Supporting Information to "Solubility of formaldehyde in mixtures of water + methanol + poly(oxymethylene) dimethyl ethers"

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1. Numerical data of the measurements

In Table S-1 an overview of all measurements of this work is given. In Table S-2 to S-33 the numerical results for the measurements are given. Each Table corresponds to one experiment according to the number given in Table S-1. In Figure S-1 to S-23 for every experiment, which could be evaluated with the kinetic model, the concentration profile of the measurement and the model is shown like in Figure 9 in the main part. Beside the best fitting value also the model results for $p = 9$ is given. The samples with two liquid phases were not evaluated.

Table S-1: Overview of the experiments carried out in this work.

Experi-ment	T / K	OME$_n$	ternary / quaternary	SLE / SLLE	$\tilde{x}^{(m)}_{OME,sol}$ / g g^{-1}	$\frac{\tilde{x}^{(m)}_{MeOH}}{\tilde{x}^{(m)}_{W}}$	$\tilde{x}^{(m)}_{NaOH}$ / g g^{-1}	Best fitting p
1	273.2	2	ternary	SLE	0.1562	0	0.0018	7
2					0.2935		0.0017	7
3				SLLE	0.4150		0.0018	n.e.
4	283.0			SLE	0.1569			≤8
5					0.2932			8
6	293.3				0.1569			≤8
7					0.2939			≤9
8				SLLE	0.4162			n.e.
9	303.4			SLE	0.1528			≤12
10	273.2	4			0.1561		0.0017	7
11				SLLE	0.2937			n.e.
12					0.4164		0.0018	
13	283.0			SLE	0.1566			8
14				SLLE	0.2930			n.e.
15					0.4162			
16	293.3			SLE	0.1584			≤9
17				SLLE	0.2929		0.0018	n.e.
18					0.4167		0.0017	

Table S-1 continued

19	303.4	4	ternary	SLE	0.1574	0	0.0017	11
20					0.2939		0.0018	
21				SLLE	0.4167			n.e.
22	273.2	2	quaternary	SLE	0.1615	0.1573		8
23					0.3024	0.1576		
24					0.1705	0.3904		≤7
25		4			0.1685	0.1579		
26					0.3020	0.1580		
27					0.1701	0.3901		
28					0.3164	0.3924		
29	293.3				0.1613	0.1576		10
30					0.3021	0.1588		≤10
31					0.1705	0.3898		11
32					0.3159	0.3896		≤10

n.e.: not evaluated

Table S-2: Measured concentration of the liquid phase over time for Experiment 1. Standard uncertainties u are $u(T)$=0.1 K, $u_r(\tilde{x}_{FA}^{(m)})$=0.01, $u_r(\tilde{x}_{W}^{(m)})$=0.02, $u_r(\tilde{x}_{FAc}^{(m)})$=0.0002

t / days	$\tilde{x}_{FA}^{(m)}$ / g g^{-1}	$\tilde{x}_{W}^{(m)}$ / g g^{-1}	$\tilde{x}_{FAc}^{(m)}$ / g g^{-1}
0	0.3571	0.5405	n.a.
11	0.1226	0.7508	0.00074
92	0.1091	0.7553	0.00182
122	0.1081	0.7589	0.00185
196	0.1074	0.7547	0.00226
590	0.1064	0.7564	n.a.

n.a. : not available

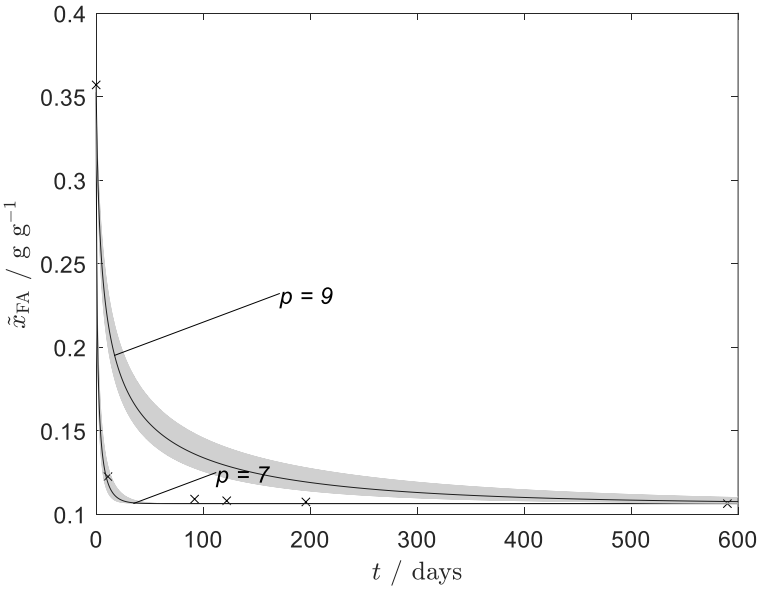

Figure S-1: Experimental and calculated overall formaldehyde concentration in the liquid phase for Experiment 1. (×) Experimental data, (−) model. The line is for pH value 11, the shaded area indicates the influence a variation of the pH in the model by ±1.5.

Table S-3: Measured concentration of the liquid phase over time for Experiment 2. Standard uncertainties u are $u(T)$=0.1 K, $u_r(\tilde{x}_{FA}^{(m)})$=0.01, $u_r(\tilde{x}_{W}^{(m)})$=0.02, $u_r(\tilde{x}_{FAc}^{(m)})$=0.0002

t / days	$\tilde{x}_{FA}^{(m)}$ / g g^{-1}	$\tilde{x}_{W}^{(m)}$ / g g^{-1}	$\tilde{x}_{FAc}^{(m)}$ / g g^{-1}
0	0.3182	0.4797	n.a.
11	0.1055	0.6510	0.00073
92	0.0941	0.6473	0.00172
122	0.0939	0.6538	0.00182
196	0.0935	0.6462	0.00213
590	0.0926	0.6456	n.a.

n.a. : not available

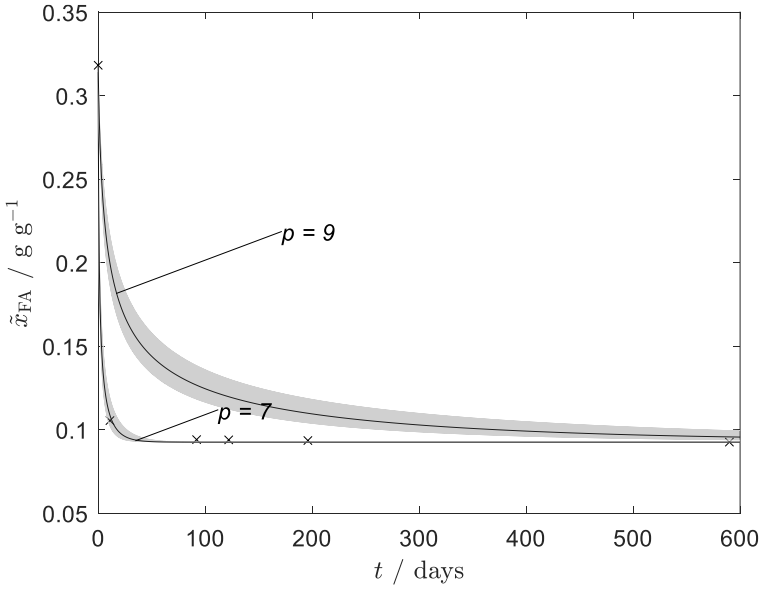

Figure S-2: Experimental and calculated overall formaldehyde concentration in the liquid phase for Experiment 2. (×) Experimental data, (−) model. The line is for pH value 11, the shaded area indicates the influence a variation of the pH in the model by ±1.5.

