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Validation of a Fuel Reactor Model for *In-situ* Gasification Chemical Looping Combustion

Alberto Abad[a,]*, Juan Adánez[a], Luis F. de Diego[a], Pilar Gayán[a], Francisco García-Labiano[a], Anders Lyngfelt[b], Pontus Markström[b]

[a] *Instituto de Carboquímica (ICB-CSIC), Miguel Luesma Castán 4, 50018-Zaragoza, Spain*
[b] *Department of Energy and Environment, Chalmers University of Technology, 41296-Göteborg, Sweden*

Abstract

The success of a Chemical-Looping Combustion (CLC) system for coal combustion is greatly affected by the performance of the fuel reactor. When coal is gasified in-situ in the fuel reactor, several parameters affect to the coal conversion, and hence to capture and combustion efficiencies. In this work a mathematical model for the fuel reactor is validated against experimental results obtained in a 100 kW_{th} CLC unit when reactor temperature, solids circulation flow rate or solids inventory are varied. The validated model can be used to evaluate the relevance of operating conditions on process efficiency.

Keywords: Chemical Looping Combustion; Coal; CO_2 capture; Modelling.

1. Introduction

In the last years increasing interest is found about the application of Chemical-Looping Combustion for the CO_2 capture from coal combustion.[1] The CLC process is based on the transfer of oxygen from air to the fuel by means of a solid oxygen carrier avoiding direct contact between fuel and air. Ideally, the CO_2 capture is inherent to this process. Fig. 1 shows a general scheme of the CLC system using coal as fuel.

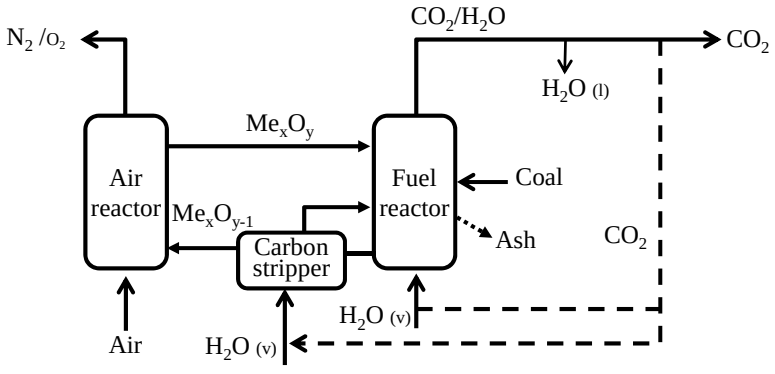

Fig. 1. Reactor scheme of the *i*G-CLC process for solid fuel using two interconnected fluidized bed reactors.

* Corresponding author. Tel.: +34-976-733977; fax: +34-976-733318.
E-mail address: abad@icb.csic.es.

A CLC system is mainly composed by two reactors, namely air and fuel reactors, with the oxygen carrier circulating between them. In the *in-situ* Gasification Chemical Looping Combustion concept (*i*G-CLC) coal is fed to the fuel reactor. The in-situ gasification of coal happens here, as well as subsequent oxidation of generated gases by reaction with the oxygen carrier, Me_xO_y. The reduced oxygen carrier, Me_xO_{y-1}, is later regenerated in the air reactor. To avoid CO_2 losses due to char entry to the air reactor, a carbon stripper is implemented to the system.

In previous works[2,3] a theoretical model describing the fuel reactor in the *i*G-CLC process was presented. The fuel reactor model can be considered as 1.5D describing the fluid dynamic of a high-velocity fluidised bed. Kinetics of chemical processes happening in the reactor are also included. In this work, this model is validated against experimental results obtained in a 100 kW_{th} CLC unit erected at Chalmers University of Technology.

2. Fuel Reactor model

In this work, the fuel reactor model is adapted to the conditions (geometry and flows) existing in the 100 kW_{th} CLC unit built at Chalmers University of Technology, see Fig. 2.[4] Table 1 shows the main dimensions of the fuel reactor, and Table 2 shows the experimental conditions -temperature, pressure drop, solids circulation flow rate and steam flow- varied during the experimental work.[5] The coal feeding rate ($\dot{m}_{coal}$ =12.6 kg/h) and flow entering in another positions were maintained constants. Experimental results obtained in this facility are used to validate the mathematical model with El Cerrejón coal as fuel and ilmenite as oxygen carrier.

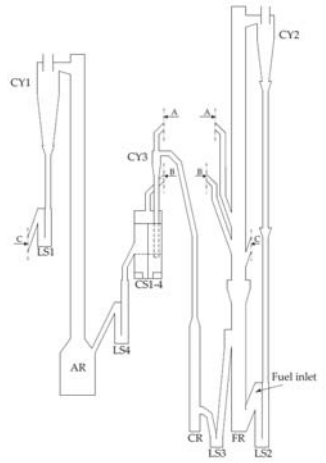

Table 1. Geometrical parameters

Reactor geometry	(m)
Height, H_r	5.0
Diameter, d_{react}	0.154
Height of stream from LS2	0.05
Height of overflow to LS3	1.0
Height of inlet in C	1.9
Height of inlet in B	2.1
Height of inlet in A	2.3

Table 2. Operational conditions.

