

USING FLUENT CODE TO PREDICT DEPOSITION DURING COMBUSTION OF SOLID FUELS

K. Waclawiak¹ and S. Kalisz²

¹ Department of Metallurgy, Silesian University of Technology, ul.Krasinskiego 8, 40-019 Katowice, Poland,
krzysztof.waclawiak@polsl.pl (Corresponding author)

² Institute of Power Engineering and Turbomachinery, Silesian University of Technology, ul.Konarskiego 20, 44-100 Gliwice, Poland

ABSTRACT

Different mechanisms describe formation of deposits, depending on thermal and flow conditions in boilers. Deposit shape and height depend on arrangement of the tubes in superheaters too. There are several kinds of deposits found in boilers firing solid fuels. In case of powdery deposition the balance of forces acting on a particle of ash impacting onto boiler superheater tubes determines if the particle bounces off the surface or stays there building the powdery deposit. On contrary, one of possible mechanisms describing formation of bonded deposit is that gaseous salts of sodium and potassium condense from flue gas onto heat exchange surfaces and produce a sticky layer capturing impacting particles of ash, so called "wet impaction". The build-up of bonded deposits is further enhanced by plastic ash particles which stick to the surface on impact.

The paper presents examples of numerical, two-dimensional modeling of the above mentioned deposit kinds on heater tubes. The deposition process can be modeled with use of Fluent dynamic mesh option. This feature allows a user to move the grid vertices independently, simulating deposit formation. This way continuous calculations are possible. Formation mechanisms of these kinds of deposits and all modifications to temperature of the tube surface and its shape were performed using User Defined Files. DEFINE_DPM_EROSION procedure defines deposition flux by using mass flow rate of ash particles, area of the face being hit by the particles, and an angle of impaction. Taking into account time and deposit density one can calculate the growth of the deposit. This leads to shift of the vertices of each face of the tube hit by ash particles in DEFINE_GRID_MOTION procedure. Since formation of deposits insulates the tube, the new surface temperature is worked out and continuously modified in the DEFINE_PROFILE procedure.

INTRODUCTION

Deposits found in power boilers are formed during combustion of practically all solid fuels. The source of

deposit formation in boilers is the presence of mineral matter in the fuel. Mineral substance undergoes physical and chemical processes producing particles of ash and volatile gases which mix with the flue gas. The volatiles may condense either heterogeneously or homogeneously along boiler ducts. Ash particles floating in the flue gas strike heat exchange surfaces. Steam heaters in power boilers are covered either with powdery deposits, loosely staying on the surface, or bonded ones, stuck firmly on the surface. Spacing of boiler tube banks influences the velocity field of the flue gas and trajectories of ash particles. Typically the tube arrangements of in-line tube banks are kept in the range of $s_1/d_i=1.5-2$ and $s_2/d_i=1.5-3$ for convective, or $s_1/d_i=5-10$ and $s_2/d_i=1.05-1.1$ for radiant superheaters (Orłowski et al., 1979). Ash particle size distribution ranges from a few microns up to 200 μm . Because of this size range, inertia is the major phenomenon influencing trajectories of ash particles. In case of the smallest grains turbulent dispersion must be considered to mirror their trajectories. Typical velocity range within superheater bundles is 5-15 m/s. Typical temperature of flue gas in this area varies from 500 to 1000°C. All these highly variable features must be modeled accordingly since they constitute quite different conditions resulting in various history of deposits formation. Practical observations indicate that powdery deposit are formed by particles smaller than 30 microns, while bonded deposits may also include large particles in the form of matrix filled with small particles (Laursen and Frandsen, 1999).

