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ScienceDirect

Energy Procedia 82 (2015) 38 – 44

Energy Procedia

ATI 2015 - 70th Conference of the ATI Engineering Association

Modeling of Aqueous Urea Solution injection with characterization of spray-wall cooling effect and risk of onset of wall wetting

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Abstract

The definition of a sufficiently resolved heat transfer model with spray cooling effect as a function of each droplet kinetic and thermal parameters is a key factor in the numerical simulation of aqueous urea (AUS) based Selective Catalytic Reduction (SCR) exhaust after-treatment systems.

A consolidated spray-wall interaction model [1] has been implemented on the open source 3D finite volume software OpenFOAM and a critical investigation of its behaviour in engine representative conditions is reported.

A simplified test case is used to highlight the influence of the chosen model on the numerical simulation of the system, reducing the importance of the other spray sub-models in the Lagrangian-Eulerian computational framework. The coupling between the droplet evaporation heat flux and the gas-solid interface thermal boundary condition has been studied, pointing out the significance of each contribution.

The main focus of this work is to present reference conditions to simulate the spray-dry wall spray impingement behavior to determine the 'onset of wall wetting' thermal conditions.

Peer-review under responsibility of the Scientific Committee of ATI 2015

Keywords: Aqueous Urea Solution, Selective Catalytic Reduction, Heat Transfer, Computational Fluid Dyamics, OpenFOAM

1. Introduction

Controlling the NO_x emissions is surely a key aspect in the evolution and application of the Diesel engine in the automotive industry. The fulfillment of the brand new legislation needs a strong effort in understanding the phenomena involved in one of the most commonly accepted technologies for nitrogen oxides control: the injection of Aqueous Urea Solution (AUS) in the exhaust channels. Computational fluid dynamic plays an important role in the description of the phenomena and as an early design tool to increase

Peer-review under responsibility of the Scientific Committee of ATI 2015
doi:10.1016/j.egypro.2015.11.880

the efficiency of the systems. For practical applications, the Lagrangian-Eulerian modeling framework gives acceptable accuracy and affordable computational costs in the simulation of system-scale cases, as reported by [1], [2]. The focus of this work is put on the spray-wall kinetic and thermal interaction characterization to define a reliable base for the application of the models to real systems involving complex geometries and widely varying operating conditions.

2. Modelling

The numerical simulation campaign is carried out with the open source software OpenFOAM [3]. The liquid phase is solved according to the Discrete Droplet Model (DDM) by Dukowicz [4], which describes the spray by stochastic particles representative of identical, non-interacting droplets tracked through physical space in a Lagrangian manner. The coupling between the Eulerian and the Lagrangian phases is obtained through source terms applied in a non-iterative scheme and it involves the mass, momentum, specie and energy balances.

The solid phase is discretized and fully resolved with 3D finite volume approach.

2.1The System

A representative simplified test case is build up to reduce the influence of the Lagrangian phase sub-models in the results.

The key features of both the fluid phases are reported in Table 1.

As described by [5], a wide range of droplet sizes can be generated by low pressure injectors, mainly depending on their configuration – pressure driven or air assisted - so a constant diameter of 50 μm is chosen to represent an average spray drop.

A single parcel generator is put 15 mm above the impingement surface and injects 0.5 kg/h with constant flow rate profile and constant velocity equal to 20 m/s in the orthogonal direction to the wall surface. According to Spiteri [6] no strong deviation is experienced in the behavior of a UWS spray compared to a pure water one. Therefore, to avoid the solution of the urea chemical reactions, water is introduced in the system. The system is tested with a cross flow of 15 m/s, assuming fully developed velocity and temperature profiles. The injection direction is put both normal to the wall and with an angle of 45° relative to the cross flow direction to test the influence of the kinetic interaction effect in the wall cooling. Initial thermal equilibrium condition is supposed at 300° C and atmospheric pressure.

