Improvement of the numerical framework for selective catalytic reduction applications

J. Baleta[*,1], M. Vujanović[1], N. Duić[1], K. Pachler[2], D. Schellander[2]

[1]Faculty of Mechanical Engineering and Naval Architecture, University of Zagreb, Zagreb, Croatia
[2]Advanced Simulation Technologies, AVL List GmbH, Graz, Austria

Abstract

The focus of this work is improvement and validation of the mathematical framework of commercial computational fluid dynamics code Fire for describing selective catalytic reduction processes. First step was further development of existing model for heat conduction inside the solid by enabling multilayer simulations, in order to have more accurate temperature profile and therefore more accurate heat transfer. Validation was carried out on the well-established experimental results from PhD thesis of Felix Birkhold. Furthermore, 3D numerical simulations of UWS injection in hot flue gases was conducted with the aim of determination of new set of parameters for urea thermolysis reaction rate.

Introduction

Various environmental regulations put ever stringent requirements on the automotive industry as a part of solution to the problem of global warming and climate change. The urea-water solution (UWS) based selective catalytic reduction (SCR) is a promising method for meeting the NOx emission limitations of the current EURO 6 standard for road vehicles propelled by the diesel engine. In principle, the UWS spray is injected into a hot exhaust gas stream preceding the SCR catalyst and ammonia is generated through series of chemical reactions. Then, the generated ammonia acts in various deNOx reactions as a reductant.

Spatially uniform distribution of the reducing agent that precedes the SCR catalyst is a crucial factor for the conversion of NOx. The uniformity of distribution and the degree of processing of the reducing agent upstream of the SCR catalyst can be, besides the evaporation and decomposition, influenced also by the spray/wall interaction. Due to increasing price of experimental equipment and with increase of both the computational power and its affordability during the last two decades, numerical simulations are becoming a valuable design tool in the field of internal combustion engines. Usage of CFD simulations to investigate and improve thermochemical processes is becoming increasingly important [1].

Objective of the current work is further improvement of existing framework by upgrading thin wall module which is used for the calculation of heat transfer inside solids and optimization of urea thermolysis model parameters. These improvements should result in a more accurate representation of SCR processes and thus provide support to ever increasing industry demands for reliable design tools.

Mathematical models

In this study, as in the most engineering applications today, the Eulerian-Lagrangian method for solving the multiphase flow phenomena is used. In this approach, the spray droplets are represented by finite numbers of droplet groups called parcels. It is assumed that all the droplets within one parcel are similar in size and have the same physical properties. The motion and the transport of the parcels are tracked through the flow field using a Lagrangian formulation, while the gas phase is described by solving conservation equations using an Eulerian formulation. The coupling between the liquid and the gaseous phase is taken into account by introducing appropriate source terms for interfacial mass, momentum, and energy exchange [2].

Equations of continuum mechanics are based on the conservation laws for mass, momentum and energy. The general form of the time averaged conservation equation for any dependent variable φ of the continuous phase in the differential form is:

$$\frac{\partial}{\partial t}(\rho\varphi)+\frac{\partial}{\partial x_j}(\rho\varphi u_j)=\frac{\partial}{\partial x_j}(\Gamma_\varphi\frac{\partial\varphi}{\partial x_j})+S_\varphi \qquad (1)$$

In the above equation ρ denotes the density, u_j Cartesian velocity, Γ_φ diffusion coefficient, and S_φ represents the source term of the dependent variable. The first term is an unsteady term, the second term is convection, the third term is diffusion and the last term is source or sink. The source term S_φ is used for the coupling of the liquid and the gaseous phases.

In order to include all relevant phenomena appearing the UWS injection into confined space of mobile SCR systems suitable mathematical description of the following processes is needed:

- momentum interaction between gas phase and droplets;
- evaporation and thermolysis of droplets;
- heat transfer between wall and droplets;
- spray/wall interaction;

* Corresponding author: jakov.baleta@fsb.hr

- two-component wall film including interaction with gas phase and exhaust tube;
- secondary break-up of spray.

Boundary layer assumptions [3] lead to the implementation of the wall film model as a 2D finite volume method on the air flow wall boundaries.

