

NUMERICAL ANALYSIS OF HEAT CONDUCTION INFLUENCE ON SCR AFTERTREATMENT SYSTEMS EFFICIENCY

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Abstract

Selective Catalytic Reduction (SCR) is well known method for reducing NO_x emission in diesel engine exhaust gas. Urea-water solution (UWS) injected into hot stream decomposes due to thermolysis into ammonia and isocyanic acid which hydrolyses further into more ammonia and carbon dioxide. Resultant ammonia is the NO_x reductor, producing water vapour and carbon dioxide from the reduction reaction. To provide sufficient NO_x reduction efficiency, UWS needs to be properly atomized and mixed with exhaust gas. However, due to more and more restrictive emissions regulations provided by European Union and Close Coupled trend of aftertreatment systems in vehicles the design process is very complex and demanding. Computational Fluid Dynamics (CFD) simulations are integral part of product development, allowing save time and reduce costs of preparing prototypes for further tests. However, it is necessary to understand all the processes and problems connected with NO_x reduction in SCR system. Strong turbulent flow of hot stream gas, urea-water solution spray injection, droplets interaction with wall, wallfilm generation are included. The objective of this work is to investigate the impact of heat transfer modelling inside mixing elements of SCR system on urea mixing uniformity and wallfilm deposit on the walls of the system. Simplified and more complex approach is compared with no heat transfer cases. All the simulations were conducted using AVL FIRE™ software. Results showed that wall heat transfer might have an impact on mixing efficiency and wallfilm formulation. It is necessary to take into account the effect of mixing elements heat conduction in CFD simulations during the aftertreatment design process.

Keywords: SCR, simulation, heat conduction, aftertreatment

1. Introduction

Modern automotive industry is facing more and more restrictive emissions regulations. Especially in the diesel engine to meet these requirements is very challenging. Due to its combustion process, diesel engines have high NO_x emissions, which are regulated by Euro 6 emissions standards [4]. Hence, the design of aftertreatment system, which will fulfil the requirements, becomes a challenge.

Selective catalyst reduction (SCR) systems with urea-water solution (UWS) injection are widely used nowadays. Urea decomposes into ammonia, which is a reducing agent of NO_x. To provide high reduction efficiency of SCR system ammonia has to be distributed as uniformly as possible at the entrance of a catalyst. To reduce costs of prototyping and testing, CFD simulations are an integral part of aftertreatment design process. Such simulations may demand high computational cost due to its complexity. That is why simplified physics models are used despite the risk of losing calculations accuracy. Due to high flow temperatures, the heat exchange between hot gas streams, injected UWS and the walls of the mixing elements play an important role in CFD simulations.

The aim of the study is to investigate an impact of heat conduction of mixing element in SCR aftertreatment system on wallfilm generation and efficiency of mixing measured by ammonia

uniformity at catalyst inlet. Widely used simplified model was compared with full coupling of heat conduction in mixing element with fluid case of UWS injection in hot exhaust gas stream. Results showed that simplified model is not accurate enough in case of SCR system simulations. Taking into account heat conduction affected distinctly both wall film formation and UWS distribution at catalyst inlet.

2. Numerical setup

Two heat conduction approaches were compared: simplified calculations with adiabatic boundary conditions and thin wall model, and ACCI coupling of fluid and solid solvers.

Thin Walls module models solid wall boundaries as thin solid material with heat conduction solved in lateral direction [5] with equation (1):

$$\frac{\partial T}{\partial t} - \frac{\lambda}{\rho c_p} \frac{\partial^2 T}{\partial x^2} = 0, \quad (1)$$

where:

T – temperature,

t – time,

λ – heat conduction coefficient,

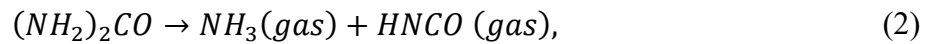
ρ – density,

c_p – heat capacity,

x – coordinate.

The second setup uses AVL Code Coupling Interface (ACCI), which allows to couple and transfer information between two and more cases [6]. For this study wall, heat transfer between fluid domain and solid mixer was simulated. Mixer wall was used as interface between fluid and solid cases, transferring temperature, and heat conduction coefficient. Each time solved step fluid case sets environment temperature and heat transfer coefficient, and transfers it to solid case, which after solving sets temperature at the interface between cases.