Table 1. Eulerian and Lagrangian phase setups

Eulerian Gaseous Phase		**Lagrangian Phase**	
Mixture	Air	Mixture	Pure Water
Turbulence Model	k-eps	Wall Interaction	Kuhnke + Wruck
Wall Functions	LowRe wall functions	Heat Transfer	Ranz Marshall
Eulerian Solid Phase		Secondary Breakup	none
Thermal capacity [J/m^{3}K]	480000	Collision	none
Thermal Cond. [W/m K]	15.1	Drag	Spheric Drag – no distorsion

2.2 Multi-region solver

The connection between the gas and solid Eulerian phases is realized by means of a mapped Conjugate Heat Transfer (CHT) boundary condition which equals both the temperatures and the heat fluxes at the interface. No momentum, mass and specie interactions are considered in the simulations.

2.3 Wall interaction Model

A strong interaction between the spray and the system walls cannot be avoided in the actual exhaust configurations because of the large mass of an average injected droplet, combined with the slow water evaporation and thermolysis of urea. The heat transfer between drops and wall can cool the solid surface below a critical temperature originating liquid film formation, increasing the risk of urea or its solid byproduct formation [7]. This work is focused on the analysis of the spray impact on dry surface, described according to the simplified approach proposed by [8], to identify the risk of onset of wall wetting. In particular, the focus will be the modeling of the thermal interaction, neglecting the contribution coming from the presence of multiphase contact interfaces or from eventual Marangoni effect

A dimensionless temperature is defined to describe the thermal behavior of the impact. Above a critical value, no liquid deposition on the wall is supposed.

$$T^* = \frac{T_{wall}}{T_{sat}}, \qquad T^*_{crit} = 1.1 \tag{1}$$

A combination of Laplace and Weber number is used in the kinetic energy description of the impinging droplet. Above a critical value defined with a uniform distribution between 20 and 40 a drop will atomize after the impact.

$$K = We^{5/8} La^{1/8} \qquad K_{crit,hot} = 20..40 \tag{2}$$

The critical value of K is defined from the normal component of the relative velocity between drop and wall because no influence of the impingement angle is reported in the definition of the model [8].

The impact of a droplet generates one or more secondary droplets - subscript 0 indicates the impinging drop, 1 indicates every ejected one - whose properties must be provided by the model according to semi-empirical correlations which involve mass, momentum and energy conservation by means of the description of:

- mass fraction ν_m
- size ratio γ_{10}
- velocity component magnitude, ejection β and deviation ψ angles

2.4 Hot wall detailed description

Two possible regimes, rebound and thermal breakup, are represented by the model. No liquid deposition is assumed in hot wall conditions, therefore ν_m is always unity.

In real systems the injected droplets usually perform a breakup interaction, so the pure rebound description is skipped. For every splashing event three secondary parcels are generated in the interaction according to [9], and each one´s size is defined by an inverse cumulative Weibull distribution around the average γ_{10} with shape parameter equal to 2. The total number of new droplets N_{tot} is determined according to mass conservation, assuming spherical shape.

The reduction of the normal component of the momentum of the splashed droplets is defined as a function of the impingement angle and introduced in the energy balance equation to extract the ejected drop Weber number,

$$We_{a,1} = \gamma_{i,10}\big(We_{a,0}(1 - \eta' sin^2\alpha) + 12\big) - \frac{12}{\nu_{32}} \tag{3}$$

assuming the ratio between Sauter Mean Diameter and geometric diameter

$$\nu_{32} = \frac{d_{32}}{d_{10}} = 2 \tag{4}$$

and an energy dissipation ratio as function of the impingement angle α

$$\eta = \eta' sin^2\alpha \qquad \eta' = 0.85 \tag{5}$$

The average ejection angle decreases with the increase of We and it is assumed proportional to α. For every secondary droplet a uniform distribution within a ±15° range around the mean value is assumed.

$$\beta_{avg} = \alpha \frac{86}{90} e^{-0.0045We_0} \tag{6}$$

For orthogonal impingement, the ejected drops leave the impingement point in random direction.
For smaller impingement angles, the trajectory deviation distribution is condensed at the leeward side [8].

2.5 Spray-Wall heat interaction

The implemented model based on the approach of Wruck[10], as suggested by Birkhold[1]. Wall and droplet are considered semi-infinite bodies exchanging energy through a contact area depending on the kinetic properties of the impinging event.

The heat exchanged by the droplet is defined as

$$Q_{w-d} = A_{cont} \frac{2\sqrt{t_{cont}}}{\sqrt{\pi}} \frac{b_w b_d}{b_w + b_d} (T_w - T_d) \tag{7}$$

where b_i is the thermal effusivity as [11] and A_{cont} is the drop contact area.

