CFD modeling and thermodynamic analysis of a concept of a MILD-OXY combustion large scale pulverized coal boiler

Wojciech P. Adamczyka, Ryszard A. Bialeckia, Mario Ditarantob, Pawel Gladysza, Nils Erland L. Haugenb, Anna Katelbach-Wozniaka, Adam Klimaneka, Slawomir Sladeka, Andrzej Szleka, Gabriel Wecela

a Institute of Thermal Technology, Silesian University of Technology, Konarskiego 22, 44-100 Gliwice, Poland
b SINTEF Energi A.S., Sem Saelands vei 11, 7034 Trondheim, Norway

ABSTRACT

A concept of a large scale pulverized coal boiler working in the oxycombustion mode has been proposed. The combustion chamber has been designed using the Moderate and Intensive Low-oxygen Dilution (MILD) combustion technology. By screening CFD solutions of several geometric configurations the best one has been selected, for which the dependence of the oxygen excess ratio and recirculation rate of the flue gases analyzed onto the efficiency of the combustion chamber has been investigated. The results of the CFD simulations have been then embedded into a process model of the entire plant. The preliminary simulations show the possibility of efficiency increase of more than 3% points.

© 2017 Elsevier Ltd. All rights reserved.

1. Introduction

Oxycombustion of coal is considered as one of the technically viable and cost effective carbon capture technologies available today [1]. It bases on replacing the combustion air by an oxidizer consisting of a mixture of nearly pure oxygen and recycled flue gases. The flue gas admixture is required to maintain low combustion temperatures in both newly built and retrofitted boilers. As a result of fuel combustion the flue gas is CO₂ rich, which after particulate mater removal, desulphurization and drying, can be compressed and transported to the storage place. As nitrogen is almost completely eliminated from the oxidant, the volume of the gases is lower, allowing for easier removal of pollutants and pumping energy savings. Moreover, the chemical energy that is used in air combustion to heat up the large amount of nitrogen in the flue gases, is saved. The price to pay when applying oxycombustion are the high capital and operation cost of oxygen production in the air separation unit. The current status of the development of oxycombustion is described in the review paper of Chen et al. [1], while comparisons of oxycombustion with other carbon capture technologies are presented in Refs. [1,2]. A review paper [3] concentrate on power plants using oxyfuel combustion and a survey of oxyfuel pilot plants is presented in Ref. [4]. An important issue that hinders the development of coal oxycombustion is the high energy penalty and the associated drop of efficiency and increase of electricity cost. Research to reduce these factors concentrate on better integration of the separation plants with the steam cycle, going to higher parameters of the produced steam and any other techniques, that would enhance the efficiency of the cycle. MILD combustion is a natural candidate to be used in this context.

MILD combustion was introduced nearly 30 year ago in the context of gas combustion in industrial furnaces [5–7]. The most important feature of the MILD technology (Moderate and Intensive Low-oxygen Dilution) is the intensive recirculation of the hot combustion products in the chamber. As a result, diluted oxidizer and fuel come to contact and the ignition and combustion occurs in regions of low oxidizer concentration. As opposed to the standard combustion process, where chemical reactions take place in a narrow flame front, MILD combustion is distributed over a significant portion of the chamber. This produces homogeneous temperature and uniform heat flux fields, while the emission of...
thermal nitrogen oxides is practically eliminated. The technology can reduce the NOx emission by 70% [8] and fuel NOx by 40–60% [9]. Reduction of the temperature and concentration gradients in the combustion chamber, reduces also the irreversibility of the heat transfer and chemical reactions, increasing the exergetic efficiency of the whole installation. These attractive features of the MILD technology resulted in spreading it among many branches of the industry. For a long time it was believed, that preheating the combustion air to temperature higher than the ignition temperature [10] is the necessary condition for MILD combustion to occur. Such high temperatures could be reached by recuperating the heat from flue gases. The equipment to accomplish this task were typically regenerators not only expensive and requiring a lot of space, but also prone to dust clogging. As a result, MILD combustion applied to coal, whose flue gases contain significant amount of dust, the preheating of air was for a longer time hindering the application of MILD technology to coal fired units. It has been shown [7,11], that MILD combustion can occur without air preheating. The necessary condition is to inject the oxidizer with high momentum so that significant flue gas entrainment and oxidizer dilution is obtained. This is associated with considerable internal flue gas recirculation development. Earlier, the question of application of MILD combustion to coal fired boilers, has been addressed in Ref. [12] while Weber at al [13] reports about first experiments using natural gas, oil and pulverized coal in a 0.58 MW installation. Reference [14] presented a concept of application of the MILD combustion in a 130 MWth supercritical pulverized coal boiler running in a MILD combustion regime. CFD simulations were used to find the best geometric configuration of the nozzles and inlet parameters. The authors report on longer residence time of coal particles, lower NOx concentrations and the possibility of reducing the oxygen excess when compared to standard designs. Parallel to this work and later, numerous papers have been published. At that point the idea of applying MILD technology in boilers has been seriously considered, also in the context of coal fired units.

The idea of MILD-OXY combustion is attractive, as the MILD combustion increases the efficiency and lowers the NOx emission, while oxycombustion is a reliable technique of CO2 separation. The joint application of these technologies would thus produce synergetic effects. It is expected that the marriage of these two technologies, due to the better mixing, longer residence time of the coal particles and internal recirculation of the flue gases would reduce the oxygen excess ratio, thereby leading to increase of the efficiency of the plant. The same effect can be expected because of the reduced production of oxygen in the ASU installation. Moreover, internal recirculation of the flue gases within the chamber, reduces the amount of flue gases that needs to be recirculated in the external loop in standard oxycombustion. This in turn results in lower pumping costs consumed in this loop. Furthermore, it is expected that better fuel flexibility of the boiler will be achieved and that it will open possibility of pulverized coal combustion in small boilers. The chance of using both oxycombustion in the context of MILD technology has been mentioned in several papers [1,7,13,16], however without reporting about any large scale application of this approach.