Investigation was conducted using relative diesel engine conditions. Tab. 1 contains the general parameters for all cases. Mass flow value was fixed to 400 kg/h and inlet gas temperature was covering the area of highest Cu/Zeolite SCR catalyst conversion performance range [2]. Four UWS injections were calculated to provide stable NH_3 uniformity value. To achieve stable calculations, the first injection starts at 0.55 s. The amount of injected UWS mass and single injection timing was calculated to provide 1:1 NH_3/NO_x ratio under defined conditions. Implemented in AVL FIRE software evaporation model with Urea decomposition was used (eq. (2) [1, 7]):



with kinetic model used by Birkhold, eq. (3):

$$\frac{dm_{\text{urea}}}{dt} = -\pi \cdot A \cdot D_d \cdot \exp\left(\frac{E_a}{RT}\right), \quad (3)$$

where:

m_{urea} – urea mass,

A – constant (Kim et al. suggests $A = 0.42 \text{ kg/ms}$ [3]),

D_d – droplet diameter,

E_a – energy of activation (Kim et al. suggests $E_a = 69000 \text{ J/mol}$ [3]),

R – gas constant,

T – temperature.

Diesel exhaust gas mixture is used as stream medium. Diesel Oxidation Catalyst (DOC) and SCR-Catalysed Diesel Particulate Filter (SDPF) zones were defined as directed porous media zones using one direction porosity type with Forcheimer pressure drop model [8]. For ACCI

coupling temperature boundary condition on mixer surface was selected in fluid case and convective boundary conditions in solid case. Polyhedral mesh cell type was used to provide high surface accuracy. Fig. 1 illustrates fluid computational domain. Global 4 mm mesh cell size was defined with 3 mm surface size. Mixer surface was refined with 2 mm surface element size. Injection cone zone was refined with 1 mm volume cell size. Solid mesh was prepared with same settings to provide accurate data transfer between both cases. Fig. 2 illustrated mixer geometry. Solid mesh was prepared with wall element surrounding the mixer. For pure fluid case and ACCI coupling the mixer surface only was selected (Fig. 2, orange).

Tab. 1. General solver setup settings

Parameter	Value
Simulation time	1.55 s
Mass flow	400 kg/h
Gas temperature	200°C, 250°C, 300°C, 350°C
Injection mass flow	0.84 mg/ms
Injection time	26.5 ms
Injection start time	0.55 s
Liquid temperature	80°C

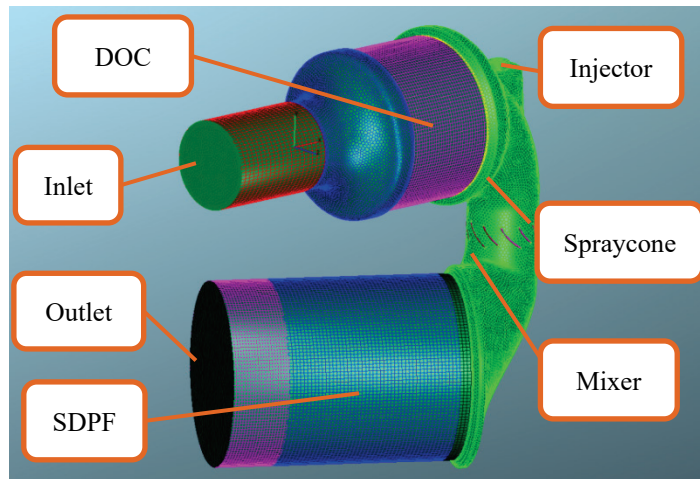


Fig. 1. Computational domain mesh view

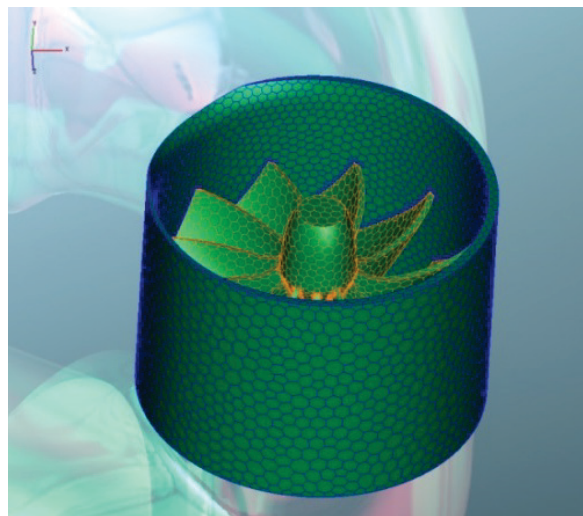


Fig. 2. Mixer mesh view with interface selection (orange)

