International Journal of Scientific & Engineering Research Volume 8, Issue 11, November-2017
ISSN 2229-5518

Thermodynamic analysis of release volatile species during pressurized combustion of biomass

Gul-e-Rana Jaffri

Abstract

High level of volatile species (e.g. Na-,K-,Cl-, and S) are released during combustion of biomass.The accumulation of these species causes eventual problems such as agglomeration, fouling, slagging and corrosion, especially in gas turbines, on super heaters and in the colder part of heat recovery systems. Thermodynamic study of high released volatile species is informative prior to carry out experimental work. Therefore, thermodynamic equilibrium was calculated using FactSage 5.2, simulating combustion conditions at elevated pressure (5, 10 and 15 bar) at 1000 °C Their releasing order of various volatile species was estimated by plotting mole fraction of each species at elevated pressure(5, 10 and 15 bar) at 1000 °C . These calculations predict that SO_2 is the most stable species for combustion. At all pressure the lowest amount of H_2S and NaCl volatilized for Rice husk while lowest volatilization of kCL for Bagasse evolution of NaCl, KCl and HCl depends on the amount of Cl present in both biomass (e.g. Bagasse and Rice husk).

Index Terms: Fact sage, Equilibrium calculations, Combustion, Biomass, release of volatile species

1 INTRODUCTION

Energy crises in Pakistan continuously haunts the country due to lengthy load shedding, growing demand supply gap, energy insecurity, Increasing reliance on imports and circular debt and acute shortage of 4,000 megawatts in power sector[1][2]. Threatening and devastating shortage of electricity adversely affected the economy of Pakistan, therefore hampering the national progress in a drastic manner [3]. Utilization of biomass such as Rice husk and Bagasse can provide a solution of this problem because Pakistan is an agrarian country and have [4] two major Biomass energy sources i.e livestock and Bagasse. These resources of biomass are capable of contributing 42% power portfolio of the country [5]. Pakistan annual production of Bagasse is 65,451 mln tones, its utilization in mills is 76.45% [6] and rice husk production is about 1,78 million tones [7]. The Pakistan can generate heat and power simultaneously from Bagasse and Rise husk from direct combustion, gasification, biomass power plants and co-firing with coal fired power plants. The biomass conversion to energy is most economical and lower capital cost than coal , wind and diesel electric power generation [7][8].Unfortunately high volatile species like Na, K, S, Cl during high temperature and pressure combustion are released and penetrate hot gas filtration unit ,super heater tubes and gas turbine blades that causes high temperature corrosion [9]. The efficiency of power plants and more satisfactory reduction for end-applications and for environmental regulations may be achieved by hot gas cleaning [10][11].

Therefor the comprehensive knowledge of released volatile species during high temperature and pressure combustion is required prior to carryout experiment by utilization of Bagasse and Rice husk biomass. Thermodynamic equilibrium calculations is the basis for obtaining such information and its method is capable of identifying species that are stable only at high temperature and pressure especially those employed in commercial combustors. The results are useful guidance for predicting the trends occurring during combustion. Therefore the present study simulates the combustion at high pressure 5 to 15) bar at 1000°C and also predict the release of volatile species for bagasse and rice husk using equilibrium calculations by Fact sage 5.2.

Dr.Gul-e-Rana Jaffri, Research Scholar, PhD in Chemical Eng (China)
& Post Doctorate in (Eng: Thermophysics and Power Engineering) (China).
Presently she is working as Senior Scientific Officer in Fuel Research Centre, PCSIR,
Off University Road Karachi-75280, Pakistan.
Ph:# 92-3153862290,Email: jaffri_gul@yahoo.com

2 MATERIAL AND METHOD

Two kinds of biomass i,e bagasse and Rice husk from Thatta sugar Mill and Hyderabad Rice Mill are mainly used. Their proximate and ultimate analysis and ash analysis is given in Table 1 and 2.

3 CALCULATION PROCEDURE

Thermodynamic equilibrium calculations were performed using Fact sage 5.2. The initial model composition is based on the data of elementary and chemical composition relate to 1 g of biomass. The fifteen (15) elements C, H, N, S, O, Cl, Al, Ca, Fe, K, Mg, Na and Si were included in the computation, as listed in Table 1 and 3. The results were calculated by plotting mole fraction of each species vs pressure (5 to 15 bar) at 1000°C for combustion process as shown in Figure 1 to 10 and calculated mole fractions are listed in Table 4.The chemical composition of Bagasse and Rice husk is included in Table 2.

4 DEFINITION OF CONDITION

To simulate the condition of combustion of Bagasse excess air, O_2=2.1319 g or (213.19 %) and N_2= 7.0176 g or (701.76%) and for Rice husk excess air, O_2=2.2426 g or (224.26%) and N_2= 7.3819 g or (738.19%) was added to system.

