INTERNATIONAL JOURNAL OF
ENERGY AND ENVIRONMENT

Volume 5, Issue 5, 2014 pp.575-582
Journal homepage: www.IJEE.IEEFoundation.org

Process simulation of oxy-combustion for maximization of energy output using ASPEN plus

Subhodeep Banerjee, Xiao Zhang, Suraj K. Puvvada, Ramesh K. Agarwal

Department of Mechanical Engineering & Materials Science, Washington University in St. Louis,
1 Brookings Drive, St. Louis, MO 63130, USA.

Abstract

Oxy-fuel combustion is a next-generation combustion technology that shows promise to address the need of low-cost carbon capture from fossil fueled power plants. Oxy-fuel combustion requires expensive pre-processing in an air separation unit to separate pure oxygen from air for the combustion process, which reduces the overall efficiency of the process. This paper employs ASPEN Plus process simulation software to model a simple oxy-fuel combustor and investigates the effect of various parameters on the energy output. The composition of the flue gas is carefully examined. The results of this study provide a starting point for optimized oxy-fuel combustion operation for maximum energy output, which will be crucial for future deployment of oxy-fuel combustion technology.

Keywords: Carbon capture; Process simulation; Oxy-fuel combustion; Optimization.

1. Introduction

Recent years have seen considerable effort devoted towards the development of carbon capture technology to prevent or significantly reduce carbon dioxide emissions resulting from the combustion of fossil fuels in electricity-generation power plants. One such technology is oxy-fuel combustion, which involves burning coal using pure oxygen instead of air. The theoretical benefits of this approach are twofold. The significant nitrogen component (around 80%) of the air does not need to be heated to the combustion temperature, which reduces the energy input into the system. Additionally, the flue gases from the combustor consist primarily of carbon dioxide and steam and are not contaminated by the presence of nitrogen and other gases; a stream of almost pure carbon dioxide can be captured without the need for expensive gas separation techniques. However, there is significant expense associated with pre-processing of the air in the air separation unit (ASU) to separate pure oxygen from air for the combustion process, as a result of which the overall efficiency of the oxy-fuel combustion process becomes relatively lower than the standard combustion and therefore the technology has not been widely accepted for deployment on a commercial scale; however the situation may change in the future.

ASPEN Plus is a process simulation software that simulates chemical processes at system level using basic engineering relationships such as mass and energy balance, and multi-phase and chemical reaction models. It consists of flow sheet simulations to calculate stream properties such as flow rate and mass composition given various chemical processes and operating conditions. In this paper, a simple model of the oxy-fuel combustor is developed to conduct parametric studies for optimal energy output; the air separation unit and the steam cycle to extract heat from the flue gases are not considered. This study provides valuable insight into the design and operating conditions required in an industrial-scale oxy-fuel plant to increase combustor efficiency and to assess the feasibility of deploying oxy-fuel combustion as an economically viable solution for electricity generation and carbon capture.

2. Materials and methods

The solid fuel used in the ASPEN Plus model is a bituminous Colombian coal “El Cerrejon”, subjected to thermal pre-treatment (i.e., heated at 180ºC in atmospheric air for 28 hours) to avoid coal swelling and bed agglomeration. The coal parameters in the model are set up based on the proximate and ultimate analysis of the pre-treated “El Cerrejon” coal; these values are obtained from the work of Zhou et al. [1] and are presented in Table 1.

Table 1. Properties of bituminous Colombian coal “El Cerrejon”

Components	Proximate Analysis (wt. %)				Ultimate Analysis (wt. %)						Energy
	Moisture	Volatile matter	Fixed carbon	Ash	C	H	N	S	O	Ash	LHV (kJ/kg)
Fresh	7.5	34.0	49.9	8.6	70.8	3.9	1.7	0.5	7.20	15.9	25880
Pre-Treated	2.3	33.0	55.9	8.8	65.8	3.3	1.6	0.6	17.6	11.1	21899

The schematic of the flow sheet of the oxy-fuel combustor used in the ASPEN Plus simulation is shown in Figure 1. The coal is pulverized and decomposed in the RYIELD reactor before it is fed into the RGIBBS reactor for combustion. It should be noted that the RYIELD and RGIBBS reactors together represent the oxy-fuel combustor since ASPEN Plus cannot model the entire process with one reactor block. The primary oxidant enters the combustor via the IN-GAS stream. The flue gases and ash are released from the combustor in the ASH and OUT-GAS streams respectively. The dashed lines connecting Q1 and Q2 in Figure 1 indicate the flow of thermal energy (heat) in the system.

