

SUPPLEMENTARY MATERIAL

Continuous hydrogen production via hydrothermal gasification of biodiesel industry wastewater: experimental optimization and energy integration simulation

Isabela R. Teixeira ¹, Isabela M. Dias ¹, Lucas C. Mourão ¹, Laiane A. Andrade ², Leandro V. Pavão ³, J. M. Abelleira-Pereira ⁵, Guilherme B. M. Souza ¹, Lucio Cardozo-Filho ³, Christian G. Alonso ¹, Reginaldo Guirardello ^{4,*}

¹ Universidade Federal de Goiás (UFG), Instituto de Química, Av. Esperança s/n, Campus Samambaia, CEP 74690-900, Goiânia, Goiás, Brazil.

² Universidade Federal do Mato Grosso do Sul (UFMS), Av. Rosilene Lima Oliveira, 64, Jardim Universitário, CEP 79750-000, Nova Andradina, Mato Grosso do Sul, Brazil.

³ Programa de Pós-Graduação em Engenharia Química, Universidade Estadual de Maringá (UEM), Avenida Colombo, 5790 - Zona 7, Maringá - PR, 87020-900, Brazil.

⁴ School of Chemical Engineering, University of Campinas (UNICAMP), Av. Albert Einstein 500, 13083-852, Campinas, SP, Brazil

⁵ Department of Chemical Engineering and Food Technology, Faculty of Sciences, University of Cádiz, International Excellence Agrifood Campus (CeiA3), 11510, Puerto Real (Cádiz), Spain.

* Correspondence: guira@feq.unicamp.br

Table S1 Effect estimates in SCWG for hydrogen production.

Factor	Effect	Std. Err. Pure Err	-95% Cnf. Limit	+95% Cnf. Limit	t(3)	p	Coeff.	Std. Err. Coeff.	-95% Cnf. Limit	+95% Cnf. Limit
Mean/Interc.	1023.611	4153.420	869.776	1177.447	21.17578	0.000230	1023.611	48.3387	869.776	1177.447
Feed flow rate (L)	282.355	106.861	1.925	562.785	3.20429	0.049170	141.177	44.0588	0.962	281.392
Temperature (L)	2717.684	12.798	2436.555	2998.814	30.76481	0.000075	1358.842	44.1687	1218.278	1499.407
Temperature (Q)	1154.088	0.010	844.769	1463.406	11.87391	0.001284	577.044	48.5976	422.385	731.703
Two-way interaction	763.270	0.177	366.573	1159.968	6.12322	0.008756	381.635	62.3258	183.286	579.984

R-sqr = 0.99283; Adj = 0.98873; 2 factors, 1 blocks, 12 runs, MS Pure Error = 15540.81

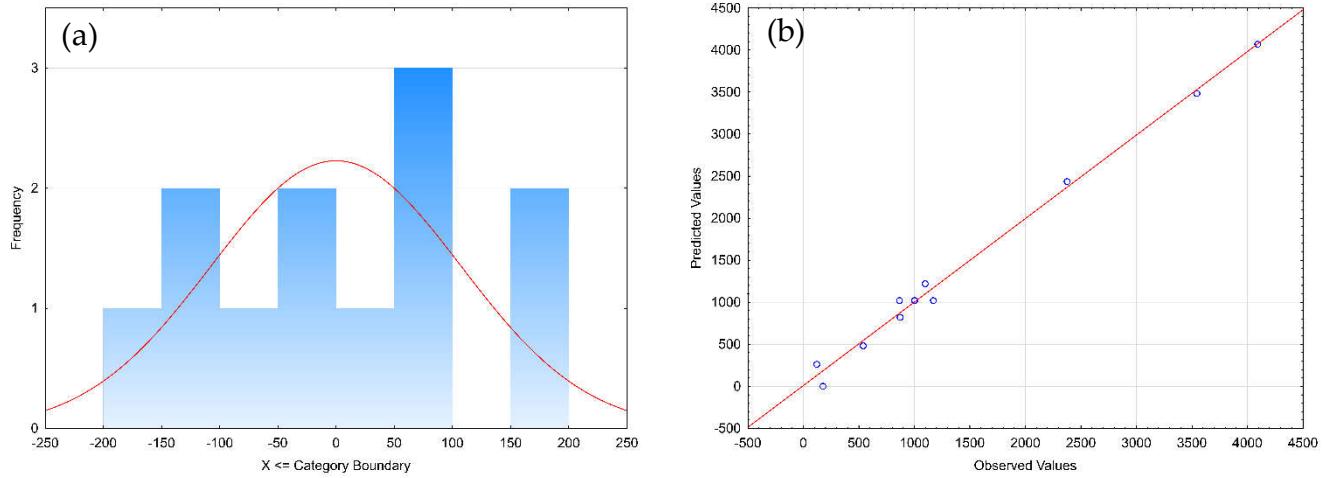


Figure S1 (a) Distribution of residual; (b) Residuals x predicted values.

