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Supplementary Materials

Thermodynamic Analysis of Biomass Gasification Using Aspen Plus: Comparison of Stoichiometric and Non-Stoichiometric Models

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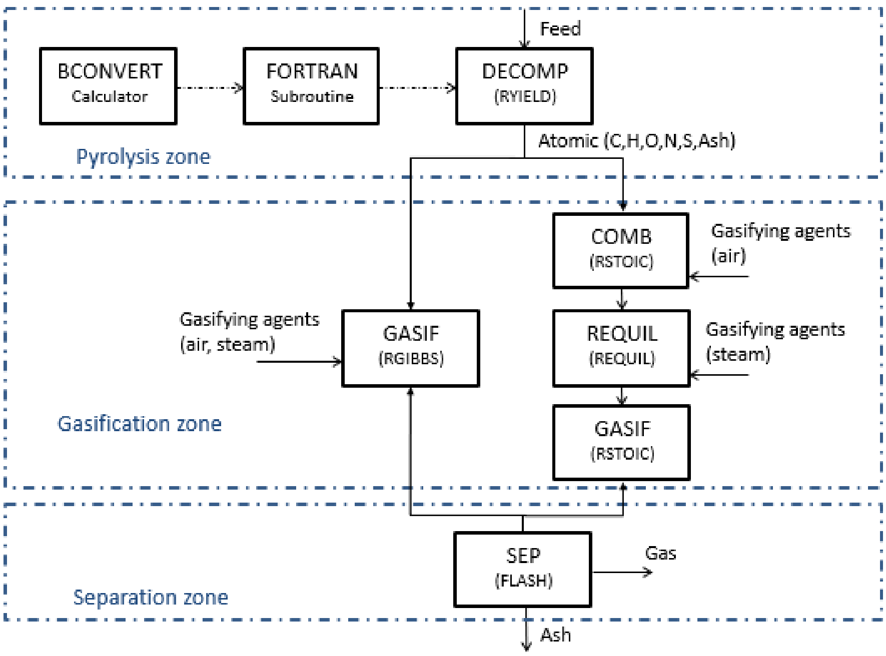

Figure S1. Flow chart of the simulation procedure for the steam gasification process.

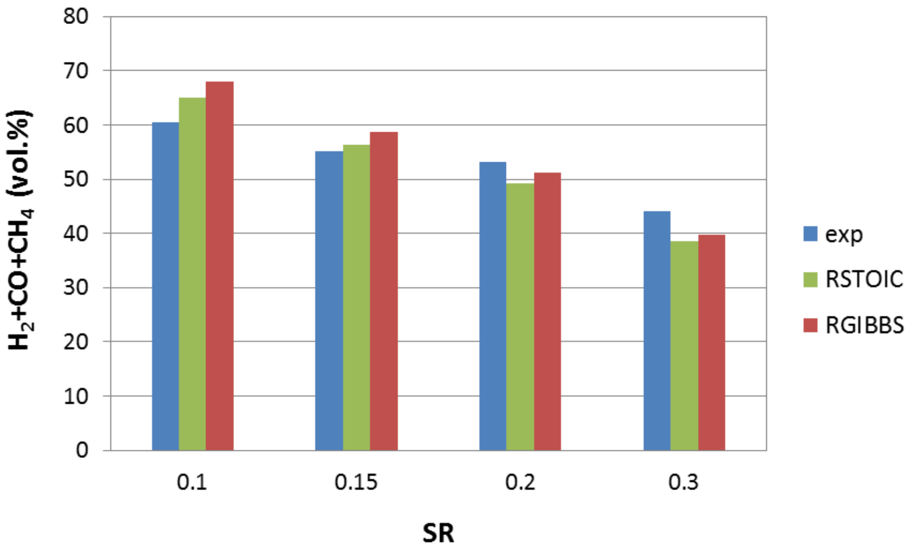

Figure S2. Comparison between experiment and simulation data of combustible gas concentration at different stoichiometric ratios, for the gasification of PKS with 70 vol.% steam at 900 °C.

