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Optimisation of Thermal Waste Treatment Plant Operation by Means of CFD-Modelling

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Optimisation of thermal waste treatment plant operation by means of CFD-modelling

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Abstract

The basic principles of the mathematical modelling for thermal waste incineration plants are indicated. For this application slagging, fouling and corrosion are of major interest. In this context, a model for the thermodynamic behaviour of ash particles is shown and tested for brown coal.

The potentials of mathematical modelling in optimisation of thermals waste incineration plants are demonstrated for a virtual plant geometry. Specially the secondary air injection between the furnace and the radiational pass of the boiler is of great interest for the operation and optimisation of a plant like this. The distribution of secondary air to the front and rear wall side is a very important influence factor. The consequences on mixing, reaction and emissions are shown as well as some effects on slagging, fouling and corrosion.

This example demonstrates the potentials of the mathematical modelling to optimise the operation of thermal waste incineration plants.

Keywords

Thermal Waste Treatment, Secondary Air Injection, Mathematical Modelling, Optimisation

0 Introduction

Mathematical modelling is a very powerful tool to analyse and optimise combustion systems. Also for thermal waste treatment plants, it is commonly used to study the influence of the shape of furnace geometry, the arrangement of secondary air injection nozzles or furnace insulation solutions. In plant operation it can be applied for optimisation of the primary to secondary air ratio, air preheating and/or flue gas recirculation. The result of such calculations is a detailed information on the temperature distribution, the CO- and O_2-concentrations and the overall flow situation (secondary flow regimes).

One of the most problematic effects in thermal waste treatment plants is the appearance of slagging, fouling and corrosion. These phenomenons can lead to a dramatic reduction in the availability of the plant and in consequence to high costs.

Slagging and fouling is the result of particle deposition or corrosion attack to the furnace walls. Ash particles in the flue gas will touch the walls by aerodynamic probabilities depending on the overall flow situation. Whether the collision of particles with the wall leads to a deposition or a reflexion is a question of the material properties. Sticky particles will deposit, whereas hard ones will be reflected. The thermodynamic probability that particles will stick on the walls is a function of the partition of molten phases in the ash. The percentage of liquid phases can be estimated via a thermodynamic real phase modelling. This equilibrium assumption allows to calculate the mineral phase composition, if data is available for these very complex systems. Data bases like FactSage in combination with equilibrium calculation schemes like ChemSage are able to calculate the equilibrium composition of the particle´s mineral phases.

1 Mathematical Modelling

The task of the mathematical modelling is to describe the physico-chemical processes in a system. Doing that, all relevant effects have to be modelled. Depending on the requirements, the model must be configurated in a suitable manner. At the same time it is evident that the complete model is just as good as the worst sub-model. It makes no sense to use a very detailed turbulence model for predicting the CO-concentrations if, on the other hand, there is no precise knowledge of the CO oxidation kinetics.

An impression of the interaction between various process and state variables gives **Fig. 1.1** [**1.1**]. The core is formed by velocity, temperature and different concentration fields. In combustion systems, the interaction is very strong. All variables are influenced by boundary conditions. As an example, the grate firing system or the furnace geometry can be indicated. Vice versa, the condition in the combustion system determines flue gas temperapture, concentrations or slagging/fouling/ corrosion at the furnace walls.

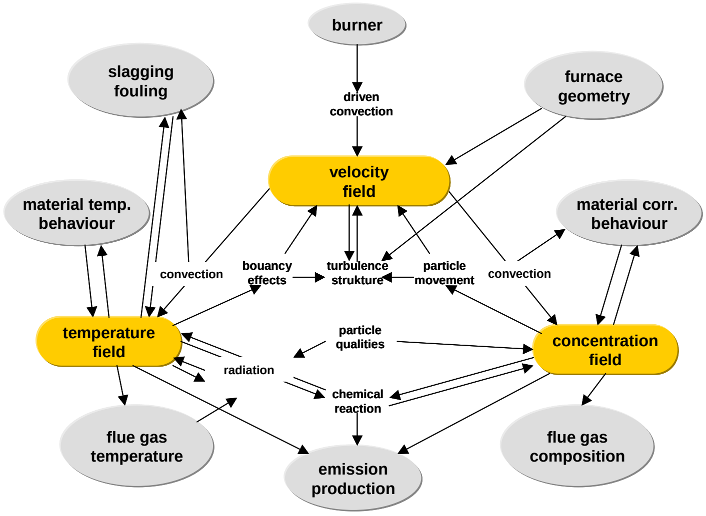


Fig. 1.1: State and process variables with its interactions

The mathematical model is based on the description of relevant state variables, like velocity, temperature and concentrations, and is balanced in very small volume elements (finite volumes) ([**1.1-1.4**]).
Doing this for the velocity ends up with the Navier-Stokes-equation which is valid for laminar as for turbulent flows (**Fig. 1.2**).