Film thickness equation is the basic governing equation for the wall film flow. It represents a slightly modified formulation of the continuity equation where, instead of mass, the wall film thickness is conserved property. The Cartesian formulation of the film thickness equation is:

$$\frac{\partial \delta}{\partial t}+\frac{\partial \delta u_1}{\partial x_1}+\frac{\partial \delta u_2}{\partial x_2}=\frac{1}{\rho A}(S_{mD}-S_{mV}) \quad (2)$$

Film thickness is represented by δ, ρ is the film density, u_1 and u_2 are film velocity components, S_{mD} and S_{mV} are source terms and A is the surface of the film. If we assume that the source terms are provided, equation (2) can be solved explicitly if the velocity components are known.

Film momentum equation describes dynamics of liquid film interaction with its environment - wall, air stream above film, impinging droplets, etc. Equation (3) gives mathematical formulation of wall film momentum conservation law:

$$\frac{dM_i}{dt}=\oint_L \rho u_i(u_i-V_j)\hat{n}_i dL=\int_L p\delta\hat{n}_i dL+mg_i+\Gamma_i+S_M \quad (3)$$

Film momentum is denoted with M_{i}, ρ is the film density, u_{i} is the film velocity, V_{j} is wall velocity, $\hat{n}_i$ is normal to the face cell facing outwards, L is length of the face cell boundary, δ is the film thickness, p is film pressure, m is film mass, g_{i} is gravity vector, Γ_{i} is the term that takes into account all shear stresses and S_{M} presents various source and sink terms such as film entrainment, spray droplets impingement and film evaporation.

Heat transfer has a major impact on the water evaporation and urea thermolysis so its accurate description is desirable. Current approach in Fire for heat conduction calculation inside the solid employs the so called thin wall module where solid is represented as a monolayer of a given thickness and linear temperature change is assumed. The mean solid temperature is used for heat transfer calculation on both sides of the solid. This approach has obvious drawbacks, especially in the case of thick or multi-material solids or in solids with pronounced temperature gradients. In order to overcome those difficulties we developed the improved model which enables multilayer solid discretization, either uniform or non-uniform and multi-material properties definition.

The 1D heat conduction modeling can be considered as accurate when the following assumptions are satisfied [4] :

- the solid is thin compared with the proportions of the computational volume;
- the solid is a stacking of homogeneous layers, i.e. with constant properties;
- lateral heat conduction is negligible with regard to normal heat conduction.

In either steady or transient calculations, the following equations are solved within a thin wall:

$$\frac{\partial T}{\partial t}-\frac{\lambda}{\rho c_p}\frac{\partial^2 T}{\partial t^2}=0 \quad (4)$$

$$\lambda_i\frac{\partial T}{\partial x}\bigg|_i=\lambda_j\frac{\partial T}{\partial x}\bigg|_j \quad (5)$$

In the above expressions λ stands for the thermal conductivity, T is temperature, ρ is density and c_p is specific heat. The 1D heat conduction is solved within the thin wall thickness, and is coupled with the fluid energy equation. The wall thickness can now be discretized in multiple layers and the number of nodes per layer could be specified. Hence, there is a constant space step per layer. This enables more accurate calculations of heat transfer with small computational time trade off.

Thermolysis of urea is modeled with Arrhenius equation which contains activation energy and frequency factor which have major influence on chemical kinetics. It is also aim of this work to obtain optimized set of this parameters and use it to predict some experimental cases.

Birkhold plate case - settings

Well established case of the plate cooling from PhD thesis of Felix Birkhold [5] is used for validation of multilayer thin module. Details of settings are given in [5], while only brief description is given here. Thin metal plate (2 mm) was placed inside the middle of rectangular channel with dimensions of 94x120x400 mm as can be seen on the Figure 1. Uniform air flow passes both above and below the plate with velocity of 30 m/s. Urea – water spray is injected into the air stream above the plate and, depending on the local conditions there will or won't be wall film formation on the plate. Thermocouples are used to measure change in the plate temperature. We will note further on cases where there is film formation as "cold" and where there is no wall film as "hot".