The principal problem when using the MILD-OXY technology is the optimal organization of the flow and mixing patterns withing the chamber. This can be done by employing CFD tools. Several papers addressed this question. Reference [17] describes the CFD simulations applied to a small pilot $\Phi = 0.2 \, m \cdot L = 2 \, m$ cylindrical chamber using high velocity oxygen jets. Spacing of the O2 nozzles and CO2 jet carrying coal particles, ignition delay and the influence of the particle diameters have been investigated. Tu et al. [18] discusses another CFD study within a cuboid $2 \times 2 \times 6.25 \, m$ chamber with two oxygen nozzles and a central fuel nozzle. Air combustion and four O2 concentrations ranging from 21 to 30% in the flue gases are analyzed and the results compared with the available IFRF experiments [13]. Good agreement between simulations and measurements is reported. Perrone and Amelio [16] used the same furnace geometry as in the previous study [18] to investigate numerically MILD and MILD-OXY combustion of coal. One of the conclusions was the observation that the energy consumption of external flue gas recirculation in standard oxy-combustion can be considerably reduced by applying the MILD-OXY combustion with its strong internal flue gas recirculation. All the aforementioned contributions concerned MILD-OXY combustion of coal in small, pilot scale installations.

The purpose of the present study is to investigate the MILD-OXY combustion process in a large scale industrial pulverized coal unit, which will be in this paper referred to as the MILD-OXY Fuel Combustion (MOFC) boiler. Specifically, the optimal location of the oxygen and fuel nozzles, the momentum of the oxidizer and fuel jets and the geometry of the chamber is sought. The possibility of using low excess oxygen ratios and the influence of the rate of externally recirculated flue gas are then verified. The peak and outflow temperatures, char conversion and thermal efficiency are monitored. These analyses are performed using a CFD model of the furnace. In order to examine the global effects of the introduced boundary data to the CFD model, and verify the concept of synergetic effects of MILD-OXY combustion, the study is extended by a thermodynamic analysis of the whole power plant. This allowed for determining plant performance parameters like gross and net power, net energy efficiency and for comparing the MOFC boiler based power plant with a reference oxycombustion plant.

2. Description of the model

The new supercritical industrial boiler fueled with pulverized coal running under MILD-OXY combustion conditions is proposed. Comparing to classical OXY combustion boilers, where the oxidizer is mixed with externally recirculated flue gases (RFG), in the analyzed case the oxidizer is supplied by separate high speed jets, as shown in Fig. 1. The basis for the design was: thermal input which was assumed to be 1000 MW and composition of the oxidizer containing 95% of O2 and 5% of N2 by volume. The transport of the pulverized coal to the furnace is forced by externally recirculated flue gas. The flue gas is conditioned prior to its supply to the mills, i.e. it is purified by desulfurization and particulate matter removal systems, and dried. Furthermore, it is assumed that the water vapor content in the RFG is 4% and the temperature of the oxygen, coal and RFG at the boiler inlet is 100 °C. As shown in Fig. 1, the CFD model of the MOFC boiler is restricted to the furnace alone, thus the convective evaporator and economizer are not modeled. The input data for the cases analyzed within this study were based on the above mentioned assumptions and the recirculated flue gas composition (except the water vapor content) was calculated from mass and energy balances of the boiler.

The CFD model of the furnace was developed using commercial software ANSYS® Release 16.2, where ANSYS® FLUENT [19] was
used as the solver. The standard functions of the solver were extended by applying the user defined function (UDFs) mechanism for tracking particles and controlling the particle distribution over the boiler during solution procedure. The coal particles were treated as discrete phase embedded in continuous gas phase. The particle motion was modeled in Lagrangian frame of reference. The interactions between continuous and discrete phases were predicted using a two-way coupling procedure. The exchange between phases appears as source/sink terms in the governing equations for the continuous and discrete phase.

As at this stage it is not possible to compare the units based on experiments, simulated solutions are compared. The models and numerical approaches used in this paper belong to standard engineering toolbox used when simulating pulverized coal boilers. Such an approach has been selected as the aim of the paper was to compare the proposed design with the reference boilers encountered in the industry and designed using standard methods.

2.1. Governing equations

The following transport equations written for the continuous phase are solved:

- mass conservation equation of the multicomponent fluid
  \[
  \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = S_{\text{mas}}
  \] (1)

- species mass conservation equations
  \[
  \frac{\partial (\rho Y_k)}{\partial t} + \nabla \cdot (\rho \mathbf{u} Y_k) = -\nabla \cdot \mathbf{J}_k + R_k + S_k
  \] (2)

- momentum conservation equations
  \[
  \frac{\partial}{\partial t} (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \mathbf{\sigma} + \rho \mathbf{g} + S_{\text{mom}}
  \] (3)