$$\frac{\partial}{\partial t}(\rho u_i)+\frac{\partial}{\partial x_j}(\rho u_i u_j)=\frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial u_j}{\partial x_i}+\frac{\partial u_i}{\partial x_j}\right)-\frac{2}{3}\mu\frac{\partial u_1}{\partial x_1}\delta_{ij}\right]-\frac{\partial p}{\partial x_i}+\rho g_i$$

By means of the continuity equation it can be transformed to:

$$\rho\left(\frac{\partial}{\partial t}u_i+u_j\frac{\partial u_i}{\partial x_j}\right)=\frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial u_j}{\partial x_i}+\frac{\partial u_i}{\partial x_j}\right)-\frac{2}{3}\mu\frac{\partial u_1}{\partial x_1}\delta_{ij}\right]-\frac{\partial p}{\partial x_i}+\rho g_i$$

Fig. 1.2: General form of the Navier-Stokes-equation for the momentum (velocity) balancing

Turbulent flow and mixing behaviour are often described by the k-ε-model of turbulence, where k is the kinetic energy of turbulence and ε its dissipation rate.

All the other scalar variables, like temperature of the gas phase and the species concentrations (e.g. for fuel, oxygen, carbon monoxide, carbon dioxide, water vapour, nitrogen oxides and others) are to be balanced, too. For that the modelled transport equation **Fig. 1.3** can be written.

In high temperature processes, like combustion, energy transfer, mainly by radiation, has to be modelled.

Special emphasis has to be taken to the characterisation of the fuel and its kinetic transfer in the fuel bed on the grate in thermal waste treatment plants. In [**1.6**] a method for analysing the release of volatiles in the different primary combustion zones is described. Based on this, the implementation of a detailed zone model for the fuel bed ([**1.7**]) is possible. Using this gives the boundary conditions of the gas outlet from the bed. Up to now, just simple one-dimensional release models are used.

$$\frac{\partial}{\partial t}\left(\overline{\rho}\,\overline{\varphi}\right)+\frac{\partial}{\partial x_j}\left(\overline{\rho u_j \varphi}\right)=\frac{\partial}{\partial x_j}\left(\frac{\mu_{eff}}{\sigma_{\varphi,eff}}\frac{\partial\overline{\varphi}}{\partial x_j}\right)+S_\varphi$$

Fig. 1.3: Modelled transport equation for a scalar variable ϕ e.g. temperature or species concentration

Around this main model a lot of detailed models can be arranged which have no or just some minor influence on the main describing variables. In this context, the NO_x-model can be named, where the heat effect of the reactions has no influence on the temperature of the gas phase.

For slagging, fouling and/or corrosion behaviour a detailed model can be build up, too. This will be described to some extent. Doing that, the particle phase has to be modelled beside the gas phase.

Fuel and ash particles are transported by gas phase flow and touch the firing walls or some convective components like heat exchanger surfaces.

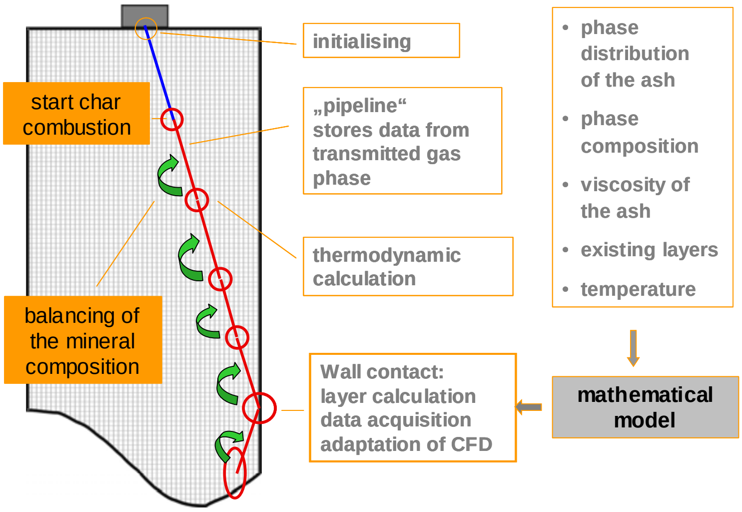


Fig. 1.4: Tracking of a fuel/ash particle through the calculation area with an online coupling to the gas phase for the calculation of the mineral phase composition

$$H_{tot} = H_{particle} + (1 - H_{particle}) \cdot H_{wall}$$

Fig. 1.5: Total probability for sticking as a complementary assumption

Inside the particles, reactions take place, like drying, pyrolysis, gasification, char combustion and mineral phase reactions. Exothermal reactions can lead to high particle temperatures and, caused by that, to sticking of particles. This quality is caused by the fact that some mineral phases get molten at higher temperatures. The higher the temperature the more molten phases are present. This property is modelled by a probability for sticking and is a function of two influencing factors: the stickiness of the particles and the stickiness of the existing ash layer. The composition of the mineral phase can be calculated via:

- description of the kinetics of the mineral phase transition [**1.8**] and
- equilibrium calculations via thermodynamic mineral phase modelling [**1.9, 1.10**].