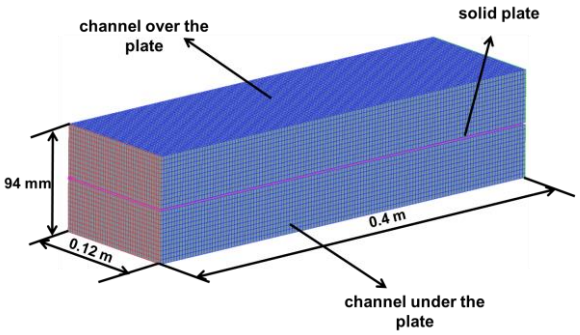

Figure 1. Mesh representation of computational domain

During the grid dependency simulations it was found that the uniform computational mesh consisting of 2 208

000 orthogonal cells with size of 1 mm produces sufficiently accurate results. For the simulation advanced k-zeta-f turbulence model was used [6]. Implicit time discretization scheme was used with time step size of 0.001 s.

Birkhold plate case - results

Figure 2. shows results of hot cases without thin wall module modifications. As it can be seen, previous approach is perfectly capable of describing the gradual cooling of the thin plate solely by convection.

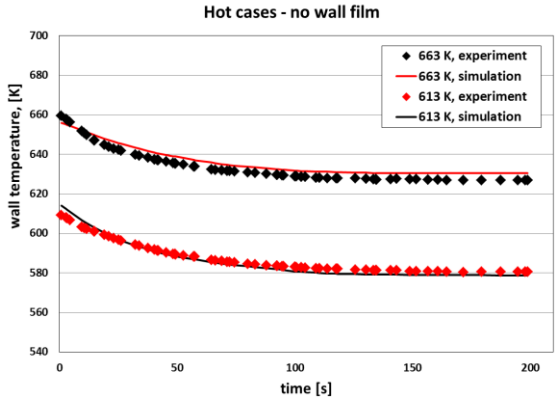

Figure 2: Plate cooling – hot cases

The same cannot be stated for the cold case in which wall film formation was observed. Liquid formed on the plate surface acts as generous heat sink and mono layer thin wall module is not capable to describe heat transfer properly which can be clearly seen as discrepancy from experimental measurements in the Figure 2.

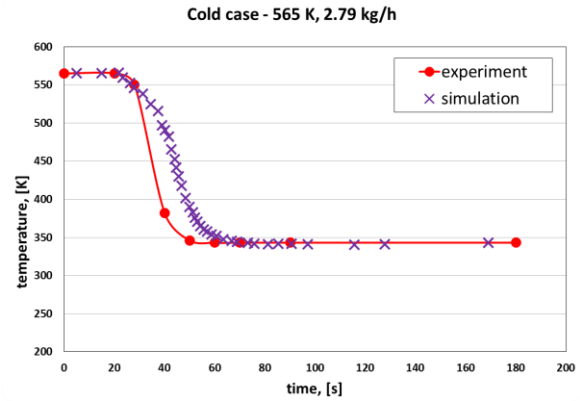

Figure 3: Plate cooling – cold case

One way to overcome this issue is using AVL Code Coupling Interface (ACCI) which enables simultaneous simulation of two domains which are connected through the common interface. After each time step, information is exchanged at the interface. This approach demands additional computational power and time for the information exchange and is therefore not suitable.

Figure 4 shows domain decomposition using developed multilayered thin wall module. It can be seen that we don't need two meshes as was the case with ACCI approach. Instead, we just make surface selection and define it as a thin wall. That way, only one equation is solved for the normal heat conduction, that way making valuable time and CPU savings.

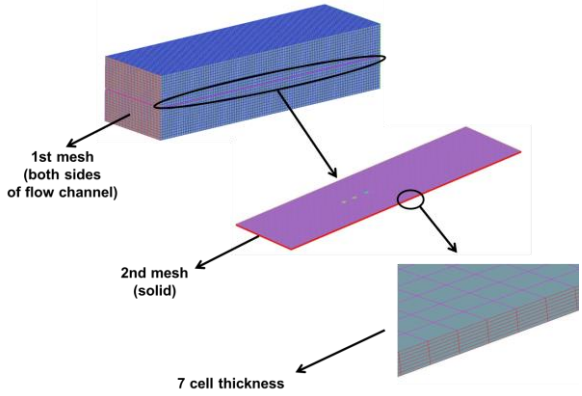

Figure 4: ACCI vs. new thin wall module

Finally, Figure 5 presents comparison of the new approach with experimental data from Birkhold which is now accurately describing plate cooling.