Table S2 Removal of total organic carbon after SCWG process

Run	Feed flow rate (mL/min)	Temperature (°C)	TOC (%)
1	12.3	529	18.99
2	12.3	671	82.62
3	22.9	529	8.31
4	22.9	671	57.27
5	10	600	48.09
6	25	600	19.11
7	17.5	500	4.48
8	17.5	700	74.07
9	17.5	600	27.86
10	17.5	600	23.95
11	17.5	600	25.54
12	17.5	600	27.00

Table S3 Effects estimate in SCWG for removal of total organic carbon.

Factor	Effect	Std. Err. Pure Err	-93% Cnf. Limit	+93% Cnf. Limit	t(2)	p	Coeff.	Std. Err. Coeff.	-93% Cnf. Limit	+93% Cnf. Limit
Mean/Interc.	25.576	1.135	21.514	29.638	22.530	0.0019	25.576	1.135	21.514	29.638
Feed flow rate (L)	-18.996	1.390	-23.970	-14.022	-13.665	0.0053	-9.498	0.695	-11.985	-7.011
Feed flow rate (Q)	10.576	1.651	4.664	16.487	6.402	0.0235	5.288	0.825	2.332	8.243
Temperature (L)	52.797	1.393	47.811	57.783	37.892	0.0006	26.398	0.696	23.906	28.891
Temperature (Q)	16.404	1.665	10.445	22.362	9.851	0.0101	8.202	0.832	5.222	11.181
Two-way interaction	-7.269	1.966	-14.304	-0.233	-3.697	0.0660	-3.634	0.983	-7.152	-0.116

R-sqr = 0.98625; Adj = 0.9725; 2 factors, 1 blocks, 11 runs, MS Pure Error = 3.8664

Table S4 Regression coefficients in SCWG for removal of total organic carbon.

Factor	Regressn Coeff.	Std. Err. Pure Err	t(2)	p	-93% Cnf. Limit	+93% Cnf. Limit
Mean/Interc.	376.0893	68.0067	5.5301	0.0311	132.7443	619.4343
Feed flow rate (L)	-2.6235	1.8816	-1.3942	0.2979	-9.3565	44.1094
Feed flow rate (Q)	0.1883	0.0294	6.4021	0.0235	0.0830	0.2935
Temperature (L)	-1.4107	0.2036	-6.9263	0.0202	-2.1394	-0.6819
Temperature (Q)	0.0016	0.0001	9.8512	0.0101	0.0010	0.0022
Two-way interaction	-0.0097	0.0026	-3.6970	0.0660	-0.0190	-0.0003

R-sqr = 0.98625; Adj = 0.9725; 2 factors, 1 blocks, 11 runs, MS Pure Error = 3.8664