In the present work, the second way is used because there is no kinetic data available for the phase transition.
The coupled calculation of the flue gas suspension and the particle mineral phase is shown in **Fig. 1.4** schematically.

particle ⇒ total probability for sticking ⇐ Wall layer

$$H_{tot} = H_{particle} + (1 - H_{particle}) \cdot H_{wall}$$

$$H_{particle} = \xi_{liquid} \cdot K_V$$

$$\xi_{liquid}(T_{particle}, p, x_i, y_i) = \frac{\sum m_{liquid}(T_{particle}, p, x_i, y_i)}{m_{particle}}$$ thermodynami

$$K_V(T_{particle}, x_i, y_i) = \frac{\mu_{ref}}{\mu_{actual}(T_{particle}, x_i, y_i)};\ K_{V,\max} = 1$$ Viscosity mo Watt & Ferec

(Walsh)

Fig. 1.6: Probability for sticking of particles which touch the walls as a function of the mineral phase composition

particle ⇒ total probability for sticking ⇐ wall layer

$$H_{tot} = H_{particle} + (1 - H_{particle}) \cdot H_{wall}$$

$$H_{wall} = \xi_{liquid} \cdot K_V \cdot C_F$$

thermodynamics $$\xi_{liquid}(T_{wall}, p, x_i, y_i) = \frac{\sum m_{liquid}(T_{wall}, p, x_i, y_i)}{m_{wall}}$$

viscosity model $$K_V(T_{wall}, x_i, y_i) = \frac{\mu_{ref}}{\mu_{actual}(T_{wall}, x_i, y_i)};\ K_{V,\max} = 1$$

present time step $$C_F(t) = \frac{\sum_{t=1}^{n}\left(\sum_{p=1}^{m}\left(\frac{\pi}{4} d^2_{particle,p}\right)\right)}{A_{cells}};\ C_{F,\max} = 1$$

Fig. 1.7: Probability for sticking of the wall layer as a function of the mineral phase composition

The probabilities for sticking of the particles $H_{particle}$ and of the wall layer H_{wall} are modelled individually and composed to a total probability for sticking H_{total}. For that a complementary assumption (**Fig. 1.5**) is used.

$H_{particle}$ and H_{wall} are modelled according to **Fig. 1.6** and **Fig. 1.7.** ξ_{liquid} is the liquid phase proportion from the real phase-equilibrium-calculation. The detailed model is described in [**1.9**].

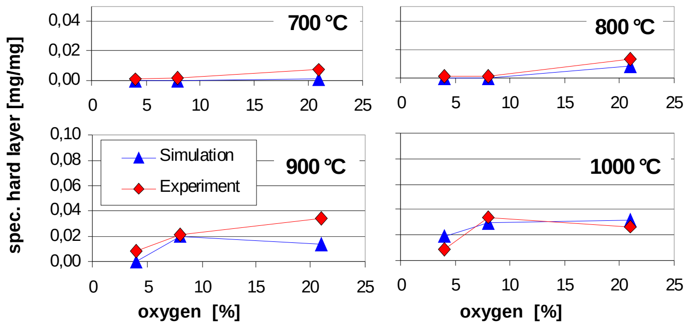


Fig. 1.8: Comparison of the calculated and measured hard layers for different temperatures and oxygen contents in the flue gas

A very good agreement between experimental data and the simulation results is achieved for brown coal (**Fig. 1.8**). The experimental data was produced in a drop tube reaction (Field pipe reactor at LUAT)

Ashes coming from thermal waste treatment have a much more complex system of mineral phases. Some amount of salts lead to a dramatic reduction of the ash softening and melting temperatures.

2 CFD-Calculation of a Model Plant

With this model, the MARS test rig at LUAT (Lehrstuhl für Umweltverfahrenstechnik und Anlagentechnik of the University of Duisburg-Essen) [**2.1, 2.2**] and a big amount of production plants [**2.2-2.8**] had been investigated. The complete model was enlarged and validated consecutively. For the validation the MARS plant is very much suitable because there are no significant operational restrictions and a very good analytical equipment is available, too.

In the following sections a fictive model plant was asssumed (**Fig. 2.1**). It works with a forward reciprocating grate firing system and a centre flow geometry. The radiational pass is followed by a vertical convective pass.

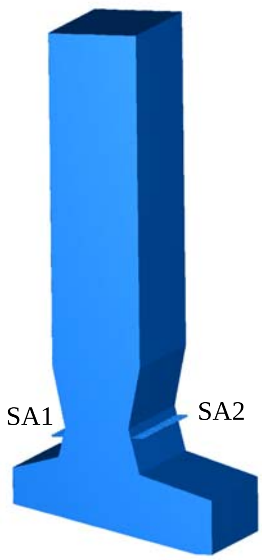
The secondary air nozzle rows 1 und 2 (SA1 and SA2) at the boiler front and rear walls consist by 16 nozzles each. They are arranged in an opposite manner (boxer arrangement) and inclined against the main flue gas flow.