Table S-4: Measured concentration of the liquid phase over time for Experiment 3. Standard uncertainties u are $u(T)$=0.1 K, $u_r(\tilde{x}_{FA}^{(m)})$=0.01, $u_r(\tilde{x}_{W}^{(m)})$=0.02, $u_r(\tilde{x}_{FAc}^{(m)})$=0.0002

t / days	$\tilde{x}_{FA}^{(m)}$ / g g^{-1}	$\tilde{x}_{W}^{(m)}$ / g g^{-1}	$\tilde{x}_{FAc}^{(m)}$ / g g^{-1}
0	0.2783	0.4202	n.a.
11	0.1039	0.6230	0.00076
92	0.0911	0.6109	0.00193
122	0.0912	0.6146	0.00210

n.a. : not available

Table S-5: Measured concentration of the liquid phase over time for Experiment 4. Standard uncertainties u are $u(T)$=0.1 K, $u_r(\tilde{x}_{FA}^{(m)})$=0.01, $u_r(\tilde{x}_{W}^{(m)})$=0.02, $u_r(\tilde{x}_{FAc}^{(m)})$=0.0002

t / days	$\tilde{x}_{FA}^{(m)}$ / g g^{-1}	$\tilde{x}_{W}^{(m)}$ / g g^{-1}	$\tilde{x}_{FAc}^{(m)}$ / g g^{-1}
0	0.3576	0.5395	n.a.
11	0.1387	0.7324	0.00108
28	0.1366	0.7408	0.00221
87	0.1332	0.7391	0.00271
120	0.1329	0.7380	0.00288

n.a. : not available

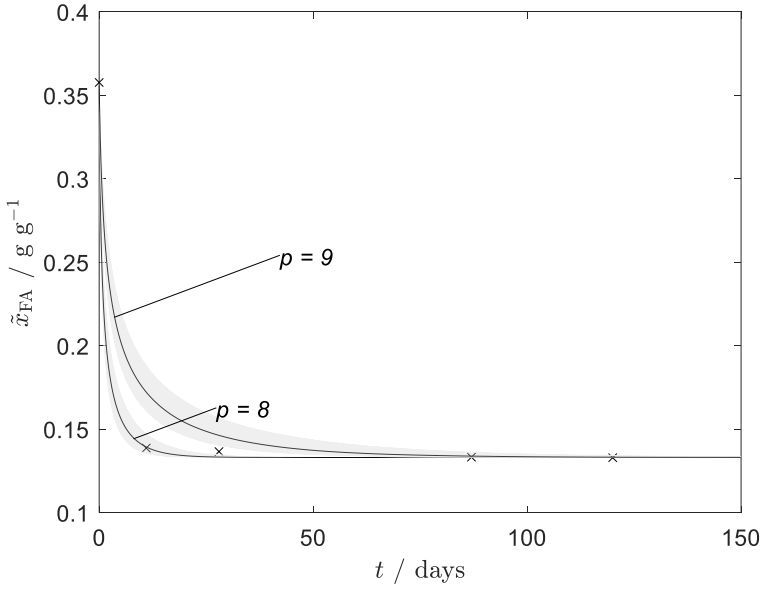

Figure S-3: Experimental and calculated overall formaldehyde concentration in the liquid phase for Experiment 4. (×) Experimental data, (−) model. The line is for pH value 11, the shaded area indicates the influence a variation of the pH in the model by ±1.5.

Table S-6: Measured concentration of the liquid phase over time for Experiment 5. Standard uncertainties u are $u(T)$=0.1 K, $u_r(\tilde{x}_{FA}^{(m)})$=0.01, $u_r(\tilde{x}_{W}^{(m)})$=0.02, $u_r(\tilde{x}_{FAc}^{(m)})$=0.0002

t / days	$\tilde{x}_{FA}^{(m)}$ / g g^{-1}	$\tilde{x}_{W}^{(m)}$ / g g^{-1}	$\tilde{x}_{FAc}^{(m)}$ / g g^{-1}
0	0.3179	0.4801	n.a.
11	0.1242	0.6288	0.00102
28	0.1178	0.6440	0.00205
120	0.1186	0.6337	0.00273

n.a. : not available

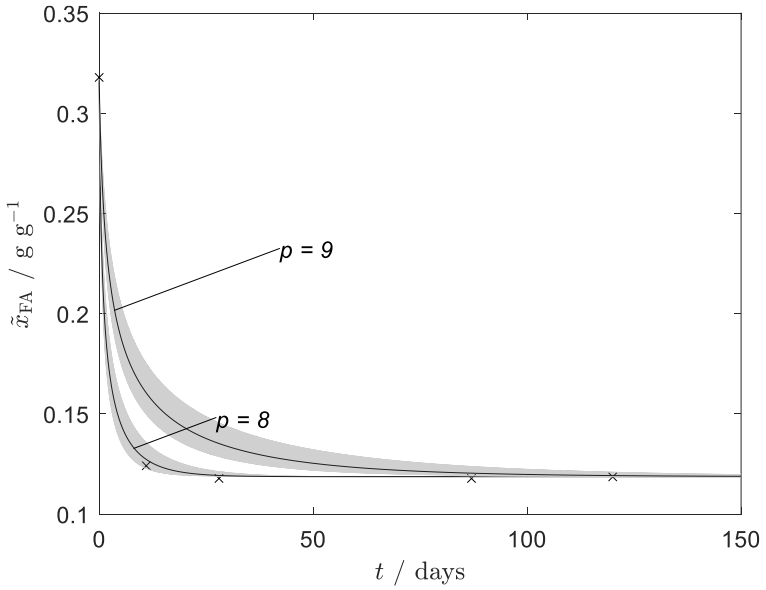

Figure S-4: Experimental and calculated overall formaldehyde concentration in the liquid phase for Experiment 5. (×) Experimental data, (−) model. The line is for pH value 11, the shaded area indicates the influence a variation of the pH in the model by ±1.5.

Table S-7: Measured concentration of the liquid phase over time for Experiment 6. Standard uncertainties u are $u(T)$=0.1 K, $u_r(\tilde{x}_{FA}^{(m)})$=0.01, $u_r(\tilde{x}_{W}^{(m)})$=0.02, $u_r(\tilde{x}_{FAc}^{(m)})$=0.0002

t / days	$\tilde{x}_{FA}^{(m)}$ / g g^{-1}	$\tilde{x}_{W}^{(m)}$ / g g^{-1}	$\tilde{x}_{FAc}^{(m)}$ / g g^{-1}
0	0.3573	0.5397	n.a.
11	0.1646	0.7161	0.00226
28	0.1642	0.7138	0.00283
94	0.1643	0.7125	0.00283
150	0.1655	0.6927	0.00284

n.a. : not available

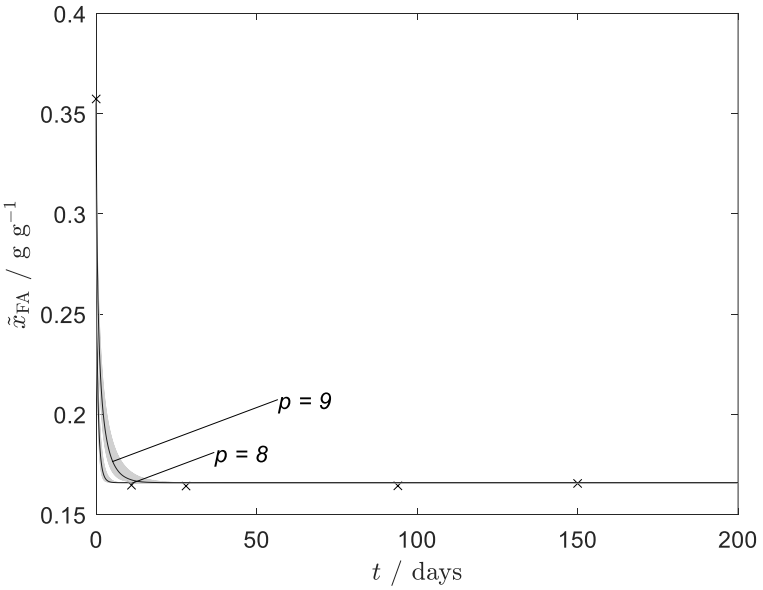

Figure S-5: Experimental and calculated overall formaldehyde concentration in the liquid phase for Experiment 6. (×) Experimental data, (−) model. The line is for pH value 11, the shaded area indicates the influence a variation of the pH in the model by ±1.5.

Table S-8: Measured concentration of the liquid phase over time for Experiment 7. Standard uncertainties u are $u(T)$=0.1 K, $u_r(\tilde{x}_{FA}^{(m)})$=0.01, $u_r(\tilde{x}_{W}^{(m)})$=0.02, $u_r(\tilde{x}_{FAc}^{(m)})$=0.0002

t / days	$\tilde{x}_{FA}^{(m)}$ / g g^{-1}	$\tilde{x}_{W}^{(m)}$ / g g^{-1}	$\tilde{x}_{FAc}^{(m)}$ / g g^{-1}
0	0.3178	0.4797	n.a.
28	0.1499	0.6175	0.00253
94	0.1483	0.6225	0.00266
122	0.1470	0.6176	0.00261

n.a. : not available

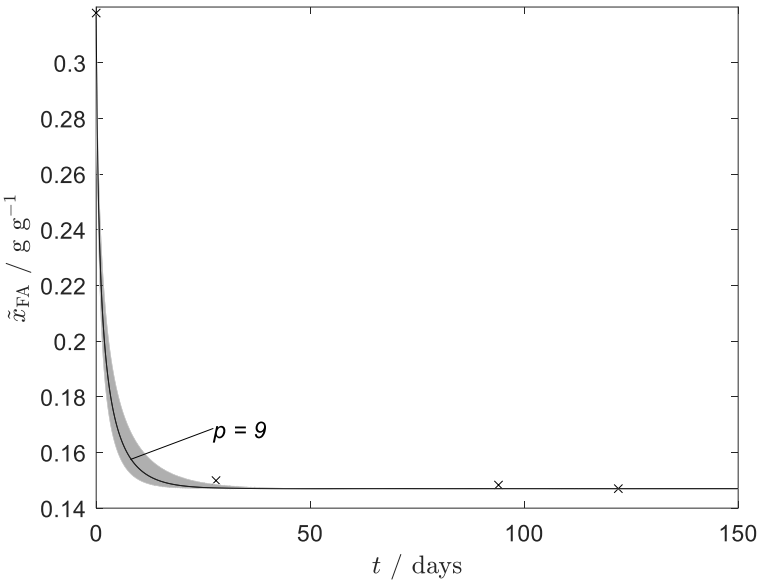

Figure S-6: Experimental and calculated overall formaldehyde concentration in the liquid phase for Experiment 7. (×) Experimental data, (−) model. The line is for pH value 11, the shaded area indicates the influence a variation of the pH in the model by ±1.5.