3. Results

Figure 3 and 4 show the comparison between Thin Wall and ACCI module in the lowest and the highest inlet temperature. For both cases, one can notice higher film evaporation rate in ACCI cases. With higher flow temperature, the difference increases. Hence, increasing evaporation rate in ACCI cases can be noticed. At the end of each injection, the wallfilm mass in ACCI cases is lower what also points at lower urea deposit risk. When comparing relative difference with reference to Thin Walls cases, ACCI coupling provides from up to 12% more mass evaporated in 200 C case and up to almost 30% in 350 C case and up to 65% difference in total film mass difference in 350 C (Fig. 5).

Higher flow temperature provides higher temperature of wallfilm and higher evaporation rate what was predicted. Wallfilm mass balance is more stable and film mass does not increase significantly in time.

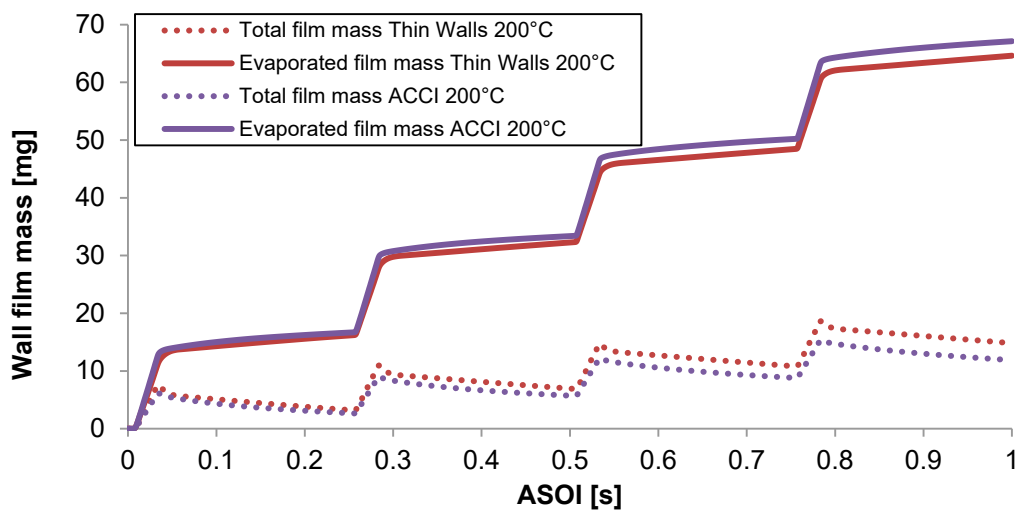


Fig. 3. Wall film mass balance at 200 C inlet flow

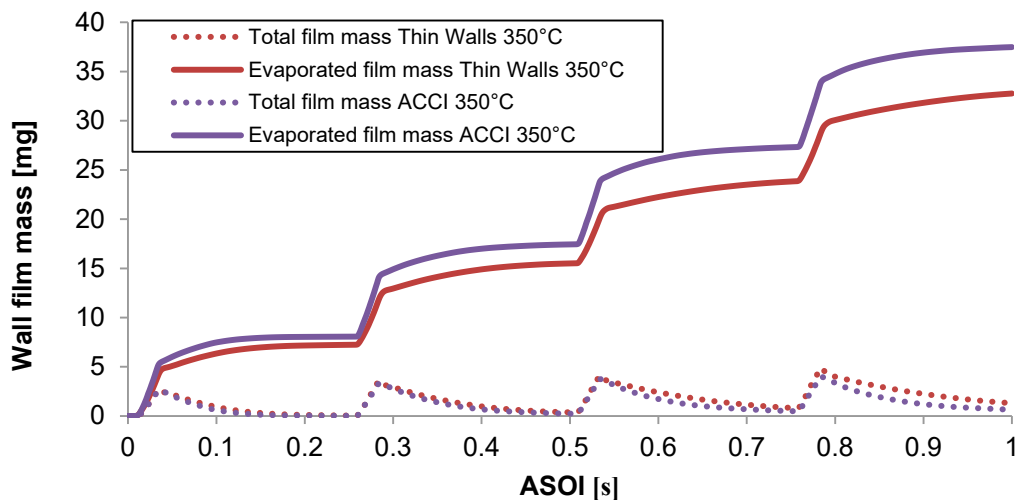


Fig. 4. Wall film mass balance at 350 C inlet flow

Figure 6 shows how the wallfilm changes with increasing temperature of the stream. One can see that nonlinear trend of decreasing wallfilm mass is saved in time after more injections. The relative difference between Thin Walls and ACCI is changing as predicted in comparison with Fig. 5.

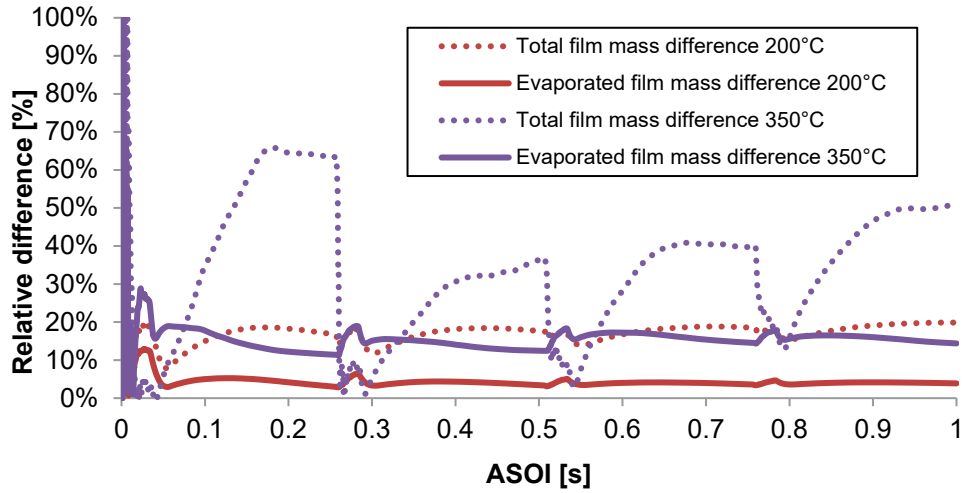


Fig. 5. Relative wallfilm mass difference between Thin Walls and ACCI models

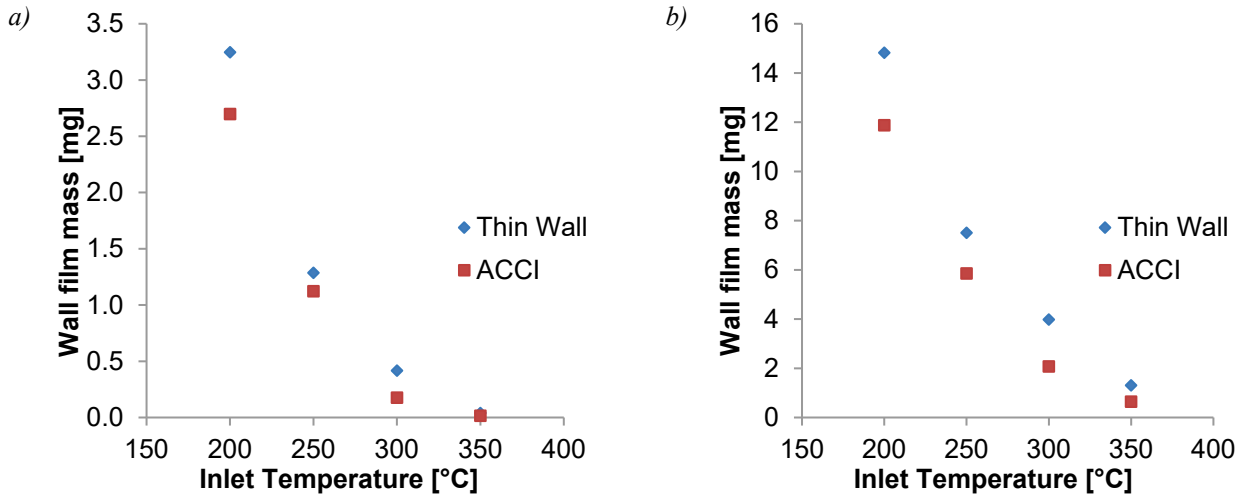


Fig. 6. Influence of inlet gas temperature on wall film mass: a) after first injection (0.25 s ASOI), b) after last injection (1 s ASOI)

