Numerical Analysis of the Impact of Parameters of Urea Solution Injection on Reagent Penetration inside the Combustion Chamber of an OP–140 Boiler

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Abstract

The implementation of new emission standards under the Industrial Emissions Directive is helping to drive the introduction of new technologies by power producers. Producers in Poland using the common OP-140 type pulverized fuel fired boilers are looking for solutions to reduce NOx emission in flue gases.

Selective Non-Catalytic Reduction (SNCR) technology is one of the de-NOx technologies tested for possible application in OP-140 type boilers. Optimization of the NOx emission reduction process in this technology consists of a selection of corresponding parameters of sprayed reagent in a boiler internal space. As part of project POIG.01.03.01 – 14 – 035/12 a simulation of thermal-flow conditions in a combustion chamber was carried out using Computational Fluid Dynamics (CFD) tools, among others simulation of thermal-fluid conditions in an OP-140 type boiler as well as the effect of operating parameters of the system that sprays out the reagent water solution and the influence of nozzle geometry on the spraying quality of this solution. This paper provides the results of aforementioned CFD simulations and experiments of SNCR technology operation for the considered optimal operating parameters (for selected levels of the OP-140 type boiler output) of this system.

1. Introduction

OP-140 is a pulverised fuel fired boiler design. These boilers are mainly operated in municipal and industrial heat and power generating plants and they have not been equipped with any flue gas cleaning systems, except for particulate matter removal. Current emission standards permit concentrations of 600 mg/Nm³ at 6% O_2 for nitrogen oxides in the exhaust gas from those boilers [10].

New legal regulations, including the Industrial Emissions Directive (IED) [5], will impose a requirement to considerably reduce emissions of pollutants, including nitrogen oxides. This has increased interest in the use of SNCR technology with OP-140 boilers.

IED requires combustion plants with capacity rating exceeding 50 MW_{th} to reduce their nitrogen oxides emission. The reduction obligation affects boilers with ratings from 15 MW upwards if they operate with a single emission stack in a group of at least 50 MW_{th}.

Depending on the type of source, the new standard will come into force in either 2016 or 2022. In Poland to date de-NOx systems are to be found exclusively at large commercial power plants. Boilers with outputs around 120 MW_{th} have not been equipped with de-NOx systems.

Selective Non-Catalytic Reduction technology for NOx emission abatement from industrial boilers involves injecting reducing an agent directly into a high-temperature zone of the combustion chamber. Reactions between the NH_2 radical and nitrogen oxides contained in the flue gas yield nitrogen, carbon dioxide and water [9], [3], [13].

The radicals are generated through the thermal decomposition of reducing agents. The following

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substances are used in this capacity in the SNCR process[4]:

- Urea (NH2)2CO in the form of an aqueous solution or solid,

- Ammonia NH3 as a gas or aqueous solution NH4OH,

- Cyanuric acid C3N3(OH)3 (cyclic trimer of the cyanic acid HNCO),

- Ammonium salts (sulphate (NH4)2SO4, carbonate (NH4)2CO3),

- Mono-, di-, trimethylamine CH3NH2, (CH3)NH, (CH3)N,

- Hydrazine N2H2.

To date, industrial applications have used urea and ammonia. The other compounds have been tested in laboratory reactors or at pilot plants, but so far have not been widely used on a larger scale and their application would require more research and development.

Literature data [3], [9], [13] reveals that the optimal temperature ranges are 900-1150°C for urea and 870-1100°C for ammonia. At lower temperature levels the reaction rates are low and ammonia is carried along unreacted with the exhaust gases causing ammonia slip. At higher temperatures the reagent oxidises, leading to additional NOx generation.

Therefore efficiency of a NOx reduction process depends on parameters such as reaction temperature and type of reagent used, but also on the characteristic of the spraying nozzles, duration of contact between the reagent and the treated gas and the chemical composition of the treated gas.

The method of introducing the reagent into the combustion chamber should be individually adapted for every boiler type, according to its design, size and combustion technology used (grate, pulverised bed).