- energy conservation equation
  \[
  \frac{\partial}{\partial t} (\rho h) + \nabla \cdot (\rho h \mathbf{u}) = \frac{\partial p}{\partial t} + \nabla \cdot \mathbf{\sigma} + \rho \mathbf{g} + S_{\text{en}}
  \] (4)

where \(\rho\) is the fluid density, \(\mathbf{u}\) the velocity vector, \(k\) is the species index, \(Y_k\) stands for the mass fraction of species \(k\), \(J_k\) is the diffusion flux of species \(k\), \(p\) is the pressure, \(\mathbf{\tau}\) is the stress tensor, \(\mathbf{g}\) is the vector of gravitational acceleration, \(h\) is the enthalpy, \(q\) is the heat flux vector, \(m\) stands for the number of species in the system. The source terms \(S_{\text{mas}}, S_k, S_{\text{mom}}\) and \(S_{\text{en}}\) are the sources due to exchange of mass (mixture), mass of species, momentum and energy between the continuous phase and the dispersed phase, respectively. \(R_k\) represents the source due to homogeneous and heterogeneous reactions in which species \(k\) are produced or consumed. The source term \(S_{\text{rad}}\) defines the contribution to the energy equation due to the radiation. The source term \(S_{\text{re}}\) stands for the amount of energy released in chemical reactions. Combustion of coal particle is divided into several steps, which include heating, evaporation, devolatilization, and finally char oxidation. To model the coal combustion the changes of particle mass and temperature need to be known. This is realized by solving the mass and energy balance equations for individual particles. The particle mass change during combustion can be defined as

\[
\frac{d m_p}{d t} = \frac{d m_{\text{char}}}{d t} + \frac{d m_{\text{vol}}}{d t} + \frac{d m_{\text{water}}}{d t}
\] (5)

where subscript \(p\) denotes the particle data (in one dispersed phase several materials with different physical properties can be tracked), \(m_{\text{char}}, m_{\text{vol}}\) and \(m_{\text{water}}\) are the masses of the char, volatiles and water in combustible particle, respectively. The motion of individual particle is modeled as

\[
\frac{d \mathbf{u}_p}{d t} = F_D (\mathbf{u} - \mathbf{u}_p) + \frac{g}{\rho_p} (\rho_p - \rho) - \frac{1}{\rho_p} \mathbf{V}
\] (6)

where \(\rho_p\) is the particle material density, \(F_D (\mathbf{u} - \mathbf{u}_p)\) is the particle acceleration due to drag. The drag coefficient \(F_D\) was calculated using the model for perfectly spherical particles by Morsi and Alexander [20]. The term \(-\nabla p/\rho_p\) defines the particle acceleration due to the pressure gradient at the particle location. The changes of particle position is calculated for its known velocity as

\[
\frac{d \mathbf{x}_p}{d t} = \mathbf{u}_p
\] (7)

The heat transfer between surrounding gases and the particle is taken into account by solving particle balance equation

\[
m_{\text{char}} \frac{dT_p}{d t} - A_p \alpha (T - T_p) + Q_c + A_p \varepsilon_p \sigma (T_h^4 - T_p^4)
\] (8)

where \(A_p\) and \(T_p\) stands for the particle heat capacity and temperature respectively, \(T\) is the temperature of gases inside a cell where the particle is located, \(\alpha\) denotes the heat transfer coefficient between particle and gases in vicinity to particle, \(\varepsilon_p\) is the particle emissivity, \(\sigma\) is the Stefan-Boltzmann constant and \(A_p\) is the external surface area of the particle. The incident radiation temperature \(\Phi\) can be calculated as

\[
\Phi = \left( \frac{C}{4\sigma} \right)^{1/4} \rightarrow G = \int_{\Omega}^{4\pi} I d\Omega
\] (9)

where \(I\) stands for the radiation intensity, \(\Omega\) is the solid angle, and \(G\) is the particle irradiation. The \(Q_c\) symbol in Eq. (8) represents the changes of energy due to the evaporation \(d m_{\text{h}_2}\), where \(h_{\text{h}_2}\) is the enthalpy of evaporation defined as

\[
h_{\text{h}_2} (T_p) = h_{\text{bp}} + \int_{t_p}^{t_{\text{bo}}} c_{\text{w}} dT - \int_{t_{\text{bo}}}^{t_{\text{bp}}} c_{\text{g}} dT
\] (10)

where the subscript \(\text{bp}\) defines the boiling point (373.15 K), \(c_{\text{w}}\) and \(c_{\text{g}}\) are the specific heats of water and water vapor, respectively. For simulation running at or near atmospheric pressure it can be assumed that the latent heat \(h_{\text{h}_2}(T_p)\) is equal to the latent heat \(h_{\text{h}_2}(T_{\text{bp}})\) at boiling temperature 2256.4 kJ/kg.

The \(Q_c\) parameter in the case of char surface combustion is defined as \(-f_{\text{d}m_{\text{H}_2} / d t}\), where \(H_{\text{H}_2}\) is the heat released by the surface reaction and \(f_{\text{d}}\) is the fraction of heat absorbed by the particle during char combustion process which in all simulations was set to 0.3. The term \(d m_{\text{H}_2}\) used for calculation of \(Q_c\) can be defined using different models representing actually considered process. High temperature and presence of participating gases, makes the heat exchange mode important in simulations of the energy transfer in the pulverized coal boiler. The gaseous phase was
modeled as an absorbing-emitting medium of temperature and composition dependent on absorption coefficient. The radiative transfer equation (RTE) for modeling radiation intensity in medium which contain particles is defined as [19].

\[
\nabla \cdot (\vec{s}I) + (a + a_p + \sigma_p)I(\vec{r}, \vec{s}) = \frac{\alpha^2 T^4}{\pi} + E_p \\
+ \frac{\sigma_D}{4\pi} \int \frac{I(\vec{r}, \vec{s}')\phi(s, s')d\Omega_f}{\sigma_{fl}}
\]

