STUDIA UNIVERSITATIS BABEŞ-BOLYAI, CHEMIA, XLV, 2, TOM I, 2010

Dedicated to the memory of Prof. dr. Ioan Silaghi-Dumitrescu marking 60 years from his birth

MATHEMATICAL MODELING AND SIMULATION OF COAL CO-GASIFICATION WITH WASTE/BIOMASS IN AN ENTRAINED-FLOW GASIFIER

VICTORIA MAXIM[a], CĂLIN-CRISTIAN CORMOŞ[a], PAUL ŞERBAN AGACHI[a]

ABSTRACT. The aim of this paper is to evaluate the ways to use coal alone or in addition with biomass (sawdust, agricultural wastes etc.) or solid waste (animal residue, municipal solid wastes, waste paper etc.) trough co-gasification to supply syngas for energy vectors poly generation in an Integrated Gasification Combined Cycle (IGCC) with Carbon Capture and Storage (CCS).

This paper analyses various cases of blending coal with different renewable energy sources by means of mathematical modeling and simulation of the gasification process using the process flow modeling software ChemCAD.

The effect of varying the feedstock and the effect of varying the blending ratio coal vs. alternative fuel on the cold gas efficiency and hydrogen production potential is studied for the gasifier performance optimization.

Keywords: *Co-gasification, Coal, Renewable energy sources, Solid wastes, Mathematical modelling and simulation*

INTRODUCTION

The climate change and the reduction of greenhouse emissions are very important and actual in the context of modern society. There are many greenhouse gases sources: transport, agriculture, power generation plants, industry etc., but the larger contributor is the power generation field, with a percentage around 24% of all greenhouse gases emissions and is set to grow by 2030 around 40% [1]. Coal accounts for around one-third of the EU's electricity production and its utilization is regarded with concern because of the larger greenhouse emissions compared with other fossil fuels (e.g. natural gas and oil).

[a] *Universitatea Babeş-Bolyai, Facultatea de Chimie şi Inginerie Chimică, Str. Kogălniceanu Nr. 1, RO-400084 Cluj-Napoca,Romania,*
Emails: vgoia@chem.ubbcluj.ro, cormos@chem.ubbcluj.ro, sagachi@staff.ubbcluj.ro

The most powerful greenhouse gas is the carbon dioxide CO_2 which is produced by the transportation, industrial and energy generating sectors. In order to prevent the increasing trend of greenhouse gas emissions the carbon capture and storage technology was developed. The carbon capture and storage (CCS) is a way of mitigating the contribution of fossil fuel emission to global warming. This is based on capturing the carbon dioxide and storing it away either in deep geological formations, in deep ocean masses, or in the form of mineral carbonates [2, 3].

In close co-operation with industries and Member States, the EU government presently supports the development of CCS (Carbon Capture and Storage) technologies in coal-fired power plants [4]. The aim is to make zero emission power generation plants using CCS commercially feasible by 2020 [1,4].

Gasification of solid fuels is a process which converts the solid feedstock by partial oxidation with oxygen and steam into syngas. The syngas can be used in a large number of applications as: power generation, manufacture of various chemicals and fuels (e.g.. hydrogen, methanol, ammonia, fertilizers etc.). The gasifiers may be designed for wide variety of solid feedstock: fossil fuels (e.g. coal, lignite peat etc.), various biomass types (sawdust, agricultural wastes etc.) and solid waste (e.g. animal residue, municipal solid wastes, waste paper etc.). The chemical composition of syngas varies based on many factors: coal composition, size and rank, feeding system (dry or slurry), gasification agent used for oxidation (air or oxygen), temperature, pressure, residence time in the gasifier, heating rate, gasification island configuration, etc. [5,6].

The conventional Integrated Gasification Combined Cycle (IGCC) is a concept regarding the conversion of solid fuels into syngas, meaning that a mixture of carbon monoxide and hydrogen, which after ash removal and desulphurization is burned in a conventional Combined Cycle Gas Turbine (CCGT) to generate electrical power. A unit can be considered capture-ready if, at some point in the future, it can be retrofitted for CO_2 capture and sequestration and still be economical to operate [7]. IGCC is a carbon capture ready technology. The design for a modified IGCC scheme for poly-generation of electricity and hydrogen with CCS is presented in Figure1.

