Supporting Information on: Conceptual design of a novel process for the production of poly(oxymethylene) dimethyl ethers from formaldehyde and methanol

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Adsorption results

Table S1 gives the mass of the liquid initial mixtures, the mass of zeolite and the composition of the mixtures prior adsorption for the experiments at $T = 298.15$ K and Table S2 gives the compositions after adsorption at $T = 298.15$ K.

Table S3 gives the mass of the liquid initial mixtures, the mass of zeolite and the composition of the mixtures prior adsorption for the experiments at $T = 311.85$ K and Table S4 gives the compositions after adsorption at $T = 311.85$ K.

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Table S1: Mass of the liquid initial mixtures, mass of zeolite and compositions of the initial mixtures prior adsorption for the experiments at $T = 298.15$ K.

			overall mass fraction / (g/g)						
Experiment	m_{Initial} / (g)	m_{Zeolite} / (g)	formaldehyde	water	methanol	methylal	OME_2	OME_3	OME_4
Ads1	20.023	9.981	0.0595	0.0054	0.0626	0.6891	0.1621	0.0003	0.0209
Ads2	20.013	10.041	0.0565	0.0555	0.0595	0.6544	0.1540	0.0003	0.0199
Ads3	20.041	10.035	0.0535	0.1057	0.0563	0.6196	0.1458	0.0003	0.0188
Ads4	19.793	10.051	0.0486	0.1879	0.0511	0.5627	0.1324	0.0002	0.0171
Ads5	20.003	9.995	0.2142	0.0095	0.1001	0.4488	0.2059	0.0003	0.0213
Ads6	20.250	10.002	0.2024	0.0640	0.0946	0.4241	0.1946	0.0003	0.0201
Ads7	20.083	10.005	0.1922	0.1109	0.0899	0.4028	0.1848	0.0003	0.0191
Ads8	19.434	9.992	0.1786	0.1741	0.0835	0.3742	0.1717	0.0002	0.0177

Table S2: Compositions of the mixtures after adsorption for the experiments at $T = 298.15$ K.

	overall mass fraction / (g/g)						
Experiment	formaldehyde	water	methanol	methylal	OME_2	OME_3	OME_4
Ads1	0.0535	0.0001	0.0549	0.7083	0.1626	0.0000	0.0206
Ads2	0.0532	0.0015	0.0530	0.7066	0.1645	0.0003	0.0209
Ads3	0.0527	0.0298	0.0588	0.6747	0.1626	0.0003	0.0212
Ads4	0.0521	0.1054	0.0557	0.6187	0.1485	0.0003	0.0194
Ads5	0.2119	0.0019	0.1035	0.4493	0.2112	0.0003	0.0220
Ads6	0.2048	0.0040	0.1035	0.4529	0.2124	0.0003	0.0221
Ads7	0.1923	0.0459	0.1086	0.4214	0.2095	0.0003	0.0220
Ads8	0.1793	0.1011	0.1018	0.4051	0.1924	0.0003	0.0200

Table S3: Mass of the liquid initial mixtures, mass of zeolite and compositions of the initial mixtures prior adsorption for the experiments at $T = 311.85$ K.

			overall mass fraction / (g/g)						
Experiment	m_{Initial} / (g)	m_{Zeolite} / (g)	formaldehyde	water	methanol	methylal	OME_2	OME_3	OME_4
Ads9	19.980	10.020	0.2104	0.0097	0.1026	0.4460	0.2092	0.0003	0.0217
Ads10	19.980	10.110	0.2000	0.0588	0.0975	0.4239	0.1988	0.0003	0.0207
Ads11	20.010	10.030	0.1893	0.1092	0.0923	0.4012	0.1882	0.0003	0.0195
Ads12	19.980	10.020	0.1747	0.1777	0.0852	0.3704	0.1737	0.0003	0.0180

Table S4: Compositions of the mixtures after adsorption for the experiments at $T = 311.85$ K.

	overall mass fraction / (g/g)						
Experiment	formaldehyde	water	methanol	methylal	OME_2	OME_3	OME_4
Ads9	0.2076	0.0015	0.0939	0.4441	0.2259	0.0026	0.0243
Ads10	0.1933	0.0289	0.1076	0.4280	0.2189	0.0003	0.0230
Ads11	0.1849	0.0675	0.1074	0.4126	0.2056	0.0003	0.0216
Ads12	0.1732	0.1307	0.1060	0.3817	0.1884	0.0002	0.0198

A flowsheet of the route producing OME via the intermediates trioxane and methylal is given in Figure S1. Compared to this route, the novel OME process saves various process units.