MODELING OF DEPOSITION ON SUPERHEATERS IN COAL-FIRED BOILERS

Constant progress in numerical methods results in wide range of utility applications including computational fluid dynamics (CFD) codes, such as Fluent, solving thermal and flow issues. This computational tool may be also applied for predicting fouling phenomena occurring at heating surfaces of power boilers. Some examples of using Fluent code for this purpose can be found in publications (Huang et al., 1996), (Yilmaz and Cliffe, 2000), (Kaer et al., 2005), (Tomeczek and Waclawiak, 2009). This work presents a summary of two-dimensional CFD modeling of deposition

of various kinds. Slagging and fouling are complex phenomena. The shape of deposit, its composition and deposition rate are influenced by a number of factors and the major influence is associated with composition and particle size distribution of original mineral matter in the fuel as well as the gasdynamic and thermal conditions in the flue gas duct.

Although it is unlikely to describe precisely all kinds of deposition mechanisms, some attempts can be made. In this paper 3 formation mechanisms were analyzed contributing to build up of powdery (loose) and bonded deposits. In the latter case either by condensing salts or by plastic (sticky) ash particles.

The basic equation (Eq. 1) for each deposition flux includes mass flow rate \dot{m}_p of particulate matter striking the deposition surface A and the angle of impaction γ

$$\dot{m}_{f,A} = P_f \frac{d\dot{m}_p}{dA} \sin(\gamma) \quad (1)$$

The real superheater is a tube bank composed of several tube rows. Nevertheless, in order to shorten the computational time, the mesh shown in Fig. 1 has been prepared. The mesh is a simplified 3-tube representation of an in-line (parallel) real tube bank array. Such a size limitation is sufficient for quantitative and qualitative modeling of fouling at all sides of tubes in the bank, nevertheless the flow direction. It must be stressed that the mesh allows for the study of the influence of neighboring tube rows. For instance, it is possible to study the trajectories of particles rebounding from the neighboring tube rows. In case of power boilers where the deposit is in macro scale, with its height of up to tens centimeters and is built with majority of grains of more than 10-20 μm in diameter, the inertia plays the major role in particle transport, so the mesh can have larger cells. Especially, because of the dynamic mesh option, the cells should be larger in order to avoid the "negative volume error".

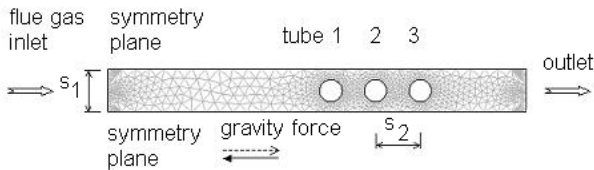


Fig. 1. Mesh for modeled in-line super heater tube bank.

Powdery deposits

Regarding powdery, loose deposits it is assumed that deposition is governed by inertial impaction and subsequent capture of certain fraction of particles at the deposition surface (Fig. 2). In contrast to "wet impaction" it could be called "dry impaction".

The capture condition is a fulfillment of a vectorial equation of forces affecting the particle on impact (Eq. 2). These forces are the normal elastic rebound force $F_{s,n}$, Van

der Waals adhesion force F_{vw} and normal component of gravity F_G

$$F_{s,n} \vec{\leq} (\vec{F}_{vw} + \vec{F}_G) \quad (2)$$

The gravity force may enhance or hinder the particle capture depending on the flue gas flow direction. For the specific case of powdery deposits the probability of deposition P_f has been calculated upon the following assumptions:

$$P_f = \begin{cases} 0, & \text{if } (F_{S,n} > (F_{VW} \pm F_{G,n})) \\ 1, & \text{if } (F_{S,n} \leq (F_{VW} \pm F_{G,n})) \end{cases} \quad (3)$$

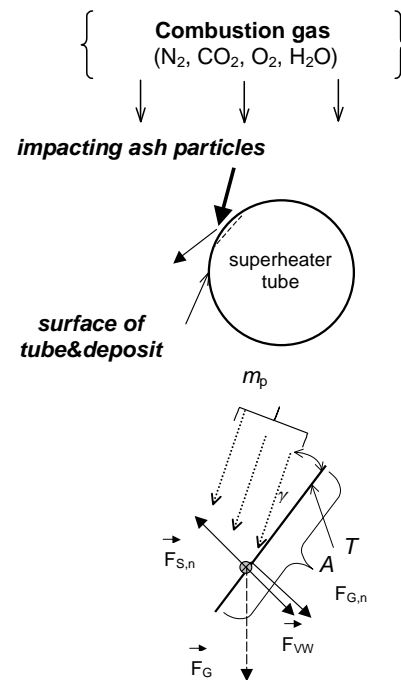


Fig. 2. A schematic view of the powdery deposition.