In terms of relative total mass difference for 200 ° C, case stable periodic change up to about 18% can be noticed. For 350 ° C, relative difference of total mass changes every injection. The difference goes up to about 65% at the end of the first injection, then goes down to almost 40% at the end of the second injection and then it increases at the end of each injection.

Figure 7 illustrates temperature distribution on mixer wall for both ACCI and Thin Walls models for 350°C case. In the Thin Wall module, where there is no physical calculation of solid domain, there is no heat conduction between both sides of the mixer blades. This is the main difference between the models. When UWS is injected and the droplets hit the mixer, it cools down the blades from the top. Due to heat conduction, also bottom side of the mixer is cooled. ACCI coupling calculates it.

Due to existing solid mesh, there is more heat energy to be absorbed by the droplets hitting the mixer blade. That is why evaporation is stronger in ACCI cases and the difference increases along with gas temperature.

The mixing efficiency of the system is determined by NH_3 distribution uniformity at SDPF inlet calculated from eq. (4):

$$UI_{\text{NH}_3} = 1 - \frac{\sum_i |NH_{3i} - NH_{3\text{avg}}| A_i}{2 NH_{3\text{avg}} A_{\text{total}}}, \quad (4)$$

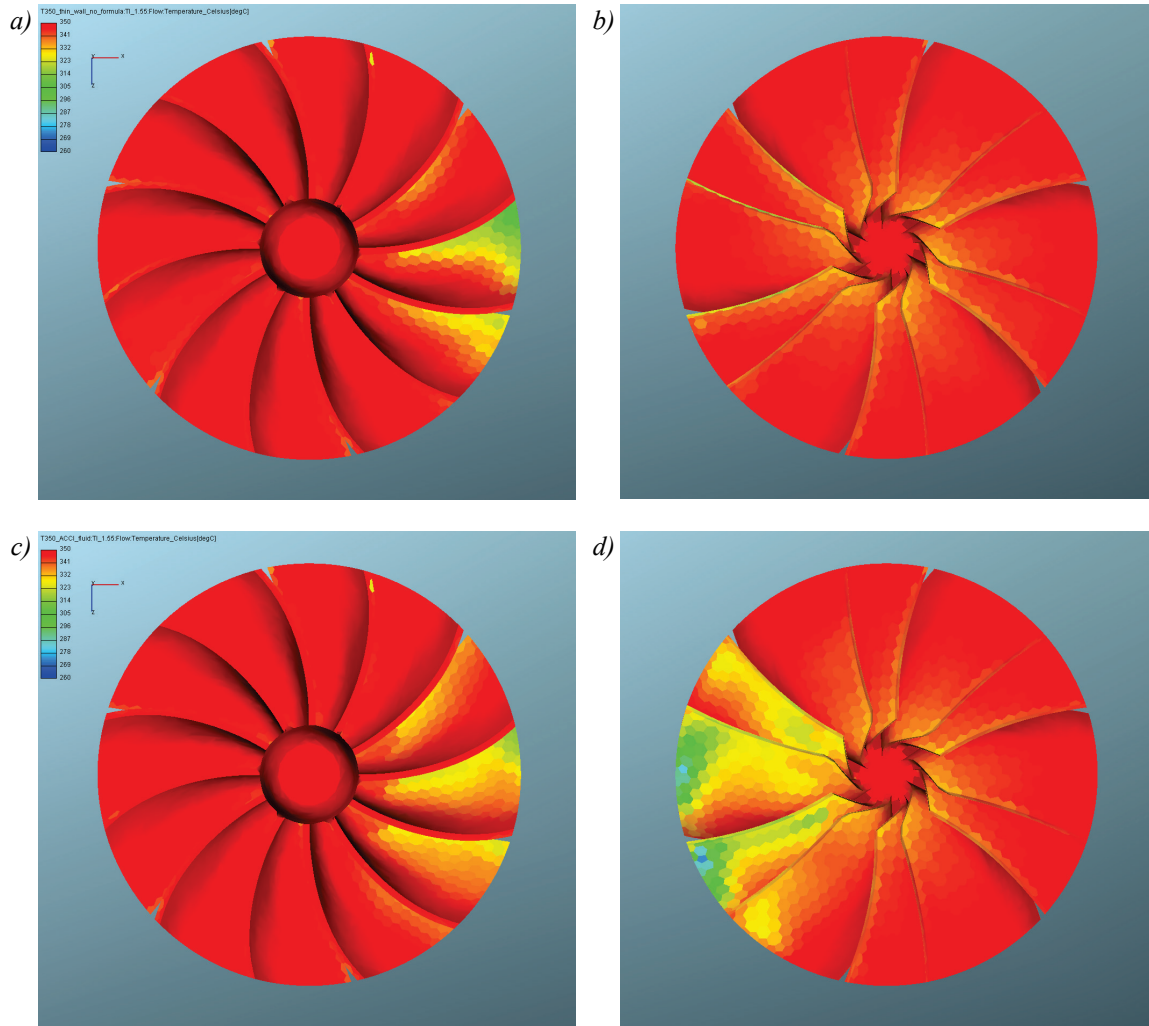


Fig. 7. Mixer wall temperature for 350 C case: Thin Walls mixer top (a) and bottom (b), ACCI mixer top (c) and bottom (d)

where:

- UI_{NH_3} – ammonia uniformity index,
