ANALYSIS OF INFLUENCE OF MODEL INPUT PARAMETERS ON ASH FOULING RATE PREDICTED BY CFD

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Abstract: *The study of particulate matter deposition on solid surfaces is an important subject for development of technologies for combustion of solid alternative fuels such as municipal solid waste (MSW). For this purpose, new experimental facility was build and available mathematical models of particulate matter fouling were examined. One of the two main parts of experimental facility is a deposition chamber, which became a subject to a subsequent simulations of initial stage of fouling process. We consider MSW as a testing fuel. A simple fouling model from group of critical velocity models was selected. Model parameter values were obtained from literature. Influence of variations of one of these parameters (reference diameter) on predicted deposition mass flux was studied. For considered size distribution the overall deposition mass flow shows only a little dependence on chosen reference diameter. Also simulation yielded the deposition chamber efficiency, showing ability to retain 15 % of overall particulate matter mass flux for considered size distribution.*

Keywords: MSW combustion, Ash fouling, Deposit formation, CFD, Particulate matter.

1. Introduction

One of the main problems in solid fuel combustion facilities is particulate matter fouling. This is true especially in the case of using solid alternative fuels, including very wide range of different materials and compared to the conventional fuels like coal, we have still relatively little experience from operation of large industrial facilities. The fouling prediction is strongly dependent on empirical data. Although most of individual mechanisms are known, the sufficiently accurate determination of particulate matter and surface properties and of the local conditions is necessary for correct evaluation of their influence. Computational Fluid Dynamics (CFD) has already been shown as very useful tool for fouling prediction.

Commonly, three main groups of fouling models are mentioned in literature (Cai et al., 2018). *Molten fraction models* estimate the sticking probability of a particle, as the name suggests, from the fraction of melted particle mass. Usually a non-zero melt fraction is assumed, until the particle is considered non- sticky and similarly the non- unit value, when the particle is able to rebound. *Critical viscosity models* relate sticking probability and particle viscosity. The probability usually increases with decrease in viscosity and from certain value is equal to one. *Critical velocity models* determine the sticking probability from energy or force balance during the particle impact.

Both the molten fraction and critical viscosity models are more empirically based compared to the group of critical velocity models using body contact mechanics. Each of those models to some extent requires the properties of particles, impacted surface and local conditions. Particle properties can be determined from fly or bottom ash analysis or it is possible to connect the fouling model to the combustion model and this case obtain required properties from predicted combustion conditions and fuel properties. The advantage of this approach is possibility of simulating the influence of fouling on the combustion process.

Fouling criterions used in molten fraction and critical viscosity models use empirical parameters and coefficients related to relatively narrow range of fuel compositions compared to solid alternative fuels like the Municipal Solid Waste (MSW). Critical velocity models use to some extent the ash or fly ash composition and properties of individual components and wall or deposit surface properties. However, these values can be with some uncertainty determined in advance. Additionally, those models consider

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particle impact velocity and deposit surface structure. In spite of difficulties in determination of some of mechanical properties necessary in many critical velocity models (Kær, 2001), we are going to use models from this group, offering possibility to consider large scale of physical and chemical processes.

2. Methods

A model described in (Wacławiak and Kalisz, 2012) was originally used for simulations of several tubes of superheater in pulverized coal boiler. They assumed gravitational force F_g and Van der Waals force F_{VW} to act on a particle. Authors supposed that the condensation of gaseous compounds is already finished and does not influence deposition in the superheater. In our case of fouling non-cooled walls, we considered only inertial transport to the walls. The sticking probability is given by following simple function

$$P = \begin{cases} 1, & F_{VW} + F_g \sin \theta \geq F_{el} \\ 0, & \end{cases},$$ (1)

where F_{el} is elastic force and θ angle between surface normal and gravitational force $\vec{F}_g$ actig on a particle. The Van der Waals force is given by Eq. (2), where d_p is the particle diameter.

$$F_{VW} = B \, d_p/(6 \, \delta^2)$$ (2)

Elastic rebound force is estimated using Eq. (3).

$$F_{el} = G \left(d_p/d_{ref} \right)^n d_p^2 \left| v_{i,n} \right|^{6/5}$$ (3)