The core of the IGCC technology is the gasification process of a solid fuel either fossil fuels alone or in addition with various biomass types and solid waste having energetically value. The IGCC is one of the power generation technologies having the highest potential to capture CO_2 with the lowest penalties in energy efficiency and cost. The IGCC technology is very attractive for energy vectors poly-generation: electricity, hydrogen, heat and chemicals [8, 9].

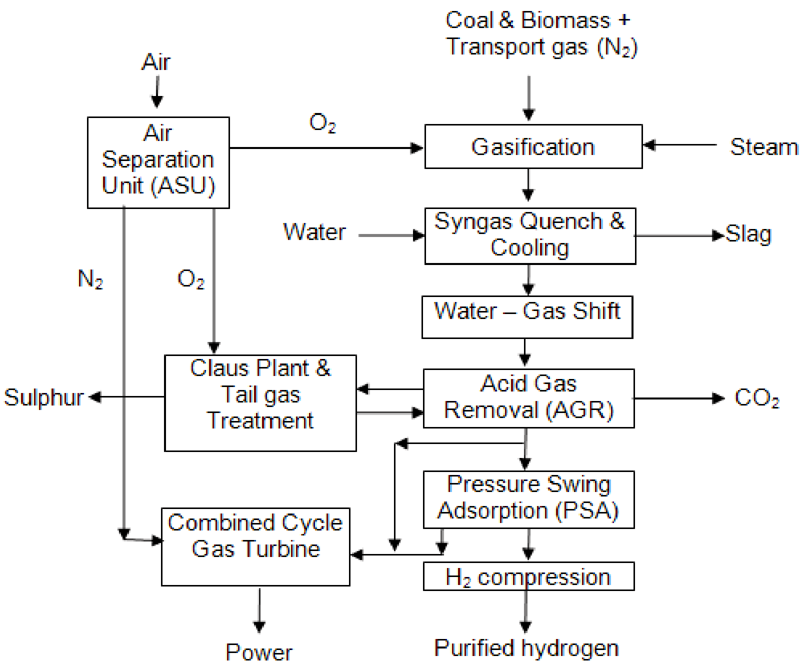

Figure 1. The IGCC scheme modified for poly-generation of electricity and hydrogen with carbon capture and storage (CCS)

The next section of this paper presents the gasifier concept, the feedstock caracteristics and the modeling and simulation of gasification process. The co-gasification of coal alone or in addition with biomass (sawdust, agricultural wastes) or solid waste (animal residue, municipal solid wastes, waste paper) will be analyzed by mathematical modeling and simulation using the process flow modeling software ChemCAD. The most appropriate mixture will be chosen by analyzing the syngas composition, Cold Gas Efficiency (CGE) and the hydrogen production potential. The behavior of co-gasification of coal with various sorts of biomass or solid wastes will be studied by varying the blending ratio.

RESULTS AND DISCUSSION

The main system component of the gasification process is the gasifier. It is a pressure vessel in which a fuel (coal or biomass/waste) togheter with air (or oxygen) and water are heated to high temperatures, above 900°C, to produce syngas (mainly a mixture of hydrogen and carbon monoxide). The syngas after cleaning is used to generate electricity in a gas turbine [10].

The gasification reactors can be grouped in one of the three main categories: moving-bed gasifiers, fluidised-bed gasifiers, and entrained-flow gasifiers. The caracteristics of these reactors can be found in the literature [6,11].

Based on several criteria such as: oxygen purity, gasifier throughputs, reliability and experience, cold gas efficiency (CGE), carbon conversion efficiency (CCE), syngas cooling options, influence of oxygen purity and gasifier feed system for hydrogen purification step, hydrogen production potential, capital cost etc., from the large range of gasifiers, as the most promising reactor for energy vectors poly-generation (mainly hydrogen and electricity) with Carbon Capture and Storage, a Shell gasifier has been chosen.