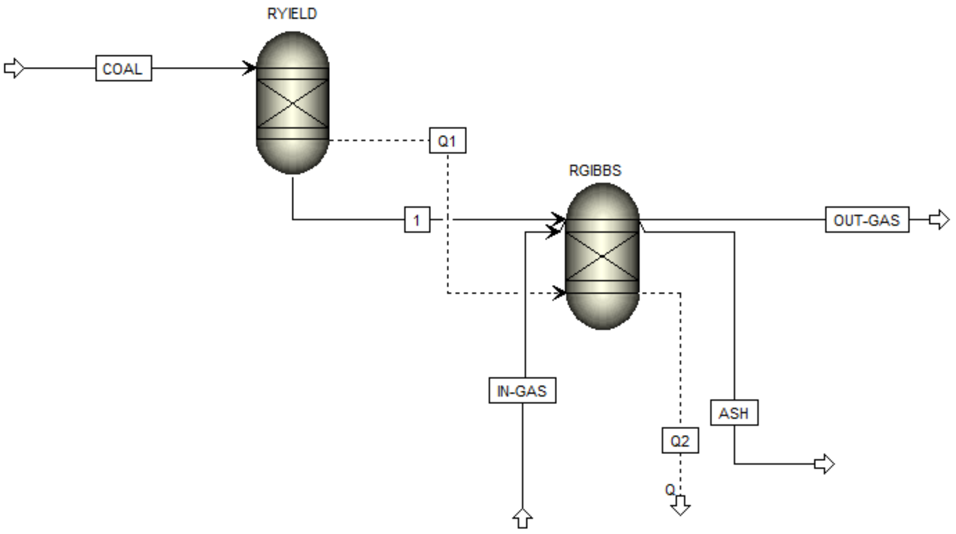

Figure 1. Schematic of the oxy-fuel combustor model in ASPEN Plus

The ASPEN Plus simulations are conducted with both air and oxygen as the primary oxidant. The mass of oxygen required for the stoichiometric ratio is obtained by summing the oxygen requirements for combusting each component of the coal except nitrogen, which is effectively inert at the temperatures considered, minus the mass of oxygen already present in the coal. The ASPEN Plus model uses 100kg of “El Cerrejon” coal for which the stoichiometric mass of oxygen is approximately 212kg. When air is used as the primary oxidant, the same mass of oxygen is used while nitrogen and argon are added such that their relative proportions are correct for air. Considering a ratio of 78% nitrogen, 21% oxygen, and 1% argon, the corresponding mass of air required is 1014kg.

The mass of oxygen in the IN-GAS stream is maintained at the stoichiometric ratio in all cases unless otherwise indicated. Similarly, the temperatures of the RGIBBS reactor and the IN-GAS stream are set at

1000 K and 500 K respectively, unless otherwise indicated; the pressures are set at 1.6 MPa and 1 atm respectively, in line with the work of Gopan et al [2]. The temperature and pressure of the RYIELD reactor are inconsequential since its output is solely based on the proximate and ultimate analysis of the coal. For each case considered, the net energy output of the system corresponding to stream Q2 in Figure 1 is recorded along with the molar composition of the OUT-GAS stream. The parameters that are varied to investigate their effects on the net energy output and flue gas composition are listed in Table 2.

Table 2. Operating parameters considered using ASPEN Plus simulation

Parameter varied	Variation range	Results section
Temperature of RGIBBS reactor	500–1500 K	03.1
Mass of IN-GAS stream	25–175% of stoichiometric O_2	3.2
Temperature of IN-GAS stream	500–1500 K	03.3

3. Results and discussion

3.1 Effect of variation in temperature of RGIBBS reactor

The variation in net energy output of the oxy-fuel combustor model with the RGIBBS reactor temperature is given in Table 3 and Figure 2. According to Figure 2, the relationship between the temperature and the energy output is inversely proportional. The net heat produced by the combustion reaction depends only on the chemical energy stored in the coal; it is independent of temperature. However, as the reactor temperature increases, the temperature of the flue stream increases, which takes away more heat from the reactor. Hence, the net heat output of the reactor decreases with temperature. Furthermore, using pure oxygen as the primary oxidant yields higher energy than using air at all temperatures except at 500 K. At 500 K, there is no energy lost due to heating of the additional components in air to the reactor temperature; therefore the net energy output is the same for both oxygen and air. At higher reactor temperatures, more and more energy is lost due to heating of the nitrogen fraction in air. Consequently, the energy output deficit using air compared to oxygen increases with temperature.