As an example, the ratio of secondary air at the front and rear wall had been investigated and will be presented in the following section. In „case A“ (left hand side of each figure) the secondary air to the front wall (SA1) is 35 % and 65 % goes to the rear wall (SA2). In „case B“ this ratio is 50 % / 50 %.

geometry

centre flow firing with a secondary air nozzle row at the front and rear wall

SA secondary air
1 front wall
2 rear wall



Furnace and radiational pass with secondary air injection nozzles

Secondary air injection nozzles at the rear wall

Detail of the secondary air injection at the rear wall (boxer arrangement of the nozzles concerning the front wall).

Fig. 2.1: Geometrical conditions of the furnace and the radiational pass and details of the secondary air injection

The velocity distribution in a cross-section through nozzles of the front and rear wall near the symmetry plane is shown in **Fig. 2.2**. It can be seen that in "case A" SA1/SA2=35%/65% the flue gas flow touches the boiler front wall. Whereas in „case B“ the flow is centered in the radiational pass. Also the penetration depth of the secondary air jets can be estimated by this plot. In **Fig. 2.3** the velocity value „10 m/s“ is shown in an iso-surface-plot.

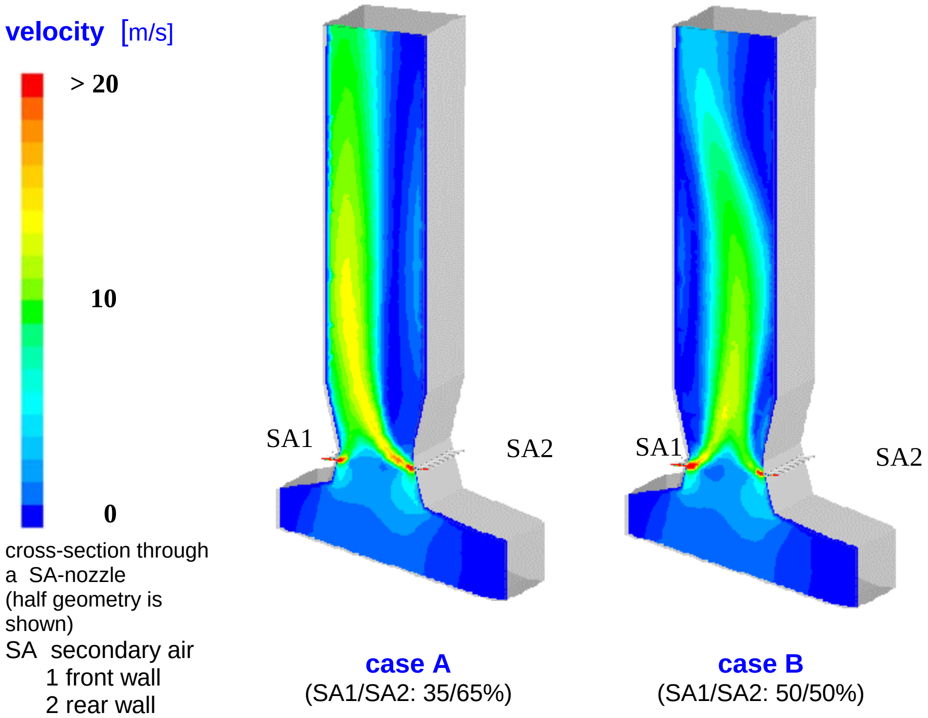


Fig. 2.2: Velocity distribution in a vertical cross-section (furnace and radiational pass)

In „case A“ the momentum flow from SA1-nozzle row is very small. So, just a small penetration depth is reached. SA2-jet enters up to the opposite wall. In total, a very bad mixing behaviour is seen.
A much better mixing is achieved in „case B“. Both secondary air jet streams (from front and rear wall) penetrate nearly the same distance.
The optimisation of the SA1/SA2-ratio just makes sense for a special thermal load and fire position case. If there are some changes in these conditions the SA1/ SA2-ratio has to be adopted again. It is no problem doing this by means of simulation. In practical plant operation it is not easy because of missing indication for the fire position, respectively. Therefore a guiding variable for a closed loop operation for the SA1/ SA2-control is missing. To some extend an information by an infrared camera (**[2.9]**) can be generated.