Correct installation of a Selective Non-Catalytic Reduction system reducing nitrogen oxides emission from an industrial boiler requires proper selection or design of injection equipment, taking into account properties defined by flow characteristics, spraying angle, droplet diameter, spray range, mutual interference between sprays from different nozzles and the influence of flue gas lift. Before injectors can be selected or designed, it is necessary to specify their desirable operating parameters, taking into account the local conditions of individual boilers (furnace geometry, flue gas velocity and temperature).

The aim of this study was to determine optimal spray nozzle operating parameters, such as average reagent droplet diameter, initial droplet velocity and spray angle, to ensure best if not full coverage of the furnace's cross-section for specified boiler geometry. Computational Fluid Dynamics methods and *ANSYS Fluent Software* [1] were used to achieve this aim.

The geometrical and operational parameters used in the modelling process were sourced from actual boilers and they were as follows:

- Furnace dimensions (width/depth/height): 6 m / 6 m / 27 m,

- Air-fuel mixture injection velocity: 25 m/s,

- Secondary air injection velocity: 35 m/s,

- Total fuel mass rate: 3.27 kg/s,

- Water walls temperature: 627 K.

The simulation results provided information concerning the influence of nozzle operating parameters on reagent evaporation rates, and therefore also the spray range in realistic temperature conditions. They also made it possible to observe the influence of exhaust gas velocity on reagent droplet trajectory, depending on droplet size. Those relations are very important in the context of achieving the ultimate objective: ensuring reagent supply at optimal concentration to every point of a cross-section of the furnace.

2. Calculation methodology

The following algorithm was used to achieve the defined aim of the study:

- Performing thermal flow calculations for the processes occurring inside the furnace of a OP 140 boiler in order to pre-determine the desired temperature window and to find exhaust gas velocity and temperature distribution in that area.

- Separating part of the furnace volume where the temperature conditions are favourable for reagent injection, together with assigning proper boundary conditions at relevant boundaries;

- Running a number of reagent injection simulations in a domain which is a separated part of the furnace of the analysed boiler for different:

- Average reagent droplet sizes,

- Injection velocities,

- Injection angles.

The simulations were performed for a single injector feeding the reagent into the boiler. This approach was chosen, as the aim of the research was determining reagent behaviour (in the form of droplets and upon

Figure 1: Computational geometry used to analyse the impact of injection parameters on reagent behaviour in the boiler volume (marked green)
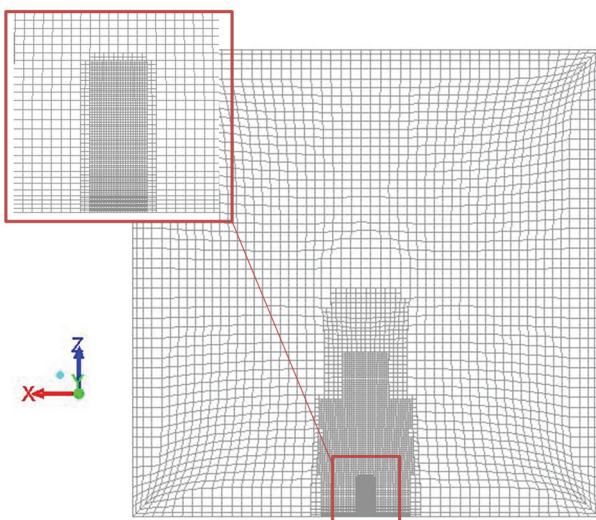

Figure 2: Computational grid used to analyse the impact of injection parameters on reagent behaviour in the boiler

evaporation) in the boiler rather than analysing NOx content reduction. Result analysis informed conclusions about the influence of injection parameters on the spray range and reagent concentration distribution in the boiler.

3. Simulation parameters

The geometry used for analysing influence of injection parameters on reagent behaviour in the boiler was separated from the whole furnace volume; the part with temperature conditions for reagent feeding deemed favourable was selected. The separated geometry is marked in green in Figure 1.

Relevant boundary conditions were specified for the side, top and bottom surfaces of the modelled volume (i.e. walls temperature, flue gas inlet and outlet respectively). The flue gas conditions involved:

- Velocity distribution,
- Pressure distribution,
- Temperature distribution,
- Turbulence distribution.

