

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

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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 SO₂ 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 CO₂ and H₂O, 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 SO₂ 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 SO₂ 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 (O₂/CO₂ 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 (O₂/CO₂ 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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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 SO₂ 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 SO₂ prediction from coal and biomass combustion under different 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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References

1. D. R. McIlveen-Wright, F. Pinto, L. Armesto, M. A. Caballero, M. P. Aznar, A. Cabanillas, Y. Huang, C. Franco, I. Gulyurtlu, and J. T. McMullan, *Fuel Processing Technology* **87**, 793 (2006)
2. W. Muskała, J. Krzywański, R. Sekret, and W. Nowak, *Chemical and Process Engineering - Inżynieria Chemiczna i Procesowa* **29**, 473 (2008)
3. T. Klajny, J. Krzywanski, and W. Nowak, in *Proceeding of the 6th International Symposium on Coal Combustion* (Huazhong Univ Sci Technol, Wuhan, Peoples R. China, Dec 01-04 2007, 2007), pp. 148–153
4. K. Idziak, T. Czakiert, J. Krzywanski, A. Zylka, M. Kozłowska, and W. Nowak, *Fuel* **268**, 117245 (2020)
5. A. Abad, P. Gayán, F. García-Labiano, L. F. de Diego, and J. Adánez, *Fuel Processing Technology* **171**, 78 (2018)
6. I. Majchrzak-Kuceba and D. Wawrzyńczak, *Advanced CO2 Capture Technologies for Clean Coal Energy Generation* (Publishing Office of Czestochowa University of Technology, Czestochowa, 2016)
7. T. Czakiert, *Spalanie Paliw Stałych w Układach z Pętlą Chemiczną (Solid Fuels Combustion in Chemical Looping Systems)* (Wydawnictwo Politechniki Czestochowskiej, 2019)
8. A. Zylka, J. Krzywanski, T. Czakiert, K. Idziak, M. Sosnowski, K. Grabowska, T. Prauzner, and W. Nowak, *Fuel* **255**, 115776 (2019)
9. J. Krzywanski, T. Czakiert, T. Shimizu, I. Majchrzak-Kuceba, Y. Shimazaki, A. Zylka, K.

- Grabowska, and M. Sosnowski, *Energy Fuels* **32**, 6355 (2018)
10. J. Krzywański and W. Nowak, *Journal of Power Technologies* **97**, 75 (2017)
 11. J. Krzywanski, K. Grabowska, M. Sosnowski, A. Żyłka, K. Sztekler, W. Kalawa, T. Wojcik, and W. Nowak, *Thermal Science* **23**, 1053 (2019)
 12. T. J. Ross, *Fuzzy Logic with Engineering Applications*, 3rd ed (John Wiley, Chichester, U.K., 2010)
 13. J. Krzywanski, *Energies* **12**, 4441 (2019)
 14. J. Krzywanski, K. Grabowska, M. Sosnowski, A. Żyłka, K. Sztekler, W. Kalawa, T. Wójcik, and W. Nowak, *MATEC Web of Conferences* **240**, 1 (2018)
 15. J. Krzywanski, A. Żyłka, T. Czakiert, K. Kulicki, S. Jankowska, and W. Nowak, *Powder Technology* **316**, 592 (2017)
 16. J. Adanez, A. Abad, F. Garcia-Labiano, P. Gayan, and L. F. de Diego, *Progress in Energy and Combustion Science* **38**, 215 (2012)
 17. K. Idziak, T. Czakiert, J. Krzywanski, A. Żyłka, and W. Nowak, *J. Energy Resour. Technol* **142**, (2020)
 18. I. Adánez-Rubio, A. Pérez-Astray, T. Mendiara, M. T. Izquierdo, A. Abad, P. Gayán, L. F. de Diego, F. García-Labiano, and J. Adánez, *Fuel Processing Technology* **172**, 179 (2018)
 19. M. L. de Souza-Santos, *Energy* **120**, 959 (2017)
 20. Q. Liu, W. Zhong, J. Gu, and A. Yu, *Powder Technology* **373**, 522 (2020)
 21. L. Zhou, K. Deshpande, X. Zhang, and R. K. Agarwal, *Energy* **195**, 116955 (2020)
 22. M. Sosnowski, J. Krzywanski, and R. Scurek, *Entropy* **21**, 1047 (2019)
 23. J. Krzywanski, *Entropy* **21**, 919 (2019)
 24. J. Krzywanski, D. Urbaniak, H. Otwinowski, T. Wyleciał, and M. Sosnowski, *Materials* **13**, 3303 (2020)
 25. J. Krzywanski, A. Blaszczyk, T. Czakiert, R. Rajczyk, and W. Nowak, in (CFB-11: Proceedings of the 11th International Conference on Fluidized Bed Technology, 2014), pp. 619–624
 26. M. R. H. Mohd Adnan, A. Sarkheyli, A. Mohd Zain, and H. Haron, *Artif Intell Rev* **43**, 345 (2015)
 27. A. Żyłka, J. Krzywański, T. Czakiert, K. Idziak, K. Kulicki, S. Jankowska, and W. Nowak, *E3S Web of Conferences* **13**, 04002 (2017)