Test	T_{FR} (ºC)	ΔP (kPa)	$\dot{m}_{OC}$ (kg/h)	$F_{g,FR}$ (Nm^3/h)
1	956	15.4	990	18.7
2	957	20.2	1566	18.7
3	957	22.6	2142	18.7
4	957	23.4	2610	18.7
5	959	20.3	2424	6.2
6	969	19.6	2376	6.2
7	976	15.6	3210	6.2
8	969	18.3	2190	6.2
9	963	18.8	2166	18.7

Fig. 2. Schematic picture of the 100 kW_{th} CLC system at Chalmers University of Technology and operating conditions.[4,5]

3. Results

Fig. 3(a) compares dry concentration of CO_2, CO, H_2 and CH_4 predicted by the model and measured during the experimental campaign. In general, good fitting between experimental and model prediction values are found. Also the tendency on the gas concentration values is adequately predicted. Thus, the effect of varying the reactor temperature, pressure drop, solids circulation flow rate or inlet gas flow is properly predicted by the model.

The performance of the fuel reactor is evaluated by analysing the oxygen demand, Ω_{OD}, and the carbon capture efficiency, η_{CC}. Ω_{OD} represents the ratio of oxygen required to fully oxidize unburnt compounds to the total oxygen required by the fuel, i.e. is a measure of the combustion degree. To calculate the η_{CC} value, the model needs to know the value of the efficiency of the carbon stripper separating char particles from oxygen carrier particles, η_{CS}. Inputs regarding the carbon flows to and from the carbon stripper are required to calculate the η_{CS} value, but they are not available.[5] The solution adopted in this work is to use the carbon capture efficiency, η_{CC}, as a target parameter; thus the experimental η_{CC} value is reproduced by the model by fitting the value of the carbon stripper efficiency. Once η_{CS} value is fixed, the rest of parameters can be calculated.

Fig. 3(b) shows that a good agreement is found between the oxygen demand obtained during the experimental campaign and values predicted by the model. Oxygen demand decreased during experiments 1 to 4 because a higher amount of solids is present in the fuel reactor. In the rest of experiments, the oxygen demand is barely changed when

temperature, solids circulation flow rate or/and steam flow into the fuel reactor is varied, and it averaged a value of 17.5%. In some cases, it seems that there is a trade-off between different effects. For example, in experiments 5 to 7 the temperature is increased but the solids inventory, which is related to ΔP, decreased. Both variations are compensated, because an increase in temperature gives a decrease in the oxygen demand, whereas the opposite happens when the solids inventory decreases.

High experimental values of the carbon capture efficiency were obtained, about 98%.[5] The mathematical model replicates these results by using the carbon stripper efficiency as a tunable parameter. Worth noting that an average value of η_{CS} = 99.4% is needed to fit the experimental η_{CC} values. This means that the carbon stripper implemented into the 100 kW_{th} unit is very effective, allowing the separation of most char exiting the fuel reactor. The good performance of the carbon stripper is the main reason to have high CO_2 capture values with a low solids inventory, corresponding to 450 kg/MW_{th}. The low solids inventory is the main responsible for the high oxygen demand, i.e. low combustion degree, obtained during the experimental work.

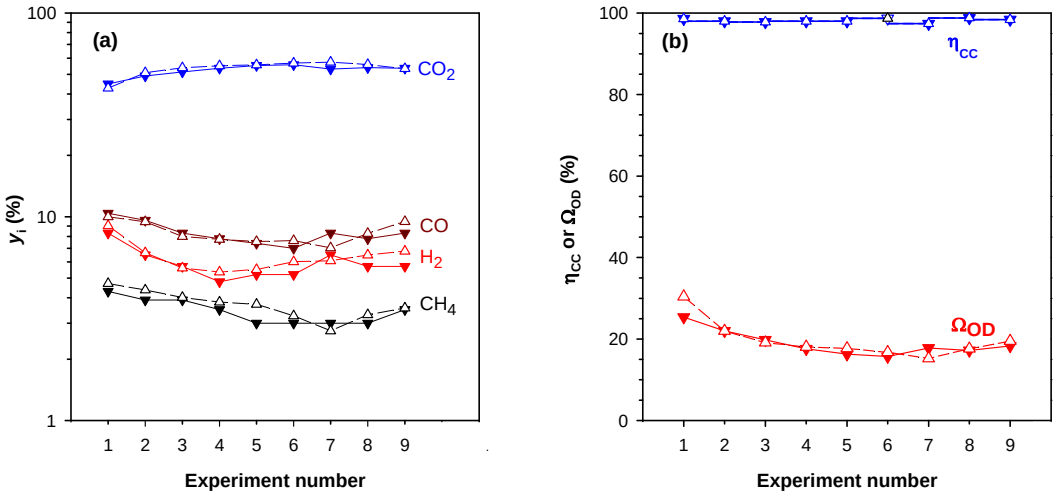

Fig. 3. (a) Dry concentration of CO_2, CO, H_2 and CH_4 at the fuel reactor exit and (b) oxygen demand and carbon capture efficiency for tests evaluated in this work. Filled symbols: experimental results;[5] empty symbols: model predictions.

4. Conclusions

A model to predict the behaviour of the fuel reactor in a CLC process with coal is validated against results obtained in a 100 kW_{th} CLC unit erected at Chalmers University of Technology. Good agreement is found between theoretical and experimental values, and the general tendency on the gas concentrations is adequately predicted. The oxygen demand in the fuel reactor (Ω_{OD}) due to unconverted gases is also properly predicted in all cases. High values were due to the low solids inventory used in the plant. The high values of the carbon capture efficiency obtained, about 98%, were due to the high efficiency of the carbon stripper.

Acknowledgments

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