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COMPUTATIONAL FLUID DYNAMIC METHOD IN COAL COMBUSTION MODELING: POLLUTANTS FORMATION IN AIR AND OXY ATMOSPHERE

ZASTOSOWANIE NUMERYCZNEJ MECHANIKI PŁYNÓW W MODELOWANIU SPALANIA WĘGLA W ATMOSFERZE POWIETRZA I OXY

Abstract: Despite the fact that alternative energy sources sector has been rapidly developed since last years, coal combustion as a major fossil-fuel energy resource (especially in Poland) will continue being a major environmental concern for the next few decades. To meet future targets for the reduction of toxic and greenhouse gases emission new combustion technologies need to be developed: pre-combustion capture, post-combustion capture, and oxy-fuel combustion (the process of burning a fuel using pure oxygen instead of air as the primary oxidant). This paper deals with the air-fired and oxy-fuel hard and brown coal combustion (pulverized coal) combustion, and its impact on pollutants (NO_x and SO₂) formation.

For CFD modeling of media flows and hard and brown coal combustion process the laboratory model of combustion reactor was applied. The material input was set based on technical-elementary analysis of pulverized coal used in experiment and sieves grain-size analysis. Boundary conditions (media flows intensities and temperatures), was set based on laboratory experimental measurements. Radiation case-sensitive WSGGM model (weighted – sum – of – gray – gases model) was used for calculation. The modeling was proceed for different combustion parameters in air and OXY atmosphere in oxygen/fuel ratio variation and fuel humidity variation function. The results was presented in tables and in figures

Keywords: CFD modeling, coal combustion, radiation model, hard coal, brown coal

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Introduction

The role of coal as an energy source has attracted renewed interest due to the stability of its supply and its relatively low cost, which will probably guarantee its inclusion in the energy mix in the foreseeable future [1, 2]. However, coal combustion produces a large amount of CO₂, which is the chief contributor to global climate change. To meet future targets for the reduction of greenhouse gas emissions, CO₂ must be captured and stored [2]. Oxy-coal combustion is a carbon abatement technology that can be used for the capture of carbon dioxide (CO₂) from coal-fired power plants. The amount of unburnt carbon or the Loss on Ignition (LOI) depends on the particle residence time in the furnace, the temperature and the availability of oxygen along the particle path [3].

Considerable knowledge of the fundamentals of heat and mass transfer, combustion processes and pollutant formation under CO₂ – rich conditions has been acquired through extensive experiments and modeling efforts in recent years. However, many fundamental issues remain uninvestigated [4]:

- Oxy-combustion characteristics of different coal types;
- Models for sub-processes (models for devolatilization, char formation, agglomeration and coal group combustion under the oxy-combustion conditions are mostly based on air combustion studies);
- Scaling characteristics of oxy-combustion;

Pressure effect (when operating under elevated pressure, the gas phase flowfield and coal particle residence time may change significantly).

An important issue of implementation this technology is also its impact on problem of pollutants formation, *ie* thermal NO_x due to the absence of nitrogen gas in the combustion atmosphere and SO₂ formation from contaminated fossil fuel.

The authors presents results of simulation witch aim was investigation of NO_x and SO₂ forming during hard and brown coal combustion process in the laboratory reactor using numerical tools.

Methodology

For CFD modeling of media flows and coal combustion process the laboratory model of combustion reactor was applied. The material input was set based on technical-elementary analysis of pulverized coal used in experiment and sieves grain-size analysis. Boundary conditions (media flows intensities and temperatures). was set based on laboratory experimental measurements. Radiation case-sensitive WSGGM model (weighted – sum – of – gray – gases model) was used for calculation. The modeling was proceed for different combustion parameters in air and OXY atmosphere in oxygen/fuel ratio variation and fuel humidity variation function.

Boundary conditions

In Table 1 the results of technical-elementary analysis of applied fuel are presented.

Table 1

Technical-elementary analysis of applied fuel (pulverized hard and brown coal)

Coal proximate analysis	Hard coal	Brown coal
Moisture content [wt. %]	13.23	7.22
Ash [wt. %, db]	4.96	16.2
V.M. [wt. %, db]	30.64	70.0
F.C. [wt. %, db]	51.17	6.58
Heating value [MJ/kg, db]	25.5	19.2
Ultimate analysis [wt. %, daf]		
C	73.60	66.6
H	5.26	6.50
N	1.44	0.74
S	0.80	0.18
O	18.9	26.0
Sieves grain-size analysis: fraction [%]		
< 63 μm	34.08	28.05
63–80 μm	26.51	11.58
80 μm – 0.106 mm	25.29	15.15
0.106 mm–0.160 mm	7.39	36.02
> 0.2 mm	6.73	9.2

Five lambda coefficient value (λ : 0.83; 1.0; 1.1; 1.3; 1.35) and four values of humidity (φ : 0, 7, 14, 21) was chosen to the modeling.