Table S-9: Measured concentration of the liquid phase over time for Experiment 8. Standard uncertainties u are $u(T)$=0.1 K, $u_r(\tilde{x}_{FA}^{(m)})$=0.01, $u_r(\tilde{x}_{W}^{(m)})$=0.02, $u_r(\tilde{x}_{FAc}^{(m)})$=0.0002

t / days	$\tilde{x}_{FA}^{(m)}$ / g g^{-1}	$\tilde{x}_{W}^{(m)}$ / g g^{-1}	$\tilde{x}_{FAc}^{(m)}$ / g g^{-1}
0	0.2782	0.4194	n.a.
11	0.1376	0.5629	0.00214
28	0.1375	0.5691	0.00270
94	0.1373	0.5576	0.00266

n.a. : not available

Table S-10: Measured concentration of the liquid phase over time for Experiment 9. Standard uncertainties u are $u(T)$=0.1 K, $u_r(\tilde{x}_{FA}^{(m)})$=0.01, $u_r(\tilde{x}_{W}^{(m)})$=0.02, $u_r(\tilde{x}_{FAc}^{(m)})$=0.0002

t / days	$\tilde{x}_{FA}^{(m)}$ / g g^{-1}	$\tilde{x}_{W}^{(m)}$ / g g^{-1}	$\tilde{x}_{FAc}^{(m)}$ / g g^{-1}
0	0.3465	0.5519	n.a.
128	0.2023	0.6856	n.a.
215	0.2039	0.6837	n.a.

n.a. : not available

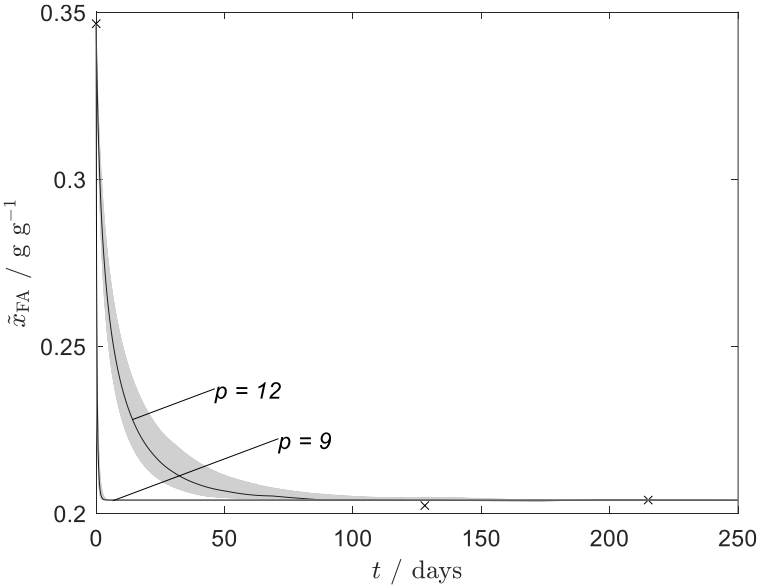

Figure S-7: Experimental and calculated overall formaldehyde concentration in the liquid phase for Experiment 9. (×) Experimental data, (−) model. The line is for pH value 11, the shaded area indicates the influence a variation of the pH in the model by ±1.5.

Table S-11: Measured concentration of the liquid phase over time for Experiment 10. Standard uncertainties u are $u(T)$=0.1 K, $u_r(\tilde{x}_{FA}^{(m)})$=0.01, $u_r(\tilde{x}_{W}^{(m)})$=0.02, $u_r(\tilde{x}_{FAc}^{(m)})$=0.0002

t / days	$\tilde{x}_{FA}^{(m)}$ / g g^{-1}	$\tilde{x}_{W}^{(m)}$ / g g^{-1}	$\tilde{x}_{FAc}^{(m)}$ / g g^{-1}
0	0.3577	0.5401	n.a.
11	0.1295	0.7529	0.00074
26	0.1199	0.7628	0.00081
92	0.1140	0.7615	0.00175
220	0.1125	0.7512	0.00199

n.a. : not available

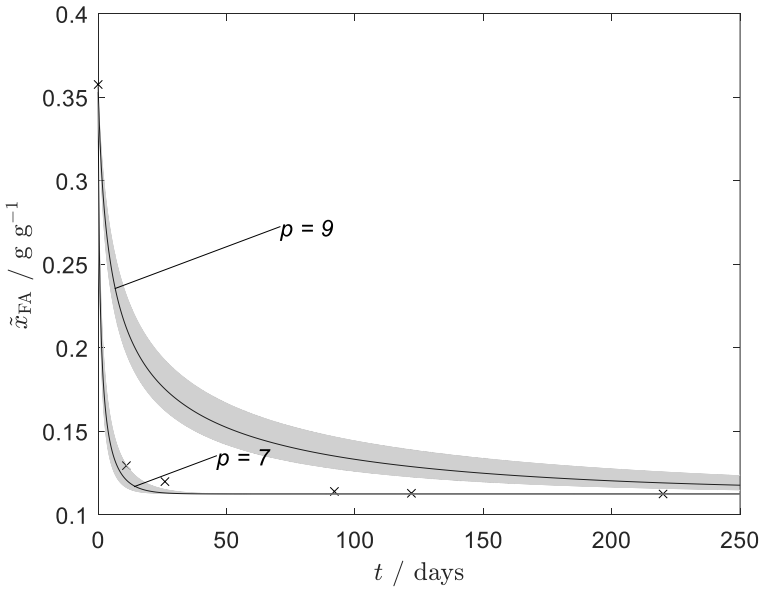

Figure S-8: Experimental and calculated overall formaldehyde concentration in the liquid phase for Experiment 10. (×) Experimental data, (−) model. The line is for pH value 11, the shaded area indicates the influence a variation of the pH in the model by ±1.5.

Table S-12: Measured concentration of the liquid phase over time for Experiment 11. Standard uncertainties u are $u(T)$=0.1 K, $u_r(\tilde{x}_{FA}^{(m)})$=0.01, $u_r(\tilde{x}_{W}^{(m)})$=0.02, $u_r(\tilde{x}_{FAc}^{(m)})$=0.0002

t / days	$\tilde{x}_{FA}^{(m)}$ / g g^{-1}	$\tilde{x}_{W}^{(m)}$ / g g^{-1}	$\tilde{x}_{FAc}^{(m)}$ / g g^{-1}
0	0.3179	0.4798	n.a.
11	0.1237	0.6758	0.00067
26	0.1105	0.6780	0.00078
92	0.1102	0.6744	0.00160
150	0.1082	0.6539	0.00183
455	0.1020	0.6515	n.a.

n.a. : not available

Table S-13: Measured concentration of the liquid phase over time for Experiment 12. Standard uncertainties u are $u(T)$=0.1 K, $u_r(\tilde{x}_{FA}^{(m)})$=0.01, $u_r(\tilde{x}_{W}^{(m)})$=0.02, $u_r(\tilde{x}_{FAc}^{(m)})$=0.0002

t / days	$\tilde{x}_{FA}^{(m)}$ / g g^{-1}	$\tilde{x}_{W}^{(m)}$ / g g^{-1}	$\tilde{x}_{FAc}^{(m)}$ / g g^{-1}
0	0.2781	0.4193	n.a.
11	0.1258	0.6782	0.00080
26	0.1145	0.6897	0.00097
92	0.1076	0.6865	0.00206
122	0.1065	0.6888	0.00219
455	0.1022	0.6621	n.a.