Equations of forces needed for calculating probability P_f have been taken after an author of a book in Russian (Tekenov, 1985). The author explains that in a zone of contact between grain and surface some microscopic deformation takes place which results in reaction called a rebounding force. The equations were cited later in a publication (Pronobis, 1986) together with further considerations on fouling. The normal elastic rebound force is given as

$$F_{S,n} = Kd_p^2 w_p^{1,2} \quad (4)$$

where: K is a proportionality constant depending on elasticity of particle and deposition surface.

In order to obey the relationship $F_s < F_g$ for smaller particles and $F_s > F_g$ for larger particles, an effort has been

made to develop an own approach linking constant K with particle diameter d_p in the following form

$$K(d_p) = G \left(\frac{d_p}{d_{ref}} \right)^n \quad (5)$$

where: G is a constant, d_{ref} is a reference diameter and n is an exponent, which should be assumed and tested in the course of computational runs to verify their correctness in predicting the deposit height.

The Van der Waals force is calculated upon

$$F_{VW} = \frac{Bd_p}{6\delta^2} \quad (6)$$

where: B is a molecular interaction constant and δ is a distance between particle and deposition surface.

The gravity force affecting particle is given by

$$F_G = \frac{1}{6} \pi d_p^3 \rho_p g \quad (7)$$

where: g is gravitational acceleration.

In another paper (Bouris and Bergeles, 1996) a similar approach describing deposit formation by the impact-adhesion model is presented, this time using the energy balance at the point of impaction and consider the material properties of the particle and surface.

Formation of loose deposits requires only major flue gas constituents to be considered (vol.%): $\text{CO}_2=13.6$, $\text{O}_2=4.7$, $\text{H}_2\text{O}=10.0$, rest N_2 . The velocity of flue gas has been 7 m/s and its temperature in the range of 500-550 C. The concentration of fly ash in the flue gas ranged from 6 to 8 g/m^3 . The initial velocity of particles was equal to flue gas velocity.

From results reported by Kalisz and Pronobis (2005), the steam reheater was chosen for modeling. It is an in-line arranged heating surface composed of $d_t=51$ mm horizontally aligned tubes, with transverse and longitudinal pitches $s_1/d_t=1.68$ and $s_2/d_t=1.49$. The particle-laden flue gas flows downwards following the gravity force direction. The deposit height measurement was carried out at the upwind side of the first, upper tube in the bank. The maximum height was reported to be 12 mm after about 32 hours of deposition. For numerical prediction of fouling the assumptions were made: flue gas temperature 550°C and the surface temperature 440°C. In order to produce the expected deposit growth, in Eq. (5) describing constant K in the elastic rebound force, the reference particle diameter was set as $d_{ref}=20 \mu\text{m}$, the exponent $n=2$ and $G=1$. The modeling results are shown in Fig. 3, i.e. the shape and the progress of fouling.