Table 1. Design assumptions for Shell gasifier

Parameters	Shell gasifier
Maximum pressure (bar)	40
Temperature (°C)	1400-1600
Carbon conversion (%)	>99

The Shell gasifier is a carbon steel vessel that contains a gasification chamber enclosed by a non-refractory membrane wall, which operates at 30-40 bar pressure, temperature range of 1500-1600°C, dry feed and one stage. The pulverized coal is stored under nitrogen, where it is pressurized and then pneumatically transported into the gasifier. The syngas is quenched with cooled recycled product gas and further cooled in a syngas cooler. Raw gas is cleaned in ceramic filters. A Shell gasifier configuration is shown in Figure 2. The image represents a dry-feed, pressurized, entrained-flow, slagging gasifier which can be operated on a wide variety of feedstocks [12].

The Shell gasifier used for the coal co-gasification with waste/biomass considered was the Gibbs Free Energy Reactor (GIBS). The Gibbs reactor model uses an equilibrium model based on equilibrium constants. Product rates, compositions, and thermal conditions are calculated by the minimization of Gibbs free energy This method has to define the specific chemical reactions used in the calculation [13].

The gasifier is operating at high temperatures with a high fuel conversion. Other gasifier design assumptions are: pressure drop 1 bar, operating pressure 40 bar and heat duty -22990 MJ/h.

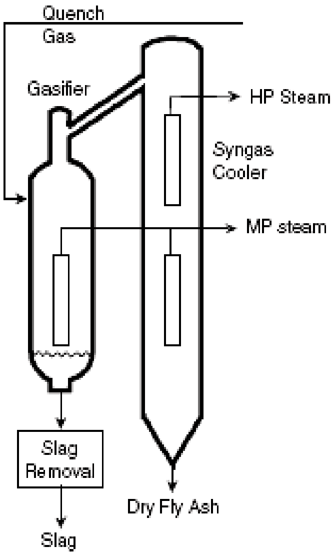

Figure 2. Schematic diagram of Shell gasifier

Figure 3 represents the flowsheet for a Shell gasification block mathematically modeled and simulated using ChemCAD software.

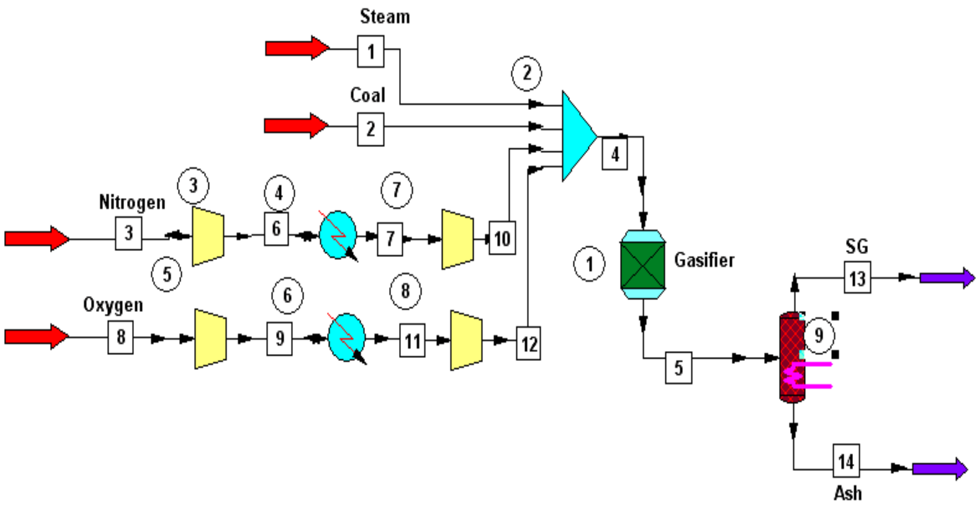

Figure 3. The Shell gasification diagram

Feedstocks

Coal is mainly the result of slow anaerobic transformation of biomass (wood, vegetation etc.) over millions of years. Coal is often classified in terms of its rank, which is determined by the degree of this anaerobic transformation from brown coal to anthracite [6, 14].

The most important biomass fuel is wood, but the trees are too valuable to be burned, instead residues from the woodworking industries as sawdust, could be a very valuable feedstock. Another biomass fuels are the agricultural residues such as: wheat straw, corn stalks, husks from rice, coconuts etc. Different solid wastes, such as: municipal solid wastes, waste paper, sewage, animal residues, can be used as feedstock to a gasification process as well.