These parameters were assigned following results of the earlier furnace modelling.

A base grid consisting of ca. 140,000 box elements, with density additionally increased near the domain boundaries, was defined for the modelled volume. The density of the base grid was also increased in the area adjacent to the selected reagent injection location. Grid independence tests were performed, and following a series of preliminary calculation runs one variant – optimal in terms of calculation time and accuracy – was selected. The element count of the final grid was ca. 265,000 (Fig. 2).

The settings used for solving the problems included activation of energy equation and discrete ordinates (DO) radiation model [11].

The Discrete Phase Model was used to model reagent injection [2]. The reagent is introduced into the furnace at high velocity, which may lead to secondary droplet disintegration due to aerodynamic forces. SSD Breakup Model was used to take this possibility into account [7]. The introduced droplets were considered as Multicomponent elements (mixture of urea and water).

In order to determine the amount of reagent introduced by a single injection nozzle into the boiler it was necessary to make a number of assumptions. It was assumed that:

- The average content of nitrogen oxides in the exhaust gas of an OP-140 boiler is 600 mg/Nm³, which upon conversion into dry gas and 6% oxygen content yields 447.8 ppm;

- Reagent would be injected through six injectors;

- Amount of generated flue gas is ca. 170,000 kg/h.

The general reaction between the urea and nitrogen oxide may be defined as follows [9]:

$$CO(NH_2)_2 + 2NO + 0.5O_2 = 2N_2 + CO_2 + 2H_2O$$

According to this equation, in stoichiometric conditions 1 mole of urea reacts with 2 moles of NO. As the molar mass of the urea is 60 g/mol and molar mass of NO is 30 g/mol, in stoichiometric conditions their masses are equal.

Therefore urea demand for an OP-140 boiler running at nominal load (assuming stoichiometric proportions) is ca. 0.0214 kg/s, i.e. ca. 77 kg/h.

If six injectors are used to deliver a 15% urea solution, the reagent flow through single injector is ca. 0.0253 kg/s.

4. Calculation results

Selected modelling results shown in this paper apply to a simulation of reagent injection into a volume which is a part of an OP-140 boiler furnace for various:

- Reagent average droplet sizes – 100 µm, 200 µm and 500 µm;

- Injection velocities – 50 m/s, 100 m/s and 200 m/s;

- Injection angles – 20° and 40°.

In order to evaluate the quality and usefulness of reagent injection for a certain set of injection parameters, it is necessary to observe reagent behavior both in liquid phase (urea solution droplets) and in gaseous phase (urea upon evaporation).

The results shown below, which refer to the movement of urea solution droplets in the flue gas, specify:

- Horizontal and vertical droplet penetration;

- Droplet velocity;

- Changing droplet diameter as the penetration progresses.

Nevertheless, what is essential for the course of NO_x reduction into N_2 using urea is the urea behaviour after evaporation, i.e. in gaseous phase. Therefore it was decided to perform a detailed analysis of urea concentration distribution in the modelled volume for individual analysed injection scenarios. In order to do that:

- A number of isosurfaces was created, representing points of constant urea concentration for values,

- Equal to the required stoichiometric concentration ensuring reduction to the assumed nitrogen oxides content of 600 mg/Nm³,

- Two times higher than stoichiometric,

- Four times higher than stoichiometric,

- Eight times higher than stoichiometric;

- Exhaust gas volumes contained in the isosurfaces defined above were calculated.

In reality, the urea decomposes into ammonia and cyanic acid [8], [12]. Observed isosurfaces of urea concentration should be treated as a visualization of gaseous reagent products.

Analysis of shapes, placement and volumes of the flue gas contained in individual isosurfaces provides much useful information concerning urea behaviour (in the gaseous phase) in the boiler. It was assumed that the flue gas volume between the isosurfaces would be one of the tangible parameters describing the quality of injection for a certain set of parameters. It was assumed that the growth of volume contained in a specific isosurface should be interpreted as a higher potential of uniform urea supply to the flue gas contained in the furnace.