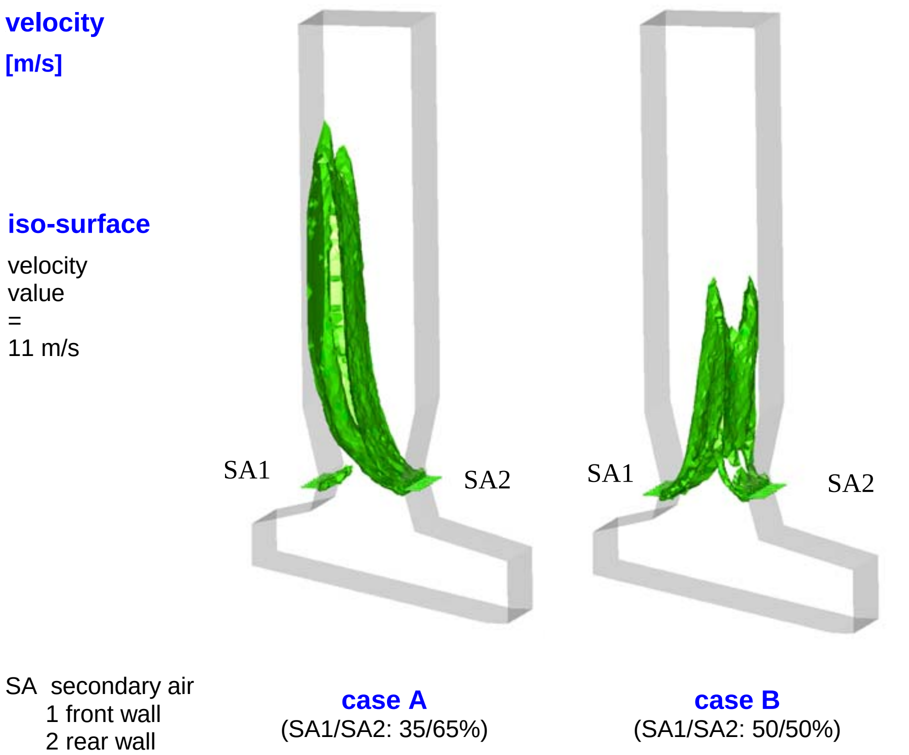


Fig. 2.3: Secondary air injection (11 m/s-iso-surface of the velocity)

The consequences of this mixing behaviour can directly be observed by the temperature distribution in the flue gas (**Fig. 2.4**). In this figure also a vertical cross-section through a secondary air injection nozzle (1 nozzle from SA1 and SA2) near the symmetry plane of the boiler is shown. The temperature in the flue gas suspension in „case A" is extremely lopsided. The high flue gas temperatures can be detected in the whole radiational pass and also reach the after combustion chamber. Also for „case B" the temperature distribution is much better and no strands can be detected in the after combustion chamber.

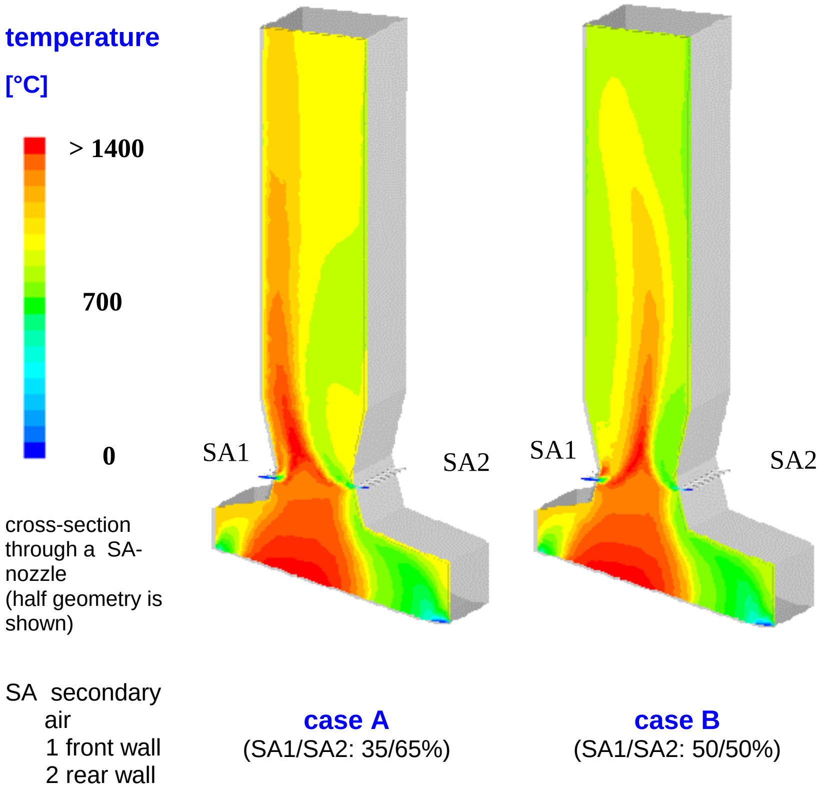


Fig. 2.4: Temperature distribution in a vertical cross-section through the furnace and the radiational pass

In **Fig. 2.5** the flue gas temperatures near the boiler walls are shown. The high temperatures at the side walls are not to be avoided. Nevertheless, „case A" shows higher temperatures in the lower part of the radiational pass. This fact can lead to fouling up to slagging in this area.

