

Electronic Supplementary Material

A New Approach to Dehydration of xylose to 2-furfuraldehyde Using a Mesoporous Niobium-based Catalyst

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Tables: 04

Supplementary Table 1. Regression coefficients for the responses evaluated in the 2³ experimental design.

Yield (%)	Regressn Coeff.	Std.Err. Pure Err	t(2)	p-value	-95% Cnf.Limt	+95% Cnf.Limt
Mean/Interc.	-164.677	45.06818	-3.65395	0.067413	-358.590	29.23576
(1) <i>T</i> (°C)(L)	1.813	0.50669	3.57756	0.070024	-0.367	3.99284
(2) <i>t</i> (min)(L)	0.171	0.10624	1.60764	0.249168	-0.286	0.62792
(3) <i>CXR</i> (%) (L)	0.062	0.13972	0.44714	0.698535	-0.539	0.66363
<i>T</i> (°C)(Q)	-0.004	0.00140	-3.01523	0.094636	-0.010	0.00180
2L by 3L	-0.001	0.00056	-1.90745	0.196703	-0.003	0.00133
1L by 3L	-0.001	0.00073	-1.00189	0.421923	-0.004	0.00241
1L by 2L	-0.000	0.00056	-0.84347	0.487764	-0.003	0.00192
Conversion (%)	Regressn Coeff.	Std.Err. Pure Err	t(2)	p-value	-95% Cnf.Limt	+95% Cnf.Limt
Mean/Interc.	-732.552	20.20425	-36.2573	0.000760	-819.484	-645.620
(1) <i>T</i> (°C)(L)	7.776	0.22715	34.2309	0.000852	6.798	8.753
(3) <i>CXR</i> (%) (L)	1.177	0.06264	18.7887	0.002821	0.907	1.446
(2) <i>t</i> (min)(L)	0.563	0.04763	11.8240	0.007077	0.358	0.768
<i>T</i> (°C)(Q)	-0.018	0.00063	-29.1661	0.001173	-0.021	-0.016
1L by 3L	-0.006	0.00033	-17.0717	0.003414	-0.007	-0.004
1L by 2L	-0.002	0.00025	-9.6939	0.010475	-0.003	-0.001
2L by 3L	0.000	0.00025	0.5492	0.638018	-0.001	0.001
Selectivity (%)	Regressn Coeff.	Std.Err. Pure Err	t(2)	p- value	-95% Cnf.Limt	+95% Cnf.Limt
Mean/Interc.	306.5686	46.98692	6.5246	0.022694	104.4002	508.7370
(1) <i>T</i> (°C)(L)	-2.3608	0.52826	-4.4690	0.046598	-4.6338	-0.0879
(3) <i>CXR</i> (%) (L)	-1.7158	0.14567	-11.7790	0.007130	-2.3426	-1.0891
1L by 3L	0.0074	0.00076	9.7094	0.010442	0.0041	0.0107
<i>T</i> (°C)(Q)	0.0051	0.00146	3.4756	0.073742	-0.0012	0.0113
(2) <i>t</i> (min)(L)	-0.0037	0.11076	-0.0334	0.976409	-0.4803	0.4729
2L by 3L	-0.0012	0.00058	-2.0215	0.180603	-0.0037	0.0013
1L by 2L	0.0003	0.00058	0.5041	0.664239	-0.0022	0.0028

Supplementary Table 2. ANOVA results for response yield (%) evaluated in the 2³ experimental design.

Factor	ANOVA; Var: Yield (%); $R^2=0.93033$; $R^2_{adj}:0.76777$ (Spreadsheet5) 3 factors. 1 Blocks. 11 Runs; MS Pure Error=10.9099 DV: Yield (%)				
	SS	df	MS	F	p-value
(1) <i>T</i> (°C)(L)	662.116	1	662.1161	60.68947	0.016081
<i>T</i> (°C)(Q)	99.188	1	99.1883	9.09159	0.094636
(2) <i>t</i> (min)(L)	24.500	1	24.5000	2.24567	0.272723
(3) <i>CXR</i> (%)(L)	253.575	1	253.5752	23.24267	0.040433
1L by 2L	7.762	1	7.7618	0.71145	0.487764
1L by 3L	10.951	1	10.9512	1.00379	0.421923
2L by 3L	39.694	1	39.6941	3.63835	0.196703
*Lack of Fit	60.390	1	60.3900	5.53534	*0.142921
Pure Error	21.820	2	10.9099		
Total SS	1179.996	10			

*When p -value > 0.05, lack of fit of mathematical model is no significant.

Supplementary Table 3. ANOVA results for response conversion (%) evaluated in the experimental design.