Similarly to (Wacławiak and Kalisz, 2012) we used values $B = 10^{-17}$ and $\delta = d_p/2$ for Van der Waals force and $G = 1$ and $n = 2$ for elastic rebound force. We chose d_{ref} as a parameter to be examined.
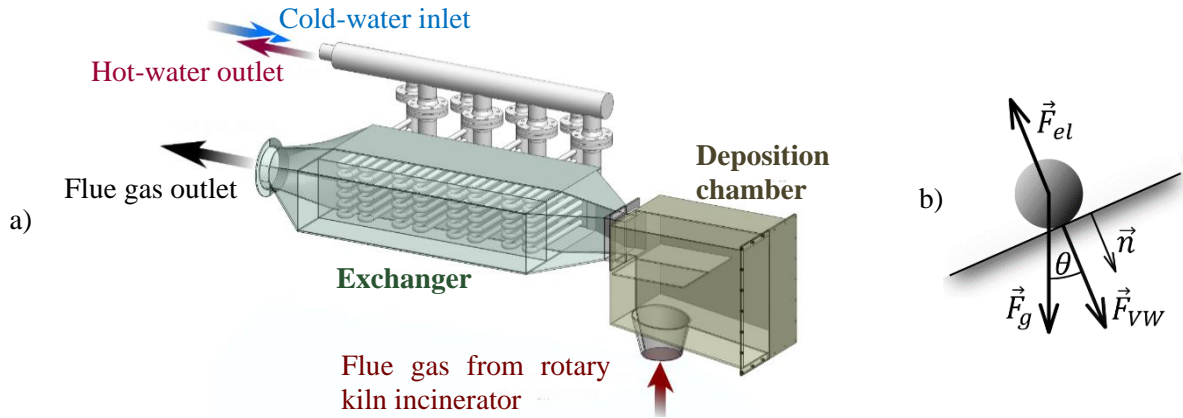

Fig. 1: a) Flue gas system scheme; b) forces considered in model of (Wacławiak and Kalisz, 2012).

In order to evaluate the influence of input parameters to deposit formation, a technological model able to simulate conditions in industrial facilities was designed. The model includes a rotary kiln incinerator for combustion of given test fuel and a flue gas system consisting of two main parts (see Fig. 1). The first part is a deposition chamber, which represents the mechanical part for PM retaining. It is made of welded metal sheets and equipped with demountable rear wall. The second part is a heat exchanger consisting of four modules, each containing a removable tube bundle. The design of the whole assembly enables good access and detailed measurements, providing information about fouling process. This information can be used for optimisation of industrial facilities with similar configuration as the model and for determination of boundary conditions in CFD simulations and validation of used methods and models.

3. Fouling model test

For this simulation test, we decided to use data from literature (Raclavská et al., 2017) describing MSW ash properties. While setting up the model parameters, we also decided to use different value of d_{ref} than (Wacławiak and Kalisz, 2012) considering different fuel and facility type. Instead, the average diameters were calculated for all 3 samples described in (Raclavská et al., 2017) and their arithmetic

average was set as a initial guess for d_{ref}. There were 6 ash size fractions described, with mean diameters 6, 14, 19.5, 28.5, 41.5 and 74.5 μm and also particles larger than 100 μm. As initial simulations shown (see Fig. 2), the largest particles were unable to enter the chamber and so the average diameter was estimated only from six smaller fractions, giving $d_{ref} = 17.53\ \mu m$. For this value we subsequently tested its variation ±50 %.The initial phase of deposit growth was examined assuming negligible influence of created deposit on deposition rates. The case solved as a steady state. We used as ANSYS® Fluent® for computing both the fluid flow and subsequently the particle trajectories as a post-process. Realizable k-ε model combined with Enhanced Wall Treatment was used for turbulent flow calculation. We used Discrete Phase Model (DPM) combined with Discrete Random Walk Model and Random Eddy Lifetime for particle tracking. The influence of particle on fluid flow was neglected.

At first, we tested 5 meshes with different boundary layer refinements. The mesh containing 588 677 cells was selected with average value of $y^+ \approx 1.7$ in the deposit chamber. Only 0.75 % of boundary cells had value $y^+ \geq 4$. We considered the minimum allowable cell height to be equal to the largest particle radius as it prevents unrealistic particle submersion under the wall surface. Only 0.5 % of total number of cells were below this value (e.g. 36.25 μm). The total deposition mass flow simulated on each of the five meshes varied no more than 7 % compared to the coarsest mesh. For surfaces with highest deposition mass flows, e.g. front and side walls, those differences were approximately 4 and 10 % compared to the coarsest mesh. These five simulations used value $d_{ref} = 17.53\ \mu m$.