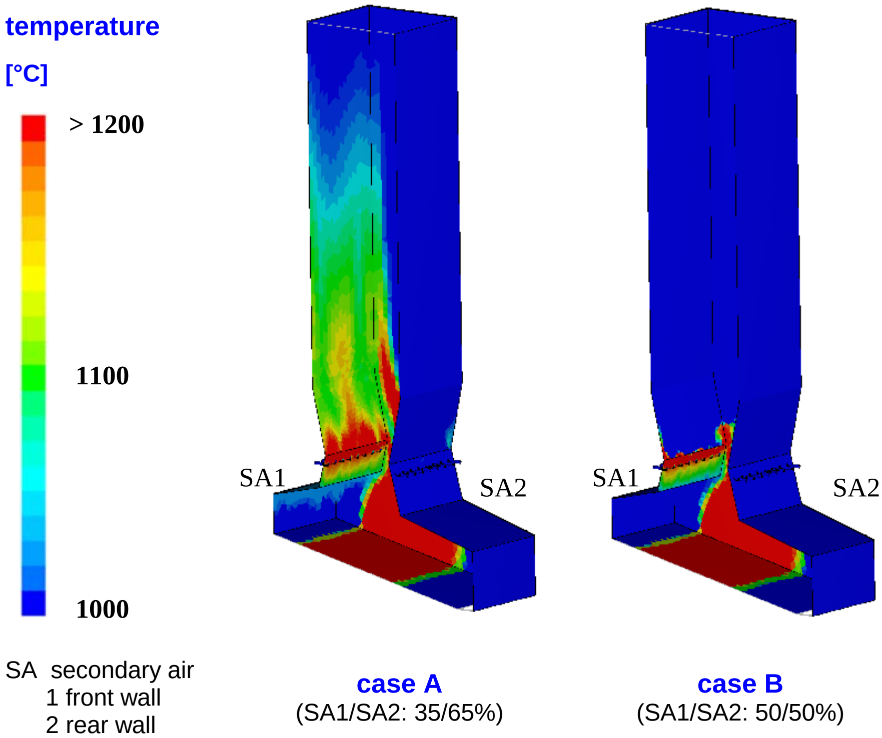


Fig. 2.5: Temperature distribution near the walls on the flue gas side

As shown in Fig. 2.2 and 2.3 the secondary air mixing in „case A“ is very poor. This also has consequences to the oxygen distribution in the flue gas (**Fig. 2.6**) which is important for the complete burn-out of carbon monoxide and hydrocarbons.
For both reaction systems mixing and kinetics are important influencing factors for the present reaction rates.

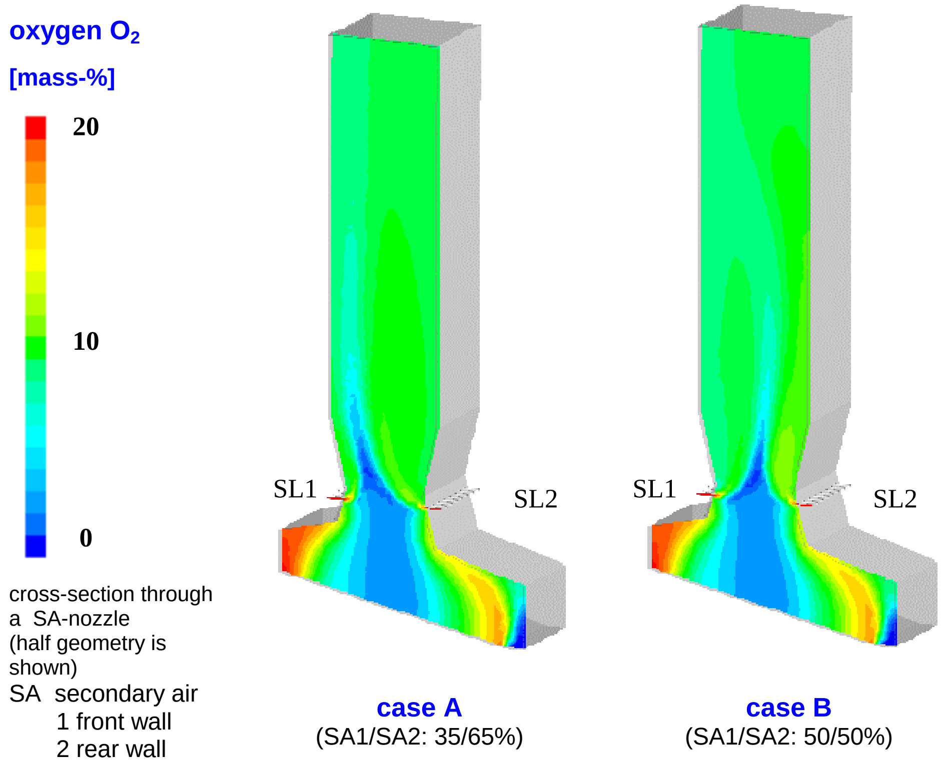


Fig. 2.6: Oxygen distribution in a vertical cross-section through the furnace and the radiational pass

Very important for a corrosion attack to the boiler walls and the reactions in the wall ash layers is the flue gas oxygen content near the walls (**Fig. 2.8**).
In „case B“ values of more than 9 mass-% can be detected above the secondary air injection location. “Case A“ shows values near the walls in the area of 0 mass-%.

