A comprehensive model of NOx and SO₂ emissions from advanced coal combustion in a complex geometry CLC equipment

Jaroslaw Krzywanski[1*], *Tomasz* Czakiert[2], *Anna* Zylka[1] , *Kamil* Idziak[2], *Karol* Sztekler and *Wojciech* Nowak[3]

[1]Jan Dlugosz University in Czestochowa; A. Krajowej 13/15, 42-200 Czestochowa, Poland
[2]Czestochowa University of Technology, Dabrowskiego 73, 42-200 Czestochowa, Poland
[3]AGH University of Science and Technology, A. Mickiewicza 30, 30-059 Cracow, Poland

Abstract. The paper describes experiences in the modeling of complex geometry CLC equipment. The facility consists of two reactors: the air reactor and the fuel reactor. The fuzzy logic (FL) methods are used in the study for the prediction of NO_x and SO_2 from the solid fuels combustion in CLC equipment. Maximum errors between measured and predicted results are lower than 10 %.

1 Introduction

Fluidized bed technology is a convenient method for co-firing of coal and biomass [1,2]. Different combustion atmospheres can be applied in such systems, including air-firing mode and oxy-combustion conditions [3–5], generating flue gas, mainly composed of CO_2 and H_2O, which is almost suitable for geological storage [6,7]. Similar applies to CLC and CLOU technologies [6,8]. However, since solid fuels contain nitrogen and sulfur, NO_x and SO_2 emissions should be considered before this combustion technology is put into practice [7,9,10].

The manuscript demonstrates an application of the Fuzzy Logic approach as one of the leading artificial intelligence methods [11–14] to predict NO_x and SO_2 emissions from CLC equipment. The performed model was successfully validated against experimental results.

2 Experiments

The necessary data were acquired from experiments carried out on a hot CLC facility at Czestochowa University of Technology, Poland [15,16]. The unit consists of two reactors: an air reactor and a fuel reactor (Figure 1). A detailed description of the system can be found elsewhere [8,15,17]. The experiments were conducted using coal and biomass as a renewable energy source [18–21], described in Table 1.

Different operating conditions are considered in this study, i.e., Test 0 (air-fired conditions), Test 1 (O_2/CO_2 mode) Tests 2 – 6 (CLC and CLOU) conditions. Detailed characteristics of all OCs used in the study can be found in [7].

Fig. 1. The hot CLC facility.

Different operating conditions are considered in this study, i.e., Test 0 (air-fired conditions), Test 1 (O_2/CO_2 mode) Tests 2 – 6 (CLC and CLOU) modes. Various kinds of OCs are taken into account, ilmenite (OC1) in Tests 2, 5, and 6, copper oxide (60% wt.) with the supports (OC2, OC3) in Tests 3 and 4. Detailed characteristics of all OCs used in the study can be found in [7].

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* Corresponding author: j.krzywanski@ujd.edu.pl

Table 1. Fuel's characteristics.

Fuel		coal	biomass
LHV MJ kg^{-1}		26.16	17.25
Proximate analysis/wt., %	M	6.6	6.2
	V.M.	35.7	77.0
	A	5.5	1.4
	F.C.$^{by\ diff.}$	52.2	15.4
Ultimate analysis/wt., %	C	68.2	47.7
	H	4.90	5.47
	S	1.02	0.11
	N	1.01	0.27
	O$^{by\ diff.}$	12.77	38.85

3 Results

The Qtfuzzylite fuzzy logic control application was used to develop the model [22–24].
The following input parameters are employed to develop the model:

- ID$_{mode}$ tag defining the combustion mode,
- the kind of oxygen carrier OC,
- oxygen excess OE,
- average fuel reactor temperature T,
- F.C.^{ad}/ V.M.^{ad} ratio, and N^{ad}/C^{ad} molar ratio,
- sulfur S^{ad} and ash A^{ad} contents in the fuel,
- ID$_{fuel}$ tag, defining the kind of fuel.

Such selected input variables allow describing the outputs in the developed FL-based model [19,25]. The model uses triangular and constant terms for inputs and outputs, respectively [26].
The validation procedure was successfully performed on the hot facility [27] (Table 2).

Table 2. Comparison of calculated and experimental results

Test		SO$_2$	NO$_x$	SO$_2$	NO$_x$	ERR	
		exp.		calc.		NO$_x$	SO$_2$
		ppm		ppm		%	
Test 0	-	627	393	595	371	5.1	5.6
Test 1	-	843	379	769	351	8.8	7.4
Test 2	OC1	85	56	77	56	9.4	0.0
Test 3	OC2	40	116	42	106	-5.0	8.6
Test 4	OC3	61	176	56	173	8.2	1.7
Test 5	OC1	21	57	20	62	4.8	-8.8
Test 6		8	125	8	114	0.0	8.8

Comparing measured and predicted SO$_2$ and NO$_x$ emissions revealed that the maximum relative error is lower than 10 %. This confirms the good accuracy of the model, allowing for the correct prediction of the emission of sulfur and nitrogen oxides.

4 Conclusions

A comprehensive FL-based model was shown in this paper for NO$_x$ and SO$_2$ prediction from coal and biomass combustion under differen**t** combustion modes. Air-fired, oxyfuel, CLOU, and iG-CLC conditions are considered in the study. The model's accuracy was successfully confirmed by the validation process. with the maximum error below 10 %.

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