Results

The results was presented in tables and in figures below.

Simulation of hard coal combustion process

In Table 2 the simulation results for hard coal are presented for each lambda value and humidity function.

In Fig. 1 the chosen results of particular exhaust gases components concentrations are presented in lambda coefficient function on example of 7 % humidity content in the fumes.

Combustion process in OXY atmosphere caused almost 70 % increase in dicarbon oxide concentration. The highest values was observed during the fuel combustion in 20/80 oxy-atmosphere, the insignificant decrease (~8 %) of CO₂ concentration was noticed for all oxy-coal combustion processes. The oxygen share increase in OXY-combustion caused few-percent CO₂ concentration reduction.

Table 2
Simulation results for pulverized hard coal combustion: NO_x, SO₂, CO₂, O₂ concentrations in λ and humidity function

p. %	NO _x [ppm]						SO ₂ [ppm]						CO ₂ [% vol.]						O ₂ [% vol.]					
	0	7	14	21	0	7	0	7	14	21	0	7	0	7	14	21	0	7	0	7	14	21		
λ	air																							
0.83	0	0	9	87	1545	1453	1400	1308	169	16.9	16.9	14.9	14.9	16.5	14.9	0	0	0	0.1	1.8				
1.00	53	75	114	255	1321	1251	1177	1104	16	14.9	14	12.9	12.9	14	12.9	1.3	2.4	3.4	3.4	4.4				
1.10	104	137	229	290	1219	1157	1091	1019	14.7	13.8	13	12.1	12.1	13	12.1	2.9	3.8	4.6	4.6	5.5				
1.20	163	208	288	367	1123	1068	1007	942	13.4	12.7	11.9	11.1	11.1	11.9	11.1	4.4	5.11	5.9	5.9	6.8				
1.35	288	342	400	430	1012	957	902	844	11.9	11.4	10.6	10	10	10.6	10	6.2	6.7	7.6	7.6	8.2				
λ	OXY 20/80																							
0.83	40	54	72	100	1139	1087	1015	953	90.3	88.6	86.9	85.1	85.1	86.9	85.1	1.9	3.1	4.2	4.2	5.5				
1.00	81	93	150	190	955	904	852	799	87.7	86.4	85	83.5	83.5	85	83.5	5.8	6.6	7.6	7.6	8.6				
1.10	132	175	204	215	880	835	786	738	86.6	85.3	84	82.8	82.8	84	82.8	7.4	8.2	9.2	9.2	9.8				
1.20	154	194	232	300	812	768	725	680	85.7	84.5	83.3	82.1	82.1	83.3	82.1	8.7	9.6	10.4	10.4	11.2				
1.35	193	267	297	304	726	688	649	609	84.5	83.5	82.4	81.4	81.4	82.4	81.4	10.5	11.2	11.9	11.9	12.6				
λ	OXY 25/75																							
0.83	45	55	88	119	1156	1096	1033	970	84.6	83.2	81.4	79.6	79.6	81.4	79.6	7.6	8.5	9.8	9.8	11				
1.00	84	124	143	185	971	921	868	813	82.1	80.7	79.5	77.9	77.9	79.5	77.9	11.4	12.4	13.1	13.1	14.1				
1.10	117	142	192	256	895	849	800	750	81.1	79.8	78.6	77.3	77.3	78.6	77.3	12.9	13.7	14.5	14.5	15.4				
1.20	147	209	242	287	825	782	738	691	80.1	79	77.8	76.6	76.6	77.8	76.6	14.4	15.1	15.9	15.9	16.6				
1.35	198	258	289	346	738	700	660	619	78.9	77.9	76.8	75.7	75.7	76.8	75.7	16.2	16.8	17.6	17.6	18.2				
λ	OXY 30/70																							
0.83	52	62	83	117	1175	1114	1051	984	79.4	77.7	76.2	74.5	74.5	76.2	74.5	12.8	14.1	15	15	16.2				
1.00	90	126	152	205	987	935	882	826	76.8	75.5	74.1	72.7	72.7	74.1	72.7	16.8	17.6	18.5	18.5	19.4				
1.10	119	176	209	232	909	862	813	762	75.7	74.5	73.2	71.9	71.9	73.2	71.9	18.3	19.1	19.9	19.9	20.7				
1.20	138	199	262	300	838	794	749	702	74.7	73.5	72.4	71.2	71.2	72.4	71.2	19.8	20.6	21.3	21.3	22				
1.35	214	276	326	390	749	710	670	627	73.4	72.4	71.4	70.3	70.3	71.4	70.3	21.7	22.3	22.9	22.9	23.6				