Table: 1 Proximate and ultimate analysis of Bagasse and Rice husk

Biomass Type	**Proximate analysis**				**Ultimate analysis**				
	M_{ad}%	A_{ad}%	V_{ad}%	$FC_{ad\%}$	$S_{t,ad}$%	H_{ad}%	C_{ad}%	N_{ad}%	O_{ad}%
Bagsase	9.58	3.07	70.05	17.3	0.25	6.21	61.068	0.18	19.642
Rice husk	5.75	20.6	57.36	16.29	0.063	6.924	59.01	5.004	2.65

Note： $O_{ad}\%=100-A_{ad}\%-S_{t,ad}\%-C_{ad}\%-H_{ad}\%-N_{ad}\%-M_{ad}\%$

Table: 2 The ash composition of Bagasse and Rice husk

Biomass sort		**Bagasse**	**Rice husk**
A_{ad} %		3.07	20.6
Ash	SiO_2/ Al_2O_3	1.32	2.13
Composition analysis of ash, %	SiO_2	45.71	52.5
	Al_2O_3	16.42	10.5
	Fe_2O_3	15.15	5.25
	CaO	5.55	3.23
	MgO	4.44	1.54
	TiO_2	3.62	0.58
	SO_3	0.18	10.55
	k_2O	5.65	11.65
	Na_2O	0.95	1.15
	P_2O_5	1.73	2.53

Table: 3 Chemical Composition of Bagasse and Rice husk

Biomass Type	**Si**	**Al**	**Fe**	**Ca**	**Mg**	**Ti**	**K**	**Na**	**P**	**Cl**
Bagasse	0.66	0.133	0.16	0.12 2	0.08	0.07	0.12	0.01	0.015	0.00004
Rice husk	5.05	0.57	0.37	0.47	0.191	0.075	1.7	0.09	0.145	0.00002

Table:4 Calculated mole fraction at pressure 5 to 15 bar and temperature 1000°C for combustion of Biomass

Alkali Species	Mole Fraction		
	P(bar)	**Bagasse**	**Rice husk**
SO_2	5	2.2063E-04	5.4148E-05
	10	2.1683E-04	3.5526E-05
	15	2.1399E-04	1.9350E-05
H_2S	5	2.5127E-20	3.0180E-20
	10	1.7464E-20	1.4031E-20
	15	1.4075E-20	6.2501E-21
NaCl	5	5.8183E-10	1.3690E-09
	10	4.1421E-10	1.1536E-09
	15	3.3923E-10	7.9721E-10
KCl	5	1.5292E-10	7.4485E-09
	10	1.0886E-10	6.2765E-09
	15	8.9157E-11	5.6873E-09
HCl	5	3.2534E-08	7.2379E-09
	10	3.2755E-08	8.6255E-09
	15	3.2854E-08	9.5716E-09

