catalysts

Supplementary Material

CO_2 methanation over hydrotalcite-derived nickel/ruthenium and supported ruthenium catalysts

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Reduction temperature of $Ru/Al_2O_3^{com.}$

The catalyst $Ru/Al_2O_3^{com.}$ was tested in the screening conditions after reduction at 300°C and 600 °C. The CO_2 conversion and CH_4 selectivity obtained are presented in **Fig. S.1** and **Fig. S.2**, respectively.

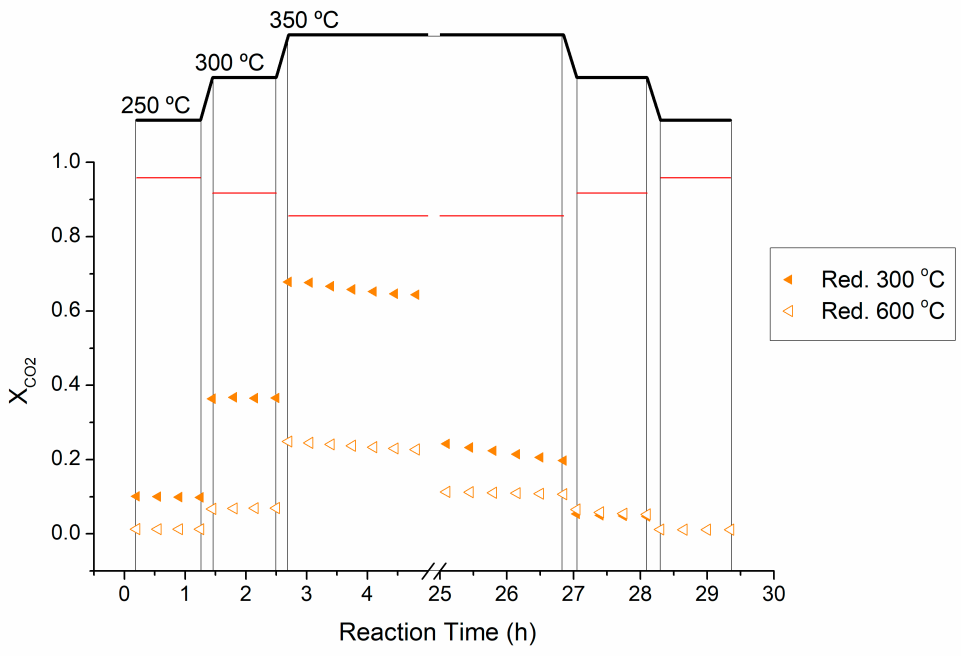

Fig. S.1 - CO_2 conversion of Ru/Al_2O_3 reduced at 300 °C and 600 °C, during the screening test. Red line shows the equilibrium conversion.

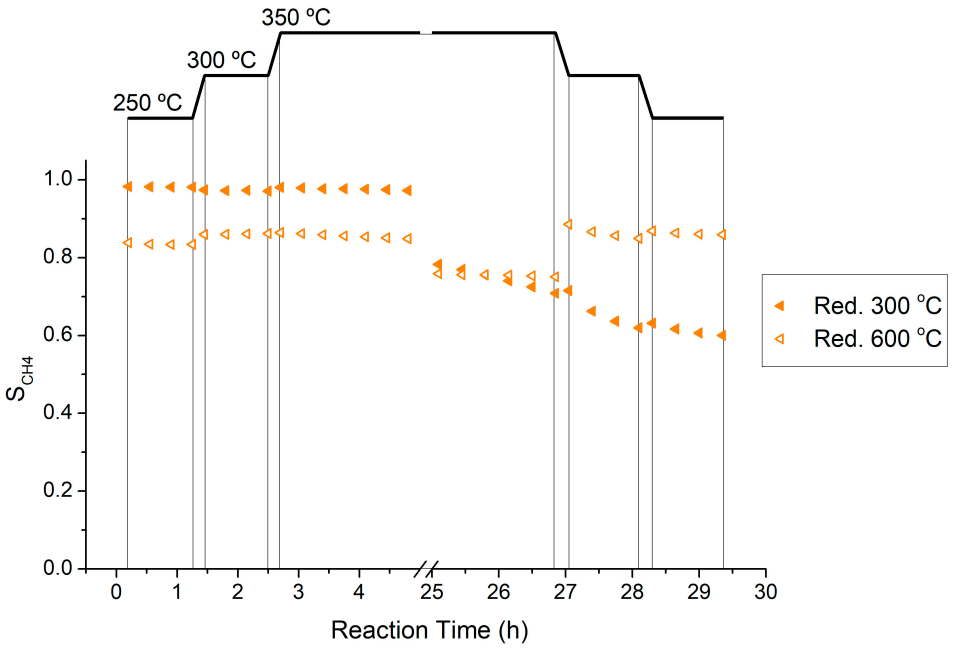

Fig. S.2 – CH_4 selectivity of Ru/Al_2O_3 reduced at 300 °C and 600 °C, during the screening test.

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Catalysts Price estimation

The price of the prepared catalysts was estimated using the CatCost tool [1]. The selected price estimation method was the simple step-based method (details can be found in [1]) that requires inputting to the CatCost tool both synthesis and business data. The former is data related to the catalyst composition, raw materials consumption, synthesis steps and other information that can be obtained from the laboratory-scale reaction. The latter is the annual demand, order frequency and order size. However, when using the simple step-based method only the order size is required, which was considered the same for all the catalysts (i.e. 1 ton). **Table S.1** summarizes the necessary inputs to the CatCost tool. **Table S.2** summarizes the outputs generated by the CatCost Tool, in U.S. dollars per kilogram.

Table S.1 - Price estimation inputs required for the single-step method in the CatCost tool.

	Inputs
Synthesis Campaign Size	
Order size (1-1000 tons)	1 ton
Overhead and Selling Margin	
General & administrative	5 %
Sales, Admin, Research, Distribution	5 %

The hydrotalcite derived materials (prepared by coprecipitation with or without Ru impregnation) were estimated to be the most expensive to synthesize. Both the materials used and processing steps executed showed higher prices in these catalysts, than in the ruthenium in silica catalyst (prepared by impregnation). The impregnation of NiMgAl with ruthenium adds circa 35 $/kg to the synthesis expenses.

The total price (including synthesis costs, overheads and selling margin) of Ru/NiMgAl, the most expensive catalyst, was estimated to be 1 023 $/kg, followed by NiMgAl, 962.55 $/kg and then Ru/$SiO_2$ (266.40 $/kg).

Table S.2 - Prices in U.S. dollars for producing 1 kg of catalyst calculated using the CatCost tool.

	Ru/NiMgAl	NiMgAl	Ru/SiO_2
Synthesis Costs			
Raw material	561.27	529.82	140.86
Processing steps	15.62	12.53	9.25
Subtotal ($/kg)	**576.88**	**542.36**	**150.10**
Overheads & Margin			
General & administrative	28.84	27.12	7.51
Sales, Admin, Research, Distribution	30.29	28.47	7.88
Selling Margin	387.82	364.60	100.91
Total Overheads & Margin ($/kg)	**446.95**	**420.20**	**116.29**
Total Catalyst Price ($/kg)	**1 023.83**	**962.55**	**266.40**

References

[1] F. G. Baddour, L. Snowden-Swan, J. D. Super and K. M. Van Allsburg, Estimating Precommercial Heterogeneous Catalyst Price: A Simple Step-Based Method, Org. Process Res. Dev., vol. 22, pp. 1599–1605, 2018.