For the gasification process the proximate analysis (fixed carbon, volatile matter, moisture, ash), the ultimate analysis (elemental, apart from ash) and ash composition must be known prior evaluation. These fuel characteristics mainly determine the key performance indicators of the gasification process (e.g. cold gas efficiency, oxygen and stream consumptions, hydrogen production potential etc.)

Case studies

This paper analyses eight different case studies of coal blending with different renewable energy sources, which use the same configuration for the gasification process, as follows:

- Case 1 - coal alone used as feedstock;
- Case 2 – coal in addition with sawdust (SWD) blending ratio 80/20% wt.;
- Case 3 – coal in addition with wheat straw (WS) blending ratio 80/20% wt.;
- Case 4 – coal in addition with corn stalks (CS) blending ratio 80/20% wt.;
- Case 5 – coal in addition with municipal solid wastes (MSW) blending ratio 80/20% wt.;
- Case 6 – coal in addition with waste paper (WP) blending ratio 80/20% wt.;
- Case 7 – coal in addition with sewage sludge (SWG) blending ratio 80/20% wt.;
- Case 8 – coal in addition with meat and bone meal (MBM) blending ratio 80/20% wt.

The fuel characteristics are presented in Table 2 [15].

Table 2. Fuel characteristics

Parameter	Coal	SWD	WS	CS	MSW	WP	SWG	MBM
Proximate analysis (% wt)								
Moisture (a.r.)	8.10	10.00	10.00	8.00	10.00	6.00	10.00	1.90
Volatile matter (dry)	28.51	80.05	69.94	73.40	72.70	82.50	54.50	73.40
Ash	14.19	0.98	14.48	7.00	13.90	8.21	37.56	18.80
Ultimate analysis (% wt dry)								
Carbon	72.04	49.20	41.11	44.80	41.20	49.25	36.19	46.20
Hydrogen	4.08	5.99	5.20	5.39	5.50	6.97	4.46	6.70
Nitrogen	1.67	0.82	1.01	0.85	0.50	0.34	5.63	9.70
Oxygen	7.36	42.98	37.36	41.75	38.70	35.00	15.00	17.07
Sulphur	0.65	0.03	0.24	0.21	0.20	0.20	1.06	0.65
Chlorine	0.01	0.00	0.60	0.00	0.00	0.03	0.10	0.88
Ash	14.19	0.98	14.48	7.00	13.90	8.21	37.56	18.80
Calorific value (MJ/kg dry)								
HHV – Gross	28.704	19.436	16.091	17.206	16.425	21.664	15.264	21.163
LHV – Net	27.803	18.113	14.943	16.016	15.211	20.125	14.279	19.683
Ash composition (%wt)								
SiO_2	52.20	9.44	54.64	63.30	52.45	19.44	39.80	0.00
Al_2O_3	27.30	1.56	5.73	0.00	16.21	63.97	11.70	0.00
Fe_2O_3	5.10	1.88	6.16	4.70	7.17	0.42	14.20	2.90
CaO	6.40	62.00	5.02	0.60	16.92	8.37	8.00	66.28
MgO	2.10	2.18	2.45	4.80	0.00	1.68	0.00	0.00
TiO_2	1.50	0.10	0.23	0.00	0.00	3.81	0.00	0.00
K_2O	1.00	15.00	14.09	8.40	0.00	0.23	0.80	13.00
Na_2O	0.30	0.61	2.16	0.50	7.25	0.83	0.60	17.82
SO_3	2.40	2.72	3.03	7.20	0.00	1.14	0.00	0.00
P_2O_5	1.30	1.23	2.43	2.10	0.00	0.10	0.00	0.00
SrO	0.00	0.15	0.00	0.00	0.00	0.00	0.00	0.00

The effects of coal blending with renewable energy sources (wood, agricultural wastes etc.) or alternative fuels (various wastes) are analyzed using the following key gasification process parameters[6,16]:

- *Cold gas efficiency (CGE):* is desirable that this indicator to be as high as possible on condition that hydrocarbons (mainly methane) present in syngas must be as low as possible (hydrocarbons negative influence the carbon capture plant capabilities). CGE represents the energy efficiency of the gasification process and it is defined as follow:

$$CGE = \frac{Syngas\ thermal\ energy\ [MW]}{Feedstock\ \ thermal\ energy\ [MW]} * 100 \quad (1)$$

