INVESTIGATING THE ACIDITY EFFECT OF NIOBIA AS CATALYTIC SUPPORT FOR FURFURAL CONVERSION

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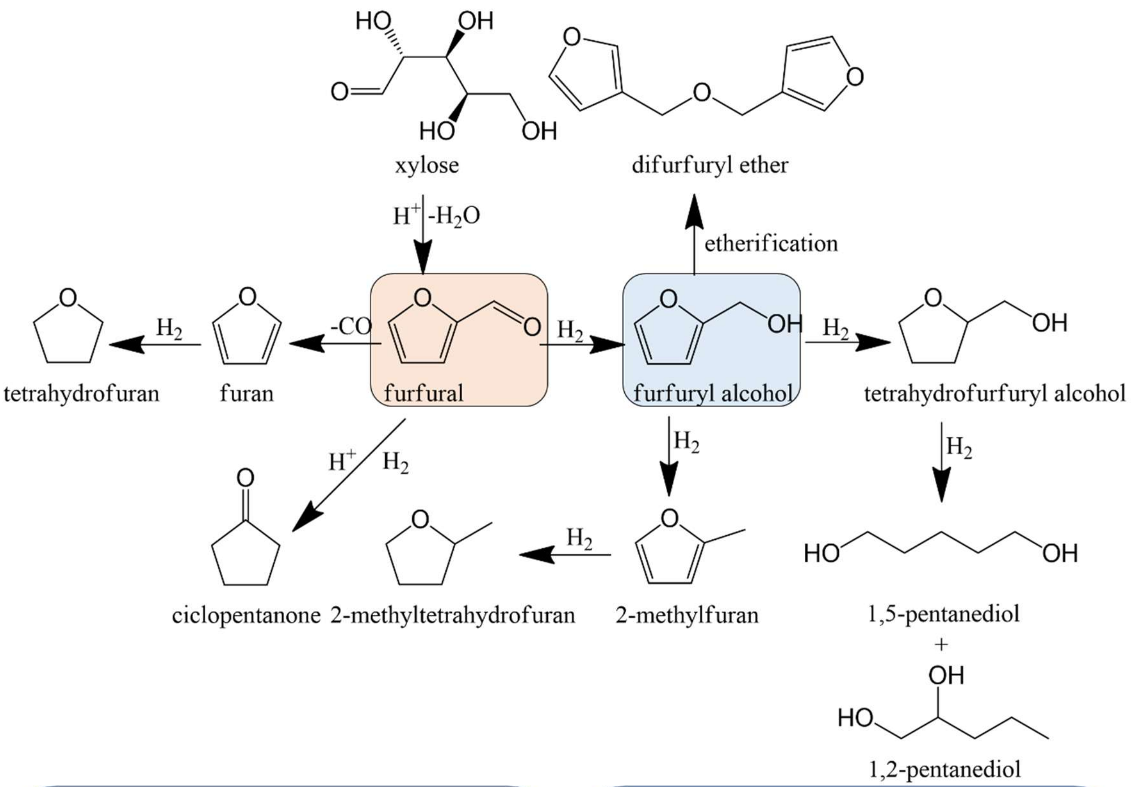


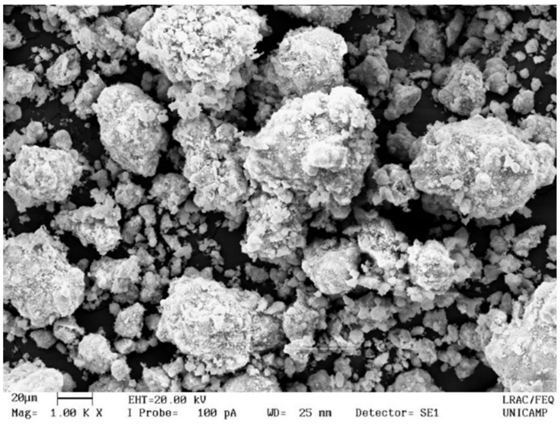
Furfural:

- Production via fossil-based materials is not economically competitive
- Precursor of more than 80 furan-based chemicals and solvents
- Applications: selective solvent for aromatics and unsaturated molecules; used in transportation, pharmaceutical and agrochemical industries
- Common reactions: hydrogenation, decarbonylation and hydrodeoxygenation