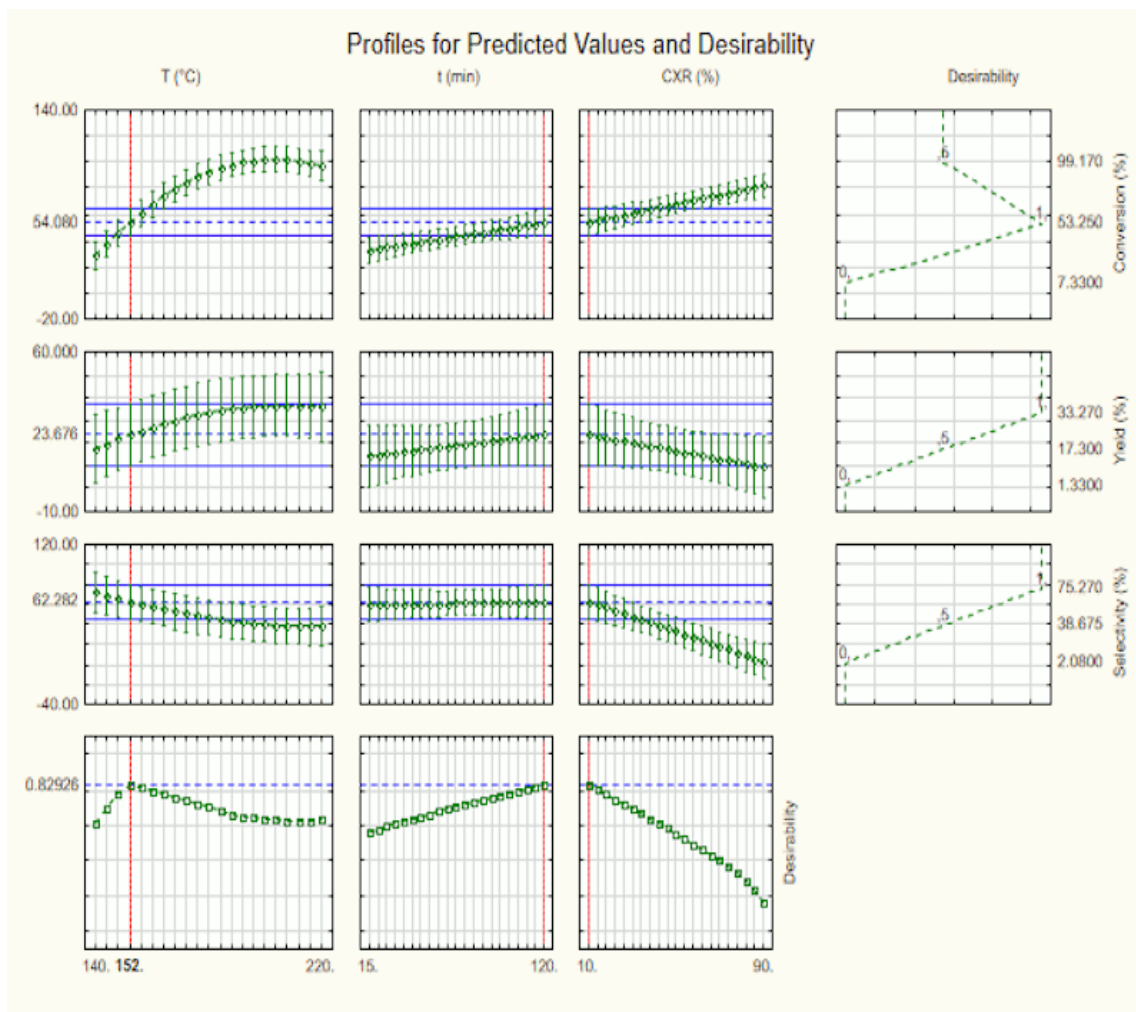
Factor	ANOVA; Var.:Conversion (%); $R^2=0.99627$; $R^2_{adj}=0.98756$ (Spreadsheet5) 3 factors. 1 Blocks. 11 Runs; MS Pure Error=2.192633 DV: Conversion (%)				
	SS	df	MS	F	p -value
(1) T (°C)(L)	7287.87	1	7287.866	3323.796	0.000301
T (°C)(Q)	1865.19	1	1865.193	850.663	0.001173
(2) t (min)(L)	401.86	1	401.861	183.278	0.005412
(3) CXR (%)(L)	417.60	1	417.605	190.458	0.005210
1L by 2L	206.05	1	206.045	93.971	0.010475
1L by 3L	639.03	1	639.031	291.445	0.003414
2L by 3L	0.66	1	0.661	0.302	0.638018
*Lack of Fit	36.13	1	36.125	16.476	*0.055675
Pure Error	4.39	2	2.193		
Total SS	10858.77	10			

*When p -value > 0.05, lack of fit of mathematical model is no significant.

Supplementary Table 4. ANOVA results for response selectivity (%) evaluated in the 2³ experimental design.

ANOVA; Var.:Selectivity (%); $R^2=0.97024$; $R^2_{adj}=0.90079$ (Spreadsheet5) 3 factors. 1 Blocks. 11 Runs; MS Pure Error=11.85863 DV: Selectivity (%)					
Factor	SS	df	MS	<i>F</i>	<i>p</i> -value
(1) <i>T</i> (°C)(L)	282.388	1	282.388	23.8128	0.039521
<i>T</i> (°C)(Q)	143.252	1	143.252	12.0800	0.073742
(2) <i>t</i> (min)(L)	2.071	1	2.071	0.1746	0.716638
(3) <i>CRX</i> (%)(L)	2768.052	1	2768.052	233.4208	0.004257
1L by 2L	3.014	1	3.014	0.2541	0.664239
1L by 3L	1117.936	1	1117.936	94.2719	0.010442
2L by 3L	48.462	1	48.462	4.0866	0.180603
*Lack of Fit	110.187	1	110.187	9.2917	*0.092873
Pure Error	23.717	2	11.859		
Total SS	4499.078	10			

*When *p*-value > 0.05, lack of fit of mathematical model is no significant.



Supplementary Figure 1. Predicted values by the desirability tool for all responses studied.