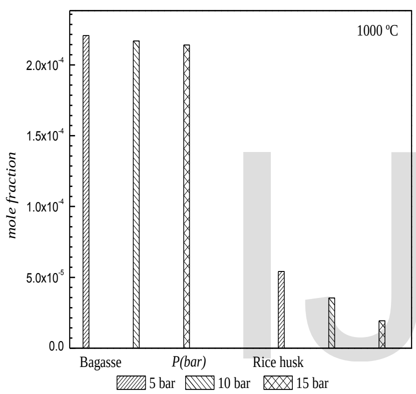

Fig:1 pridicted results of SO_2 at high Pressure combustion

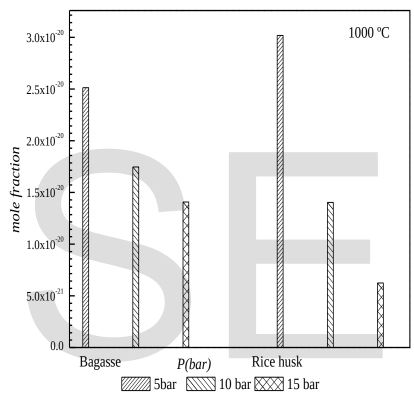

Fig:2 pridicted results of H_2S at high Pressure combustion

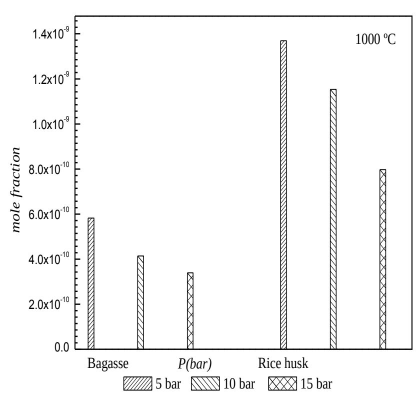

Fig:3 pridicted results of Nacl at high Pressure combustion

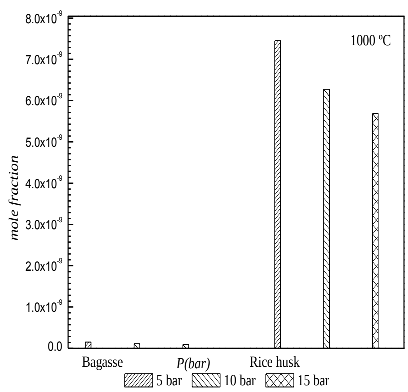

Fig:4 pridicted results of KCl at high Pressure combustion

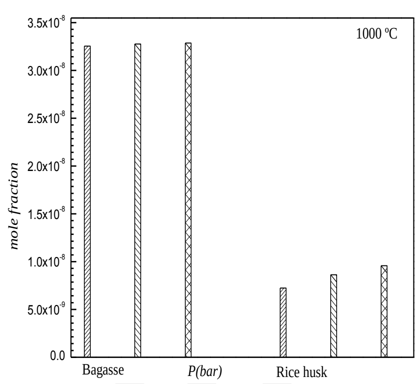

Fig:5 Pridicted results of HCl at high Pressure combustion

5 RESULTS AND DISCUSSION

5.1 Release of volatile species during high pressure Combustion

The computed release of SO_2, H_2S, NaCl, KCl and HCl under pressurized combustion is listed in Table 4.
On the basis of the calculated mole fraction the release of SO_2 gradually decreases with increasing the pressure from 5 to 15 bar, as shown in Figure 1, but higher than H_2S due to higher combustion product while release of H_2S gradually decrease with increasing pressure during combustion, as indicated in Figure 2.The decrease in volatilization of H_2S may shift the equilibrium to the left side of the reaction. Such changes are mainly as a consequence of the Le Chatelier-van't Hoff Law.
Therefore, lower release of SO_2 to the gas phase occurs for Bagasse and rice husk and even a sharp decrease were observed at 15 bar. The release of H_2S is showing little lower at 15 bar for Bagasse and Rice husk.
The results of NaCl and KCl are depicted in Figures 3 and 4. The release of NaCl, KCl strongly decreases with increasing pressure from 5 to 15 bar for Bagasse and Rice husk. The sharp decrease of NaCl, KCl was observed in Bagasse at 15 bar.
The release of HCl gradually increases with increasing pressure 5 to 15 bar for Bagasse and Rice husk as obviously indicated in Figure 5. The sharp increase in mole fraction of Bagasse and Rice husk was observed at 15 bar. The decrease and increase volatilization in Bagasse and Rice husk may be lower content of Cl in Bagasse and little high content in Rice husk but the system is in equilibrium and no effect on reaction will takes place because no of moles of the gas are same on each side of chemical equation of NaCl, KCl and HCl (Lechatelier Principle).

$$Na + Cl \rightarrow NaCl \quad (1)$$
$$K + Cl \rightarrow KCl \quad (2)$$
$$H + Cl \rightarrow HCl \quad (3)$$

6 COMPARISON OF PREDICTED COMBUSTION RESUTS OF BAGASS AND RICE HUSK AT ELEVATED PRESSURE

Thermodynamic equilibrium calculations were used to compare the predicted results of combustion both Bagasse and Rice husk at elevated pressure. The comparison of predicted combustion results at elevated pressure as shown in Figure 6. It is found that the release of SO_2 is very sharply reached at maximum value for Bagasse at 5bar in Figure 6(A), as compared to pressure 5 bar for Rice husk in Figure 6(B), moreover the release of SO_2 at 5 bar also greater than the release of H_2S, NaCl, KCl and HCl at elevated pressure.
On the basis of calculated mole fractions, the order of release species SO_2, H_2S, NaCl, KCl and HCl for Bagasse and Rice husk during combustion at elevated pressure are predicted as follows:

6.1 Releasing order of species at elevated pressure:

Bagasse $(SO_2 > H_2S < NaCl > KCl < HCl)$
Rice husk $(SO_2 > H_2S < NaCl < KCl < HCl)$

On the basis of releasing order, the SO_2 release is higher at elevated pressure both in Bagasse and Rice husk. The release of SO_2 is highest for Bagasse at 5 bar and lowest for Rice husk at 15 bar, the order of release at elevated pressure is Bagasse $>$ Rice husk.
For H_2S the higher and lower release at 5 bar for Bagasse and at 15 bar for Rice husk. The order of release is Bagasse $>$Rice husk at elevated pressure.
The higher and lower release of NaCl is observed at 15 bar for Rice husk and Bagasse. The order of release at elevated pressure is Rice husk $>$ Bagasse.
The KCl release is higher for Rice husk at 5 bar and lower for Bagasse at 15 bar, the order of release is Rice husk $>$Bagasse at elevated pressure.
The HCl release is higher for Bagasse at 15 bar and lower at 5 bar for Rice husk, the order of release is Bagasse $>$ Rice husk at elevated pressure.