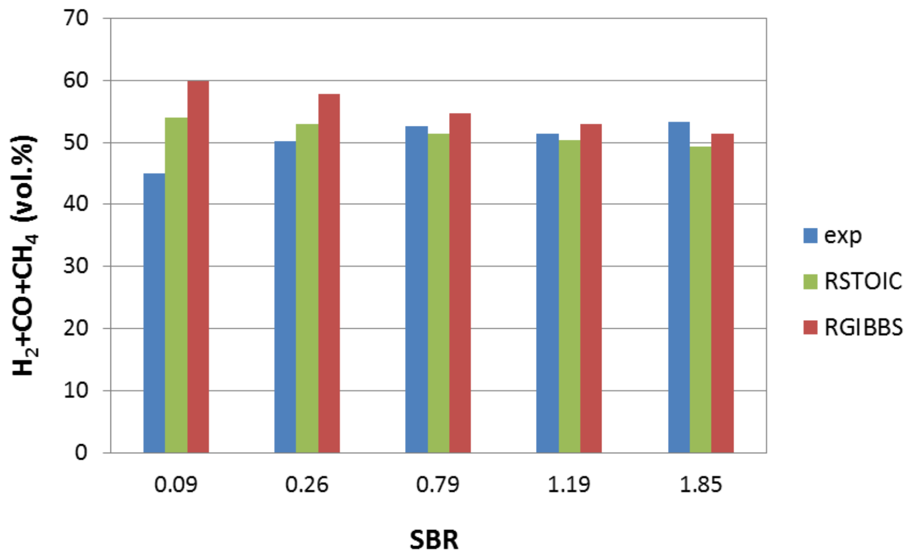

Figure S3. Comparison between experiment and simulation data of combustible gas concentration at different steam to biomass ratios, for the gasification of PKS at 900 °C with SR = 0.2.

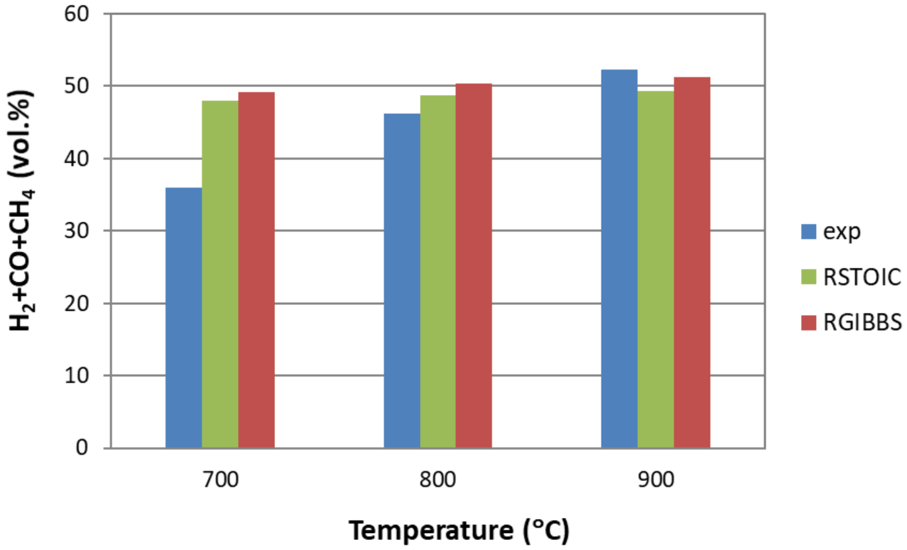

Figure S4. Comparison between experiment and simulation data of combustible gas concentration at different temperatures, for the gasification of PKS at SR = 0.2 and 70 vol.% steam.

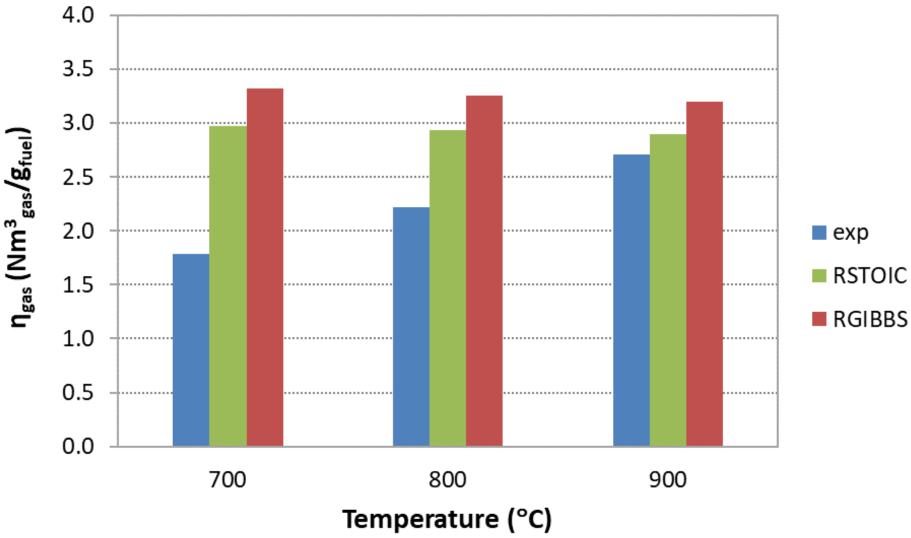

Figure S5. Effect of the variation of η_{gas} with temperature for the gasification of PKS with SR = 0.2 and 70 vol.% steam.

