A comprehensive model of NO\textsubscript{x} and SO\textsubscript{2} 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\textsubscript{x} and SO\textsubscript{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\textsubscript{2} and H\textsubscript{2}O, 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\textsubscript{x} and SO\textsubscript{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\textsubscript{x} and SO\textsubscript{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 Częstochowa 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\textsubscript{2}/CO\textsubscript{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].
### 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:
- IDmode 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,
- IDfuel 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 1. Fuel’s characteristics.

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

### Table 2. Comparison of calculated and experimental results

| Test | SO$_2$ (ppm) | NO$_x$ (ppm) | SO$_2$ (%) | NO$_x$ (%) | ERR (%) |
|------|--------------|--------------|------------|------------|---------|
| exp  | calc.        | NO$_x$ | SO$_2$ |          |         |         |
| 0    | 627 | 393 | 595 | 371 | 5.1 | 5.6 |
| 1    | 843 | 379 | 769 | 351 | 8.8 | 7.4 |
| OC1  | 85  | 56  | 77  | 56  | 9.4  | 0.0 |
| OC2  | 40  | 116 | 42  | 106 | -5.0 | 8.6 |

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 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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develop the model: The following input parameters are employed to used to develop the model [22–24].

3 Results
The validation procedure was successfully performed on model uses triangular and constant terms for inputs and Such selected input variables allow describing the Table 2.

| Test | OC1 | OC2 | OC3 |
|------|-----|-----|-----|
| ID   | Mode | Tag | Defining | Combustion | Time | Temperature | Oxide | Carrier | OC | Fuel |
| Test 0 | 627 | 393 | 595 | 371 | 5.1 | 5.6 |
| Test 1 | 843 | 379 | 769 | 351 | 8.8 | 7.4 |
| Test 2 | 21 | 57 | 20 | 62 | 4.8 | -8.8 |
| 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 | 255 | | | |
| Test 6 | 8 | 125 | 8 | 114 | 0.0 | 8.8 |

Comparison of calculated and experimental results successfully confirmed by the validation process. with considered in the study. The model's accuracy was fired, oxyfuel, CLOU, and iG-CLC conditions are t emission of sulfur and nitrogen oxides. model, allowing for the correct prediction of the lower than 10 %. This confirms the good accuracy of the 9.  J. Krzywanski, T. Czakiert, T. Shimizu, I. Majchrzak-Kucęba and D. Wawrzyńczak, 8.  A. Zylka, J. Krzywanski, T. Czakiert, K. Idziak, 7.  T. Czakiert, 6.  I. Majchrzak-Kuceba and D. Wawrzyńczak, 5.  A. Abad, P. Gayán, F. García-Labiano, L. F. de Diego, and J. Adánez, Fuel Processing Technology 4 Conclusions

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