_upg}}{\tau_{WT}}$
0.5	6975	9294	22983	1.3	3.3
1.4	5764	5641	8137	1.0	1.4
3.5	1706	1553		0.9	
5.0	937	802		0.9	

Comparison of CFD and MELCOR with 4 particle sizes

- To further illustrate effect of thermophoresis in the MELCOR model
  - The temperature gradients were extracted from the LES data and new thermophoretic deposition velocities were calculated at each MELCOR heat structure surface.
  - New depletion rates were estimated for the MELCOR model, assuming uniform particle distribution in the cavity.



Time constants from the LES, from MELCOR and the relative difference of the two

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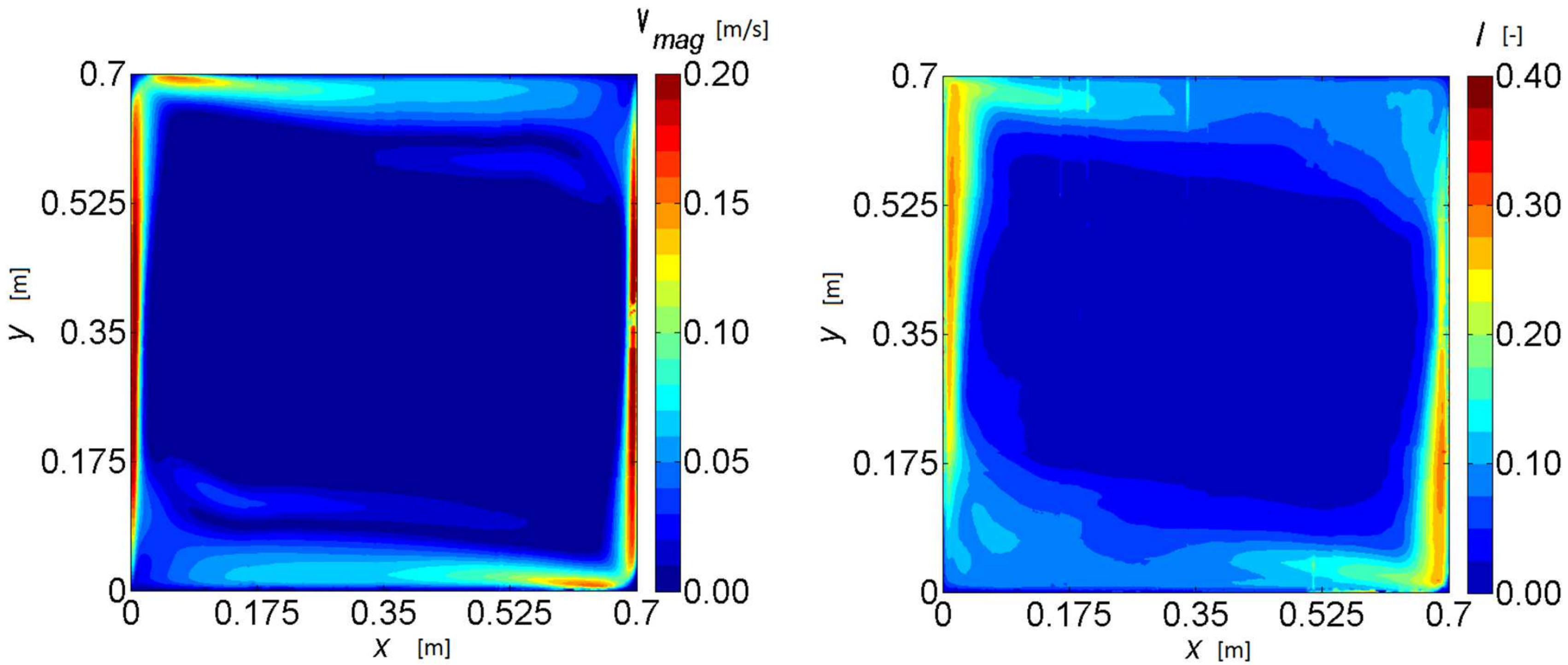
Conclusions