4.1. Influence of injection velocity on reagent behaviour in the boiler

Three values of injection velocity were considered in this study: 50 m/s, 100 m/s and 200 m/s. Modelling results indicate that the injection velocity has only limited impact on the reagent droplet range. Of course increasing injection velocity increases the range, but only until a certain point. At a certain velocity, the Weber number exceeds the critical value and aerodynamic forces acting on droplets cause secondary disintegration [6]. This leads to a rapid reduction in average droplet size in the stream and faster evaporation. This in turn reduces range. This phenomenon is presented in the diagram below (Figure 3).

It can be seen that for the 200 µm droplets the range at the injection velocity of 200 m/s is shorter than for velocity of 100 m/s. This effect is caused by secondary droplet disintegration. This phenomenon is not observed for 100 µm droplets, as for such a small value the Weber number does not exceed critical value in the analysed velocity range.

As for droplet stream movement, the influence of injection velocity on droplet range is not great below the critical value of the Weber number.

Increasing velocity, just like increasing droplet size, moves the zone in which the reagent turns into gas further away. Accordingly, the gaseous reagent cloud appears further from the injection point (Figure 4).

4.2. Influence of droplet size on reagent behaviour

Modelling results lead to the conclusion that the biggest factor affecting range is reagent droplet size. As is shown in Figure 5, reagent droplet size change roughly doubles if the diameter is increased from 100 to 200 microns. The figure below presents a comparison of reagent droplet diameter distribution in a stream for injection velocity of 50 m/s, spray angle of 20° and two different initial droplet diameters of 100 μm (Fig. 5a) and 200 μm (Figure 5b).

Figure 3: Range of reagent droplets as a function of injection velocity
and average droplet size – modelling results

Considerable differences may be seen not only in droplet range, but also their lift. Larger diameter droplets, prior to full evaporation, slow down sufficiently to be lifted with the flue gas. This may be a harmful phenomenon, pushing the reaction zone outside the optimal temperature range. At smaller diameters, the droplet evaporation zone is placed lower.

Additionally, this phenomenon intensifies along with increasing injection velocity, but only up to the value where secondary droplet disintegration starts.

Figure 6 presents the behavior of reagent droplets in secondary disintegration conditions. Due to disintegration, droplet diameter drops rapidly, thus leading to quick reagent evaporation and considerable range reduction, regardless of initial injection parameters.

Modelling also revealed (Figure 7) that 500 μm droplets are definitely too large for use in the analyzed boiler type (at injection velocities in the investigated range). Even at injection velocity of 100 m/s those droplets approach the opposite boiler walls.

In such a case the evaporation zone is lifted to a level considerably above the injection level, thus placing the gaseous phase of the reagent beyond the desired flue gas temperature range.

Figures 8 and 9 present exemplary droplet velocity and temperature distributions for the following injection conditions: initial velocity 50 m/s, initial droplet diameter 200 μm, and spray angle 20°.

The presented results show that the velocity of sprayed droplets drops quite quickly. When the velocity drops below a certain value, the droplets in their final life period – when their diameters are reduced in reference to the initial value – are lifted by the flue gas flow.
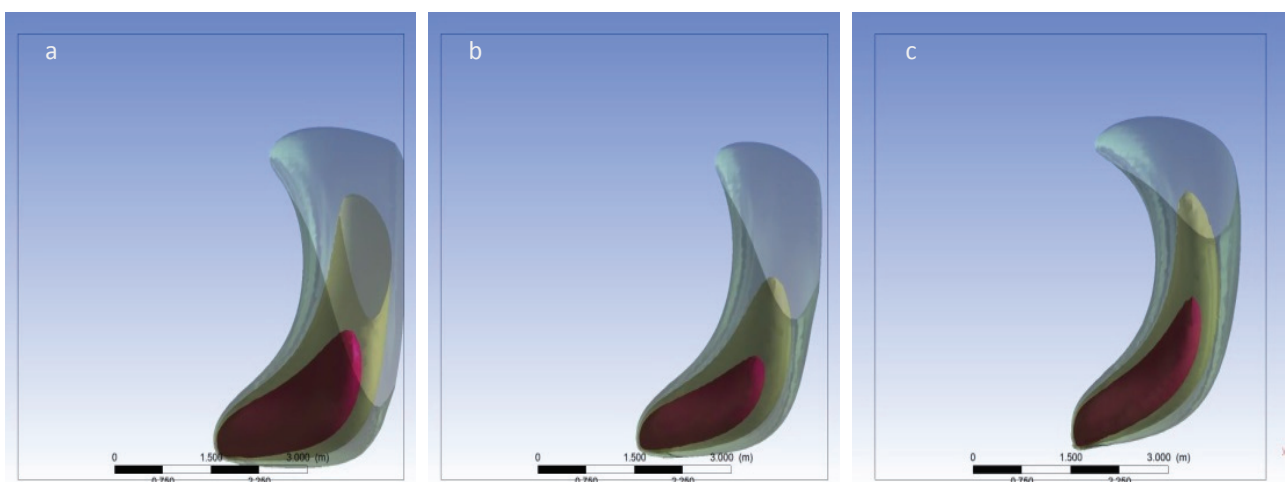