(11)

where \(a\) is the absorption coefficient, \(n\) refractive index, \(\vec{r}\) position vector, \(\vec{s}\) direction vector, \(\vec{s}'\) scattering direction vector, \(\phi\) is the phase function, \(\Omega_f\) is the solid angle, \(I\) stands for the radiation intensity which is function of position and direction. The \(a_p\) is the equivalent absorption coefficient, \(E_p\) is the equivalent emission, and \(\sigma_n\) is the equivalent particle scattering factor due to the presence of particles. Integration of the RTE (11) equation over angle was performed using the Discrete Ordinates (DO) method [21], while the spectral radiation properties of the optically active gases, i.e. CO2 and H2O were modeled with a constant absorption coefficient equal to 0.15, which has been evaluated using a stand alone 1D code for testing influence of radiative active gases on the heat transfer process [22], where spectral emissivity data of CO2 and H2O molecules were taken form HITEMP 2010 base [23]. Undoubtedly, to accurately simulate the spectral radiation properties of the optically active gases, the Weighted Sum of Gray Gases (WSGG) model should be used. Due to the long calculation time, the application of exact radiation model will be the subject of our further work.

The turbulence-chemistry interaction was modeled using the standard k-\(\varepsilon\) model, with a wall function approach [19,24].

The turbulence-chemistry interaction was modeled using the finite rate/eddy-dissipation model [19]. Combustion of volatiles was simulated using two homogeneous reactions (12) and (13). The set of reactions is supplemented with hydrogen combustion reaction (14).

\[
C_kH_{10}O_{m}N_{n}S_{o} + \frac{1}{2}O_{2} \rightarrow \frac{1}{2}CO + \frac{1}{2}H_{2}O + \frac{1}{2}SO_{2} + \frac{1}{2}N_{2}
\]

(12)

\[
CO + 0.5O_{2} \rightarrow CO_{2}
\]

(13)

\[
H_{2} + 0.5O_{2} \rightarrow H_{2}O
\]

(14)

where \(k, l, m, n, o\) are the stoichiometric coefficients and \(C_kH_{10}O_{m}N_{n}S_{o}\) is a fictitious species representing the volatiles, for which the subscripts \(k, l, m, n, o\) were calculated based on mass balances and their values along with the stoichiometric coefficients are given in Table 1.

It was assumed that the carbon content in the volatiles is the difference between the carbon content C from the ultimate analysis and fixed carbon (char) from the proximate analysis. The general rate expression for the finite rate model can be written as

\[
R_i = A_i T^{\beta_i} \exp \left( -\frac{E_i}{RT} \right) \prod_{j=1}^{n} \left( \frac{c_j}{\eta_j} \right)^{\eta_j}
\]

(15)

where \(A_i\) is the preexponential factor, \(E_i\) is the activation energy, \(n\) is the number of species taking part in the reaction \(i\), \(c_j\) is the molar concentration of species \(j\) expressed in mol/m^3 and \(\eta_j\) is the reaction order with respect to species \(j\). The rate constants for the homogeneous reactions are given in Table 2, where the volumetric reaction rate \(R_i\) is given in kmol/m^3 s.

The char combustion process was modeled using three reactions Eqs. (19)–(21), where the char gasification process in presence of CO2 and water vapor H2O is taken into account. This is important in case of modeling coal combustion process in oxidizer atmosphere containing high concentrations of CO2 and water vapor H2O [25,26]. To model multiple-surface reactions the rate of individual reaction \(i\) of surface species \(j\) can be expressed as

\[
\frac{dm_{p_{ij}}}{dt} = A_p \eta_j Y_j \frac{1}{1/R_{dif_{ij}} + 1/R_{kin_{ij}}}
\]

(16)

where \(p\) is the bulk partial pressure of the gas phase species reacting with surface species \(j\), \(\eta_j\) is the effectiveness factor which is related to the particle surface area, \(Y_j\) is the mass fraction of surface species \(j\) in the particle (if the particle contains only one species e.g. carbon this fraction is equal to 1), \(R_{dif_{ij}}\) is the diffusion rate coefficient for reaction \(i\) defined as

\[
R_{dif_{ij}} = C_j \frac{\beta_j}{d_{p}^{0.75}} \left( \frac{T_{p} + T}{2} \right)^{j}
\]

(17)

and \(R_{kin_{ij}}\) is the kinetic rate of reaction \(i\) expressed in the Arrhenius form as

\[
R_{kin_{ij}} = A_i T^{\beta_i} \exp \left( -\frac{E_i}{RT} \right)
\]

(18)

where \(A_i\) is the pre-exponential factor, \(\beta_i\) is the temperature exponent and \(E_i\) is the activation energy. The kinetic data \((A_i, \beta_i, \text{ and } E_i)\), as well as the diffusion rate constant \(C_j\) need to be provided for each reaction \(i\). In this study the required data were adapted from the work of Toporov et al. [27]. The data are summarized in Table 3.

<table>
<thead>
<tr>
<th>Reaction</th>
<th>(A_i) units vary</th>
<th>(\beta_i)</th>
<th>(E_i) J/kmol</th>
<th>(\eta_1)</th>
<th>(\eta_2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(12)</td>
<td>5.01e+11</td>
<td>0</td>
<td>2.0e+8</td>
<td>0.7</td>
<td>0.8</td>
</tr>
<tr>
<td>(13)</td>
<td>5.42e+9</td>
<td>0.75</td>
<td>1.26e+8</td>
<td>1</td>
<td>0.25</td>
</tr>
<tr>
<td>(14)</td>
<td>9.87e+8</td>
<td>0</td>
<td>3.1e+7</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

2.2. Fuel

The fuel used in the simulations is a bituminous coal from a Polish coal mine Janina. Reserves of this coal mine are the largest of

Table 1

| Volatiles formula coefficients and stoichiometric coefficients of the volatiles combustion reaction. |
|-----------------|--------|----------|----------|
| \(C_{k}H_{l}O_{m}N_{n}S_{o}\) | \(n_i\) | \(k\) | \(l\) |
| \(m\) | \(n\) | \(o\) | \(1.0340\) | \(2.6824\) | \(0.0034\) |
| \(O_{2}\) | \(CO\) | \(SO_{2}\) | \(N_{2}\) | \(0.7413\) | \(1.0340\) | \(0.0137\) | \(0.0034\) | \(0.0034\) | \(1.3412\) | \(0.0034\) | \(0.0137\) |
all existing coal mines in Poland, therefore this coal was selected as the prototype fuel. The proximate and ultimate analyses of the Janina coal is presented in Table 4.