n.a. : not available

Table S-14: Measured concentration of the liquid phase over time for Experiment 13. Standard uncertainties u are $u(T)$=0.1 K, $u_r(\tilde{x}_{FA}^{(m)})$=0.01, $u_r(\tilde{x}_{W}^{(m)})$=0.02, $u_r(\tilde{x}_{FAc}^{(m)})$=0.0002

t / days	$\tilde{x}_{FA}^{(m)}$ / g g^{-1}	$\tilde{x}_{W}^{(m)}$ / g g^{-1}	$\tilde{x}_{FAc}^{(m)}$ / g g^{-1}
0	0.3578	0.5397	n.a.
11	0.1423	0.7309	0.00109
28	0.1357	0.7434	0.00216
87	0.1342	0.7419	0.00271
120	0.1343	0.7427	0.00282
196	0.133	0.7303	0.00272

n.a. : not available

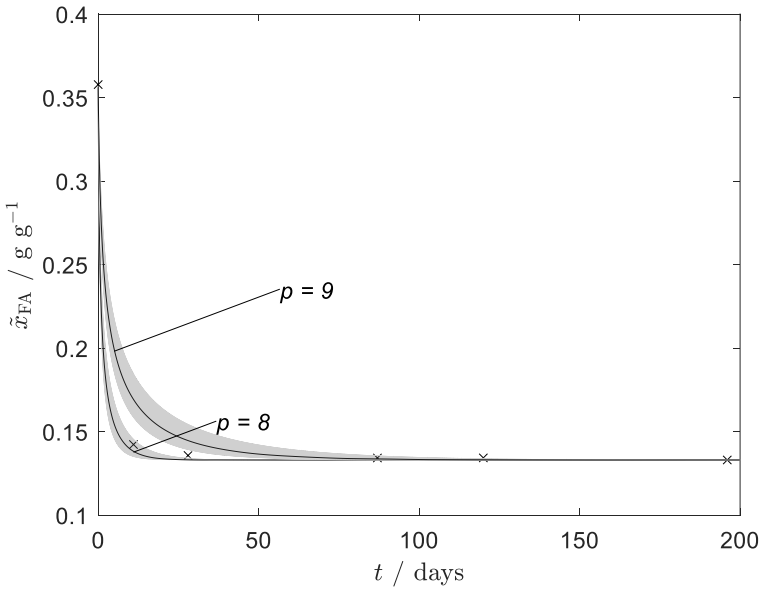

Figure S-9: Experimental and calculated overall formaldehyde concentration in the liquid phase for Experiment 13. (×) Experimental data, (−) model. The line is for pH value 11, the shaded area indicates the influence a variation of the pH in the model by ±1.5.

Table S-15: Measured concentration of the liquid phase over time for Experiment 14. Standard uncertainties u are $u(T)$=0.1 K, $u_r(\tilde{x}_{FA}^{(m)})$=0.01, $u_r(\tilde{x}_{W}^{(m)})$=0.02, $u_r(\tilde{x}_{FAc}^{(m)})$=0.0002

t / days	$\tilde{x}_{FA}^{(m)}$ / g g^{-1}	$\tilde{x}_{W}^{(m)}$ / g g^{-1}	$\tilde{x}_{FAc}^{(m)}$ / g g^{-1}
0	0.3181	0.4800	n.a.
11	0.1293	0.6630	0.00107
28	0.1230	0.6575	0.00220
87	0.1228	0.6718	0.00278
150	0.1260	0.6390	0.00274
193	0.1255	0.6347	0.00278
490	0.1249	0.6306	n.a.

n.a. : not available

Table S-16: Measured concentration of the liquid phase over time for Experiment 15. Standard uncertainties u are $u(T)$=0.1 K, $u_r(\tilde{x}_{FA}^{(m)})$=0.01, $u_r(\tilde{x}_{W}^{(m)})$=0.02, $u_r(\tilde{x}_{FAc}^{(m)})$=0.0002

t / days	$\tilde{x}_{FA}^{(m)}$ / g g^{-1}	$\tilde{x}_{W}^{(m)}$ / g g^{-1}	$\tilde{x}_{FAc}^{(m)}$ / g g^{-1}
0	0.2778	0.4195	n.a.
11	0.1300	0.6631	0.00128
28	0.1234	0.6591	0.00259
87	0.1232	0.6684	0.00332
196	0.1221	0.6494	0.00324

n.a. : not available

Table S-17: Measured concentration of the liquid phase over time for Experiment 16. Standard uncertainties u are $u(T)$=0.1 K, $u_r(\tilde{x}_{FA}^{(m)})$=0.01, $u_r(\tilde{x}_{W}^{(m)})$=0.02, $u_r(\tilde{x}_{FAc}^{(m)})$=0.0002

t / days	$\tilde{x}_{FA}^{(m)}$ / g g^{-1}	$\tilde{x}_{W}^{(m)}$ / g g^{-1}	$\tilde{x}_{FAc}^{(m)}$ / g g^{-1}
0	0.3571	0.5390	n.a.
11	0.1652	0.7073	0.00214
28	0.1636	0.7008	0.00270
94	0.1636	0.7161	0.00276
150	0.1639	0.7083	0.00272
193	0.1636	0.7030	0.00272

n.a. : not available

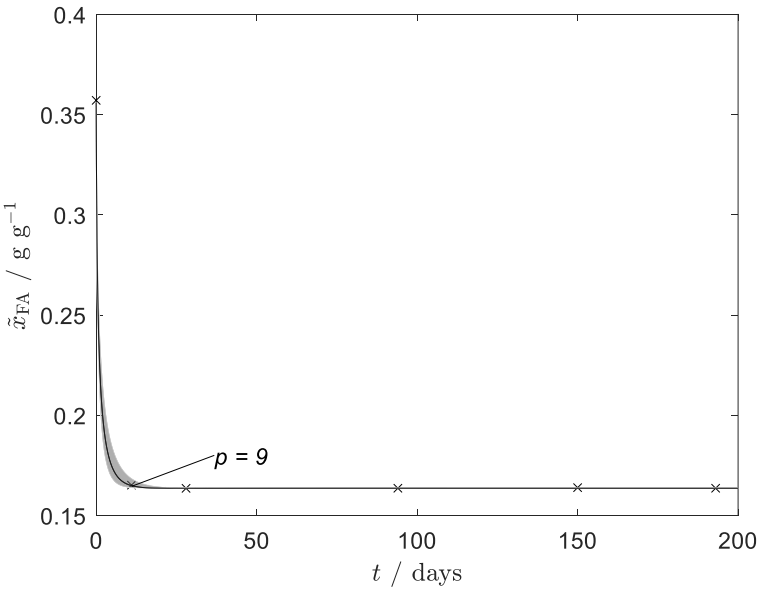

Figure S-10: Experimental and calculated overall formaldehyde concentration in the liquid phase for Experiment 16. (×) Experimental data, (−) model. The line is for pH value 11, the shaded area indicates the influence a variation of the pH in the model by ±1.5.

Table S-18: Measured concentration of the liquid phase over time for Experiment 17. Standard uncertainties u are $u(T)$=0.1 K, $u_r(\tilde{x}_{FA}^{(m)})$=0.01, $u_r(\tilde{x}_{W}^{(m)})$=0.02, $u_r(\tilde{x}_{FAc}^{(m)})$=0.0002

t / days	$\tilde{x}_{FA}^{(m)}$ / g g^{-1}	$\tilde{x}_{W}^{(m)}$ / g g^{-1}	$\tilde{x}_{FAc}^{(m)}$ / g g^{-1}
0	0.3177	0.4805	n.a.
11	0.1500	0.6240	0.00216
94	0.1478	0.6337	0.00269
193	0.1478	0.6118	0.00267

n.a. : not available

Table S-19: Measured concentration of the liquid phase over time for Experiment 18. Standard uncertainties u are $u(T)$=0.1 K, $u_r(\tilde{x}_{FA}^{(m)})$=0.01, $u_r(\tilde{x}_{W}^{(m)})$=0.02, $u_r(\tilde{x}_{FAc}^{(m)})$=0.0002

t / days	$\tilde{x}_{FA}^{(m)}$ / g g^{-1}	$\tilde{x}_{W}^{(m)}$ / g g^{-1}	$\tilde{x}_{FAc}^{(m)}$ / g g^{-1}
0	0.2779	0.4191	n.a.
11	0.1504	0.6366	0.00248
28	0.1490	0.6391	0.00311
94	0.1483	0.6402	0.00306
150	0.1492	0.6027	0.00303
193	0.1486	0.6035	0.00303

n.a. : not available

Table S-20: Measured concentration of the liquid phase over time for Experiment 19. Standard uncertainties u are $u(T)$=0.1 K, $u_r(\tilde{x}_{FA}^{(m)})$=0.01, $u_r(\tilde{x}_{W}^{(m)})$=0.02, $u_r(\tilde{x}_{FAc}^{(m)})$=0.0002

t / days	$\tilde{x}_{FA}^{(m)}$ / g g^{-1}	$\tilde{x}_{W}^{(m)}$ / g g^{-1}	$\tilde{x}_{FAc}^{(m)}$ / g g^{-1}
0	0.3573	0.5395	n.a.
11	0.2430	0.6429	0.00248
28	0.1989	0.6825	0.00254
87	0.1991	0.6919	0.00253
120	0.1991	0.6891	0.00275
196	0.1989	0.6789	0.00256