- NH_{3i} – ammonia mass in i-th element,
- NH_{3avg} – area averaged ammonia mass,
- A_i – area i-th element,
- A_{total} – total area.

Uniformity is decreasing with higher gas temperature with an exception of ACCI 250 C case. Stronger evaporation in fluid-solid coupling results in more gas phase ammonia in domain, which mixes with exhaust gas stream easier than liquid. Fig. 9 shows NH_3 distribution at SDPF inlet. For both low and high inlet temperatures the trend are similar. The highest concentration of NH_3 is in the upper right side of the SDPF inlet. In both ACCI cases, the high NH_3 concentration area is larger. However, generally the ammonia distribution is more uniform. It is due to more vapour ammonia in the domain. Diffusion makes gas mix with another gas easier than liquid with gas.

4. Conclusions

Simplified thin walls heat transfer model was compared with ACCI fluid-solid wall heat transfer coupling. Results showed that coupling UWS injection into hot exhaust gas stream case in fluid domain with heat conduction of mixing element in solid domain provides more physical prediction of temperature distribution. Due to that, evaporation of wallfilm generated by the droplets hitting

the hot blade surface is enhanced. In SCR application, every percentage point is important along with accurate wallfilm formation prediction. Hence, proper model of heat transfer between hot exhaust gas stream, injected UWS, and solid mixer wall is an important element of SCR aftertreatment design process.