### 2.3. Geometry of the model

The scheme of the MOFC boiler is taken from the design proposed by Schaffel et al. [14], which is a down fired MILD combustion boiler. The fuel and oxidizer (air) are supplied through the top wall of the boiler by a set of specially arranged jets. The inlets are located in such a way that fuel and oxidizer are separated by the distance which does not allow for fast mixing of both streams. The flue gases outlets from the boiler combustion chamber located at the top of the boiler forces to intensify boiler internal gases recirculation. The selected fuel and oxidizer inlets cross sections result in gas velocities in the range of 40–70 m/s. The resulting flow profile generates large internal recirculation. At the same time combustion products can reach the bottom of the boiler, which extends the fuel residence time. Oxidizer inlets inject the oxidizer directly into the internally recirculated flue gases stream. The final locations of the fuel and oxidizer jets were found by simulation of about 50 configurations and selecting the best one. The final dimensions of the boiler are 36 m long, 19 m high, and 20 m deep (see Fig. 2), which are selected to keep the firing density in the range of 50–70 kW/m³ and the average wall heat flux in the range of 100–140 kW/m². The boiler consists of 8 identical segments separated by heat release screens, allowing for firing each segment independently and facilitating the control of the boiler load. Each of the segments contain 2 fuel inlets, 2 oxidizer inlets and 1 outlet. The fuel inlet diameter is 0.327 m and the oxidizer inlet diameter is 0.298 m. The dimensions of the outlet are 2 m x 4 m. The segment is surrounded by heat release screens, which prevents mixing of combustion products with other neighboring segments. A single segment is shown in Fig. 3. Fuel jets are located close to the screen, creating a symmetry plane along the height of the boiler. The oxidizer jets are located roughly in the middle of the 1/8th segment of the boiler. Outlet of a rectangular cross section is located near the side wall of the boiler.

### 2.4. The mesh

The computational mesh was created using the ANSYS Meshing application. The generated mesh was composed of 712 thousand hexahedral and small fraction of tetrahedral cells. The quality of the mesh was monitored by checking following criteria: Minimum Orthogonal Quality equal to 0.22, and Maximum Ortho Skew equal to 0.66. The mesh configuration applied in this study is presented in Fig. 4.

### 2.5. Solution procedure

The SIMPLE pressure-velocity coupling scheme was used and the second order discretization schemes for all transport equations were applied to discretize the convective terms. Linear pressure interpolation scheme was used. All simulations were run in steady state.

### 3. Boundary data

As mentioned earlier, the model input data were calculated based on mass and energy balances coming from the simulations of the remaining portion of the plant, assuming 1000 MW thermal input (chemical energy in fuel) to the boiler. Mixture of 95% oxygen and 5% nitrogen (by volume) is used as the oxidizer. Additionally it is assumed that the recirculated flue gases used to transport the

---

### Table 3

<table>
<thead>
<tr>
<th>Reaction</th>
<th>$A_i$ kg/m² sPa</th>
<th>$\delta_i$</th>
<th>$E_i$ kJ/mol</th>
<th>$C_i$ s/K⁰.⁷⁵</th>
</tr>
</thead>
<tbody>
<tr>
<td>(19)</td>
<td>0.005</td>
<td>0</td>
<td>74</td>
<td>4.13 x 10⁻¹²</td>
</tr>
<tr>
<td>(20)</td>
<td>0.00192</td>
<td>0</td>
<td>147</td>
<td>4.12 x 10⁻¹²</td>
</tr>
<tr>
<td>(21)</td>
<td>0.00635</td>
<td>0</td>
<td>162</td>
<td>1.69 x 10⁻¹²</td>
</tr>
</tbody>
</table>

### Table 4

<table>
<thead>
<tr>
<th>Proximate analysis</th>
<th>Ultimate analysis</th>
</tr>
</thead>
<tbody>
<tr>
<td>wt %</td>
<td>wt % daf</td>
</tr>
<tr>
<td>Moisture</td>
<td>ar 10.7 c</td>
</tr>
<tr>
<td>Ash</td>
<td>ar 9.0 h</td>
</tr>
<tr>
<td>Volatiles</td>
<td>daf 55.59 o</td>
</tr>
<tr>
<td>LHV</td>
<td>MJ/kg ar 21.39 n</td>
</tr>
<tr>
<td></td>
<td>s 0.20</td>
</tr>
</tbody>
</table>

ar - as received; daf - dry ash free.
fuel through the mills to the furnace are purified by desulfurization and particulate matter removal systems. Finally they are dried to a level of 4% of moisture by mass. The RFG also contains a fraction of oxygen. Drying of the fuel in mills was assumed, which leads to reduction of the water content in coal to 0.04 kg H2O/kg dried fuel and an increase of moisture in the recirculated flue gas. A flue gas recirculation ratio \( mpr \) is defined, which is the ratio of dried recirculated flue gas mass flow rate \( m_{RFG,d} \) to the raw fuel mass flow rate \( m_{coal} \).