Table 3. Effect of varying RGIBBS temperature on net energy output

Oxidant	500K	750K	1000K	1250K	1500K
O_2	800627 W	774404 kW	745732 kW	715255 kW	683524 kW
Air	800341 W	713490 kW	621540 kW	525577 kW	426270 kW

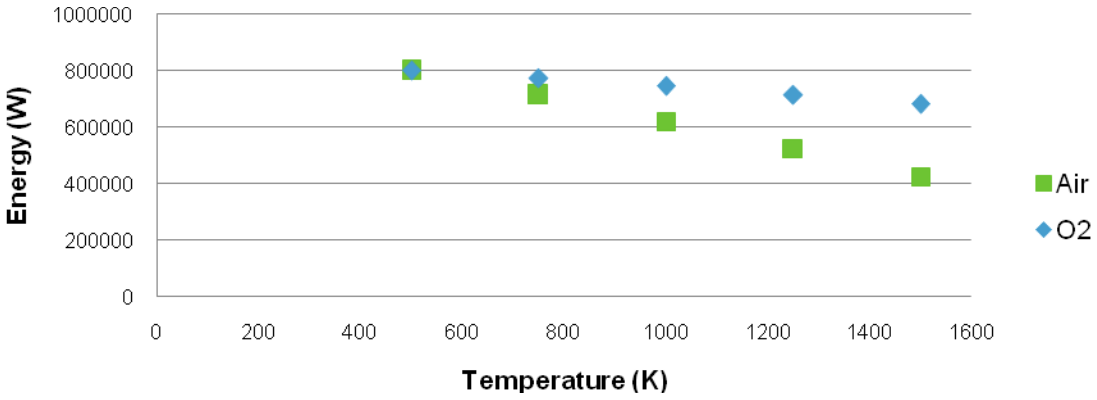

Figure 2. Effect of varying RGIBBS temperature on net energy output

Figure 3 shows the relative distribution of the flue gases in the flue stream of the oxy-fuel combustor model at all temperatures. The most significant products are carbon dioxide and steam. Although the mass of oxygen was prescribed in the stoichiometric ratio, some unused oxygen is observed in the flue stream. The nitrogen originally present in the coal is also present in the flue stream in both cases, although it gets overshadowed by the nitrogen in the air when air is used as the oxidant.

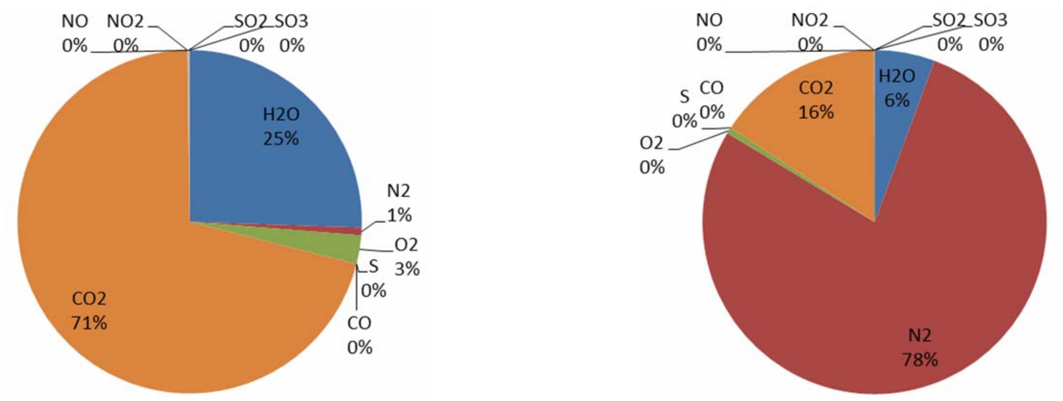

Figure 3. Flue stream composition with oxygen (left) and air (right) using stoichiometric mass of oxygen

NOx and SOx concentrations in the flue stream are negligible according to Figure 3. However, their flow rate variations with temperature, as shown in Figure 4, provide insight into the formation of these pollutants and how they may be reduced. The reaction between nitrogen and oxygen is virtually non-existent at the temperature range considered in the study. The rate of formation of NOx products increases with temperature for both air and oxygen. The formation of SOx products is slightly faster, and there is an inverse relationship in the formation of SO_2 and SO_3. Complete combustion is more favorable at higher reactor temperatures, therefore the molar flow rate of SO_3 decreases and SO_2 increases as the temperature increases.