- Particle depletion in a cubic differentially heated cavity was investigated experimentally and using a CFD simulations.
- MELCOR was used to produce a model of DHC and the results were compared to CFD and experiments.
- Using 16 control volumes in MELCOR, stratified temperature distribution and encircling natural convective flow similar to experiments and CFD were produced.
- The depletion rates obtained from MELCOR coincided reasonably well with the CFD and measurement data.
- The large effect of non-homogeneity of the turbulent flow in DHC in particle deposition, shown in the CFD simulations with different boundary conditions was not observed in MELCOR.
  - ➢ Particle depletion rate in MELCOR dependent on gravitational settling, thermophoresis and Brownian diffusion.
  - ➢ The effects of thermophoresis on particle depletion rate in MELCOR simulations differs considerably from the CFD simulations.
    - ✓ For d_p = 0.5 µm and 1.4 µm particles, MELCOR overestimated the temperature gradients near the cold wall, resulting to a significantly larger deposition velocities compared to the LES of the cavity.

Thank you for your attention.

Additional slides



$$V_{mag} = \sqrt{(u)^2 + (v)^2}$$

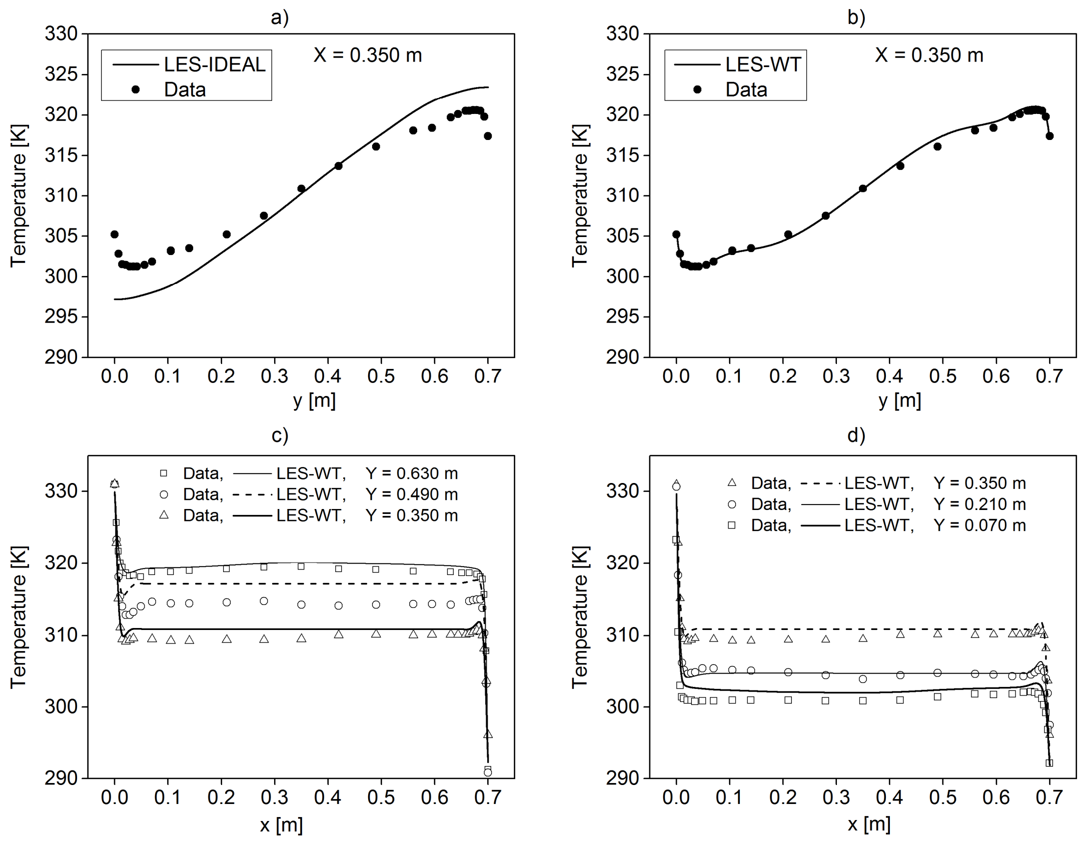
$$I = \frac{\sqrt{u_{rms}^2 + v_{rms}^2}}{max\left(\sqrt{u^2+v^2}\right)}$$

Mean velocity magnitudes and the turbulence intensity at the cavity center plane.