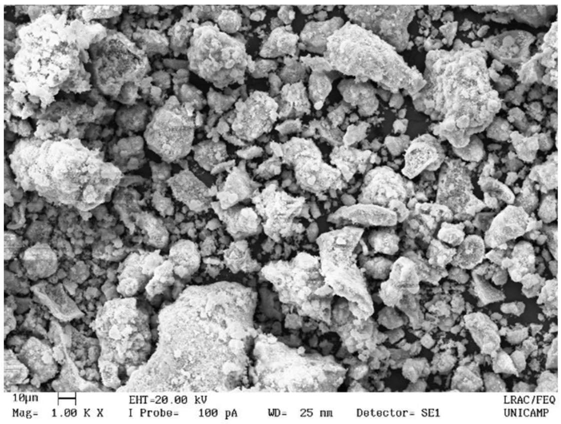
Furfuryl alcohol:

- Obtained by the hydrogenation of the aldehyde group in furfural
- About 65% of all furfural produced is directed towards obtaining furfuryl alcohol
- Application: production of furan resins, with excellent chemical, thermal and mechanical properties, as well as resistance to corrosion and to solvent action
- Industrial synthesis with a copper-chromite catalyst, which is toxic and deactivating

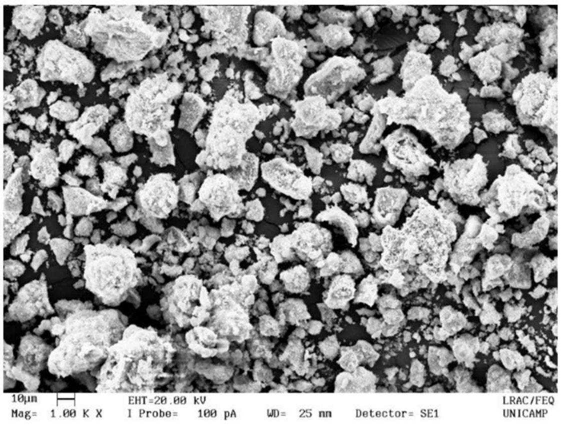
Fig. S1 - Most common furfural conversion routes and main information about furfural and furfuryl alcohol.