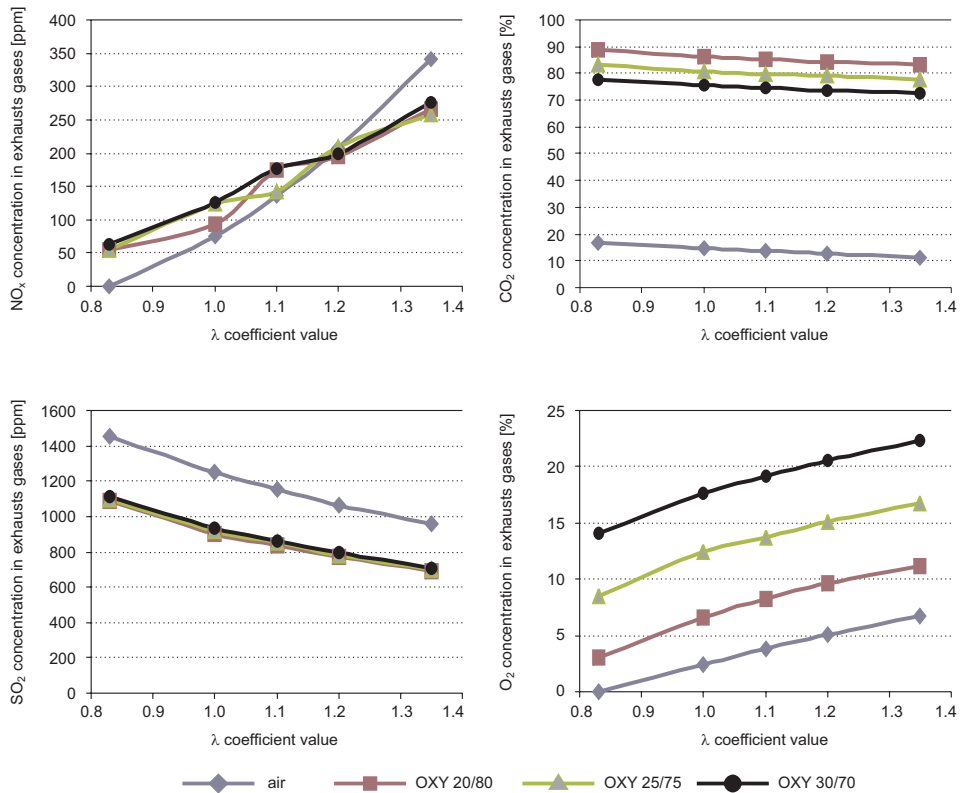


Fig. 1. The concentration of NO_x, SO₂, O₂ and CO₂ in lambda coefficient function for various OXY atmosphere (7 % humidity content in the fumes) during pulverized hard coal combustion

The nitric oxides concentration was rapidly rising due to lambda coefficient increase – in case of all oxy-coal combustion processes a concentration range was reduced and its maximum level is lower more than 100 ppm in comparison to air combustion.

Despite the fact that SO₂ concentration pattern is similar for all oxy-atmospheres and for the air-atmosphere, the SO₂ contents in the exhausts in case of oxy-coal combustion is about 400 ppm lower in comparison to air-combustion process.

Simulation of brow coal combustion process

In Table 3 the simulation results for brown coal are presented for each lambda value and humidity function.

In Fig. 2 the chosen results of particular exhaust gases components concentrations are presented in lambda coefficient function on example of 7 % humidity content in the fumes.

Similarly to hard coal, the highest carbon dioxide concentration was observed during the fuel combustion in 20/80 oxy-atmosphere, the insignificant decrease of CO₂ concentration was noticed for other oxy-coal combustion processes (the oxygen share

Table 3
Simulation results for pulverized brown coal combustion: NO_x, SO₂, CO₂, O₂ concentrations in λ and humidity function