7 CONCLUSION

The high volatilization of SO_2 at elevated pressure can be predicted that SO_2 is the most stable specie for Combustion.
The volatilization of SO_2 is predicted higher for Bagasse (5 bar)) and lowers for Rice husk (15 bar) at elevated pressure during combustion.
The volatilization of H_2S is predicted lower for Bagasse and Rice husk (15 bar) at elevated pressure than SO_2, NaCl, KCl and HCl.
The predicted release of NaCl, KCl is lower for Bagasse (15 bar) at elevated pressure while volatilization of HCl for Bagasse is higher (15 bar) at elevated pressure.
The volatilization of NaCl, KCl and HCl is dependent on Cl content present in the Bagasse and Rice husk

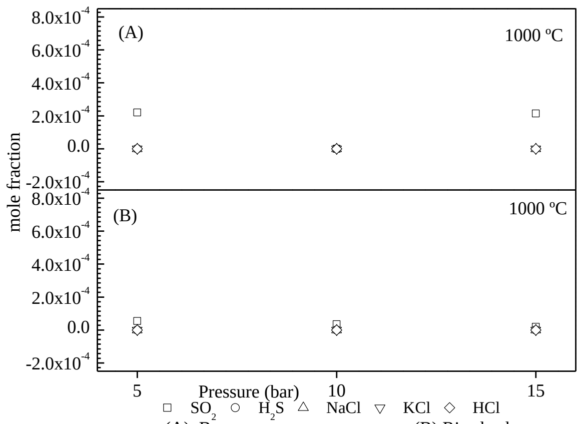

Fig: 6 Comparision of predicted equilibrium calculation results of combustion at elevated pressure.

8. References

[1] M.Asif, "The Energy Crises" https://www.dawn.com/news/1326795/2017-04-09.

[2] A.S.Azhar, "Will Energy Shortage be overcome" , https://www.dawn.com/news/1324565/2017/04/03.

[3] K.Perveen,"Energy Crises hurting economy", http://nation.com.pk/business/18-May-2016/energy-crisis-hurting-economy

[4] M.Amer and T.U.Daim, " Selection of renewable energy technologies for a developing country:A case of Pakistan." *J.Energy for Sustainable Development*, vol.15, pp.420-435.

[5] M.J.S.Zuberi,S.Z.Hasany,M.A.Tariq and M.Fahrioglu, "Assesment of biomass energy resources potential in Pakistan for Power generation" *Proc, IEEE 4th International Conference on Power engineering, energy and electrical drives (POWERENG)*,pp.1301-1306, 2013. **DOI:** 10.1109/PowerEng.2013.6635801

[6] M.K.Iskander, "Annual Review of Pakistan Sugar Mills Association, 51st Annual General Meeting", pp.1-12,Oct: 2016. http://www.psmacentre.com/aboutus.php?id=6&type=annual_review&status=1#top

[7] A.A.Mirani, A.Munir, K.A.Shabbir and A.Tanveer, " A Rice Husk Gasifier for Paddy Drying" *J.Sci.Tech and Dev.vol.*32,no,2,pp.120-125,2013. docsdrive.com/pdfs/std/std/2013/120-125.pdf

[8] M.A.Saeed, A.Irshad,H.Sattar,G.E.Andrews, H.N. Phylaktou & Gibbs B.M, "Agricultural Waste Biomass Energy Potential in Pakistan". Proc, International Bioenergy (Shanghai) Exhibition and Asian Bioenergy Conference Shanghai, P.R.China. Oct, 2015. http://dx.doi.org/10.5071/BSCE2015-ICO.1.2

[9] M.Deepa ,S.Surendra and P.Satya, " Corrosion Problems in Incinerators and Biomass-Fuel-Fired Boilers"*J. International Journal of Corrosion volume(2014),* Article ID 505306,pp.1-14, 2014. http://dx.doi.org/10.1155/2014/505306

[10] W.Zhang, H.Liu,I.U.Hai, Y.Neubauer, P.Schroder, H.Oldenburg, A.Seilkopf and A.Kolling, "Gas Cleaning strategies for biomass gasification product gas." *J. International Journal of Low-Carbon Technologies*,Vol.7, pp.69-74, 2017. http://dx.doi:10.1093/ijlct/ctr046 Advance Access Publication 8 February 2012

[11] . Blacing, M. Muller, "Influence of pressure on release of inorganic species during high Temperature gasification of coal". *J. Fuel*, Vol.90, pp, 2326-233, 2011. http://dx.doi.org/10.1016/j.fuel.2011.02.013