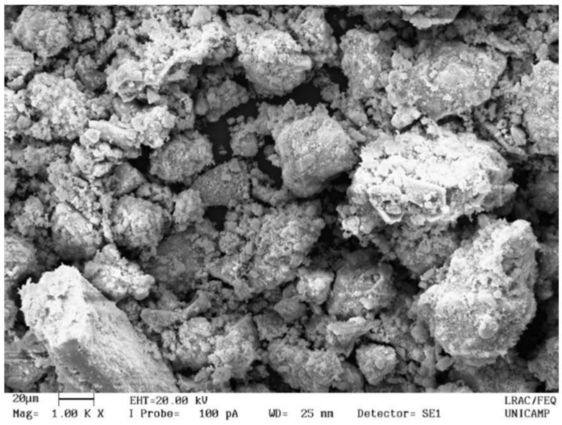
a) Nb_2O_5



b) 5% Ni/Nb_2O_5

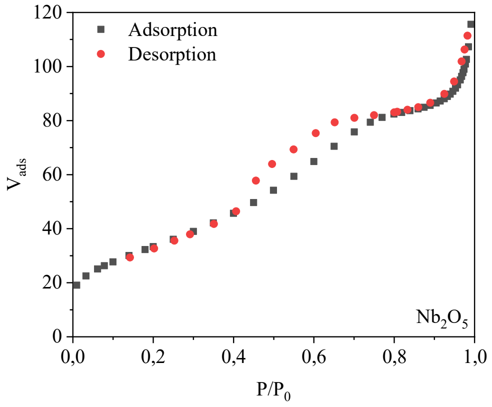


c) 10% Ni/Nb_2O_5

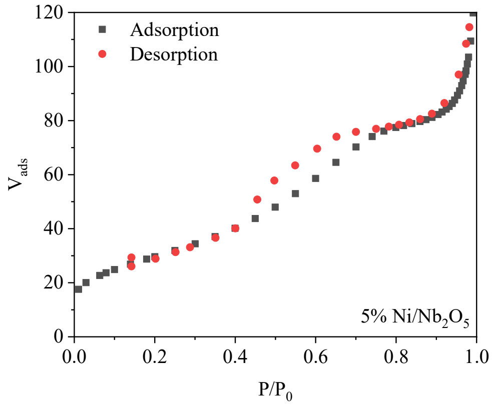


d) 15% Ni/Nb_2O_5

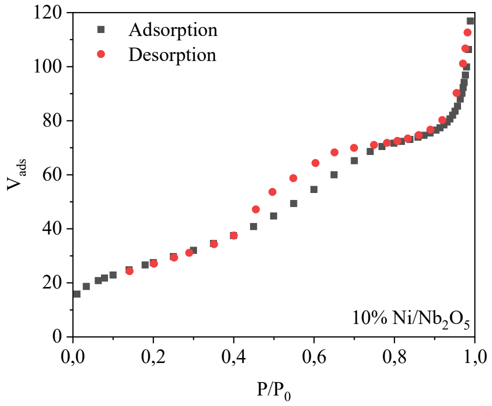
Fig. S2 - SEM images for Nb_2O_5 (a), 5% Ni/Nb_2O_5 (b), 10% Ni/Nb_2O_5 (c) and 15% Ni/Nb_2O_5 (d). SEM conditions: electrical current of 100 pA and 20 kV, with 25 mm focus (magnification 1000x).



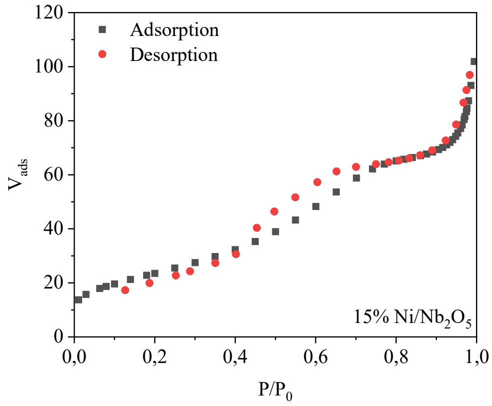
a) Nb_2O_5



b) 5% Ni/Nb_2O_5



c) 10% Ni/Nb_2O_5



d) 15% Ni/Nb_2O_5

Fig. S3 - Isotherm plots obtained in N_2 physisorption for Nb_2O_5 (a), 5% Ni/Nb_2O_5 (b), 10% Ni/Nb_2O_5 (c) and 15% Ni/Nb_2O_5 (d). N_2 physisorption conditions: -196°C, samples pretreated under vacuum at 200°C for 12 hours.

Table S1 – Ni catalysts applied in furfural hydrogenation to furfuryl alcohol previously reported in the literature.

Reference	Catalyst	Temperature (°C)	H_2 pressure (MPa)	Solvent	Time (h)	Furfural conversion (%)	Furfuryl alcohol selectivity (%)
This work	**Ni/Nb_2O_5**	**150**	**5**	**2-propanol**	**5**	**47**	**60-80**
[1]	Ni/SiO_2	100	1	2-propanol	8	31	76
[2]	Ni/Fe_2O_3	180	CTH	2-propanol	7.5	46	72
[3]	Ni/SiO_2	110	3	2-propanol	3	99.5	50.3
[4]	Ni/CN	200	1.3	2-propanol	5	100	75
[5]	Ni/AC	200	3	2-propanol	5	85	6
[6]	Ni/R-Ca	140	CTH	ethanol	4	39.9	58.2
[7]	Ni-MFC-400	160	2	methanol	4	92.3	59.3
[8]	$Ni_{0.15}$/Al_2O_3-C-400	160	4	ethanol	6	55.5	85.8
[9]	Ni@CG	150	0.5	2-propanol	5	19	29
[10]	Ni@OMC	180	3	2-propanol	12	51	92
[11]	Ni/bentonite	150	2.5	2-propanol	15	100	70
[12]	Ni/CL	160	3	ethanol	2	100	51
[13]	Ni/TiO_2-350	120	2	water	4	85.2	64.2
[14]	Ni/HNPC	110	2	2-propanol	4	95.2	94.8
[15]	Ni/TiO_2-A2	50	2	methanol	2	65.7	66.7
[16]	Ni/TiO_2-400-350R	140	2	2-propanol	6	80	85
[17]	Ni/γ-Al_2O_3	150	CTH	2-propanol	2	98	27
[18]	Ni/hydrotalcite	140	5	water	4	45	98