\[
mpr = \frac{m_{RFG,d}}{m_{coal}} \tag{22}
\]

To keep a constant thermal load of the boiler the mass flow rate of the raw coal was kept constant and equal to \( m_{coal,r} = 46.73 \) kg/s. The moisture released during drying of the raw coal in mills is therefore transferred to the recirculated flue gas, which changes the mass flow rate of coal to \( m_{coal} \) and of the RFG to \( m_{RFG} \). \( m_{coal} \) and \( m_{RFG} \) are the flow rates of gases introduced to the furnace in the CFD model. Calculations were performed for the selected geometry for three different excess oxygen ratios \( \lambda \) (1.05, 1.10, 1.15) and two flue gases recirculation ratios \( mpr \) (1.5, 2.0). It should be stressed that the excess oxidizer ratio \( \lambda \) is defined globally and thus includes the oxygen supplied in the oxidizer stream and in the recirculated flue gas. Assuming ideal mixing and long residence time of the coal particles in the chamber, the oxygen excess ratio one would lead to best boiler efficiency. In reality such an approach would lead to incomplete combustion and presence of combustible components in the flue gases. Thus, the quality of combustion as a constraint, the optimal oxygen excess is sought for. Similarly, the recirculating ratio should be as small as possible to reduce the pumping work. Too small values of the RFG would not allow for drying the fuel and driving it into the chamber. It would also be difficult to organize intensive internal recirculation within the chamber, with too low stream of recirculated flue gases. The parameters at inlets of the model for each of the analyzed cases are presented in Table 5.

4. CFD modeling results

Appropriate selection of the furnace geometry and arrangement of fuel and oxidizer inlets causes internal recirculation inside the combustion chamber. Furthermore, the position of the oxidizer jets closer to the side walls of the chamber was selected such that the recirculated flue gas dilutes and heats up the oxidizer (cf. Fig. 3). The fuel inlets are placed near the central wall and closer to the center of the chamber. In Fig. 6 the obtained flow patterns of gas flow inside the chamber are shown. As can be seen the desired internal mixing of flue gas with injected oxidizer is obtained. Both, the fuel and the oxidizer jets, penetrate deeply into the chamber expanding the volume of the reaction zone. This brings the combustion in the furnace close to the MILD conditions. The flue gases flow is then turned upward. A portion of the gas leaves the chamber through the outlet, while the remaining part dilutes the oxidizer inlet. This effect has been obtained by an introduction of high momentum jets entraining the flue gases. The diameters of the fuel and oxidizer inlets were selected to achieve this goal. Velocity profiles in cross sections of combustion chamber are shown in Fig. 5. It can be seen that the oxidizer stream bends towards the fuel stream.

A typical property of MILD combustion is a more equilibrated temperature distribution than in regular combustion. This is achieved by a diluted and heated up oxidizer stream. In the combined MILD and OXY combustion realized within this study, the task of diluting the oxidizer is particularly difficult due to the high oxygen content (95% vol.) in the oxidizer. In Fig. 7 the contours of oxygen mole fraction in the fuel inlet plane is presented. The internal recirculation, which causes dilution of the oxygen allows for obtaining a maximum of 30% vol. of oxygen close to the fuel jet. As can be seen this is the only region of such high oxygen content and in the remaining of the space, typical concentrations for MILD combustion occur. In Fig. 8 the obtained temperature distributions for the analyzed cases are presented. As can be seen the occurrence of high temperature regions is not completely avoided, however the maximum temperatures do not exceed 1800 °C. Apparently, the reaction zone occupies a large portion of the furnace volume. The flue gas recirculation ratio \( mpr \) is considerably affecting the overall flow pattern in the furnace. For the \( mpr = 2 \) the fuel and oxidizer jets penetrate deeper to the bottom of the furnace.

Selected global results obtained from the computations are presented in Table 6, where furnace outlet \( T_{out} \) and maximum \( T_{max} \) temperatures, heat transferred \( Q \), heat flux densities \( q \) and thermal efficiencies \( \eta_{th} \) of combustion chamber are summarized for all of the analyzed cases. The heat transferred is calculated for the entire boiler, which included the 8 segments and the thermal efficiency is defined as the ratio of heat transferred in the furnace to the

<table>
<thead>
<tr>
<th>( \lambda )</th>
<th>( mpr )</th>
<th>inlet mass flow rates</th>
<th>RFG composition</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>( m_{coal} )</td>
<td>( m_{RFG} )</td>
</tr>
<tr>
<td>1.05</td>
<td>1.5</td>
<td>77.96 43.47 73.35</td>
<td>79.19 2.50 13.34</td>
</tr>
<tr>
<td>1.10</td>
<td>1.5</td>
<td>80.23 43.47 73.35</td>
<td>76.86 4.90 13.28</td>
</tr>
<tr>
<td>1.15</td>
<td>1.5</td>
<td>82.54 43.47 73.35</td>
<td>74.64 7.21 13.22</td>
</tr>
<tr>
<td>1.05</td>
<td>2.0</td>
<td>79.68 43.47 96.72</td>
<td>81.46 2.26 11.19</td>
</tr>
<tr>
<td>1.10</td>
<td>2.0</td>
<td>81.71 43.47 96.72</td>
<td>79.33 4.45 11.15</td>
</tr>
<tr>
<td>1.15</td>
<td>2.0</td>
<td>81.71 43.47 96.72</td>
<td>77.28 6.56 11.10</td>
</tr>
</tbody>
</table>
chemical energy introduced in the fuel. As discussed earlier, location of the convective part of the boiler, which is not considered in CFD model, was assumed downstream of the furnace outflow to improve thermal efficiency. Increase of flue gas recirculation ratio from 1.5 to 2.0 leads to decrease of outflow temperature, however the peak temperatures are higher. The highest thermal load and efficiency was obtained for excess ratio $\lambda = 1.15$ and recirculation ratio $mpr = 1.5$.