n.a. : not available

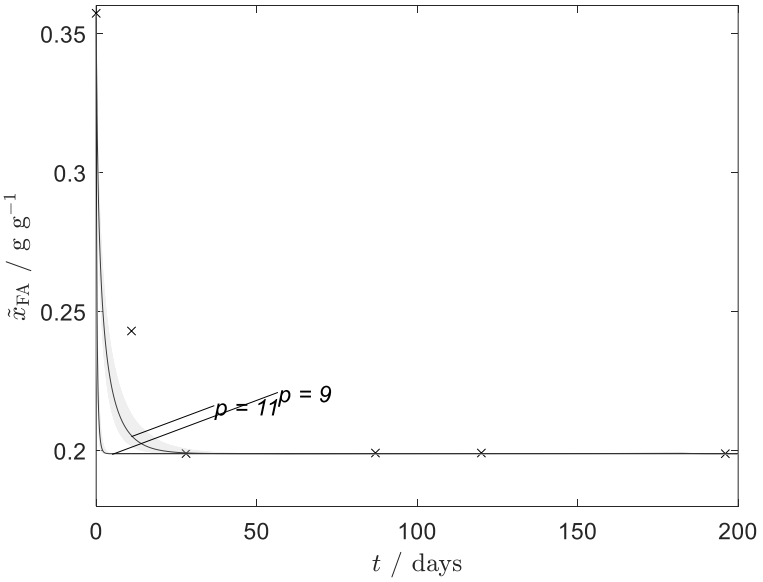

Figure S-11: Experimental and calculated overall formaldehyde concentration in the liquid phase for Experiment 19. (×) Experimental data, (−) model. The line is for pH value 11, the shaded area indicates the influence a variation of the pH in the model by ±1.5.

Table S-21: Measured concentration of the liquid phase over time for Experiment 20. Standard uncertainties u are $u(T)$=0.1 K, $u_r(\tilde{x}_{FA}^{(m)})$=0.01, $u_r(\tilde{x}_{W}^{(m)})$=0.02, $u_r(\tilde{x}_{FAc}^{(m)})$=0.0002

t / days	$\tilde{x}_{FA}^{(m)}$ / g g^{-1}	$\tilde{x}_{W}^{(m)}$ / g g^{-1}	$\tilde{x}_{FAc}^{(m)}$ / g g^{-1}
0	0.3178	0.4796	n.a.
11	0.2360	0.5439	0.00152
28	0.1790	0.5958	0.00260
87	0.1801	0.603	0.00258
120	0.1796	0.5999	0.00283
196	0.1796	0.5855	0.00261

n.a. : not available

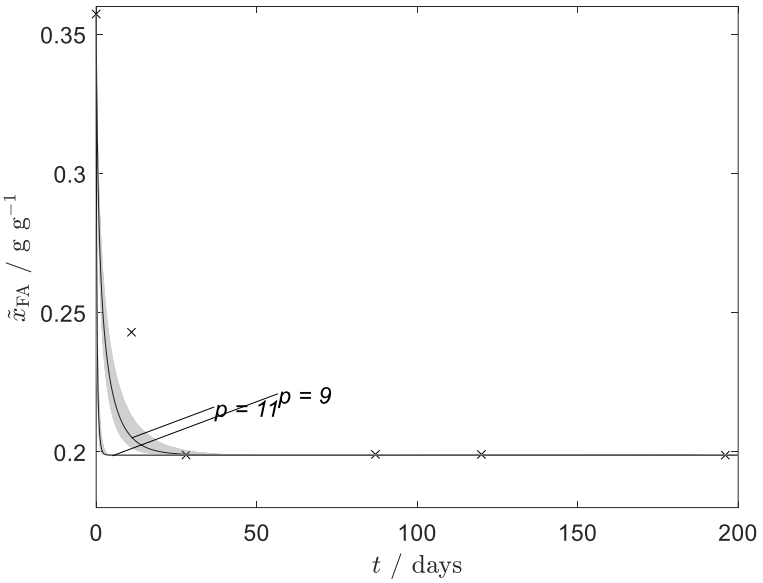

Figure S-12: Experimental and calculated overall formaldehyde concentration in the liquid phase for Experiment 20. (×) Experimental data, (−) model. The line is for pH value 11, the shaded area indicates the influence a variation of the pH in the model by ±1.5.

Table S-22: Measured concentration of the liquid phase over time for Experiment 21. Standard uncertainties u are $u(T)$=0.1 K, $u_r(\tilde{x}_{FA}^{(m)})$=0.01, $u_r(\tilde{x}_{W}^{(m)})$=0.02, $u_r(\tilde{x}_{FAc}^{(m)})$=0.0002

t / days	$\tilde{x}_{FA}^{(m)}$ / g g^{-1}	$\tilde{x}_{W}^{(m)}$ / g g^{-1}	$\tilde{x}_{FAc}^{(m)}$ / g g^{-1}
0	0.2777	0.4192	n.a.
28	0.1776	0.5899	0.00301
87	0.1768	0.5923	0.00300
150	0.1670	0.5706	0.00299

n.a. : not available

Table S-23: Measured concentration of the liquid phase over time for Experiment 30. Standard uncertainties u are $u(T)$=0.1 K, $u_r(\tilde{x}_{FA}^{(m)})$=0.01, $u_r(\tilde{x}_{W}^{(m)})$=0.02, $u_r(\tilde{x}_{FAc}^{(m)})$=0.0002, $u_r(\tilde{x}_{MeOH}^{(m)})$=0.02

t / days	$\tilde{x}_{FA}^{(m)}$ / g g^{-1}	$\tilde{x}_{W}^{(m)}$ / g g^{-1}	$\tilde{x}_{MeOH}^{(m)}$ / g g^{-1}	$\tilde{x}_{FAc}^{(m)}$ / g g^{-1}
0	0.3801	0.4478	0.07043	n.a.
64	0.1839	0.5350	0.13764	
128	0.1736	0.6004	0.09411	
215	0.1721	0.6027	0.10045	
350	0.1710	0.5977	0.09934	

n.a. : not available

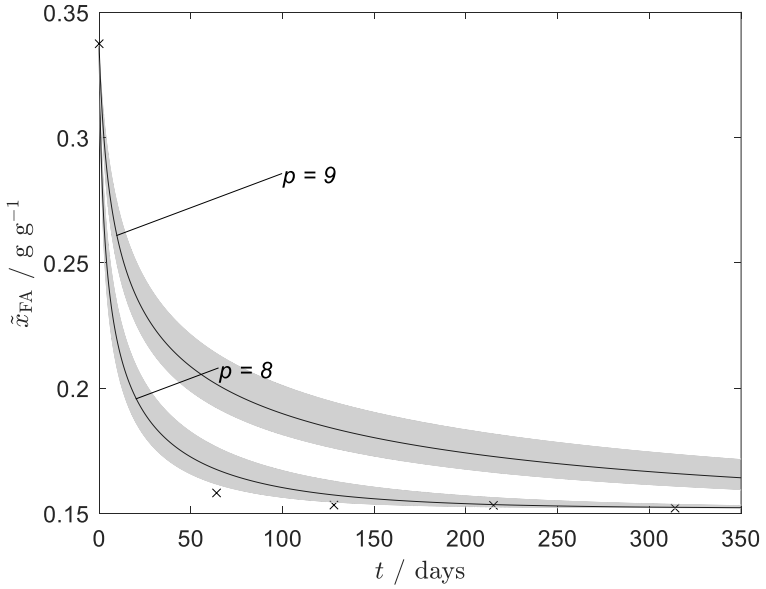

Figure S-13: Experimental and calculated overall formaldehyde concentration in the liquid phase for Experiment 30. (×) Experimental data, (−) model. The line is for pH value 11, the shaded area indicates the influence a variation of the pH in the model by ±1.5.