The maximum spreading diameter is calculated according to the results of Akao [12] as a function of the impinging droplet We.

The contact time is a function of the kinetic parameter K as reported below, where σ is the surface tension and *u* the velocity and the subscript *d* refers to the droplet properties:

$$t_{cont} = \begin{cases} \frac{\pi}{4}\sqrt{\left(\frac{\rho_d d_d^3}{\sigma_d}\right)} & K \leq 40 \\ \sqrt{\frac{\pi}{2}}\left(\frac{\rho_d d_d^5}{\sigma_d u_d^2}\right)_d^{0.25} & K > 40 \end{cases} \tag{8}$$

3. Results

The setup of the test case generates a stream of droplets that impinges always the same wall computational face, taking to the extreme level the wall cooling effect and pointing out the numerical behavior of the system. No influence of the injection direction is shown with the very simple velocity field tested. Therefore the following results refer only to the 45° droplets injection angle.

3.1 Application of the Conjugate Heat Transfer

The effect of the CHT between the gaseous phase and the wall has been tested, comparing the pure spray evaporation heat flux application with adiabatic interface and the fully coupled system. Starting from thermal equilibrium conditions, the effect of the impingement heat flux on the wall temperature is strongly dominant. Fig. 1 shows the temperature profile over the wall thickness in the condition of onset of liquid film formation for the fully coupled case. Only a slight shift in the values also for a wall face where no direct impingement happens. It means that the strong droplet momentum dissipation ejecting the secondary ones closer to the surface doesn't directly affect the wall cooling.

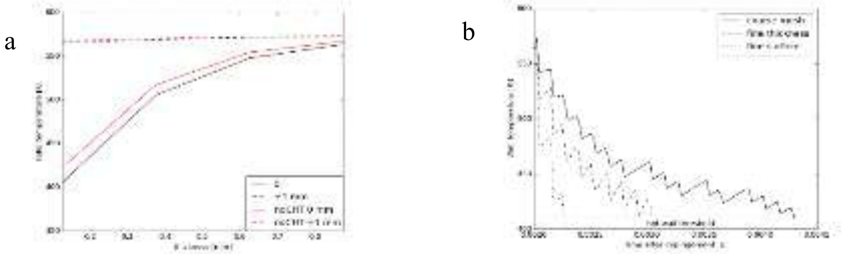

Fig.1. (a)Temperature profiles over wall thickness: effect of the Conjugate Heat Transfer on base mesh – spray cooled cell; (b) Temperature profiles over wall thickness: Effect of the Mesh Refinement

3.2 Grid Refinement effect

The simulation campaign included a solid mesh refinement analysis to estimate the effect of the heat source contribution applied in the first wall cell layer. The base mesh involves a 1 mm thick foil discretized into four uniform sized cell layers. The bottom boundary is adiabatic and each thermally coupled face has 1 mm^2 area. The spray evaporation heat flux is located always in the same cell with constant mass and frequency impingement events. The temperature profile generated along the solid thickness is much steeper than the one affecting the neighbor surface cells, which temperature profile is almost unaffected by the energy sink, as show in Fig.1a.

The time scale of the spray cooling effect is much smaller than the conduction heat flux one, and it is possible to notice that the effect of a grid refinement goes almost proportionally to the cold cell volume, independently from the mesh tightening direction. In Fig. 1b the temperature profiles are plotted against the time for two different refinement levels: half thickness – *fine thickness* - and half surface side – *fine surface*.

Fig. 2a shows the temperature profile along the foil increasing the grid refinement in the condition of onset of liquid film formation.

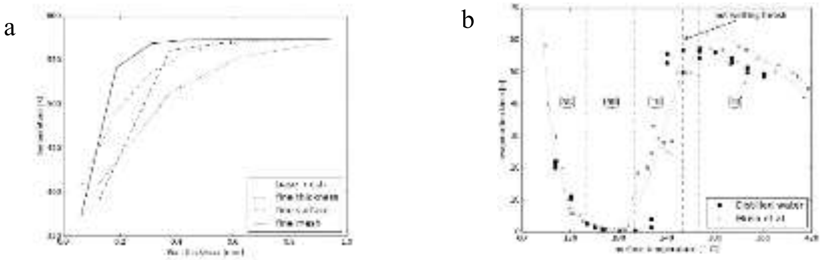

Fig.2. (a) Effect of the grid refinement on the temperature profile over the wall thickness; (b). Evaporation times of a 2.54 mm size water drop on a hot surface.