One of objectives of performed calculations was to verify the possibility of applying small excess oxidizer ratio. In Table 7 carbon dioxide, oxygen and overall char conversion are presented. Furthermore the oxygen content at the outlet of the furnace obtained from the CFD simulation is compared to the oxygen computed from stoichiometric calculations (an.), based on the assumption of complete combustion, is shown. It can be concluded that the burnout of char in the furnace is at acceptable level in all considered cases. The highest value of over 99% was obtained for the largest excess oxidizer ratio ($\lambda = 1.15$) and $mpr = 2.0$, as expected. From the viewpoint of the desired lowest oxygen demand and energy demand for flue gas fans power supply, most profitable case is that corresponding to $\lambda = 1.05$ and $mpr = 1.5$. At these conditions the char conversion is at a satisfactory level. The relatively high temperature of the flue gases at the furnace outlet need to be recovered in the convective part of the boiler.

Results presented in Table 7 and Fig. 9 confirm, that the main part of flue gas comprises the carbon dioxide. The remaining part of the mixture is shared mainly by water vapor, oxygen and nitrogen.

In order to prove that the MOFC boiler is operated at lower temperature levels, characteristic for the MILD combustion technology, the results from this study were compared with temperature distribution obtained from a CFD simulation of another PC boiler operated at OXY combustion. The considered boiler is the OP650 boiler producing 180 kg/s of steam at 13.5 MPa and 560 °C. Details of the boiler, the model and simulation results were presented elsewhere [28]. In Fig. 10 a cumulative distribution function (CDF) representing the probability of finding a given temperature in the volume of the combustion chamber. As can be seen, much lower temperatures were obtained for the MOFC boiler and their spread is narrower, which means that the temperature is more evenly distributed in the volume of the MOFC boiler than in the standard oxycombustion case.
Thermodynamic analysis of the cycle

Based on the results obtained from the CFD modeling of the MILD-OXY Fuel Combustion boiler (MOFC), a preliminary thermodynamic evaluation of the whole power plant has been conducted. The technique used was based on mass and energy balances and input-output principle. In first step, the convective part of the boiler was added, as well as oxygen and recycled CO₂ heat exchangers. Furthermore, the coal mills were taken into account, together with primary recycle fans. The whole model of the boiler island, treating the results of the CFD modeling as input parameters, was elaborated by means of the Ebsilon Professional software. Based on the assumed input-output approach, the power plant was divided into six technological modules, viz. boiler island, steam cycle, cooling water module, flue gas quality control unit, air separation unit and CO₂ processing unit. Within the study, the CO₂ transport and storage was neglected. The detailed explanation of the proposed approach (e.g. ‘input-output’ mathematical models of direct energy and material balance) have been already discussed in Refs. [29–31].

### Table 6
Simulation results - temperatures (outflow and maximum), heat fluxes (global on screens and specific) and thermal efficiency of the boiler.

<table>
<thead>
<tr>
<th>λ</th>
<th>mpr</th>
<th>T_{out} °C</th>
<th>T_{max} °C</th>
<th>Q, MW</th>
<th>q, W/m²</th>
<th>ηₜh, %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.05</td>
<td>1.5</td>
<td>1134</td>
<td>1515</td>
<td>745.5</td>
<td>111.2</td>
<td>73.7</td>
</tr>
<tr>
<td>1.10</td>
<td>1.5</td>
<td>1111</td>
<td>1535</td>
<td>766.6</td>
<td>114.3</td>
<td>75.8</td>
</tr>
<tr>
<td>1.15</td>
<td>1.5</td>
<td>1047</td>
<td>1581</td>
<td>778.7</td>
<td>116.1</td>
<td>77.0</td>
</tr>
<tr>
<td>1.05</td>
<td>2.0</td>
<td>989</td>
<td>1539</td>
<td>740.3</td>
<td>110.4</td>
<td>73.1</td>
</tr>
<tr>
<td>1.10</td>
<td>2.0</td>
<td>982</td>
<td>1605</td>
<td>749.9</td>
<td>111.8</td>
<td>74.0</td>
</tr>
<tr>
<td>1.15</td>
<td>2.0</td>
<td>958</td>
<td>1605</td>
<td>756.3</td>
<td>112.8</td>
<td>74.6</td>
</tr>
</tbody>
</table>

### Table 7
Simulation results - carbon dioxide concentration, oxygen concentration compared to oxygen concentration for complete combustion (an.) and char conversion.

<table>
<thead>
<tr>
<th>λ</th>
<th>mpr</th>
<th>CO₂,out % vol.</th>
<th>O₂,out (CFD) % vol.</th>
<th>O₂,out (an.) % vol.</th>
<th>char conv. %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.05</td>
<td>1.5</td>
<td>67.71</td>
<td>3.16</td>
<td>2.18</td>
<td>96.5</td>
</tr>
<tr>
<td>1.10</td>
<td>1.5</td>
<td>66.53</td>
<td>4.87</td>
<td>4.28</td>
<td>97.8</td>
</tr>
<tr>
<td>1.15</td>
<td>1.5</td>
<td>65.04</td>
<td>6.75</td>
<td>6.33</td>
<td>97.9</td>
</tr>
<tr>
<td>1.05</td>
<td>2.0</td>
<td>70.09</td>
<td>2.72</td>
<td>1.97</td>
<td>96.5</td>
</tr>
<tr>
<td>1.10</td>
<td>2.0</td>
<td>68.83</td>
<td>4.31</td>
<td>3.89</td>
<td>98.4</td>
</tr>
<tr>
<td>1.15</td>
<td>2.0</td>
<td>67.63</td>
<td>5.84</td>
<td>5.75</td>
<td>99.5</td>
</tr>
</tbody>
</table>

Fig. 8. Temperature field in the cross sections through the fuel inlet of boiler segment for the analyzed cases.