Turbulent flow encircling a stagnant core next to the isothermal and horizontal walls.

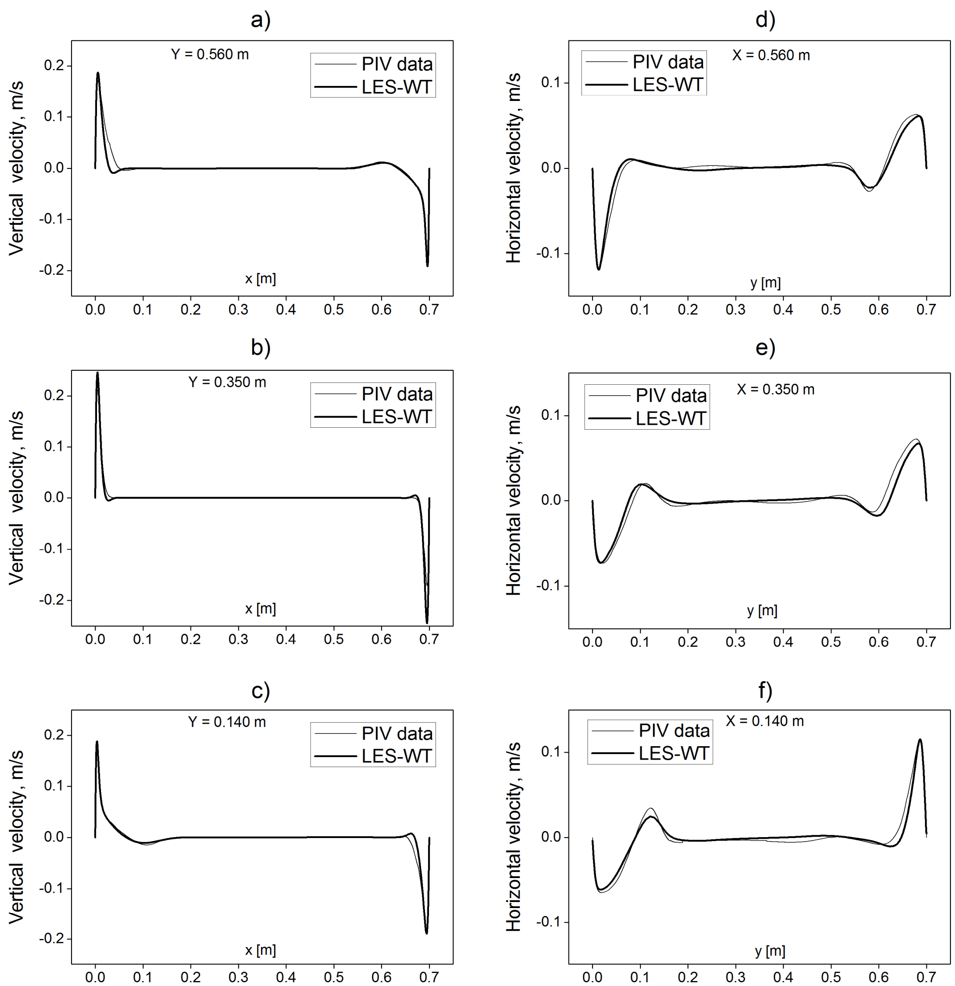
Additional slides

- Two LES with different BCs at the horizontal wall were used in the particle tracking simulations.
- In the first LES (LES-WT), the thermal BCs for isothermal and horizontal walls were obtained from the wall temperature measurement data.
- The second simulations using idealized adiabatic BCs on horizontal walls (LES-IDEAL), was validated against the DNS data by Puragliesi (PhD thesis, EPFL, 2010) with similar conditions.
- The LES-WT validated using the measurement data.
- Flow and temp. field differed with LES-IDEAL – Flow geometry different, less turbulent.