φ %	NO _x [ppm]			SO ₂ [ppm]			CO ₂ [% vol.]			O ₂ [% vol.]						
	0	7	14	21	0	7	14	21	0	7	14	21				
λ	air															
0.83	230	338	395	491	378	361	340	319	15.5	14.6	13.7	12.7	1.6	2.4	3.4	4.3
1.00	397	444	582	608	320	305	287	270	13	12.3	11.5	10.8	4.6	5.3	6.1	6.8
1.10	479	503	656	855	296	282	265	249	12	11.3	10.6	9.9	5.8	6.5	7.22	7.9
1.20	599	617	731	814	274	261	245	230	11.1	10.4	9.8	9.2	7	7.6	8.2	8.9
1.35	747	708	828	845	244	233	220	206	9.9	9.4	8.8	8.3	8.4	8.9	9.5	10.1
λ	OXY 20/80															
0.83	213	305	336	372	277	263	247	233	85	83.6	82.3	80.8	5.7	6.6	7.5	8.4
1.00	357	390	470	510	233	221	208	195	83.3	82.2	81	79.8	8.9	9.6	10.4	11.1
1.10	406	458	497	644	215	204	192	180	82.6	81.6	80.5	79.4	10.2	10.8	11.5	12.3
1.20	479	510	602	677	198	188	177	166	81.9	81	80	79	11.4	11.9	12.6	13.3
1.35	569	616	774	834	178	168	159	149	81.2	80.3	79.4	78.6	12.9	13.4	13.9	14.5
λ	OXY 25/75															
0.83	217	301	352	399	282	267	252	236	79.5	78.2	76.8	75.5	11.1	12.1	12.9	13.8
1.00	327	395	423	538	237	225	212	199	77.8	76.7	75.5	74.4	14.4	15.1	15.8	16.5
1.10	400	467	587	622	218	207	196	183	77.1	76.1	75	74	15.7	16.4	17	17.7
1.20	434	535	545	707	201	191	180	169	76.4	75.5	74.5	73.6	16.9	17.5	18.1	18.7
1.35	570	742	735	864	180	171	161	151	75.6	74.8	73.9	73	18.4	18.9	19.5	20
λ	OXY 30/70															
0.83	240	273	307	452	287	272	256	239	74.2	73	71.7	70.3	16.4	17.2	18.1	19
1.00	340	404	465	584	241	228	215	201	72.5	71.4	70.3	69.2	19.7	20.4	21.1	21.7
1.10	396	423	541	581	222	210	199	186	71.7	70.7	69.7	68.7	21.1	21.7	22.3	22.9
1.20	468	540	628	690	204	194	183	172	71	70.2	69.2	68.3	22.3	22.9	23.4	24
1.35	540	660	788	787	183	173	164	153	70.2	69.4	68.6	67.7	23.8	24.4	24.8	25.4