- *Hydrogen production potential:* similar to CGE, it is defined as the sum of carbon monoxide and hydrogen content in the syngas and it must be as high as possible. It gives a better idea of how much of the thermal energy of coal can be converted into hydrogen and it is calculated with the formula:

$$Hydrogen\ production\ potential = \frac{CO\ and\ H_2\ thermal\ energy\ [MW]}{Feedstock\ thermal\ energy\ [MW]} * 100 \quad (2)$$

All the cases from 1 to 8 were simulated using the process flow modelling software ChemCAD. Table 3 presents the results of blending coal with renewable energy sources and solid wastes.

On the basis of the Cold Gas Efficiency (CGE) and the hydrogen production potential the following four cases have the highest efficiencies: Case 1 (coal alone), Case 2 (coal in addition with sawdust), Case 6 (coal in addition with waste paper) and Case 8 (coal in addition with meat and bone meal).

For Case 8 must be mentioned that the cold gas efficiency is higher on behalf of the good thermal properties of the alternative fuel used - MBM (high calorific value and carbon content, low moisture content), the relatively high methane content in the syngas compared with other cases. Figure 4 present the changes in the Cold Gas Efficiency for the considered case studies.

Table 3. The performance indicators

	UM	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6	Case 7	Case 8
Solid fuel flowrate	t/h				165.4				
Solid fuel energy	MW_{th}	1164.7	1079.29	1053.08	1061.95	1055.29	1095.94	1047.59	1092.29
Steam/fuel		0.072	0.036	0.036	0.036	0.036	0.036	0.036	0.091
O2/fuel		0.848	0.788	0.788	0.788	0.776	0.788	0.788	0.727
N2/Fuel					0.09				
Syngas flowrate	t/h	310.94	299.02	294.61	292.5	288.15	291.83	283.08	285.04
				Syngas composition					
CO	% vol	59.79	57.39	56.88	57.88	57.41	58.23	57.91	60.00
H_2	% vol	25.42	24.5	23.86	24.16	24.89	26.41	25.13	29.88
CH_4	% vol	0	0	0	0	0	0	0	0.06
H_2S	% vol	0.19	0.16	0.17	0.17	0.17	0.17	0.23	0.22
H_2O	% vol	5.2	6.29	8.11	7.90	7.65	6.54	6.73	4.28
Ar	% vol	0.9	0.81	0.90	0	0	0	0	0.62
Others	% vol	8.5	10.85	10.08	8.99	9.88	8.65	10.00	4.94
Syngas energy	MW_{th}	928.41	850.9	820.13	833.89	829.96	880.63	824.79	940.95
CGE	%	79.71	78.84	77.88	78.52	78.65	80.35	78.73	86.14
CO + H_2 energy	MW_{th}	924.46	847.73	816.84	830.59	826.68	877.25	820.43	935.45
H_2 prod. potential	%	79.37	78.54	77.57	78.21	78.34	80.05	78.32	85.64

As can be noticed in Figure 4, the Cold Gas Efficiency increases with the increase of the carbon percent in the feedstock.Case 2 (coal in addition with sawdust), Case 6 (coal in addition with waste paper) and Case 8 (coal in addition with meat and bone meal) have a higher carbon percent, hence a higher Cold Gas Efficiency.

Analyzing the syngas composition, the Cold Gas Efficiency (CGE) and the hydrogen production potential can be noticed that Case 8 is the most appropriate mixture, which could contribute to the reduction of fossil fuels dependency and CO_2 emissions. As a result, Case 8 was chosen for a further case study: the effect of varying the blending ratio of coal with MBM on the cold gas efficiency and syngas composition.