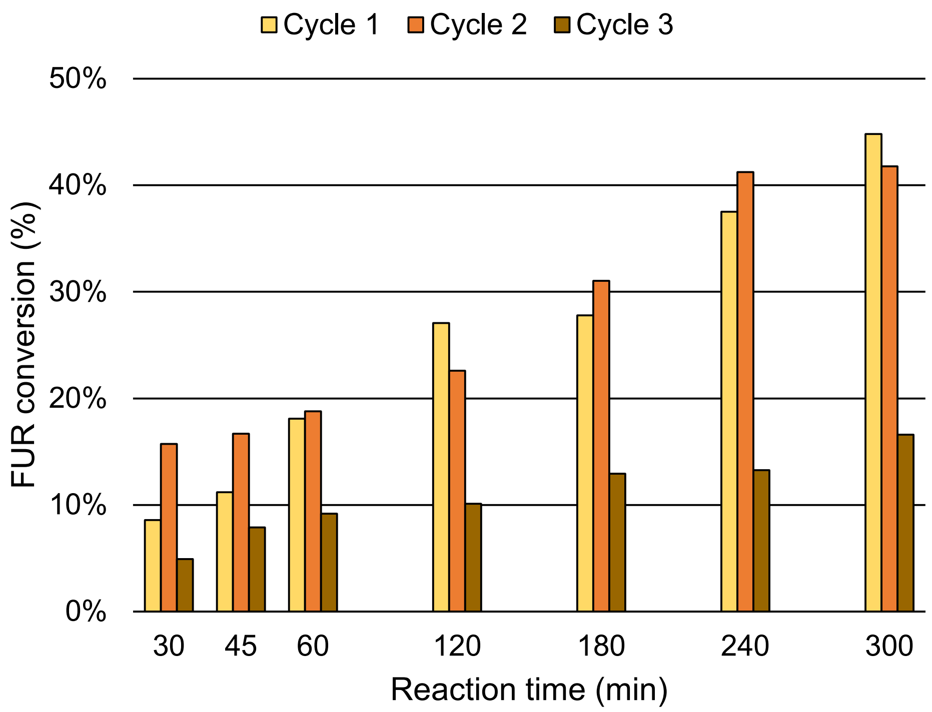


Fig. S4 - Conversion of furfural obtained with catalyst 10% Ni/Nb_2O_5 in three consecutive cycles. Reaction conditions: 5 MPa of H_2, 150°C, agitation of 1000 rpm, 300 mg of catalyst.

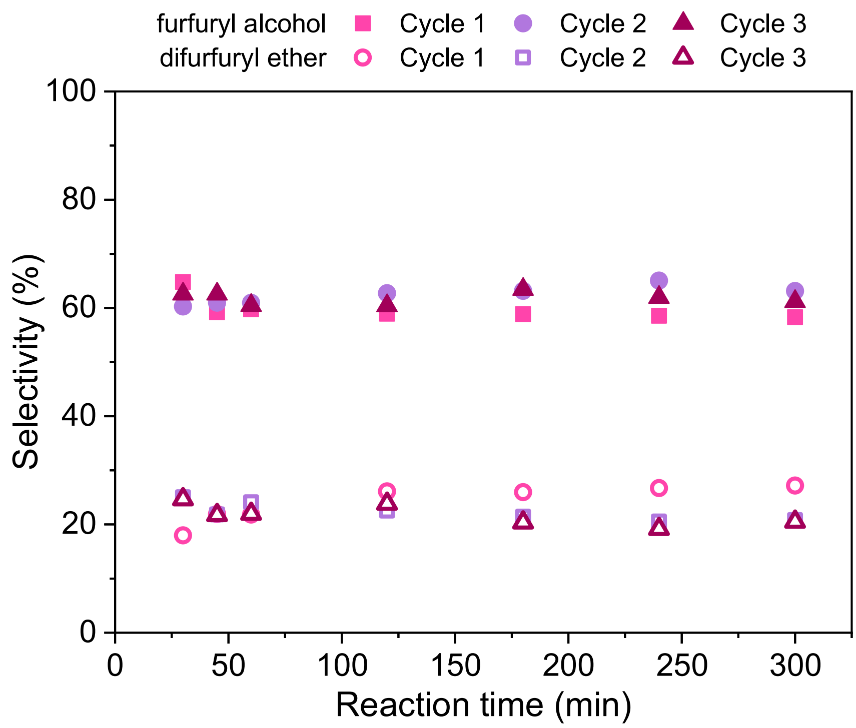


Fig. S5 - Selectivity to furfuryl alcohol and difurfuryl ether with catalyst 10% Ni/Nb_2O_5 in three consecutive cycles. Reaction conditions: 5 MPa of H_2, 150°C, agitation of 1000 rpm, 300 mg of catalyst.