3.3 Thermal boiling model behavior

As visible in Fig 1a, the implemented spray heat transfer model is dependent on the temperature difference between droplets and wall surface, as was reported by [10] for film boiling conditions and superheated liquid isopropanol. According to [13] the wetting temperature threshold for a single water or aqueous urea solution droplet evaporation is lower than the Leidenfrost minimum heat flux point as shown in Fig. 2b. Therefore the straight application of this model till the onset of liquid film formation temperature can underestimate the heat flux at low temperatures.

4. Conclusion

The goal of the presented work has been to investigate the behavior of one of the most used spray-wall interaction model in the urea-SCR systems, especially in its thermal aspects. It has been shown that:

- The application of the Conjugate Heat Transfer boundary condition between solid and gaseous phases has a limited influence on the wall temperature profile. The fast temperature fluctuation in the fluid phase due to the presence of the droplets doesn't thermally affect the metal foil.
- The application of the heat flux as a volumetric source in the solid first cell layer is strongly affected by the grid refinement level. In terms of surface temperature, which is one of the parameters affecting also the kinetic interaction, a strong grid dependency has been shown.
- The temperature range of application of this model has to be corrected according to a more extended spray boiling regime analysis.

References

[1] Birkhold F., Meingast U., Wassermann P., Deutschmann O. *Analysis of the Injection of Urea-water-solution for automotive SCR DeNOx-Systems: Modeling of Two-phase Flow and Spray/Wall-Interaction*. SAE Technical Paper (2006). 2006-01-0643.

[2] Strom H. Lundstrom A. Andersson B. *Choice of urea-spray models in CFD simulations of urea-SCR systems.* Chemical Engineering Journal 150 (2009), 69-82.

[3] www.openfoam.org.

[4] Dukowicz J.K. *A Particle-Fluid Numerical Model for Liquid Sprays.* J. Comp. Physics, vol 35 (1980), 229-253.

[5] Lokyer T., Reid B., Hargrave G., Gaynor P. et al. *Optical investigation on the Ability of a Cordierite Substrate Mixing Device to Combat Deposits in SCR Dosing Systems.* SAE Technical Paper (2015), 2015-01-1039.

[6] Spiteri A., Dimopoulos Eggenschwiler P., *Experimental Fluid Dynamic Investigation of Urea-Water Sprays for Diesel Selective Catalytic Reduction-DeNOx Applications,* Industrial & Engineering Chemistry Research (2014) 53(8), 3047-3055.

[7] Fang H.L., DaCosta H.F.M. *Urea thermolysis and NOx reduction with and without SCR catalysts.* Applied Catalysis B: Environmental, 43 (2003), 17-34.

[8] Kuhnke D. *Spray/Wall-Interaction Modelling by Dimensionledd Data Analysis.* PhD thesis (2004).

[9] Stanton D.W., Rutland C.J., *Modeling Fuel Film Formation and Wall Interaction in Diesel Engines.* SAE Technical ºPaper (1996), 1996-02-0628.

[10] Wruck N.M., Renz U., *Transient Phase-Change of Droplets Impacting on a Hot Wall.* Transient Phenomena in Multiphase and Multicomponent Systems. (2000) Wiley-VCH Verlag GmbH. ISBN: 978-3-527-27149-8.

[11] Incropera F.P., De Witt D.P., *Fundamentals of Heat and Mass Transfer.* Wiley and Sons, 7th edition, 2011. ISBN: 978-0470-50197-9.

[12] Akao J., Araki K., Mori S., Moriyama A. *Deformation behaviors of a liquid droplet impinging onto hot metal surface.* Trans. Iron and Steel Insitute of Japan, 20 (1980), 737-743.

[13] Liao Y., Nocivelli L., Dimopoulos Eggenschwiler P., Spiteri A. *Experimental investigation of urea-water sprays in selective catalytic reduction (SCR) systems.* 15th Internationales Stuttgarter Symposium (2015), 953-966.

Biography

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