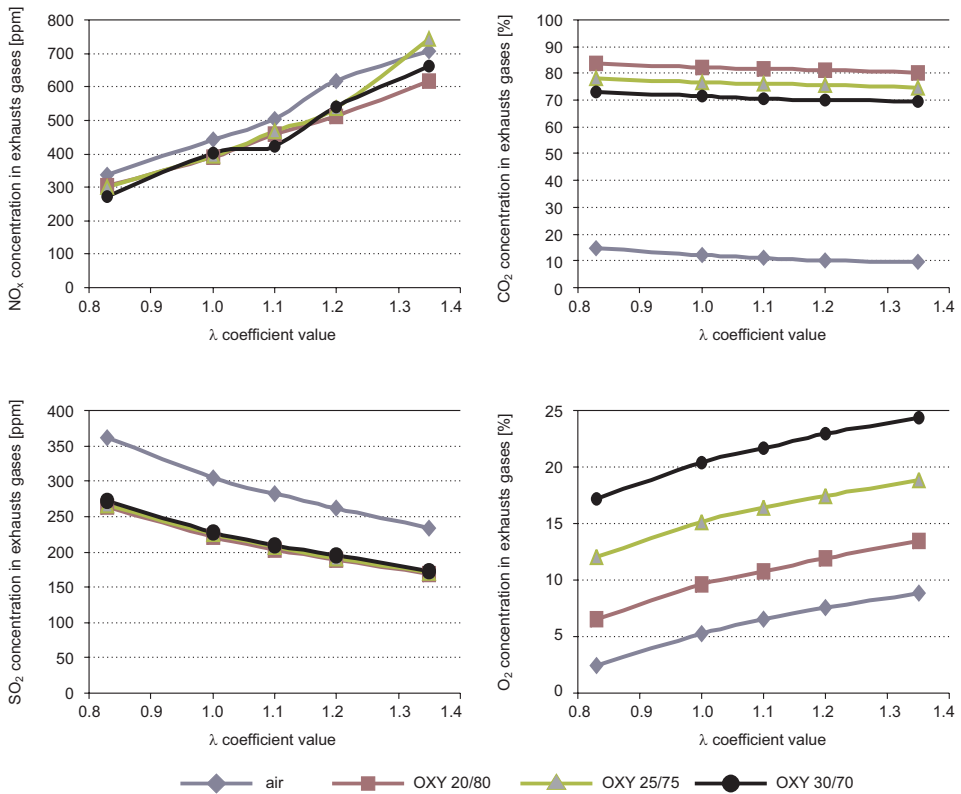


Fig. 2. The concentration of NO_x, SO₂, O₂ and CO₂ in lambda coefficient function for various OXY atmosphere (7 % humidity content in the fumes) during pulverized brown coal combustion

increase in OXY-combustion caused CO₂ concentration reduction). In case of brown coal combustion CO₂ concentrations are approximately 10 % lower than for hard coal in all atmospheres.

The nitric oxides emission in process of brown coal combustion is significantly higher than for hard coal (concentration range: near zero to 350 almost ppm for hard coal and 270 to 740 for brown coal). The highest value of NO concentration was noticed for 27/75 OXY combustion (for air combustion – in hard coal combustion process).

The lower sulfur content in the fuel caused also 4 times lower SO₂ concentration in comparison with hard coal. For all OXY-atmospheres the concentrations in function of lambda coefficient is almost 100 ppm higher than in case of air-combustion (similar situation was observed for hard coal combustion)

Summary

CFD approaches have been used in studies to better understand the flowfield and combustion processes in oxy-coal combustion and provide predictions of minor species and pollutant formations. Radiation heat transfer plays a major role in the furnace, and it

also governs the energy equation in combustion. The authors of the paper applied turbulence-radiation model for simulation.

The results of the modeling oxy-coal combustion indicate that the method is more advantageous in aspect of pollutant emission than air-combustion of coal. The fuel comparison analysis indicates that for brown coal combustion lower CO₂ but higher NO and SO₂ emission was observed than for hard coal. The pollution formation in the reactor seems to proceed in visible different mode than in air-coal combustion process. The CFD modeling of the oxy-coal combustion process is a proper tool for oxy-coal process investigation and understanding for better control of pollutant emission by combustion parameters optimization.

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ZASTOSOWANIE NUMERYCZNEJ MECHANIKI PŁYNÓW W MODELOWANIU SPALANIA WĘGLA W ATMOSFERZE POWIETRZA I OXY

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Abstrakt: Pomimo faktu gwałtownego rozwoju sektora alternatywnych źródeł energii w ostatnich dziesięcioleciach, spalanie węgla jako najważniejszego źródła energii konwencjonalnej (w szczególności w Polsce) jest bardzo istotnym zagadnieniem w aspekcie ochrony i inżynierii środowiska. Nowe wyzwania w zakresie obniżania emisji związków toksycznych, a także gazów cieplarnianych wymuszają rozwój w zakresie innowacyjnych technologii spalania węgla: pierwotnych (na etapie substratów) oraz wtórnych (na etapie produktów), a także modyfikacji procesu spalania (atmosfera OXY). W artykule zajęto się zagadnieniem formowania się zanieczyszczeń (NO_x oraz SO₂) powstających podczas procesu spalania pyłu węgla kamiennego i brunatnego w atmosferze powietrza oraz atmosferze OXY.

Do obliczeń CFD przepływu i spalania mieszanki powietrzno-węglowej wykorzystano model laboratoryjnego pieca opadowego. Jako warunki materiałowe do obliczeń posłużono się rzeczywistymi analizami techniczno-elementarnymi pyłu węglowego. Przedziały frakcyjne cząstek ustalono na podstawie analizy sitowej. Warunki brzegowe (temperaturę pieca, doprowadzanego powietrza oraz paliwa, natężenia przepływu powietrza pierwotnego i wtórnego) ustalono na podstawie pomiarów rzeczywistych w warunkach laboratoryjnych. W celu zamodelowania spalania z uwzględnieniem radiacji wykorzystano model WSGGM (weighted – sum – of – gray – gases model). Obliczenia z uwzględnieniem radiacji oraz powstawania zanieczyszczeń NO_x i SO₂ prowadzono dla warunków spalania w powietrzu oraz przyjęto różnicowane atmosfery OXY. Obliczenia prowadzono w funkcji wartości współczynnika lambda oraz dla różnych wartości wilgotności paliwa.

Słowa kluczowe: modelowanie CFD, spalanie pyłu węglowego, węgiel kamienny, węgiel brunatny, OXY, radiacyjny model spalania