Figure 4: Isosurfaces of urea mass concentration in the flue gas for the
droplet diameter of 100 μm and injection angle of 20°
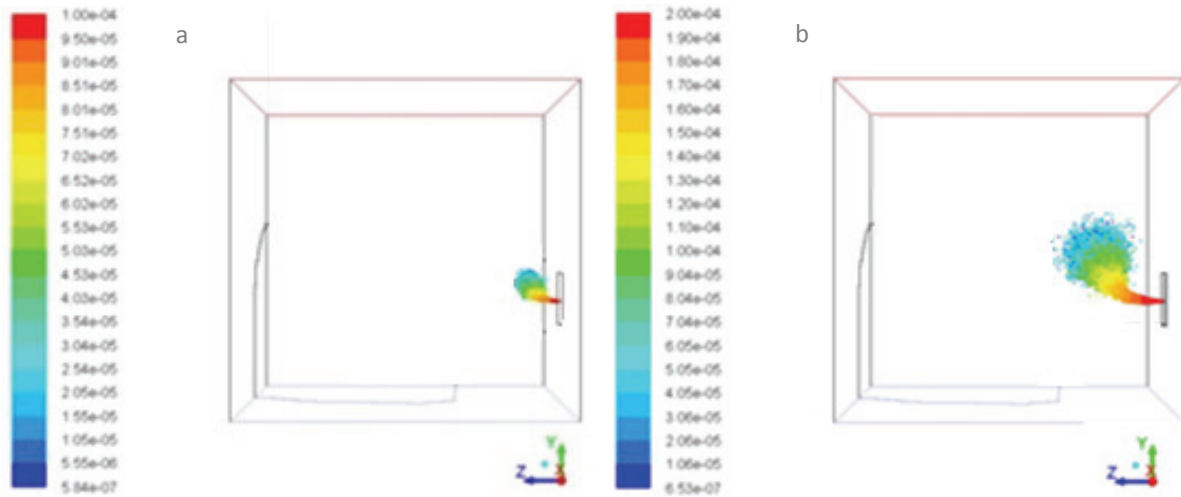(a – 50 m/s; b – 100 m/s; c – 200 m/s). View from the top of the boiler

Figure 5. Distribution of reagent droplet diameters in the stream for injection velocity of 50 m/s and spray angle of 20°
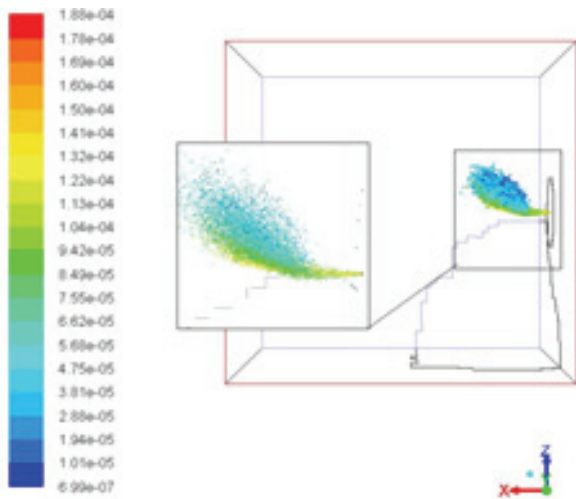(a – injection of 100 µm droplets, b – 200 µm droplets)