Table S-24: Measured concentration of the liquid phase over time for Experiment 31. Standard uncertainties u are $u(T)$=0.1 K, $u_r(\tilde{x}_{FA}^{(m)})$=0.01, $u_r(\tilde{x}_{W}^{(m)})$=0.02, $u_r(\tilde{x}_{FAc}^{(m)})$=0.0002, $u_r(\tilde{x}_{MeOH}^{(m)})$=0.02

t / days	$\tilde{x}_{FA}^{(m)}$ / g g^{-1}	$\tilde{x}_{W}^{(m)}$ / g g^{-1}	$\tilde{x}_{MeOH}^{(m)}$ / g g^{-1}	$\tilde{x}_{FAc}^{(m)}$ / g g^{-1}
0	0.3374	0.3982	0.06275	n.a.
64	0.1582	0.4712	0.10097	
128	0.1533	0.5108	0.08853	
215	0.1532	0.5082	0.08258	
314	0.1521	0.5123	0.08325	

n.a. : not available

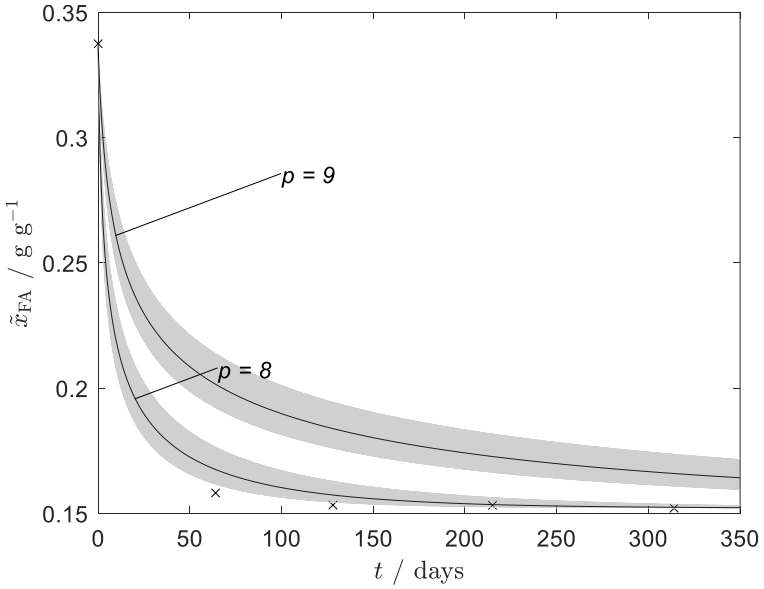

Figure S-14: Experimental and calculated overall formaldehyde concentration in the liquid phase for Experiment 31. (×) Experimental data, (−) model. The line is for pH value 11, the shaded area indicates the influence a variation of the pH in the model by ±1.5.

Table S-25: Measured concentration of the liquid phase over time for Experiment 32. Standard uncertainties u are $u(T)$=0.1 K, $u_r(\tilde{x}_{FA}^{(m)})$=0.01, $u_r(\tilde{x}_{W}^{(m)})$=0.02, $u_r(\tilde{x}_{FAc}^{(m)})$=0.0002, $u_r(\tilde{x}_{MeOH}^{(m)})$=0.02

t / days	$\tilde{x}_{FA}^{(m)}$ / g g^{-1}	$\tilde{x}_{W}^{(m)}$ / g g^{-1}	$\tilde{x}_{MeOH}^{(m)}$ / g g^{-1}	$\tilde{x}_{FAc}^{(m)}$ / g g^{-1}
0	0.4118	0.3501	0.13655	n.a.
64	0.2382	0.4387	0.19389	
128	0.2374	0.4589	0.18117	
215	0.2359	0.4546	0.17993	
314	0.2349	0.4558	0.18094	

n.a. : not available

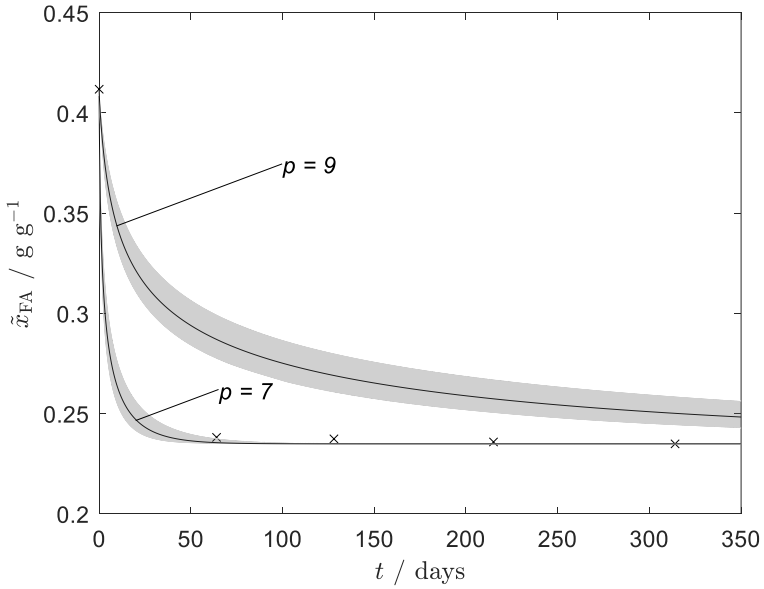

Figure S-15: Experimental and calculated overall formaldehyde concentration in the liquid phase for Experiment 32. (×) Experimental data, (−) model. The line is for pH value 11, the shaded area indicates the influence a variation of the pH in the model by ±1.5.

Table S-26: Measured concentration of the liquid phase over time for Experiment 22. Standard uncertainties u are $u(T)$=0.1 K, $u_r(\tilde{x}_{FA}^{(m)})$=0.01, $u_r(\tilde{x}_{W}^{(m)})$=0.02, $u_r(\tilde{x}_{FAc}^{(m)})$=0.0002, $u_r(\tilde{x}_{MeOH}^{(m)})$=0.02

t / days	$\tilde{x}_{FA}^{(m)}$ / g g^{-1}	$\tilde{x}_{W}^{(m)}$ / g g^{-1}	$\tilde{x}_{MeOH}^{(m)}$ / g g^{-1}	$\tilde{x}_{FAc}^{(m)}$ / g g^{-1}
0	0.3783	0.4452	0.07029	n.a.
64	0.1730	0.5742	0.11454	
215	0.1718	0.6040	0.07441	
314	0.1698	0.5956	0.09664	

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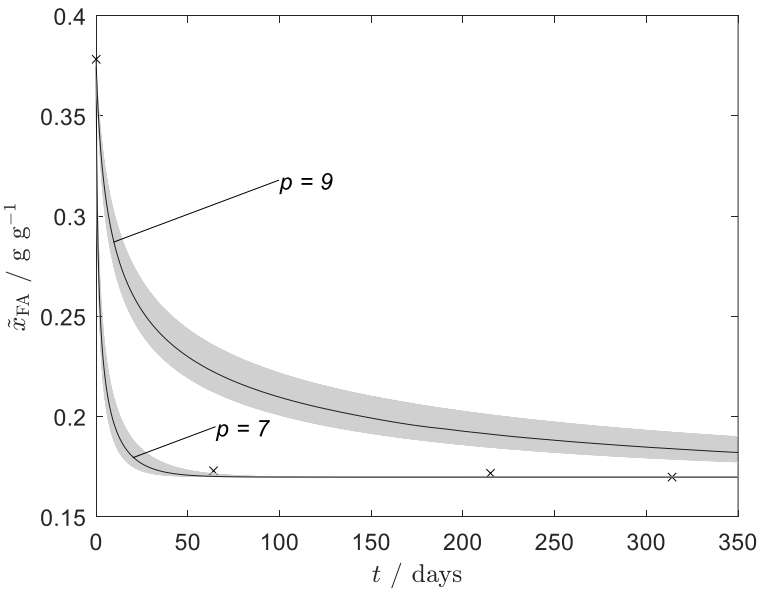

Figure S-16: Experimental and calculated overall formaldehyde concentration in the liquid phase for Experiment 22. (×) Experimental data, (—) model. The line is for pH value 11, the shaded area indicates the influence a variation of the pH in the model by ±1.5.

Table S-27: Measured concentration of the liquid phase over time for Experiment 23. Standard uncertainties u are $u(T)$=0.1 K, $u_r(\tilde{x}_{FA}^{(m)})$=0.01, $u_r(\tilde{x}_{W}^{(m)})$=0.02, $u_r(\tilde{x}_{FAc}^{(m)})$=0.0002, $u_r(\tilde{x}_{MeOH}^{(m)})$=0.02

t / days	$\tilde{x}_{FA}^{(m)}$ / g g^{-1}	$\tilde{x}_{W}^{(m)}$ / g g^{-1}	$\tilde{x}_{MeOH}^{(m)}$ / g g^{-1}	$\tilde{x}_{FAc}^{(m)}$ / g g^{-1}
0	0.3374	0.3982	0.0629	n.a.
64	0.1559	0.4929	0.0982	
215	0.1539	0.5162	0.0513	
314	0.1516	0.5119	0.0825	