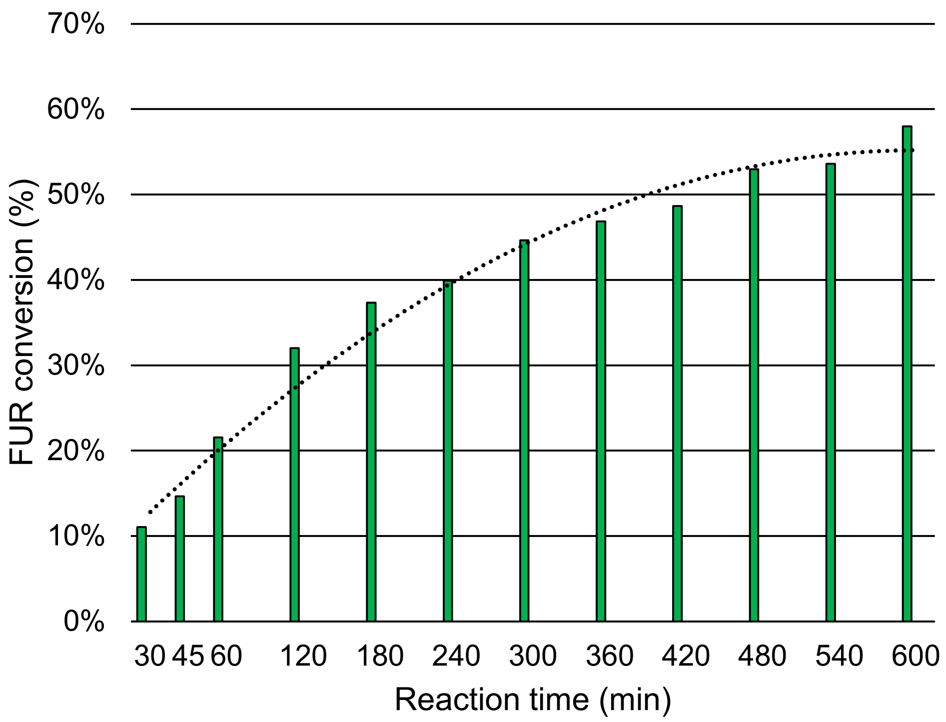


Fig. S6 - Conversion of furfural obtained with catalyst 10% Ni/Nb_2O_5 in ten hours. Reaction conditions: 5 MPa of H_2, 150°C, agitation of 1000 rpm, 300 mg of catalyst.

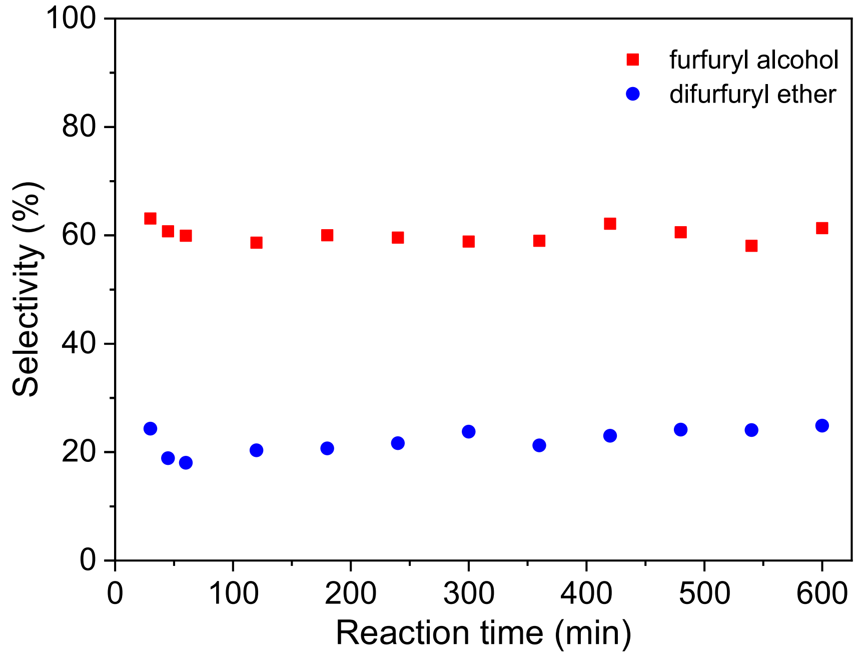


Fig. S7 - Selectivity to furfuryl alcohol and difurfuryl ether with catalyst 10% Ni/Nb_2O_5 in ten hours. Reaction conditions: 5 MPa of H_2, 150°C, agitation of 1000 rpm, 300 mg of catalyst.

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