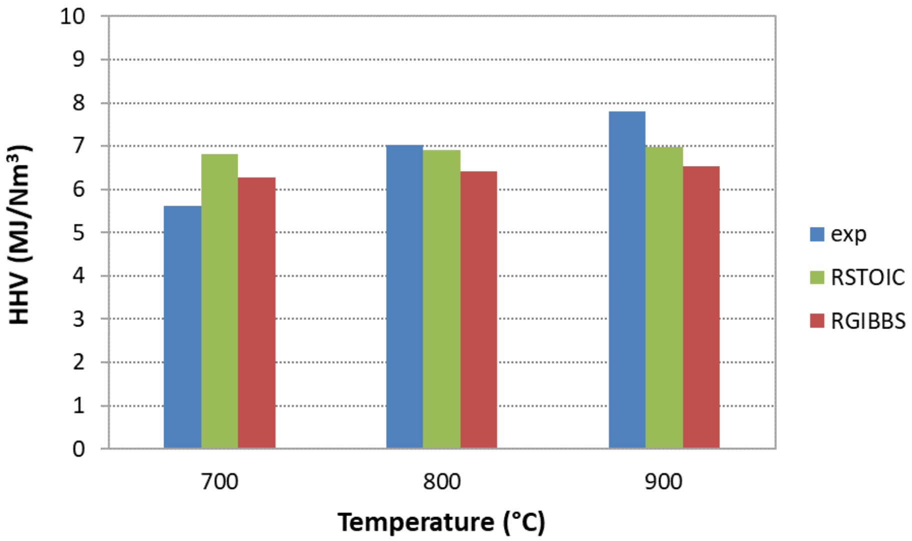

Figure S6. Effect of the variation of HHV with temperature for the gasification of PKS with SR = 0.2 and 70 vol.% steam.

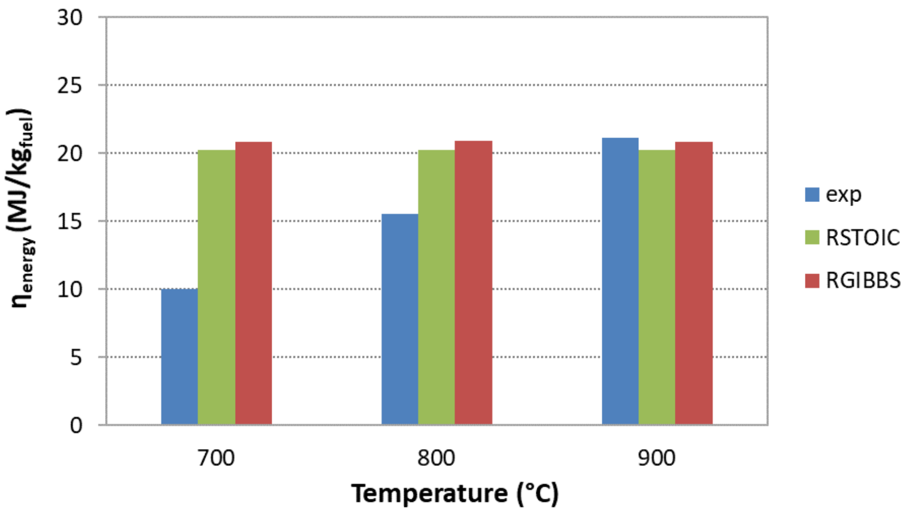

Figure S7. Effect of the variation of temperature on η_{energy} for the gasification of PKS with SR = 0.2 and 70 vol.% steam.

Table S1. Block description used in the simulation model.