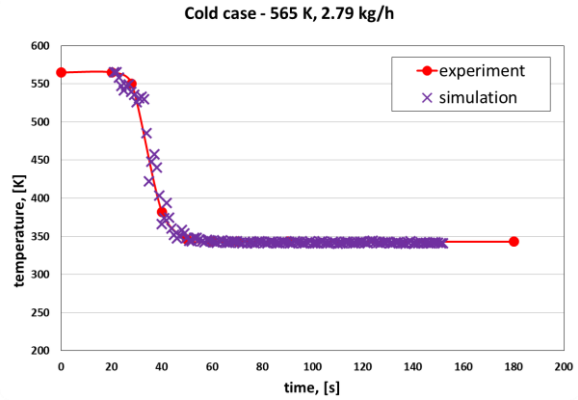

Figure 5: Plate cooling using new approach - cold case

Kim case – settings and results

Kim measured urea solution evaporation in hot exhaust gas to get values for NH_3 conversion rates [7]. Figure 6 shows scheme of experimental section with locations of sampling probes. Different distances from nozzle locations are used to calculate NH_3 conversion efficiency when quasi-steady state is reached.

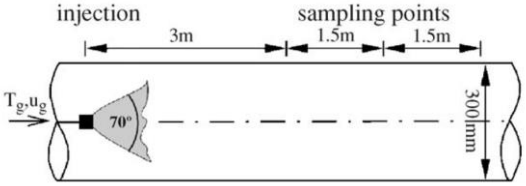

Figure 6: Schematic view of the experimental section from Kim

In Fire, an evaporation model for spray with parameters is given. The parameters E4 – activation energy and E5 frequency factor are steering thermolysis model for the droplet mass transfer whith respect NH_3 conversion rate. Figure 7 shows computational domain consisting of 65 452 hexahedral elements. Simulation settings regarding turbulence modelling and time

discretization remain the same and reader can refer to previous section for details.

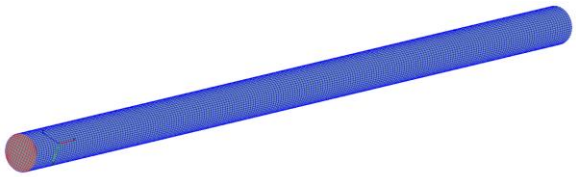

Figure 7: Kim case domain discretization

On the following figures there can be seen comparison between the old parameters, new parameters and experimental measurements from Kim. New parameters show better agreement with experiment in all cases compared to the old ones.

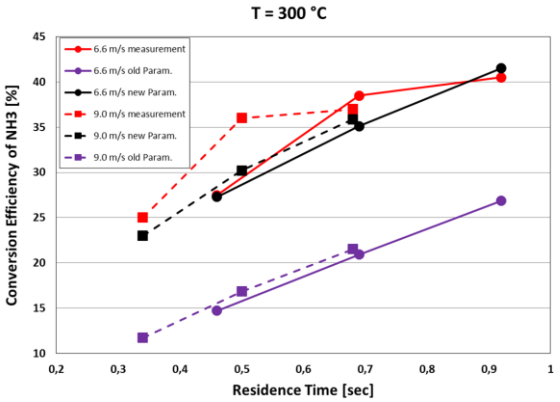

Figure 8: Comparison of results - Cases 1-3

Set of parameters, namely activation energy and frequency factor of Arrhenius equation, which was obtained by comparison of simulated results with experimental ones, yielded good agreement and was used for other cases in which exhaust gas mass flow and temperature were varied.