n.a. : not available

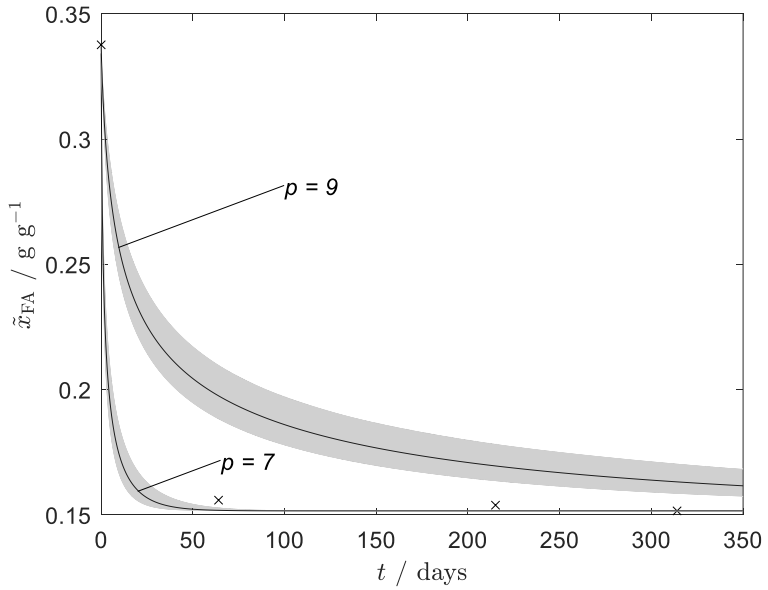

Figure S-17: Experimental and calculated overall formaldehyde concentration in the liquid phase for Experiment 23. (×) Experimental data, (−) model. The line is for pH value 11, the shaded area indicates the influence a variation of the pH in the model by ±1.5.

Table S-28: Measured concentration of the liquid phase over time for Experiment 24. Standard uncertainties u are $u(T)$=0.1 K, $u_r(\tilde{x}_{FA}^{(m)})$=0.01, $u_r(\tilde{x}_{W}^{(m)})$=0.02, $u_r(\tilde{x}_{FAc}^{(m)})$=0.0002, $u_r(\tilde{x}_{MeOH}^{(m)})$=0.02

t / days	$\tilde{x}_{FA}^{(m)}$ / g g^{-1}	$\tilde{x}_{W}^{(m)}$ / g g^{-1}	$\tilde{x}_{MeOH}^{(m)}$ / g g^{-1}	$\tilde{x}_{FAc}^{(m)}$ / g g^{-1}
0	0.4118	0.3499	0.1366	n.a.
64	0.2372	0.4395	0.1977	
128	0.2369	0.4596	0.1626	
215	0.2362	0.4600	0.1631	
314	0.2370	0.4506	0.1811	

n.a. : not available

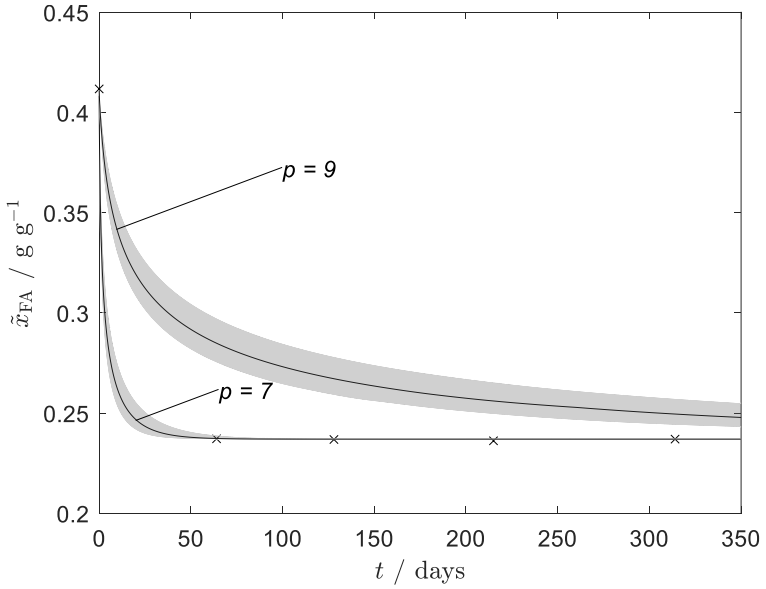

Figure S-18: Experimental and calculated overall formaldehyde concentration in the liquid phase for Experiment 24. (×) Experimental data, (−) model. The line is for pH value 11, the shaded area indicates the influence a variation of the pH in the model by ±1.5.

Table S-29: Measured concentration of the liquid phase over time for Experiment 25. Standard uncertainties u are $u(T)$=0.1 K, $u_r(\tilde{x}_{FA}^{(m)})$=0.01, $u_r(\tilde{x}_{W}^{(m)})$=0.02, $u_r(\tilde{x}_{FAc}^{(m)})$=0.0002, $u_r(\tilde{x}_{MeOH}^{(m)})$=0.02

t / days	$\tilde{x}_{FA}^{(m)}$ / g g^{-1}	$\tilde{x}_{W}^{(m)}$ / g g^{-1}	$\tilde{x}_{MeOH}^{(m)}$ / g g^{-1}	$\tilde{x}_{FAc}^{(m)}$ / g g^{-1}
0	0.3656	0.3106	0.1219	n.a.
64	0.2093	0.3757	0.1738	0.00125
215	0.2082	0.3953	0.1330	n.a.
314	0.2069	0.3975	0.1495	

n.a. : not available

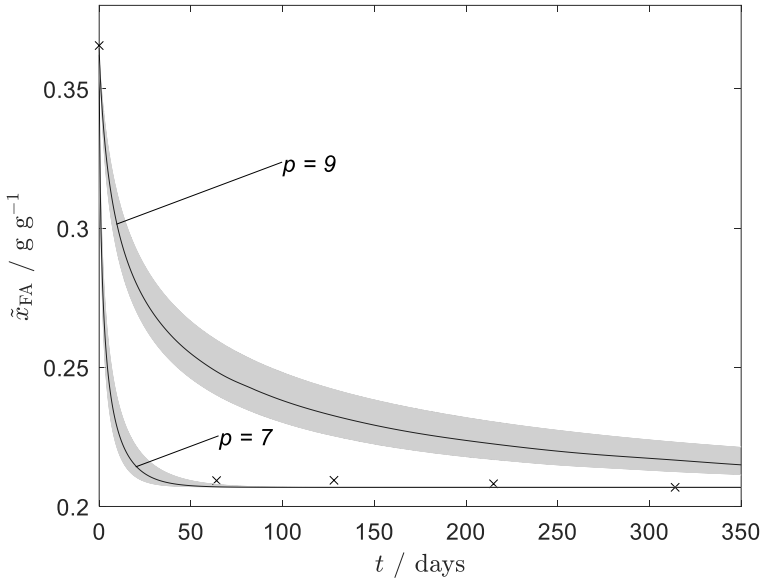

Figure S-19: Experimental and calculated overall formaldehyde concentration in the liquid phase for Experiment 25. (×) Experimental data, (−) model. The line is for pH value 11, the shaded area indicates the influence a variation of the pH in the model by ±1.5.

Table S-30: Measured concentration of the liquid phase over time for Experiment 26. Standard uncertainties u are $u(T)$=0.1 K, $u_r(\tilde{x}_{FA}^{(m)})$=0.01, $u_r(\tilde{x}_{W}^{(m)})$=0.02, $u_r(\tilde{x}_{FAc}^{(m)})$=0.0002, $u_r(\tilde{x}_{MeOH}^{(m)})$=0.02

t / days	$\tilde{x}_{FA}^{(m)}$ / g g^{-1}	$\tilde{x}_{W}^{(m)}$ / g g^{-1}	$\tilde{x}_{MeOH}^{(m)}$ / g g^{-1}	$\tilde{x}_{FAc}^{(m)}$ / g g^{-1}
0	0.3803	0.4477	0.0706	n.a.
64	0.2365	0.5340	0.0985	
128	0.2319	0.5577	0.0739	
215	0.2337	0.5553	0.0803	
314	0.2328	0.5572	0.0893	

n.a. : not available

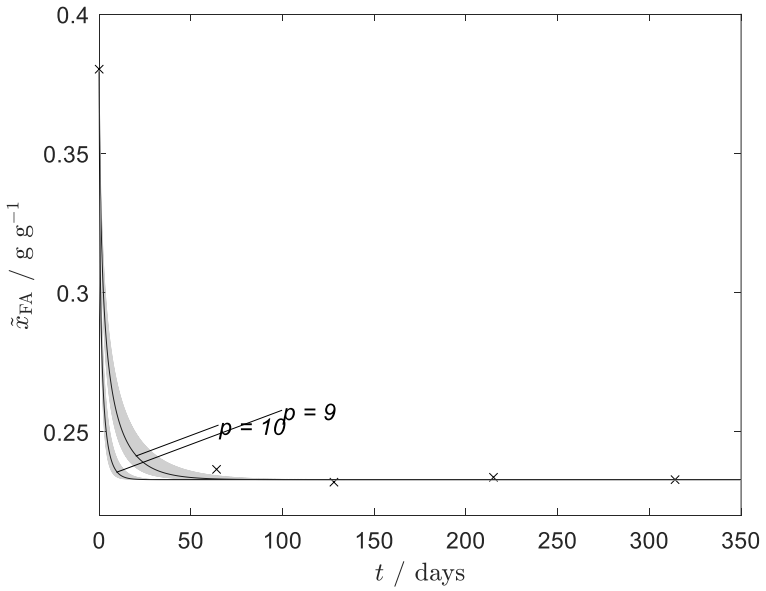

Figure S-20: Experimental and calculated overall formaldehyde concentration in the liquid phase for Experiment 26. (×) Experimental data, (—) model. The line is for pH value 11, the shaded area indicates the influence a variation of the pH in the model by ±1.5.