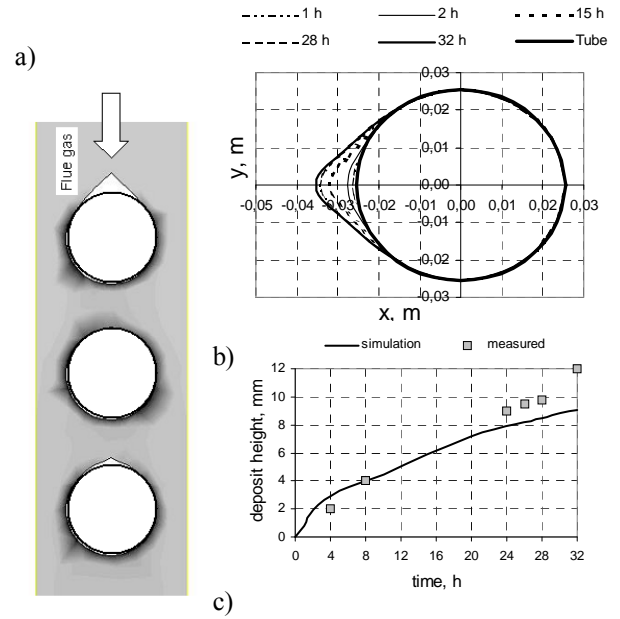


Fig. 3. Shape of predicted deposit on the steam reheater tubes of the modeled boiler after 32 hours of operation (a), change of the shape (b) and deposit height (c) on the first tube vs. time of operation.

Bonded deposits - plastic ash particles mechanism

In case of deposits made from plastic, soft ash particles, efficiency of deposition P_f of particles on a surface of tubes depends only on their temperature and is given by Eq. (8)

$$P_f = \begin{cases} 1, & \text{for } T_p \geq T_{softening} \\ 0, & \text{for } T_p < T_{softening} \end{cases} \quad (8)$$

where: $T_{softening}$ can be computed by correlations presented by Seggiani and Pannocchia (2003) or measured by standard or new (Wall et.al, 1998) methods.

A schematic view of proposed mechanism used in the modeling is presented in Fig. 4. Basic mechanism describing formation of plastic ash deposits is inertia. Ash particles move close to the tube surface, strike it and stick forming deposit there. Crucial factor in this mechanism is temperature of ash particles.

In modeling of deposition of soft, plastic ash particles the flue gas consists of 4 compounds (% vol.): $\text{CO}_2=14$, $\text{O}_2=5$, $\text{H}_2\text{O}=10$, N_2 (rest). Flue gas and ash particles velocity is 10 m/s. Gas and ash temperature is 1300°C, and it was assumed that the ash particles are plastic and perfectly (i.e. all) stick to the surface if only the threshold temperature is exceeded. Ash concentration in the flue gas is 6 g/m^3 , particle size distribution obeying Rosin-Rammler equation is characterized by $d_{min}=5 \mu\text{m}$, $d_{mean}=40 \mu\text{m}$, $d_{max}=200 \mu\text{m}$, and polydispersion parameter $n=0.8$. Temperature of the tube surface is 527°C. Calculations were done for a recurrent 3-tube section of platen superheater with tube arrangement described by relative pitches $s_1/d_t=5$, and $s_2/d_t=1.2$. Tube diameter was 38 mm.

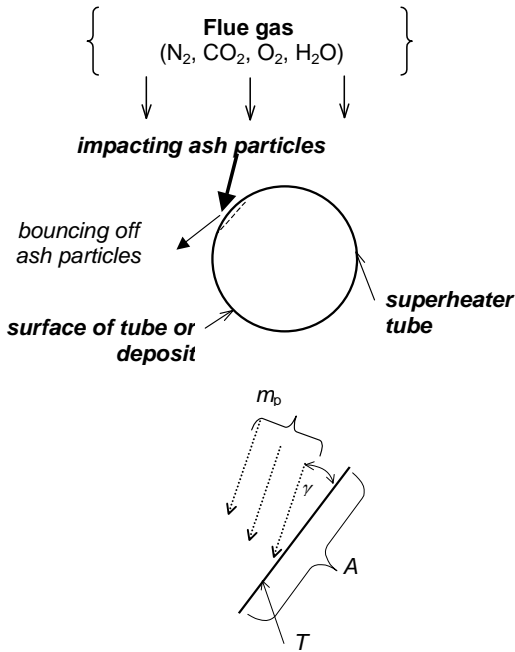


Fig. 4. A schematic view of deposition mechanism from plastic ash particles.

During the modeling it was assumed that the forming deposit had a high apparent density of 2200 kg/m^3 . An example of the simulations is shown in Figs. 5 and 6, where the deposit on the first tube grew to nearly 74 mm after 5 h of simulated operation.