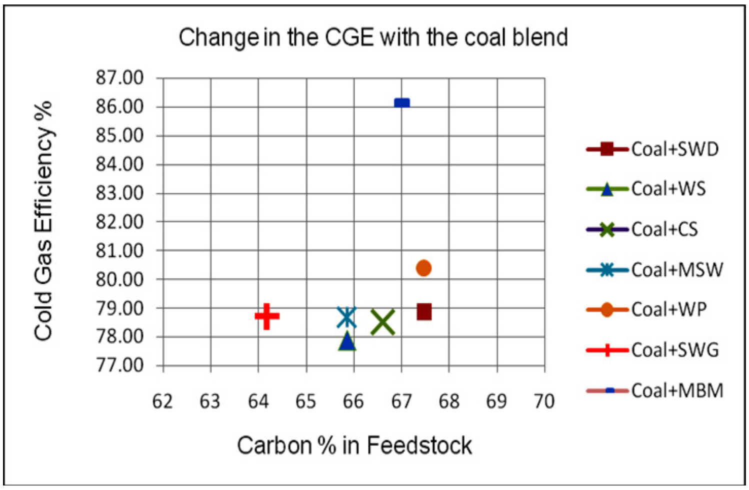

Figure 4. Changes in the CGE with the coal blend options

The blening ratio was varied from 0.1 to 0.5 (wt./wt. ratio on as received basis) and is defined by the following equation [17]:

$$\text{Blending } ratio = \frac{Biomass\ feed\ rate\ [Kg/h]}{Total\ feed\ rate\ [Kg/h]} \tag{3}$$

Figure 5 shows the change in the syngas composition with the blending ratio for Case 8 (coal in addition with meat and bone meal). With the increasing of blending ratio, the CO composition decreased from 59.79% to 52.51% and the H_2 composition increased from 25.42% to 34.84% (all syngas composition figures are expressed in molar percentages).

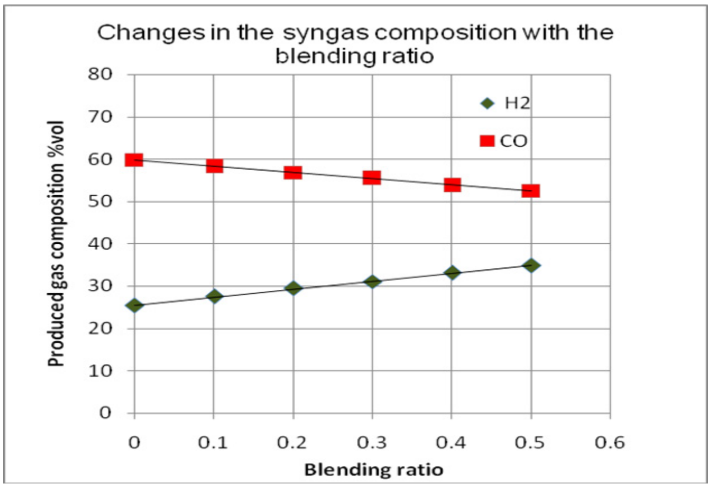

Figure 5. Change in the syngas composition with the blending ratio for Case 8

Figure 6 shows the change in the cold gas efficiency with the blending ratio for Case 8 (coal in addition with meat and bone meal), with the increasing of biomass ratio, cold gas efficiency increases from 79.71% to 90.35%.

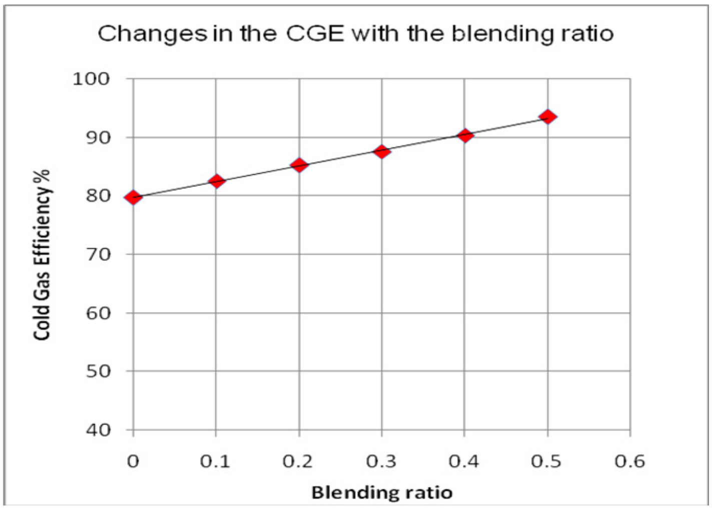

Figure 6. Change in the CGE with the blending ratio for Case 8

The results also indicate that blending coal with biomass or waste, besides the environmental benefits (conservation of fossil fuel resources and reduced CO_2 emissions with 3.58% to 17.93%, depending of the blending ratio) could provide a higher cold gas efficiency and hydrogen production potential.