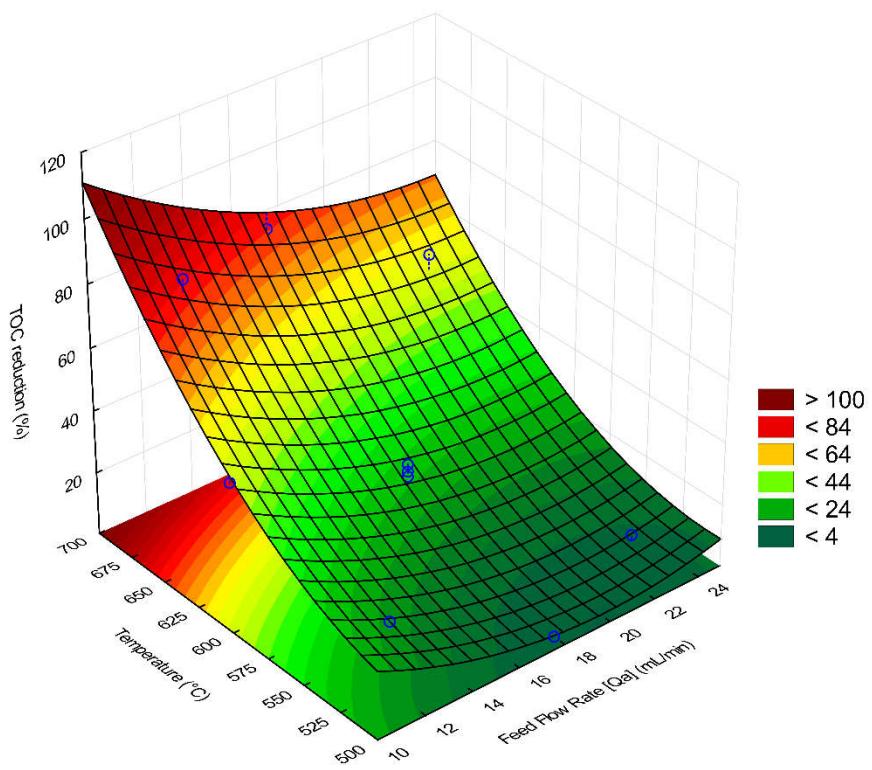


Figure S1 Response surface of TOC removal as a function of temperature and feed flow rate.

Table S5 ANOVA table in SCWG for removal of total organic carbon.

Factor	Df	Sum Sq	Mean Sq	F-value	p-value
Feed flow rate (L)	1	722.028	722.028	186.743	0.005312
Feed flow rate (Q)	1	158.4733	158.473	40.986	0.023540
Temperature (L)	1	5551.549	5551.549	1435.832	0.000696
Temperature (Q)		375.223	375.223	97.046	0.010148
Two-way interaction	1	52.848	52.848	13.668	0.066001
Lack-of-fit	3	86.791	28.930	7.482	0.120168
Pure Error	2	7.733	3.866		
Total SS	10	6874.099			

R-sqr = 0.98625; Adj = 0.9725; 2 factors, 1 blocks, 11 runs, MS Pure Error = 3.8664

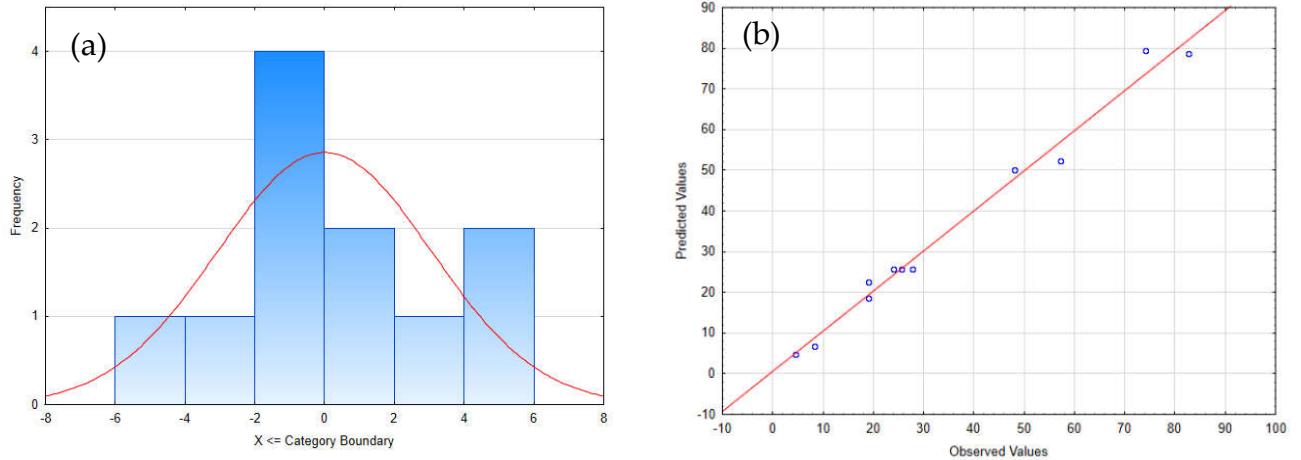


Figure S3 (a) Distribution of residual; (b) Residuals x predicted values.

Table S6 Chemical composition of Inconel 625

Chemical	Concentration (%)
Nickel (Ni)	58 - 71%
Chromium (Cr)	21 - 23%
Molybdenum (Mo)	8 - 10%
Iron (Fe)	5%
Niobium (Nb)	3.2 – 3.8%
Tantalum (Ta)	3.2 – 3.8%
Cobalt (Co)	1% max.
Manganese (Mn)	0.5 % max.
Aluminum (Al)	0.4% max.