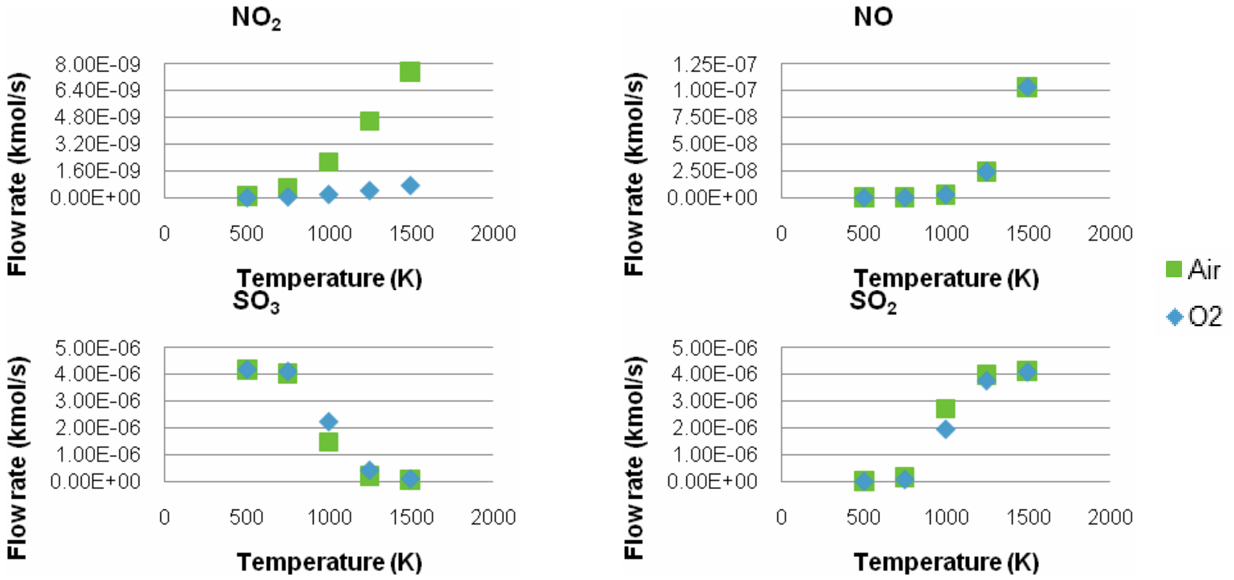

Figure 4. Effect of varying RGIBBS temperature on pollutant formation

3.2 Effect of variation in mass of oxygen in IN-GAS stream

The stoichiometric mass of oxygen required for complete combustion of 100kg of coal is 212kg. In this section, the mass of oxygen in the IN-GAS stream is varied between 25% and 175% of the stoichiometric mass. If air is used as the oxidant, the other components of air are scaled accordingly. The temperature of the oxidant stream and the RGIBBS reactor are maintained at 500 K and 1000 K respectively. Figure 5 shows the effect of the mass of oxygen on the net energy output of the oxy-fuel model. The results in Figure 5 are as expected: the net energy output increases linearly with increasing oxygen mass until the stoichiometric ratio is reached. Beyond the stoichiometric ratio, the net energy output decreases as more energy goes towards heating the excess oxygen to the reactor temperature. Similarly, the difference in the energy obtained using pure oxygen and air also increases as the mass of oxygen increases because the energy must be expended in heating the increased mass of nitrogen since the oxygen and nitrogen are in a fixed ratio in air.