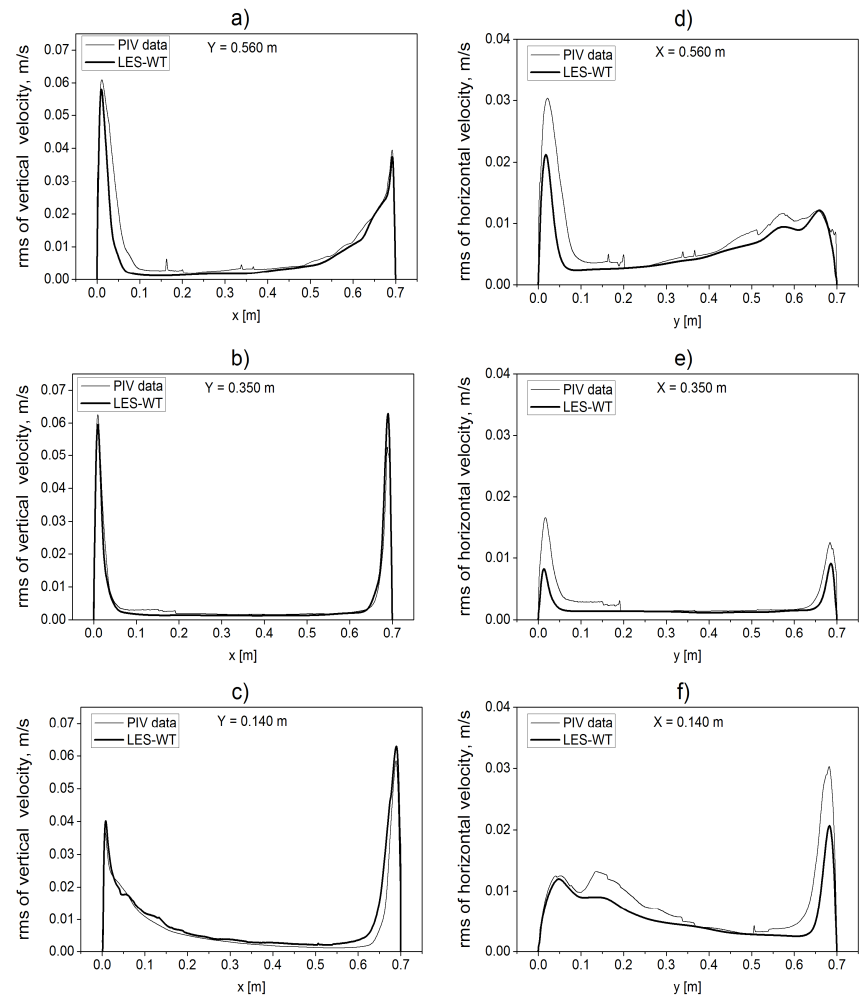


Horizontal and vertical temperature profiles from DIANA cavity, compared against LES-WT and LES-IDEAL simulation data. Both show stratified temperature distribution at cavity core.