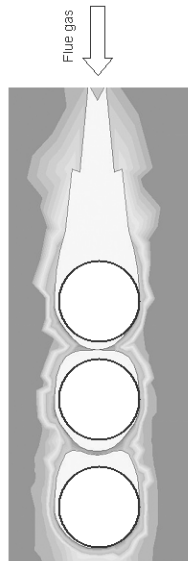


Fig. 5. Shape of predicted bonded deposit formed by plastic ash particles on the superheater tubes after 5 hours of operation.

As it can be seen in Fig. 5 in few hours, it is pretty close to a moment when the space between the tubes is filled up with the ash particles. The change of the shape leads to a change in temperature of the surface, which is shown in Fig. 7, where faces of the periphery are counted from the right, rear spot, from 1 to 30 clockwise. This kind of deposit grows the fastest, because all the particles build it up.

More on this simulations can be found in (Waclawiak and Kalisz, 2010).

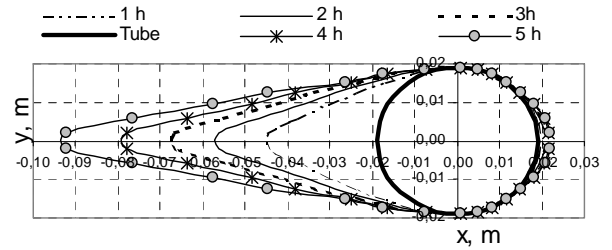


Fig. 6. Shape of predicted deposit on the first superheater tube vs. time of operation.

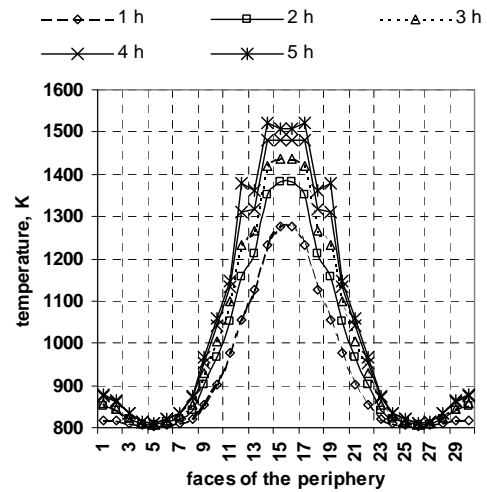


Fig. 7. Predicted surface temperature of deposit on the first superheater tube vs. time of operation.

Bonded deposits - condensation mechanism

In a paper by Tomeczek et.al (2004) one of possible mechanisms explaining how bonded deposits are created was presented. Authors assumed that as the flue gas cools down flowing through superheaters, the condensing salts (KCl , NaCl , K_2SO_4 , Na_2SO_4) diffuse towards the tube surface and condense there. This creates conditions for the solid ash particles to deposit. The particles approaching the surface may rebound or stick to it, forming deposit. The presence of a sticky layer, formed by condensed vapors, is required for the solid particles to stay on the surface (Fig. 8). As the deposit grows, its temperature increases, slowing the condensation process. This eventually terminates the deposition process. In case of bonded deposits the probability of the solid particles to remain on the surface P_f is proportional to the flux of condensing vapors:

$$P_f = S \dot{m}_{c,A}, \quad (9)$$

where constant S must be estimated on basis of final deposit size formed on a single superheater tube as shown by Tomeczek et.al. (2004). It could be computed by approach similar to “wet impaction”. However, it is not straightforward. In reality the condensing salts produce a layer which cannot grow thick, because of the gravity, tube

shape, influence of the flue gas, so the thickness of the layer is unknown. Moreover, when the deposit begins growing the surface conditions are not defined in the way as they are defined during laboratory experiments. Also the ash particles having jumped off the surface are partially wetted, so the conditions for next impactions will change as well.