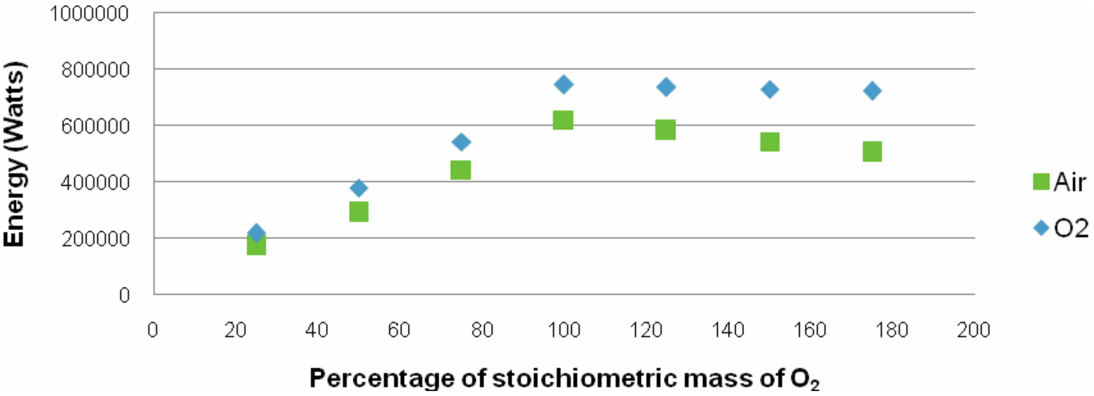

Figure 5. Effect of varying the mass of oxygen on net energy output

The distribution of products in the flue stream by varying the mass of oxygen using pure oxygen and air as oxidant is shown in Figures 6 and 7 respectively. Both figures show that for less than the stoichiometric mass of oxygen, the coal combustion is incomplete as indicated by the high percentage of CO in the flue stream. As the mass of oxygen is increased further, all the CO is converted to CO_2, and the excess oxygen is expelled with the flue stream. Similar to results in section 3.1, when the combustion occurs in air, the large fraction of nitrogen in the air offsets the remaining product fractions; however the trends for incomplete combustion when the oxygen mass is below the stoichiometric ratio are the same.

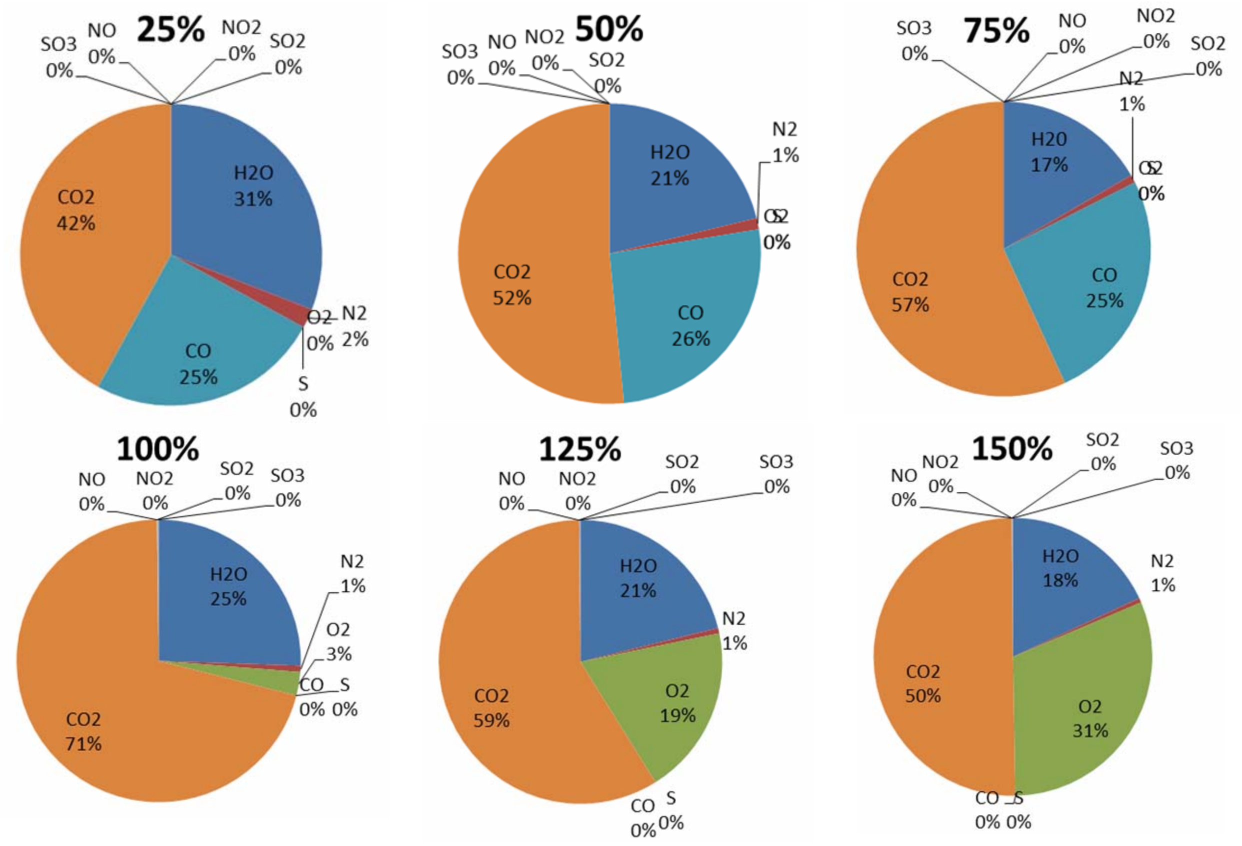

Figure 6. Effect of varying the oxygen mass on flue stream composition using pure oxygen as oxidant