Subsequently we used selected mesh for study of d_{ref} value influence on deposition flows on individual walls and for individual particle fractions. The deposition mass flow values are divided by the corresponding value for $d_{ref} = 17.53\ \mu m$. In Fig. 3 only the most significant surfaces are depicted. Deposition mass flows of particles with diameters 41.5 and 74.5 μm on these walls were zero or two orders of magnitude lower compared to other particle size fractions and so they are not reported.
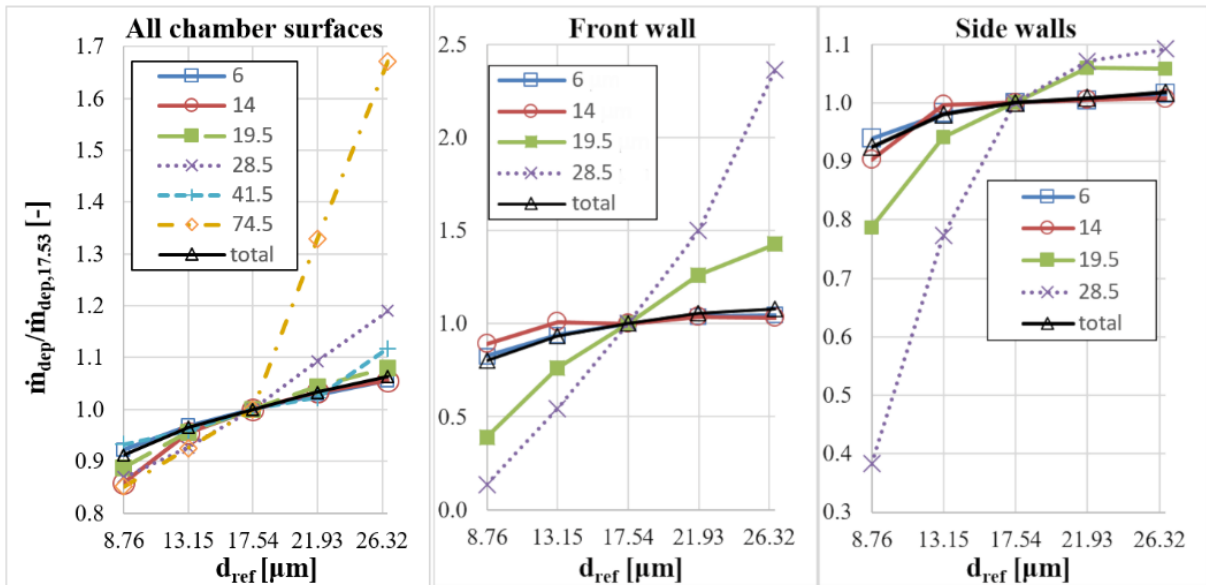

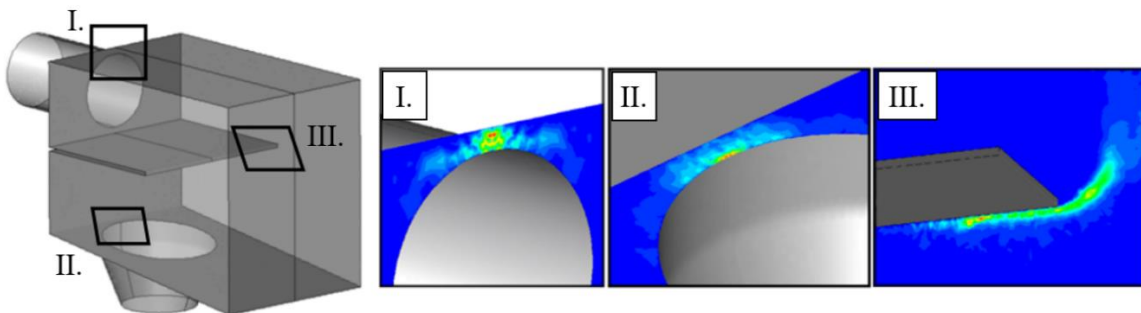*Fig. 2: Dependence of deposition flows of individual particle size fractions on reference diameter value.*

Fig. 3: Locations with high values of mass deposition flux for dref = 17.53 μm. Highest values are (I. – front wall) 2.29·10⁻², (II. - bottom) 3.85·10⁻³ and (III. – side wall) 5.67·10⁻³ kg·s⁻¹·m⁻².

By simple calculation we can obtain estimation of deposition chamber efficiency with respect to the particle diameter, as shown in Tab. 1. By efficiency we mean ratio of deposition mass flow to the particle mass inflow. Results shown that the chamber would be most efficient in case of fine particles, in contrary with original expectations.

Tab. 1: Deposition efficiencies for each particle diameter, d_{ref} = 17.53 μm.

Particle diameter [μm]	6	14	19.5	28.5	41.5	74.5	Total
Mass inflow [mg/s]	152.223	25.305	26.017	28.512	29.402	42.752	304.211
Deposited mass flow [mg/s]	36.164	4.626	3.843	1.072	0.249	0.147	46.102
Deposition efficiency [%]	**23.76**	**18.28**	**14.77**	**3.76**	**0.85**	**0.34**	**15.15**

4. Conclusions

Comparison of five meshes showed relatively low dependence of total predicted deposited mass on the number of cells in the boundary layer (approximately 5 % maximum difference compared to coarsest mesh). All the meshes showed that from considered particle size fractions only the 74.5 μm and smaller are able to reach the deposition chamber. The mesh selection for tests of reference diameter value was based on values of y^+ and on the fraction of boundary cells with height lower than maximum particle diameter, i.e. 74.5 μm.

The influence of the reference diameter value was tested for each of six particle diameters, assuming negligible dependence of deposition rate on the created deposit. The 50 % increase (or decrease) of d_{ref} value resulted only in 6 % increase (or 9 % decrease) of overall deposition rate and with increasing d_{ref} this dependence gets smaller. However, this dependence is much stronger for larger particles and the expected dependence would be much more significant in case of higher concentrations of coarser particles.

Performed simulations show seemingly reasonable results for local deposition fluxes. Oncoming experimental tests on the described technological model will be the next important step in a process of development of more sophisticated models of particulate matter fouling. When those conducted, it will be possible to verify values of the reference diameter and other four parameters in the fouling model used in for this work.

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