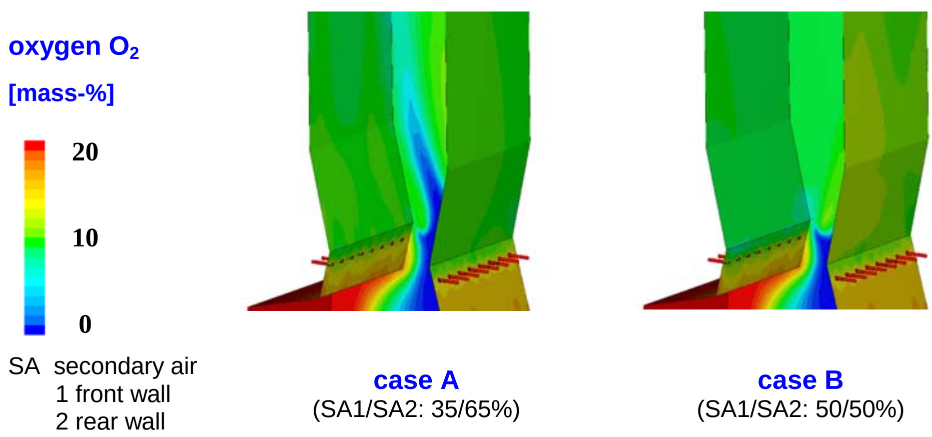


Fig. 2.7: Oxygen distribution near the walls above the secondary air injection

O_2- and CO-concentrations near the walls (see Fig. 2.7 and 2.9) have an important influence on the position of the equilibria of the mineral phases and from that on the mineral phase composition ([**2.10 to 2.13**]), which also influences the ash layer behaviour. This means reactions in the layer (e.g. sulphatisation and others), sinter processes and/or mechanical qualities (strengthness or cleanability of the ash layer).

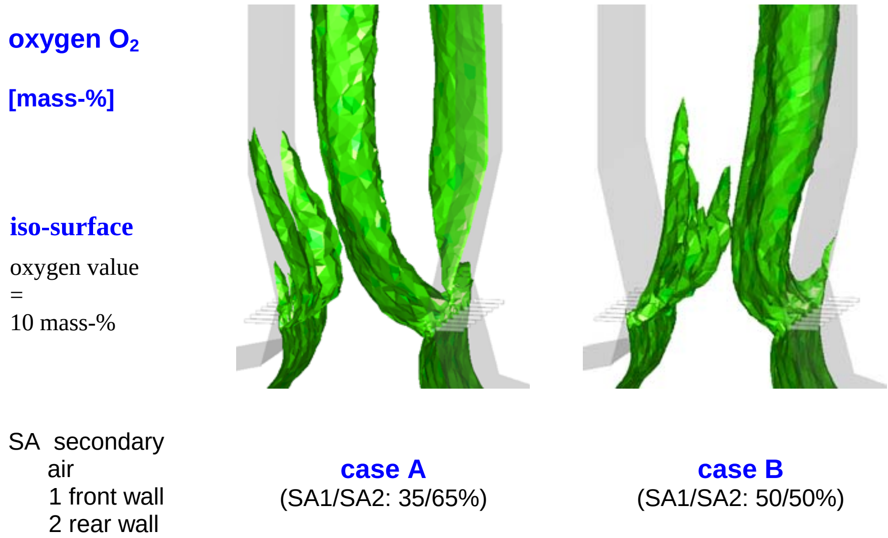


Fig. 2.8: Oxygen iso-surfaces above the secondary air injection

Fig. 2.8 shows the oxygen-iso-surfaces with a value of 10 mass-%. In „case A“ the secondary air jets penatrate very deap into the flue gas stream and are caught by a big sized flue gas recirculation flow. This leads to high O_2-values at the boiler rear wall. The jets from the front wall directly touch the front wall. This behaviour explanes the relativly high O_2-values near the front and real walls.

Some critical point can be seen from the recirculation region at the rear wall with low velocity values. In this area ash particles are advected and can lead to some wall ash layer.

Some direct consequences of the mixing quality and also for the combustion quality can be seen from the carbon monoxide distribution (**Fig. 2.9**), which shows high values in some regions of the boiler walls.

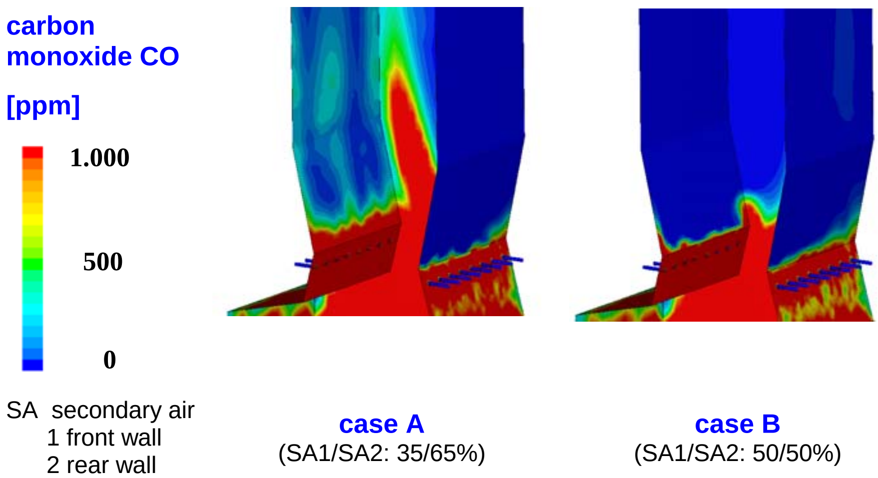


Fig. 2.9: Carbon monoxide distribution near the walls above the secondary air injection

In the present CFD-calculation also the discrete particle phase is balanced beside the continuous phase (flue gas). If particles without any mass are chosen, this is a method to visualise the flow. It allows to simulate stream lines, too.