CONCLUSIONS

The aim of this paper was to evaluate the coal co-gasification with various alternative and renewable solid fuels like wastes (animal residue, municipal solid wastes, waste paper etc.) or biomass (sawdust, agricultural wastes etc.) to supply syngas for energy vectors poly generation in an Integrated Gasification Combined Cycle (IGCC) with Carbon Capture and Storage (CCS).

In this paper was presented a study of the effect of varying different blends of feedstock (coal alone or in addition with biomass or solid waste) on the cold gas efficiency and hydrogen production potential in a entrained-flow gasifier (Shell technology was chosen based on best performances compared with other entrained-flow gasifiers). The best performances of the gasifier have been obtained for the following blends: coal in addition with meat and bone meal (MBM), coal in addition with waste paper and coal in addition with sawdust.

The technology of co-gasification of coal with renewable energy sources as waste and biomass can result in a very clean power plants using a wide range of feedstock. The use of renewable energy sources has real and tangible environmental benefits such as: the conservation of fossil fuel resources and the reduction of the CO_2 emissions with 3.58% to 17.93%, depending of the blending ratio used.

ACKNOWLEDGMENTS

The authors wish to thank for the financial support provided from the programs: (i) Investing in people! PhD scholarship, Project co-financed by the Sectoral Operational Programme Human Resources Development Contract POSDRU 6/1.5/S/3 – „Doctoral studies: through science towards society" and (ii) Romanian National University Research Council (CNCSIS) through grant no. 2455: “Innovative systems for poly-generation of energy vectors with carbon dioxide capture and storage based on co-gasification processes of coal and renewable energy sources (biomass) or solid waste”.

REFERENCES

1. European Commission, http://ec.europa.eu/energy
2. M. M. Maroto-Valer, C. Song, Y. Soong, “Environmental Challenges and Greenhouse Gas Control for Fossil Fuel Utilization in the 21st Century”, Kluwer Academic/Plenum, **2002**

3. S. Lombardi, L.K. Altunina, S.E. Beaubien, “Advances in the Geological Storage of Carbon Dioxide International Approaches to Reduce Anthropogenic Greenhouse Gas Emissions”, Springer, **2006**
4. Statistical Review of World Energy BP, www.bp.com
5. A.G. Collot, *International Journal of Coal Geology*, **2006**, *65*, 191
6. C. Higman, M. Van Der Burgt, **2008**, “Gasification”, Elsevier Science, Second edition
7. Massachusetts Institute of Technology, ”The future of coal an interdisciplinary study”, **2007**
8. E. Tzimas, A. Mercier, C.C. Cormos, S. Peteves, *Energy Policy*, **2007**, *35*, 3991
9. C C. Cormos, *Studia Universitatis Babes-Bolyai, Chemia*, **2009**, LIV, *1*, 81
10. National Energy Technology Laboratory , http://www.netl.doe.gov/
11. C.C. Cormos, “Decarbonizarea combustibililor fosili solizi prin gazeificare”, Cluj University Press, **2008**
12. B. G. Miller, “Coal Energy Systems”, Elsevier Academic Press, **2005**, chapter 5
13. Z.A. Zainal, R. Ali, C.H. Lean, K.N. Seetharamu*, EnergyConversManage* **2001**, *42*:1499
14. M. L. de Souza-Santos, ”Solid Fuels Combustion and Gasification Modeling, Simulation, and Equipment Operation”, Marcel Dekker Inc, New York, **2005**, chapter 2
15. Energy Research Centre of the Netherlands, **2010**, www.ecn.nl
16. J.C. Meerman, A.P.Faaij, W.C. Turkenburg, *Energy Procedia*, **2009***, 1*, 4241
17. K. Kumabe, T. Hanaoka, S. Fujimoto, T. Minowa, K. Sakanishi*, Fuel,* **2007**, *86*, 684