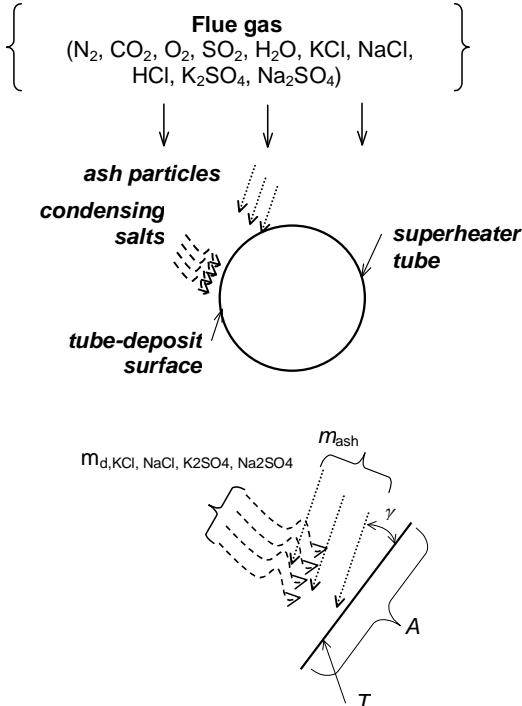


Fig. 8. A schematic view of deposition with the condensation phenomenon.

The flux of condensable gaseous i -th component of partial pressure p_i , diffusing through the tube boundary layer towards the surface area and condensing later on it can be calculated by equation

$$\dot{m}_{c,A,i} = \beta_i \frac{p_i - p_{s,i}}{p} \rho_g, \quad (10)$$

where: $p_{s,i}$ - saturation pressure of i -th component, p - flue gas pressure, and β_i - mass transfer coefficient of i -th component, calculated using the Sherwood number, diffusion coefficient D_i and tube diameter d_t , where:

$$\beta_i = ShD_i / d_t. \quad (11)$$

Surface temperature is calculated from known heat flux to the surface and assumed deposit heat transfer coefficient. Pressure p_i in Eq. (9) must be taken for the gas stream outside the boundary layer of the tube. The saturation pressure for the potassium and sodium salts was calculated by formula

$$p_{s,i} = p_n \exp(A_i - B_i / (T + C_i)), \quad (12)$$

where the A_i , B_i , C_i constants are given in Tomeczek and Waclawiak (2009) and $p_n = 10^5$ Pa.

In order to test this model in a two-dimensional geometry 10 gaseous compounds of flue gas were considered (vol.): $CO_2=13.6\%$, $O_2=4.7\%$, $H_2O=10\%$, $SO_2=500$ ppm, $K_2SO_4=3.5$ ppm, $Na_2SO_4=1$ ppm,

$KCl=18$ ppm, $NaCl=15$ ppm, $HCl=9$ ppm, rest N_2 ; inlet velocity for flue gas and ash particles- 8 m/s; inlet temperature of the flue gas and ash particles $1000^\circ C$, temperature of tube surface- $527^\circ C$; ash particles size distribution by Rosin-Rammler: minimum diameter- 1 μm , maximum diameter 200 μm , mean diameter 40 μm , and polydispersion parameter 0.80; deposit density 850 kg/m^3 ; deposit heat transfer coefficient $1.0 \text{ W/m}^2 \text{ K}$; ash concentration in the flue gas 2 g/m^3 . Basically, the shape of the deposits is similar to that shown in Fig. 5. To improve this model it is required to find out more precise data on true contents of the alkali salts in the flue gas and deposit growth in shorter periods of boiler operation.

SOME ASPECTS OF USING FLUENT CODE

The Fluent itself does not include deposition model. Only the Discrete Phase panel let a user compute in postprocessing the Accretion/Erosion rate which is in case of accretion, simply the flux of the solid matter striking the surface of any obstacles. However the deposition (accretion) rate can be modified by DEFINE_DPM_EROSION, which is a user defined file available for the code.