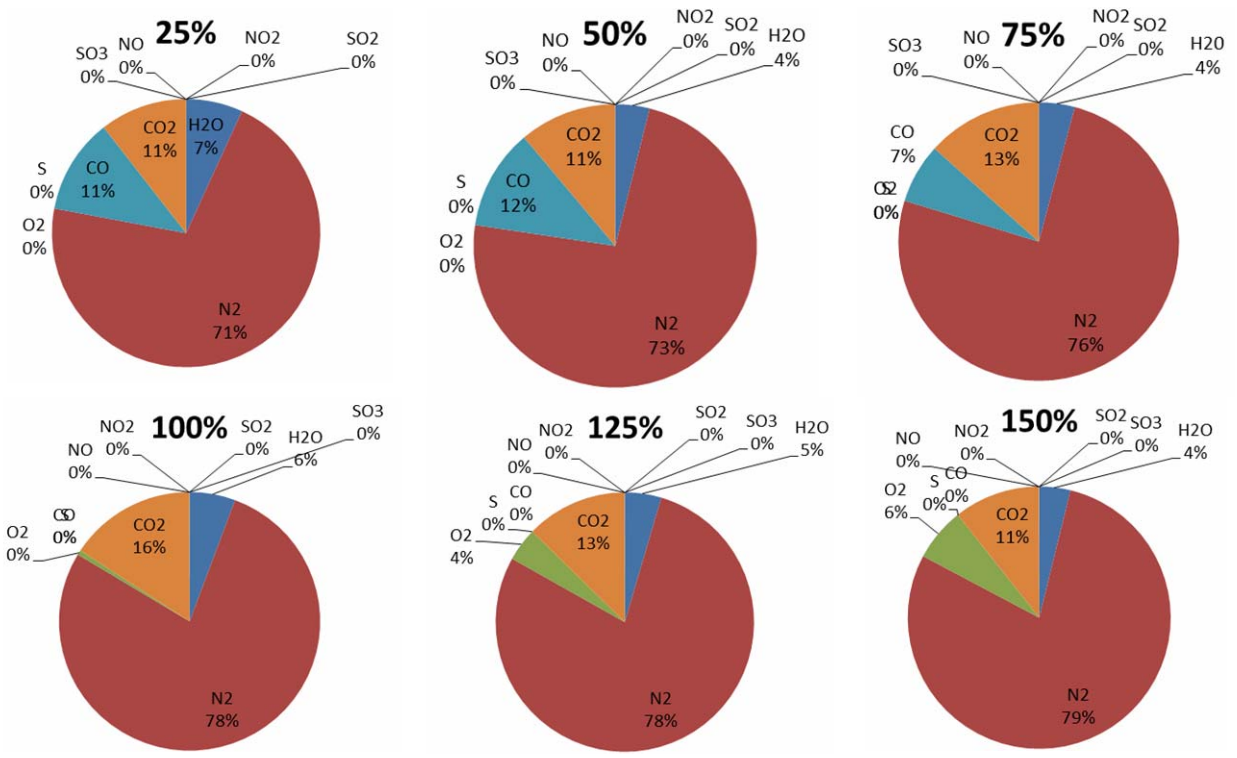

Figure 7. Effect of varying the oxygen mass on flue stream composition using air as oxidant

The detailed flow rates of CO and CO_2, and NOx and SOx products in the flue stream are presented in Figure 8. From Figure 8, it is clear that CO is only formed when the mass of oxygen is less than the stoichiometric ratio (i.e., the combustion is oxygen starved). Also, no NOx and SOx products are formed when the system is oxygen-starved. The concentrations of NO and NO_2 begin to increase when excess oxygen is supplied; this increase is more evident when the oxidant is air because of the larger nitrogen concentration in the reactor. SO_2 and SO_3 also begin to form when excess oxygen is supplied and the inverse relationship in their respective concentrations shown in Figure 4 also applies here as in section 3.1. It should be noted that the NOx and SOx product concentrations remain negligible in relation to other products even at 175% of the stoichiometric mass of oxygen.