Figure 6: Distribution of reagent droplet diameters in the stream for initial diameter of 200 µm, injection velocity 200 m/s and spray angle of 20°
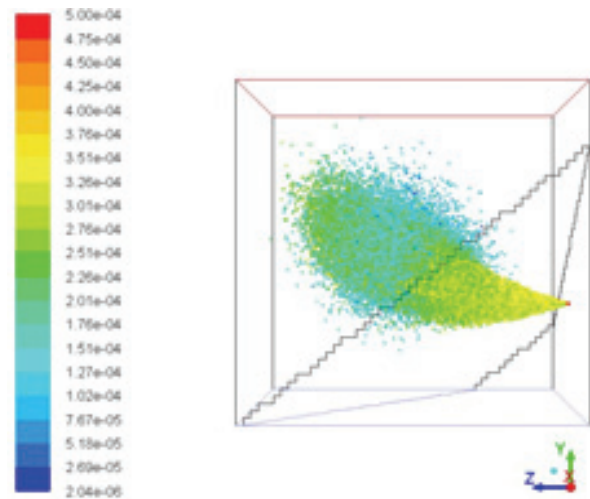
Figure 7: Reagent droplet diameters for injection velocity of 50 m/s, reagent concentration of 15%, spray angle of 40° and initial droplet diameter of 500 µm
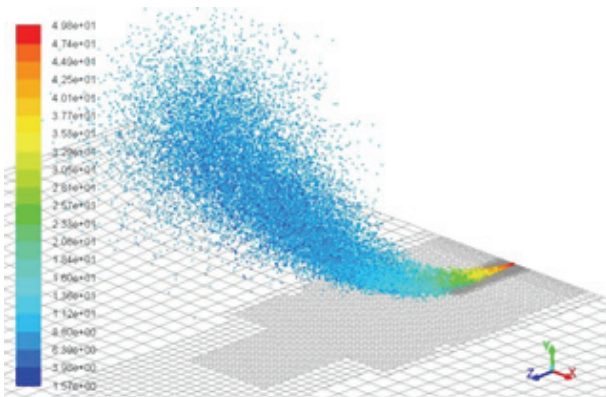

Figure 8. Reagent droplet velocity distribution for initial velocity 50 m/s, initial droplet diameter 200 µm, and spray angle 20°
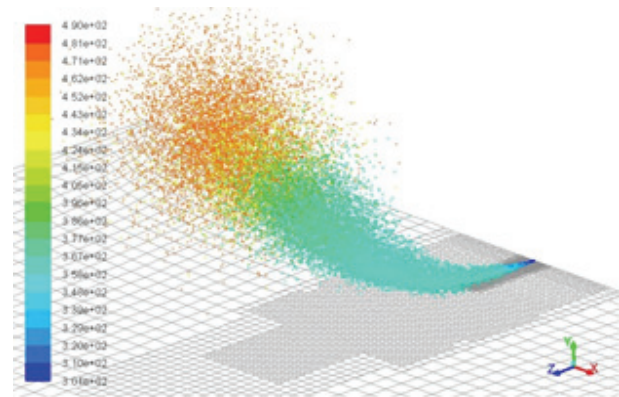
Figure 9. Reagent droplet temperature distribution for initial velocity 50 m/s, initial droplet diameter 200 µm, and spray angle 20°
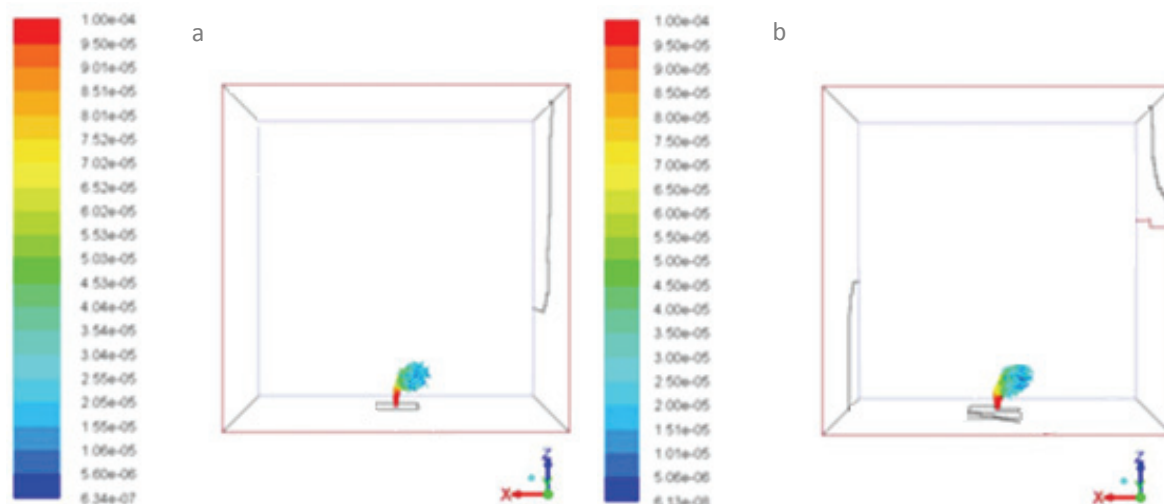
Figure 10. Distribution of reagent droplet diameters for injection velocity of 100 m/s, initial droplet diameter of 100 μm and injection angle of: a) 20°, b) 40°