The trajectories of ash particles are solved by Fluent code in a Lagrangian approach including inertia, hydrodynamic drag, the force of gravity and optionally other forces like thermophoretic, Brownian, Saffman's lift. In order to predict trajectories of small particles it is possible to include the dispersion of the particles because of the turbulence. It can be done by means of Discrete Random Walk model or "particle cloud" tracking.

The deposit growth can be modeled with Fluent dynamic mesh option. This feature allows the user to change, move the grid vertices independently, simulating formation of the deposits. This change makes continuous calculations possible, however the movement in one step must be restricted and the changing face cannot overlap the neighboring face (Fig. 9), otherwise an error- "negative volume", terminating the calculations occurs. Basically the movements are independent although a vertex drags two faces while moving. Because of the movement the most suitable grid for this kind of modeling seems to be a grid with triangles (Fig. 1). Nevertheless, possible drawbacks are lower accuracy for solving thermal and flow issues. Each described mechanism of deposition is modeled with DEFINE_DPM_EROSION procedure, where the Eq. (1) is implemented. This most important procedure defines deposition flux by using mass flowrate of ash particles, area of the face being hit by the particles, and an angle of impaction. Upon assumption of time and deposit density one can calculate the growth of the deposit for each face hit by the particles. This leads to a shift of the vertices of each face in DEFINE_GRID_MOTION procedure. In some models the surface temperature may be crucial, for instance for bonded deposits described by condensation mechanism. For all models the temperature is required to compute heat transferred from the flue gas to the steam or water in the tubes. The forming deposit insulates the tube, so the new surface temperature is worked out and modified in the procedure DEFINE_PROFILE.

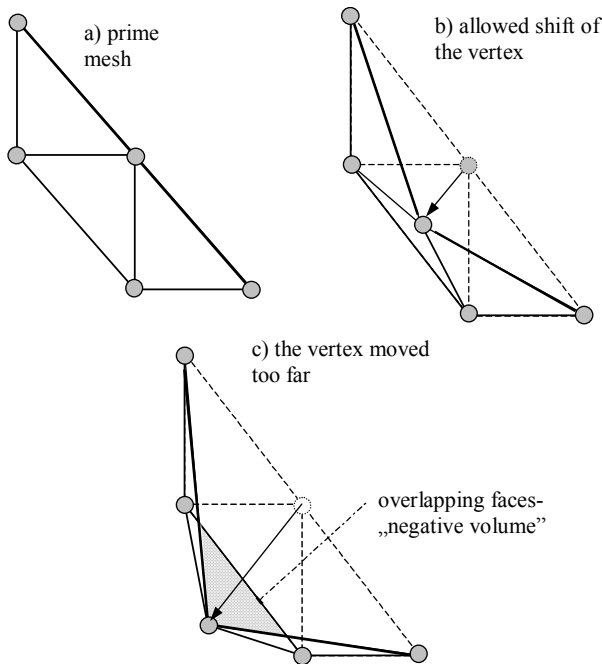


Fig. 9. Allowed and incorrect movement of face vertices.

CONCLUSIONS

This work is a survey on modeling deposit formation with use of 3 deposition mechanisms. The modeling is aiming at improving the thermal and flow calculations of steam heaters in boilers. Currently there are rare examples of predicting the shape of deposits on steam heater tube bundles in power boilers. The development of numerical methods and the availability of CFDs programs are a chance to obtain answers on optimal spacing of tubes in superheaters, flow velocities, particle size distribution of ash, gas composition so as the formation of deposits during boiler operation is properly controlled. The basic feature of the Fluent software which makes prediction of deposit formation possible is dynamic mesh, that is, possibility to change the position of the vertices at the grid during computing. Nevertheless, this feature sometimes lead to “negative volume error”, as a vertex is moved too far and overlaps any side face.

The following modeling approaches are proposed in present work:

1. In the case of powdery deposit equations of elastic rebound, adhesion and gravity forces were considered. Balance of these forces determines whether ash particle remains on the surface and builds the deposit or bounces off at the time of impact.
2. For deposits from plastic ash particles the characteristic ash fusion temperatures can be used to determine if the particles stick to or jump off the surface.
3. In the case of deposits bonded by condensing alkali salts, condensation of potassium and sodium salts is proposed as one of possible mechanisms describing their formation. Such deposit forms a sticky layer producing the binder to the impacting ash particles.