3.3 Effect of Variation of temperature of IN-GAS stream

The IN-GAS stream prescribes the chemical composition of the oxidant that is fed into the oxy-fuel combustor. The effect of varying the temperature of a pure oxygen IN-GAS stream on the net energy output of the system is shown in Figure 9. The temperature of the RGIBBS reactor is maintained at 1000 K. Figure 9 shows that the energy output increases linearly as the inlet stream temperature is increased. This is because less energy must be expended on heating the inlet stream to the reactor temperature as the inlet stream temperature increases. The composition of the flue gas stream is identical to that in Figure 3; the details of pollutant formation can be obtained from the data points in Figure 4 which correspond to a reactor temperature of 1000 K.

4. Conclusions

In this paper, ASPEN Plus software was employed to model an oxy-fuel combustor and conduct parametric studies to optimize the energy output of the system. The reactor temperature and mass inflow of oxygen were varied to investigate their effect on the net energy output of the system as well as on the composition of the flue stream of the oxy-fuel combustor. The results from the process simulations suggest that the highest energy output is obtained when the mass of oxygen is at the stoichiometric ratio for the components of the coal. Furthermore, increasing the reactor temperature lowers the energy output since more heat is lost due to the increased temperature of the flue stream. This work provides a good starting point for further studies towards improving the efficiency of an oxy-fuel combustion system.