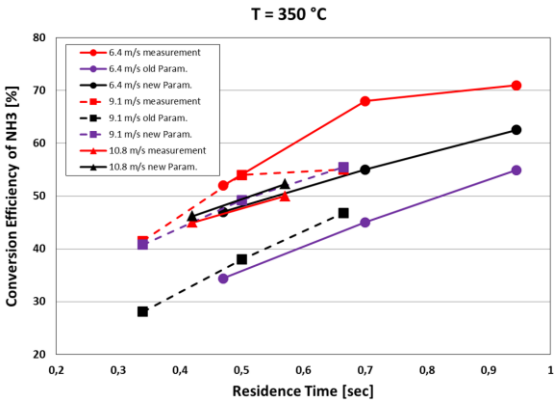

Figure 9: Comparison of results - Cases 4-6

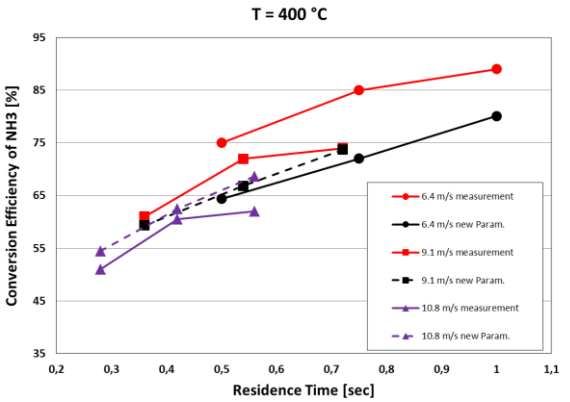

Figure 10: Comparison of results - Cases 6-9

Simulation of these cases predicted NH3 conversion efficiency with satisfactory matching with measured data. It can be concluded that new parameter show good results in range of u = 9 m/s of gas velocity.

Conclusions

After general introduction and presented details of mathematical models, including improvements in modeling of heat conduction and optimization of thermolysis parameters, two different simulation settings have been presented and described. Comparison with relevant experimental data yielded satisfactory agreement. Improved thin wall module now enables considerable savings in computational resources and/or time. Obtained optimized set of evaporation model constants favorable agreement with experimental results and gives confidence for commercial application of implemented CFD wall film module

The continuation of this work includes implementation of many new models in order to describe important phenomena such as: multicomponent evaporation of wall film, mechanism of urea deposits formation, interaction of spray with porous wall and catalyst inlet

Finally, this study concludes that mathematical models regarding spray/wall interactions and wall film formation integrated in Fire CFD code can be used as a valuable tool for the design and optimization of real mobile SCR systems.

Acknowledgements

The authors wish to thank the AVL List GmbH, Graz, Austria for the financing and opportunity to work on the research project. Authors would also wish to thank the CFD development group at AVL-AST, Graz, Austria, for their support and technical discussions during the model development.

References

[1] J.J. Klemeš, P.S. Varbanov, S. Pierucci, D. Huisingh, Minimising emissions and energy wastage by improved industrial processes and integration of renewable energy, J. Clean. Prod. 18 (2010) 843–847.

[2] H. Mikulčić, E. von Berg, M. Vujanović, P. Priesching, R. Tatschl, N. Duić, Numerical analysis of cement calciner fuel efficiency and pollutant emissions, Clean Technol. Environ. Policy. 15 (2013) 489–499. d
[3] H. Schlichting, K. Gersten, K. Gersten, Boundary-Layer Theory, 2000.
[4] AVL, FIRE ® VERSION 2013.2 manual, 2013.
[5] F. Birkhold, Selektive katalytische Reduktion von Stickoxiden in Kraftfahrzeugen : Untersuchung der Einspritzung von Harnstoffwasserlosung, Das Karlsruher Institut für Technologie (KIT), 2007.
[6] K. Hanjalić, M. Popovac, M. Hadžiabdić, A robust near-wall elliptic-relaxation eddy-viscosity turbulence model for CFD, Int. J. Heat Fluid Flow. 25 (2004) 1047–1051.
[7] J.Y. Kim, S.H. Ryu, J.S. Ha, Numerical Prediction on the Characteristics of Spray-Induced Mixing and Thermal Decomposition of Urea Solution in SCR System, in: ASME 2004 Intern. Combust. Engine Div. Fall Tech. Conf., ASME, 2004: pp. 165–170.