Block name	Aspen Plus® name	Description
DECOMP	**RYIELD**	Models a reactor by specifying reaction yields of each component. Converts the non-conventional stream "FEED" into its conventional components. Ultimate and proximate analysis of biomass are required.
BCONVRT	**CALCULATOR**	Fortran subroutine used to calculate the yields of the component attributes of the biomass feedstock. A set of different variables associated to inlet/outlet streams is required to solve this block.
HEAT-1/ HEAT-2	**EXCHANGER**	Increase the oxidizing agent temperature from ambient temperature to the gas preheater. This temperature is fixed in 650°C.
GASIF	**RGIBBS**	Gibbs free energy reactor. Simulates the partial oxidation and gasification reactions. Chemical equilibrium is restricted by specifying a temperature approach for each reaction. The operation temperature is a variable studied in the work.

SEP	**FLASH**	Separates the gas production in the gasification and the solid waste remaining in the process.
COMB	**RSTOIC**	Simulates the oxidation reactions occur in a gasification process when conventional components of biomass react with O_2 from the air stream inlet. Stoichiometric reaction is known. The operation temperature is a variable studied in the work.
GASIF		Simulates the char gasification when carbonaceous material reacts with gasifying agent no consumed in the previous steps. Stoichiometric reaction is known. The operation temperature is a variable studied in the work.
REQUIL	**REQUIL**	Simulates the equilibrium of homogeneous reactions when steam is used as gasifying agent. The operation temperature is a variable studied in the work.
MIX2	**MIXER**	Mixes the stream S1 and S with specifying temperature and pressure variables.

Table S2. Comparison of experimental and model predictions and error values for the product gas compositions (vol.%) at different stoichiometric ratios during gasification of PKS using 70 vol.% steam at 900 °C.

SR	EXPERIMENTAL				GIBBS				RMS	RSTOIC				RMS
	CO_2	CO	CH_4	H_2	CO_2	CO	CH_4	H_2		CO_2	CO	CH_4	H_2	
0.1	15.83	26.05	7.33	27.10	12.37	23.25	2.76E-03	44.76	9.82	12.60	24.21	4.88	35.88	5.09
0.15	17.02	24.43	6.53	24.13	15.60	17.18	7.83E-04	41.52	10.00	14.67	19.26	3.65	33.42	4.59
0.2	15.63	22.64	5.95	24.68	17.54	13.16	2.75E-04	38.15	8.81	16.24	15.38	2.65	31.29	3.89
0.3	17.00	17.71	4.61	21.74	19.50	8.18	4.54E-05	31.49	7.31	18.49	9.61	1.10	27.84	2.10

Table S3. Comparison of experimental and model predictions and error values for the product gas compositions (vol.%) at different steam to biomass ratios during gasification of PKS at 900 °C with SR=0.2.

SBR	EXPERIMENTAL				GIBBS				RMS	RSTOIC				RMS
	CO_2	CO	CH_4	H_2	CO_2	CO	CH_4	H_2		CO_2	CO	CH_4	H_2	
0.09	16.90	21.947	5.83	17.22	4.62	31.14	8.63E-03	28.71	10.01	6.18	29.64	4.40	19.99	6.78
0.26	15.81	24.23	6.71	19.18	7.46	27.15	4.17E-03	30.69	8.00	8.96	25.65	3.63	23.75	4.45
0.79	15.53	23.66	5.93	23.09	12.54	19.98	1.26E-03	34.68	6.93	13.09	19.65	2.81	28.87	4.04
1.19	16.91	21.30	5.77	24.38	15.00	16.68	6.45E-04	36.27	7.07	14.67	17.58	2.70	30.02	3.88
1.85	15.63	22.64	5.95	24.68	17.54	13.16	2.75E-04	38.15	8.81	16.24	15.38	2.65	31.29	5.19

Table S4. Comparison of experimental and model predictions and error values for the product gas compositions (vol.%) at different temperatures during gasification of PKS using 70 vol.% steam with SR=0.2.

T(˚C)	EXPERIMENTAL				GIBBS				RMS	RSTOIC				RMS
	CO_2	CO	CH_4	H_2	CO_2	CO	CH_4	H_2		CO_2	CO	CH_4	H_2	
700	16.67	19.081	5.38	11.57	20.66	8.83	3.08E-02	40.39	15.65	18.31	12.50	2.59	32.97	11.31
800	15.73	22.60	6.16	17.48	19.00	11.13	2.40E-03	39.22	12.78	17.23	14.00	2.62	32.10	8.70
900	15.60	22.59	5.94	23.77	17.54	13.16	2.75E-04	38.15	9.15	16.24	15.38	2.65	31.29	5.47