Particle size distributions also can be taken into account. For representative results of the whole collective a huge amount of particles have to be traced from a statistical point of view (some hundred to thousand). Taking the surface of the burning bed as starting point of the particles, the behaviour of ash particles can be simulated.

Solving an energy balance for the particle, of course as a function of the particle size, the local particle temperature can be determined. Such a calculation is shown in **Fig. 2.10.** In „case A“, very hot particles touch the boiler front wall. Normally, with higher particle temperatures larger amounts of molten mineral phases are connected. The particles become more and more sticky. The probability for sticking will be increased (see. Fig. 1.5 to 1.7) in the recirculation zone. These are areas with a higher probability for slagging and fouling.

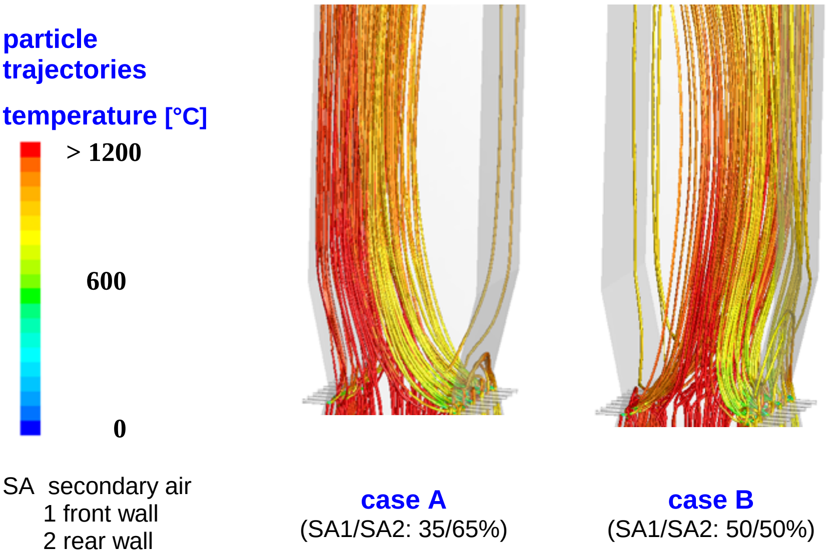


Fig. 2.10: Particle trajectories in the radiational pass after the secondary air injection coloured by particle temperature

The shown optimisation of the secondary air injection is just one example for options of a CFD-calculation for the furnace and the radiational pass of a thermal waste treatment plant. Other options concern the primary to secondary air ratio, the grate bar cooling (by air or by water), the furnace geometry (parallel, counter or centre flow) or the refractory lining. For all these options individual studies have been carried out.

3 Conclusions and Outlook

Processes taking place in thermal waste treatment plants are complex and are coupled in different ways. The fuel “waste” is very inhomogeneous and underlays big fluctuations in composition. Both facts lead to problems with an optimal operation of the plants and as a consequence to damages, which are very expensive. In this context slagging, fouling and corrosion can be mentioned. Mathematical modelling and simulation is able to contribute to a reduction of problems and damages. This is done by a „complete“ consideration of all relevant sub-processes. Such models have to be validated by experimental data. On this stage they are suitable for the engineering and optimisation of plants in real operation modes. Process and/or geometry variants are analysed and judged against each other. In the present paper this was done for the secondary air injection as an example. The slagging, fouling and corrosion behaviour could be analysed to some extent by this method. Because it is a “fictive” plant and in all real plants the conditions are different, just general information can be taken. Each plant with its geometric and operational conditions has to be analysed with the tool CFD individually. In the last years more than 30 plants have been investigated and optimised by this method. For the conception and optimisation very powerful contributions could be added. In most of the cases reality shows the same behaviour and results as the simulations.

List of symbols

A	area	[m²]	ε	dissipation of kin. Energy k	m^2/s^3
H	probability of sticking	[-]	ϕ	general state variable	[*]
k	kinetic energy of turbulence	[m^2/s^2]	μ	viscosity	[kg/(ms)]
m	mass	[kg]	ρ	density	[kg/m^3]
p	pressure	[bar]	ξ	liquid phase proportion	[-]
t	time	[s]			
T	temperature	[K]	Indices		
u	velocity	[m/s]	G	gas phase	
x	space coordinate	[m]	P	particle phase	

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