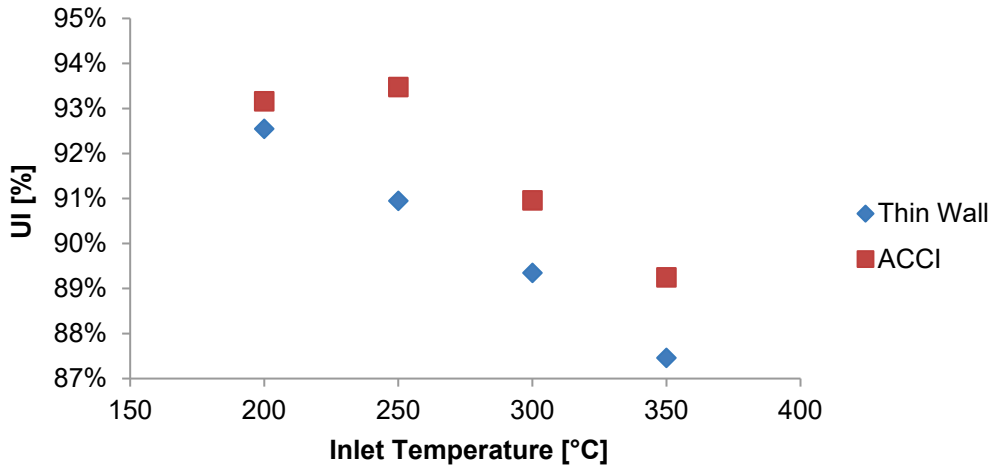


Fig. 8. Inlet gas temperature impact on NH₃ uniformity index at SDPF inlet

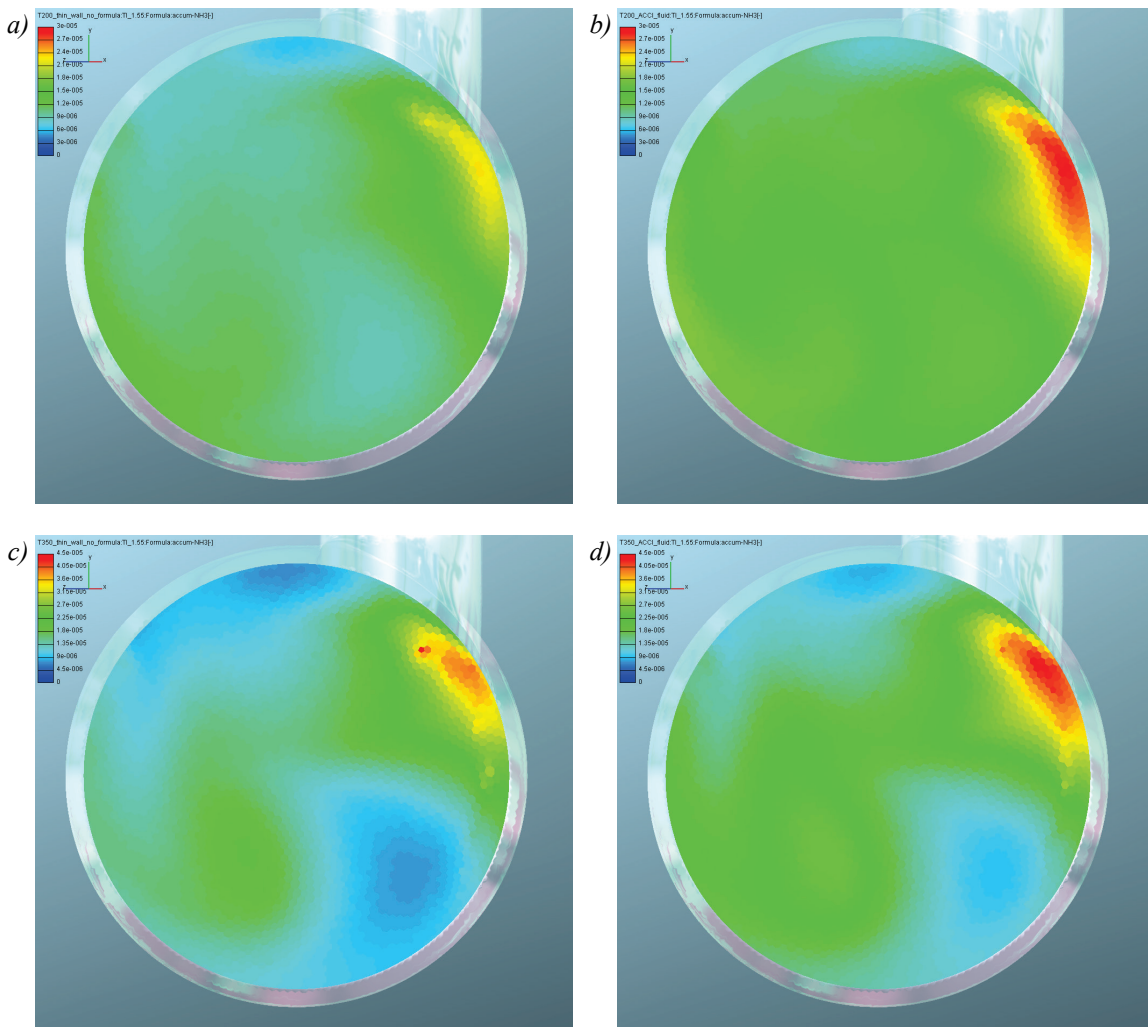


Fig. 9. NH₃ distribution at SDPF inlet, 1 s ASOI: Thin Walls 200°C (a), ACCI 200°C (b), Thin Walls 350°C (c), ACCI 350°C (d)

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