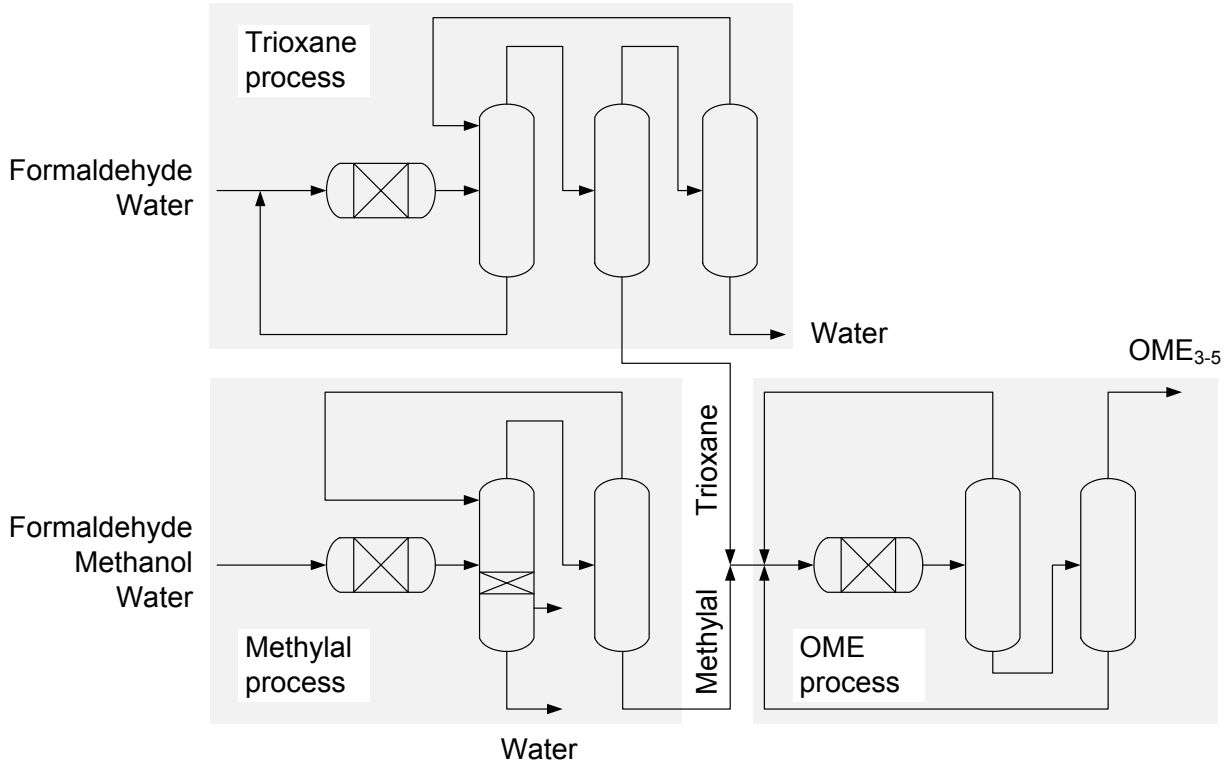

Figure S1: Flowsheet of the route producing OME via the intermediates trioxane and methylal.[1–4]

For a multicomponent distillation line at $p = 1.5$ bar and a reactor outlet as given in Table 4 of the manuscript (stream 3) , the bottom product yields are illustrated in Figure S2 showing that for this distillation line formaldehyde, methanol, water, methylal and OME_2 are not found in the bottom product, whereas 85% of OME_3 and 100% of OME with $n \geq 4$ are found in the bottom product.

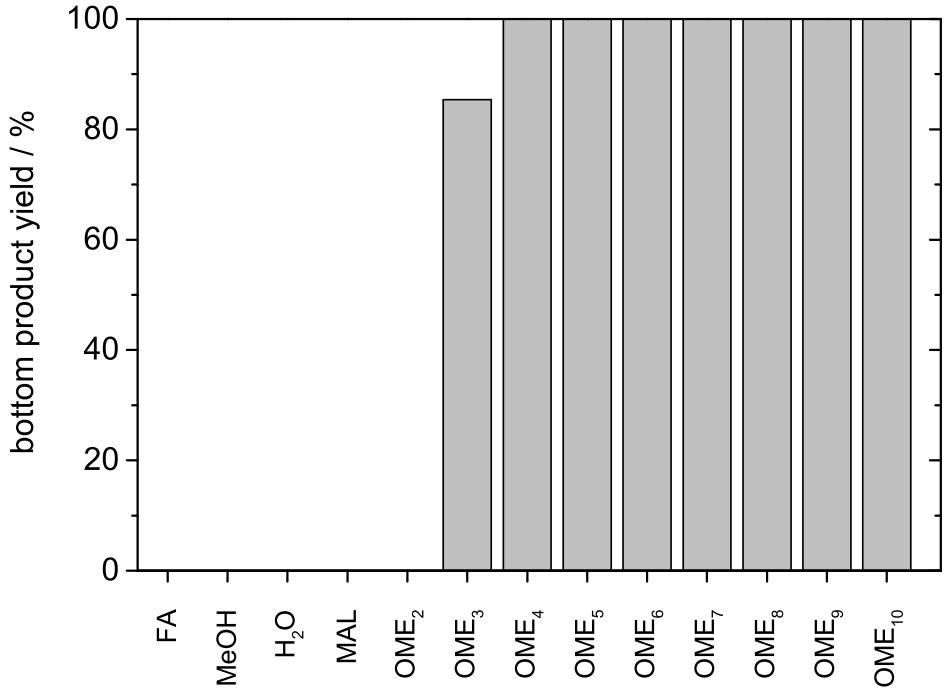

Figure S2: Bottom product yields calculated from a multicomponent distillation line at $p = 1.5$ bar for an reactor outlet (stream 3) as given in Table 4 of the manuscript. Formaldehyde, methanol, water, methylal and OME_2 are not found in the bottom product. The total bottom product yield for OME with $n \geq 3$ is 95%.

References

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