Table S-31: Measured concentration of the liquid phase over time for Experiment 27. Standard uncertainties u are $u(T)$=0.1 K, $u_r(\tilde{x}_{FA}^{(m)})$=0.01, $u_r(\tilde{x}_{W}^{(m)})$=0.02, $u_r(\tilde{x}_{FAc}^{(m)})$=0.0002, $u_r(\tilde{x}_{MeOH}^{(m)})$=0.02

t / days	$\tilde{x}_{FA}^{(m)}$ / g g^{-1}	$\tilde{x}_{W}^{(m)}$ / g g^{-1}	$\tilde{x}_{MeOH}^{(m)}$ / g g^{-1}	$\tilde{x}_{FAc}^{(m)}$ / g g^{-1}
0	0.3377	0.3978	0.0632	n.a.
64	0.2070	0.4584	0.0857	
314	0.2057	0.4786	0.0779	

n.a. : not available

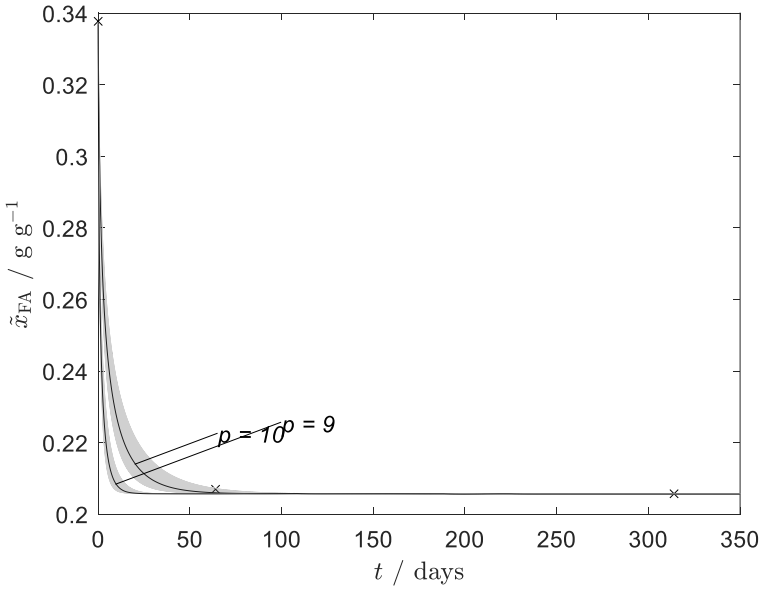

Figure S-21: Experimental and calculated overall formaldehyde concentration in the liquid phase for Experiment 27. (×) Experimental data, (−) model. The line is for pH value 11, the shaded area indicates the influence a variation of the pH in the model by ±1.5.

Table S-32: Measured concentration of the liquid phase over time for Experiment 28. Standard uncertainties u are $u(T)$=0.1 K, $u_r(\tilde{x}_{FA}^{(m)})$=0.01, $u_r(\tilde{x}_{W}^{(m)})$=0.02, $u_r(\tilde{x}_{FAc}^{(m)})$=0.0002, $u_r(\tilde{x}_{MeOH}^{(m)})$=0.02

t / days	$\tilde{x}_{FA}^{(m)}$ / g g^{-1}	$\tilde{x}_{W}^{(m)}$ / g g^{-1}	$\tilde{x}_{MeOH}^{(m)}$ / g g^{-1}	$\tilde{x}_{FAc}^{(m)}$ / g g^{-1}
0	0.4117	0.3500	0.1365	n.a.
64	0.3084	0.3983	0.1672	0.00235
215	0.3024	0.4200	0.1509	n.a.
314	0.2989	0.4219	0.1616	

n.a. : not available

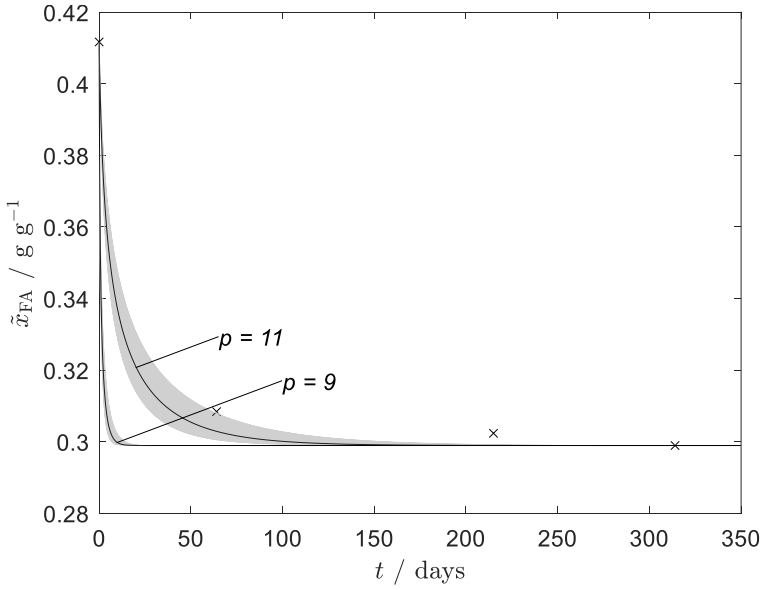

Figure S-22: Experimental and calculated overall formaldehyde concentration in the liquid phase for Experiment 28. (×) Experimental data, (—) model. The line is for pH value 11, the shaded area indicates the influence a variation of the pH in the model by ±1.5.

Table S-33: Measured concentration of the liquid phase over time for Experiment 29. Standard uncertainties u are $u(T)$=0.1 K, $u_r(\tilde{x}_{FA}^{(m)})$=0.01, $u_r(\tilde{x}_{W}^{(m)})$=0.02, $u_r(\tilde{x}_{FAc}^{(m)})$=0.0002, $u_r(\tilde{x}_{MeOH}^{(m)})$=0.02

t / days	$\tilde{x}_{FA}^{(m)}$ / g g^{-1}	$\tilde{x}_{W}^{(m)}$ / g g^{-1}	$\tilde{x}_{MeOH}^{(m)}$ / g g^{-1}	$\tilde{x}_{FAc}^{(m)}$ / g g^{-1}
0	0.3655	0.3115	0.1214	n.a.
64	0.2544	0.3528	0.1493	
215	0.2532	0.3709	0.1214	
314	0.2534	0.3706	0.1425	

n.a. : not available

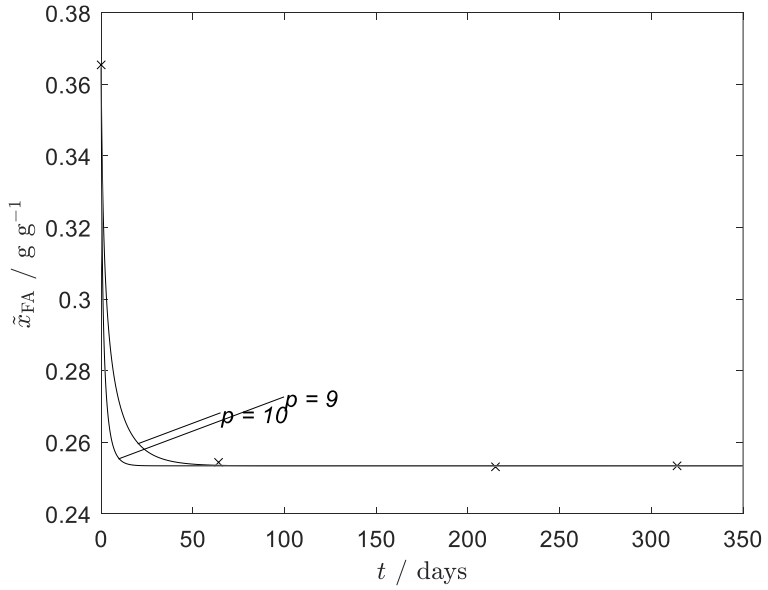

Figure S-23: Experimental and calculated overall formaldehyde concentration in the liquid phase for Experiment 29. (×) Experimental data, (−) model. The line is for pH value 11, the shaded area indicates the influence a variation of the pH in the model by ±1.5.