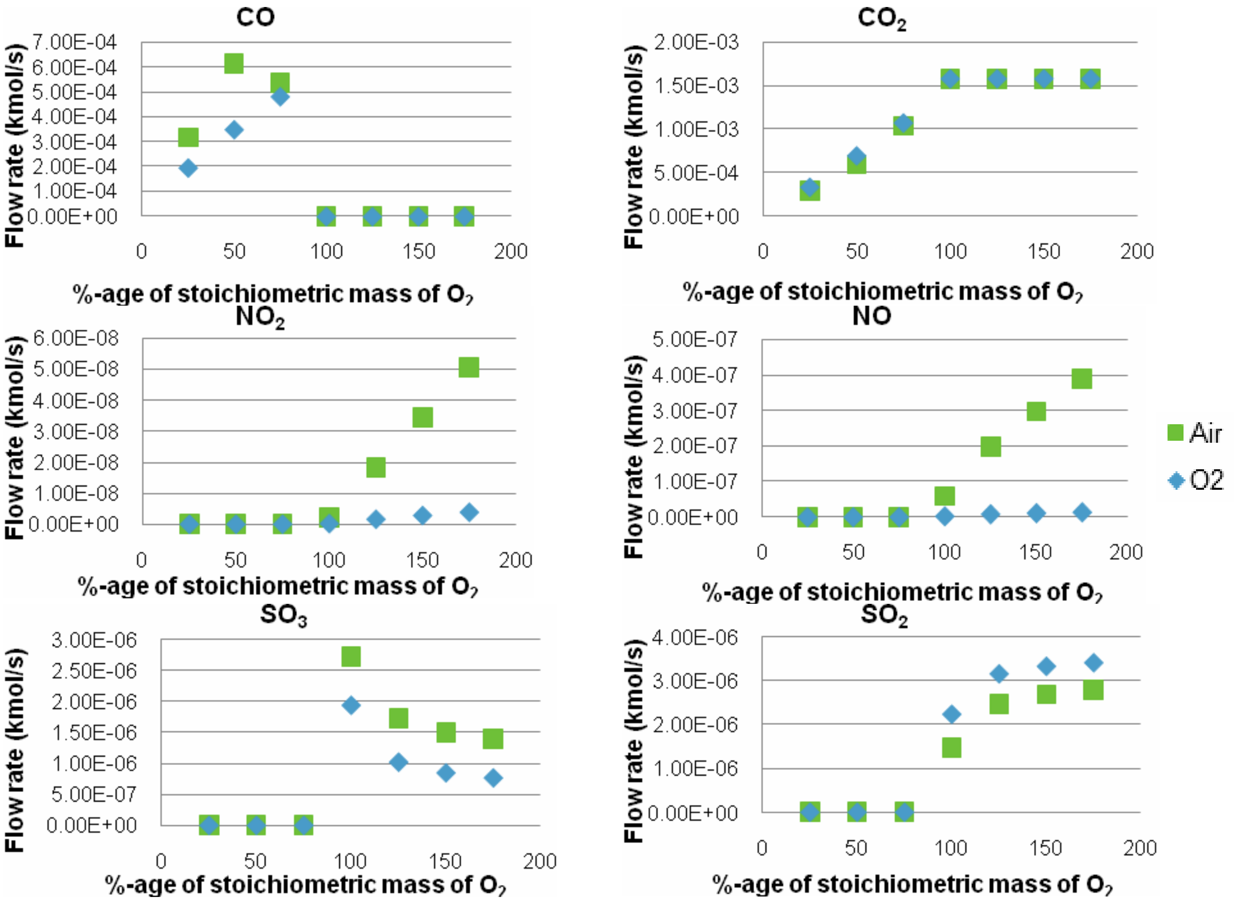

Figure 8. Effect of varying the oxygen mass on pollutant formation

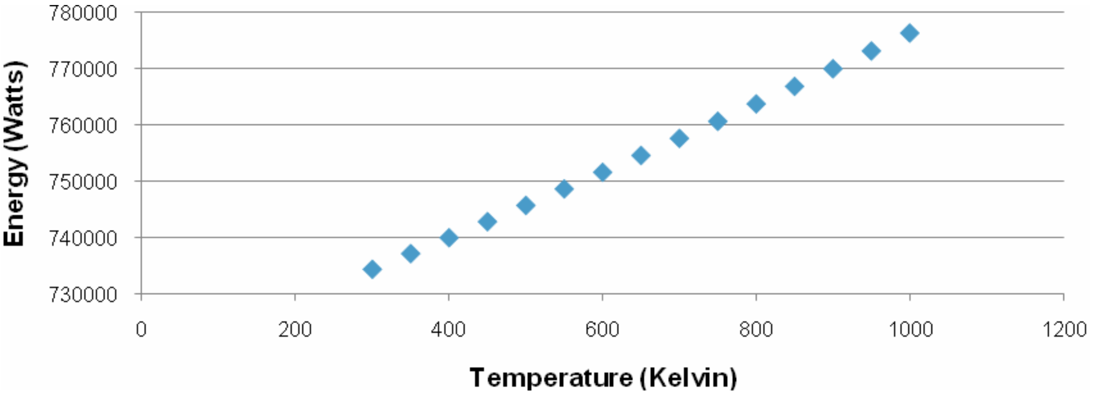

Figure 9. The effect of varying the oxygen stream temperature on net energy output

Acknowledgements
The authors would like to acknowledge the valuable inputs provided by Akshay Gopan of the department of Energy, Environment and Chemical Engineering (EECE) at Washington University in St. Louis. One of the co-authors Suraj K. Puvvada was supported by the STAR program in St. Louis.

References

[1] Zhou L., Zhang Z., Chivetta C., Agarwal R.K. Process simulation and validation of chemical-looping with oxygen uncoupling (CLOU) process using Cu-based oxygen carrier. Energy Fuels,2013, 27(11), 6906-6912.

[2] Gopan, A., Kumfer, B.M., Philips, J., Thimsen, D., Smith, R., Axelbaum, R.L. Process design and performance analysis of a staged, pressurized oxy-combustion (SPOC) power plant for carbon capture. Applied Energy, 2014,125, 179-188.

Subhodeep Banerjee is a Ph.D. student in the department of Mechanical Engineering & Materials Science at Washington University in St. Louis, USA. He holds a B.S. degree in Aerospace Engineering from University of Michigan, Ann Arbor and a M.S. degree in Aerospace Engineering from University of Southern California. His research interests are in the application of computational fluid dynamics in the study of chemical looping combustion and wind energy.
E-mail address: sb13@wustl.edu

Xiao Zhang is a M.S. student in the department of Mechanical Engineering & Materials Science at Washington University in St. Louis, USA. He holds a B.E. degree in Thermal Energy and Power Engineering from Chongqing University. His research interests are in the applications of computational fluid dynamics and chemical looping combustion. He plans to pursue Ph.D. at Washington University in St. Louis in January 2015.
E-mail address: xiaozhang@wustl.edu

Suraj K. Puvvada is a senior student at Lafayette High School in Chesterfield, MO, USA. He is interested in studying engineering and pursuing a research career. His interests include sustainable and renewable energy.
E-mail address: surajkcollege@gmail.com

Ramesh K. Agarwal is the William Palm Professor of Engineering in the department of Mechanical Engineering & Materials Science at Washington University in St. Louis. He has a PhD from Stanford University. His research interests are in Computational Fluid Dynamics and Renewable Energy Systems.
E-mail address: rka@wustl.edu