Fig. 9. Contours of carbon dioxide mole fraction in a cross section through the fuel inlet for λ = 1.05 and mpr = 2.0.
as well as the Oxy System Analysis (OSA) program, that was used within this study \[32\]. The core of the proposed analysis relays on the input-output tables of an integrated power plant, where three specific groups of energy carriers and materials have been distinguished, viz.: main products (corresponding to each technological modules), by-products and external supplies. The mathematical model of direct energy and material balance, based on the proposed input-output approach, takes the following form for main products:

\[
G + F_{\text{FG}}G + D_G = A_GG + K_G
\]  

(23)

by-products:

\[
F_{\text{FG}} = A_FG + K_F
\]  

(24)

external supplies:

\[
D_D = A_DG
\]  

(25)

where \(G\) vector of the main production; \(F_{\text{FG}}, F_F\) matrices of the coefficients of by-production supplementing and not supplementing the main production, respectively; \(D_G, D_D\) vectors of external supplies supplementing and not supplementing the main production, respectively; \(A_G, A_F, A_D\) matrices of the coefficients of consumption the main products, by-products and external supplies, respectively; \(K_G, K_F\) vectors of final production of the main products and by-products, respectively. As mentioned before, the boiler island was modeled by means of combination of CFD and process modeling. For the other technological modules of an integrated MOFC power plant, the necessary data for input-output analysis were taken over from the process models developed by means of other commercial software, as well as the data base of OSA program. Thus the set of the input data for the input-output model have been gathered (in form of the coefficients of vectors and matrices), and based on Eqs. (23)–(25), the thermodynamic assessment have be performed. At this step seven cases (integrated power plants) have been investigated, including six which were based on the results of the CFD modeling presented in this paper (MOFC power plants with different \(O_2\) excess and \(CO_2\) recirculation rates) and one reference conventional oxyfuel combustion power plant (Table 8). The results of the assessment are presented in Table 9, where the obtained net and gross powers, as well as net energy efficiencies have been presented. Additionally, the net energy efficiency increase (in comparison with the reference conventional oxyfuel combustion case) has been presented, which resulted from the MOFC boiler presence. In Fig. 11 the net energy efficiencies of the analyzed MOFC cases have been presented.

The increase of the net energy efficiency with the decreasing \(CO_2\) recirculation rate can be seen. This is the results of the lower electricity consumption for the recycle fans, as well as lower flue gas stream that enters the CPU. Additionally, a slight increase of efficiency associated with the lower oxidizer excess ratio can be noticed, as for this case the lower electricity consumption in ASU take place. The highest efficiency was obtain for the MOFC with \(\lambda = 1.1\) and \(mpr = 1.5\), which shows it might be justified to keep the oxidizer excess ratio on higher level, due to the combustion process efficiency within the boiler. It should be stressed, that the presented results should be treated as a proof of concept. Further, more detailed studies both on the level of process analysis and CFD simulation are required. The detailed process models of the whole integrated MOFC power plant with \(CO_2\) transport and storage need to be developed, and other option for the increase of net energy efficiency (e.g. heat integration) investigated. The results of this study correlates with the previous analysis by the authors \[31\], where depending on the analyzed cases, the net energy efficiency increase due to the MOFC boiler application were between 1 and 2% points (for the \(mpr = 2\) and \(\lambda = 1.15\)). Nevertheless, the presented results of the thermodynamic analysis proves that MOFC technology might be a suitable way to reduce the energy penalty associated with the \(CO_2\) capture for coal-fired power plants.

6. Conclusions

In the paper the concept of a large scale boiler operated at combined MILD and OXY combustion conditions was analyzed. The boiler of 1000 MW was divided into 8 equivalent segments and the CFD analysis was performed for a single segment only. Furthermore the convective part of the boiler was not modeled in the CFD framework. The obtained results show that appropriate organization of the flow in the combustion chamber allows for inducing internal recirculation of flue gases. This in turn considerably diluted the oxidizer stream prior to combustion, even though a high oxygen content oxidizer was introduced. The maximum temperatures in the combustion chamber did not exceed 1800 °C and the temperature was moderately well distributed throughout the furnace. Detailed examination of the results revealed that the fraction of chemical energy introduced in the fuel and recovered in the furnace was between 73.7 and 77.0%. At the same time a good carbon conversion rate was maintained (96.5—99.5%), with the lowest values corresponding to the very small excess oxidizer ratios of \(\lambda = 1.05\). Finally, the obtained results confirm, that the synergistic effects of both, MILD and OXY combustion technologies, can be used for coal combustion with several benefits coming directly from the original MILD and OXY techniques.

The whole process modeling of the entire power plant, taking the results of the CFD analysis as an input has shown that, when compared with the standard oxycombustion plant, more than 3% points increase of energy efficiency can be expected. This confirms the synergy of the MILD and OXY combustion. These preliminary results were based on several quite crude simplifications. Further research on MILD-OXY combustion to weaken these simplifications are in progress.

Acknowledgments

The research leading to these results has received funding from the Polish-Norwegian Research Program operated by the National

### References