NOMENCLATURE

A	area, m^2
d	diameter, m
D	diffusion coefficient of i -th gaseous component through flue gas, m^2/s
$F_{s,n}$	normal elastic rebound force, N
F_{vw}	Van der Waals adhesion force, N
F_G	gravity force, N
\dot{m}	mass flux, $kg/s\ m^2$
p	pressure, Pa
P_f	deposition probability, dimensionless
s_1, s_2	transverse, longitudinal pitch of tube bundle, m
Sh	Sherwood number, dimensionless
T	temperature, K
w	perpendicular component of impaction velocity, m/s
β	mass transfer coefficient, m/s
γ	angle of impaction, $^\circ$
ρ	density, kg/m^3

Subscript

A -	area
c	condensing
f	fouling
g	gas
i	i -th component
n	normal
p	ash particle
ref	reference
s	saturation
t	tube

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REFERENCES

- Bouris D., Bergeles G., 1996, Particle-surface interactions in heat exchanger fouling, *Journal of Fluid Engineering*, Vol. 118, pp.574-581.
- Huang L.Y., Norman J.S., Pourkashanian M., Williams A., 1996, Prediction of ash deposition on superheater tubes from pulverized coal combustion, *Fuel*, Vol. 75, No. 3, pp.271-279.
- Kaer S.K., Rosendhal L.A., Baxter L.L., 2005, Towards a CFD based mechanistic deposit formation model for straw-fired boilers, *Fuel*, Vol. 85, pp.833-848.
- Kalisz S., Pronobis M., 2005, Investigations on fouling rate in convective bundles of coal-fired boilers in relation to optimization of sootblower operation, *Fuel*, Vol. 84, pp. 927-937.
- Laursen K., Frandsen F.J., 1999, Classification System for Ash Deposits based on SEM Analysis, in *Impact of Mineral Impurities in Solid Fuel Combustion*, eds R.P. Gupta et al., Kluwer Academic/Plenum Publishers, New York, pp. 205-216.

Orłowski P., Dobrzański W., Szwarc E., 1979, *Kotły parowe*, WNT, Warszawa, (in Polish).

Pronobis M., 1986, *Weitere Erkenntnisse zum Einfluß der Verschmutzung auf den Wärmeaustausch in Konvektiven Kesselrohrbündeln*, VGB Kraftwerkstechnik.

Seggiani M., Pannocchia G., 2003, Prediction of coal ash thermal properties using partial least-squares regression, *Ind.Eng. Chem. Res.*, Vol. 42 (20), pp. 4919-4926.

Tomeczek J., Palugniok H., Ochman J., 2004, Modelling of deposits formation on heating tubes in pulverized coal boilers, *Fuel*, Vol. 83, pp.213-221.

Tomeczek J., Waclawiak K., 2009, Two-dimensional modelling of deposits formation on platen superheaters in pulverized coal boilers, *Fuel*, Vol. 88, pp. 1466-1471.

Waclawiak K., Kalisz S., 2010, Practical aspects of modeling of deposit formation from sticky ash particles at in-line superheater bundles, *Rynek Energii*, Vol. 6(91), pp.129-134.

Wall T.F., Creelman R.A., Gupta R.P., Gupta S.K., Coin C., Lowe A., 1998, Coal ash fusion temperatures-new characterization techniques, and implications for slagging and fouling, *Prog.Energy Combust. Sci.*, Vol. 24, pp.345-353.

Yilmaz S., Cliffe K.R., 2000, Particle deposition simulation using the CFD code FLUENT, *Journal of Institute of Energy*, Vol. 73, pp.65-68.

Текенов Ж.Т., 1985, *Адгезия пылевидных материалов*, Издательство “ИЛИМ”, Фрунзе, (in Russian).