The presented distribution of droplet temperature values shows three phases of reagent transition from the aqueous solution into gaseous form. The first short section of spray involves heating the droplets up to the water evaporation temperature. Then a constant temperature is maintained due to water evaporation. Upon complete water evaporation, urea temperature rises again to its evaporation temperature.

4.3. Influence of spray angle on reagent behaviour

Another analysed parameter was the reagent spray angle. Two values were analysed: 20° and 40°. It was shown that increasing the spray angle causes a decrease in range for all analysed injection velocities and droplet diameters.

Table 1 shows that, in addition to range, the width of the spray and droplet lift are also affected by the spray angle. If the spray angle is doubled, spray width and lift increase by several percent.

Table 1: Influence of spray angle on geometric spray parameters

Injection velocity [m/s]	Range 20°/40° [m]	Lift 20°/40° [m]	Width 20°/40° [m]
50	2.40/2.23	1.74/1.97	1.91/1.92
100	2.51/2.56	1.93/2.26	1.65/2.14
200	2.13./1.86	1.07/1.00	1.17/1.16

In contrast, spray angle was found to have no significant influence on the flue gas volume contained in individual isosurfaces of reagent concentration in the gaseous phase.

Modelling results suggest that spray angle is not an essential parameter, but it does have a considerable impact on the behaviour of sprayed droplets or gaseous reagent (Figure 10).

5. Conclusion

Having analysed a number of parameters describing reagent injection into the analysed boiler design, it may be concluded that the parameters which have an essential influence on the behaviour of reagent droplets in the boiler are primarily droplet diameter and velocity. The appropriate combinations of mentioned parameters result in wide spectrum of injection range. Spray angle is of secondary importance. According to the modelling results, to achieve a reagent droplet range sufficient to reach the middle of the analysed furnace does not require the use of droplets much larger than 200 μm. Injection velocity should be ultimately decided after verifying the correlation between the droplet size and velocity just after the injector, using an experimental facility.

Analysis of the modelling results concerning reagent spread in the gaseous phase leads to the following conclusions:

- Reagent behaviour is dependent less on injection parameters and more on the flue gas velocity profile in the furnace;

- The volume of flue gas contained between consecutive isosurfaces of reagent

concentration is relatively insensitive to the analysed injection parameters;

- The injection parameters which impact the location where the gaseous reagent appears are: droplet size and injection velocity.

Analysing such a wide spectrum of injection scenarios provided knowledge and insight on potential reagent behaviour in the boiler, both in the form of droplets and in the gaseous phase.

Acknowledgement

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