Additional slides

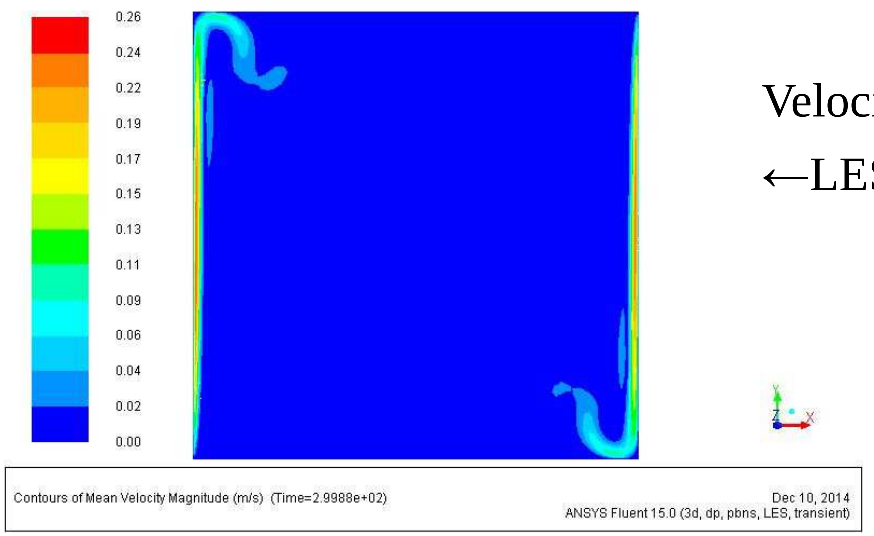


Comparison between PIV measurement of mean vertical and horizontal velocity components and LES-WT simulation.



Rms of velocity along horizontal and vertical profiles from PIV measurements and LES-WT simulations .

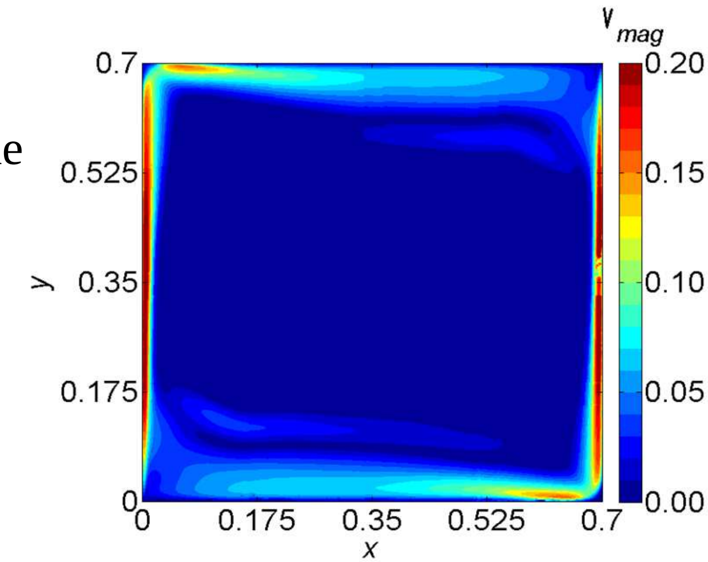
Additional slides

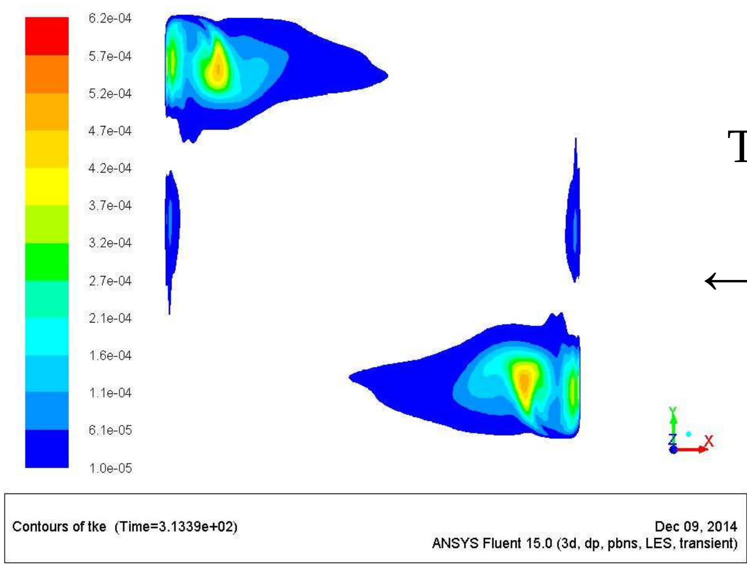


Velocity magnitude

←LES-IDEAL

PIV→





Turbulence kinetic energy

←LES-IDEAL

LES-WT→