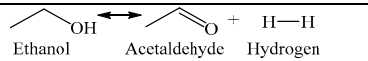
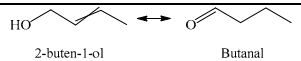
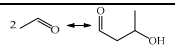
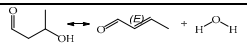
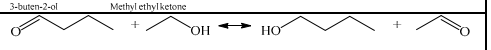
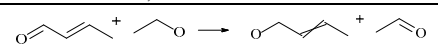
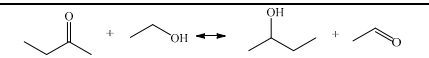
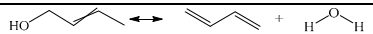
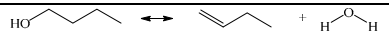
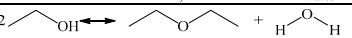
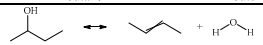
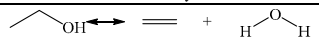
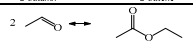
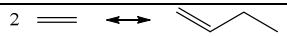
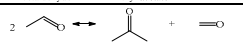
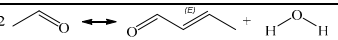
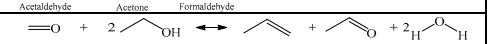
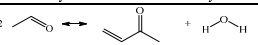
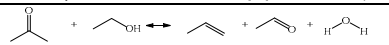
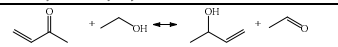
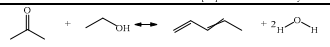
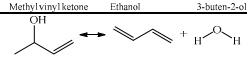
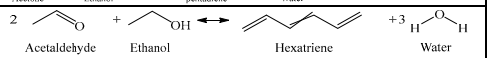
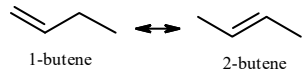
Table S1. Chemical reactions explaining the BD synthesis from ethanol

Code	Chemical reaction	Code	Chemical reaction
R1		R2	
R3		R4	
R5		R6	
R7		R8	
R9		R10	
R11		R12	
R13		R14	
R15		R16	
R17		R18	
R19		R20	
R21		R22	
R23		R24	
R25			

1. Stoichiometry and kinetic model for one-step ETB process [14]

Reaction number	Stoichiometry	Rate expression	$k_i = k_{i,m} exp\left[\frac{E_i}{R}\left(\frac{1}{T_m} - \frac{1}{T}\right)\right]; T_m = 626$	
			$k_{m,i}$, kmol/(kg·h·bar ^{ni})	E_i/R, K
R1	$C_2H_5OH \Leftrightarrow C_2H_4O + H_2$	$r_1 = k_1\left(p_{EtOH} - \frac{p_{ACH}p_{H_2}}{K_{p,1}}\right)$	$4.025 \cdot 10^{-3}$	7439.8
R11	$2C_2H_5OH \Leftrightarrow C_4H_{10}O + H_2O$	$r_2 = k_2\left(p_{EtOH}^2 - \frac{p_{DEE}p_{H_2O}}{K_{p,2}}\right)$	$3.826 \cdot 10^{-4}$	6638.2
R13	$C_2H_5OH \Rightarrow C_2H_4 + H_2O$	$r_3 = k_3 p_{EtOH}$	$5.921 \cdot 10^{-4}$	1324.5
R15	$2C_2H_4 \Rightarrow C_4H_8$	$r_4 = k_4 p_{C2H4}^2$	17.253	3008.3
R3+R5	$2C_2H_4O \Leftrightarrow C_4H_6O + H_2O$	$r_5 = k_5\left(p_{ACH} - \frac{p_{C54H6O}p_{H_2O}}{K_{p,2}}\right)$	11.312	4005.8
R26**	$C_4H_6O + C_2H_5OH \Rightarrow C_4H_6 + C_2H_4O + H_2O$	$r_6 = k_6 p_{EtOH} p_{C4H6O}$	503.75	1018.2
R27**	$C_4H_{10}O \Rightarrow 2C_2H_4 + H_2O$	$r_7 = k_7 p_{DEE}$	$5.839 \cdot 10^{-2}$	13655

Subscripts used in the rate expressions: EtOH- ethanol; AcH - acetaldehyde; DEE -diethyl ether; C4H6O -crotonaldehyde;

***) ni=1 for i=1,3 and 7 ; ni=2, for i=2,4,5 and 6.**

****) specific steps considered in this kinetic model**

2. Data for calculating Economic Potential values (inert fraction 0.2)

Table S2. Flowrates, EtOH conversion and BD Yield (inert fraction 0.2)

Catalyst weight/ [kg]	BD flowrate/ [kmol/h]	Recycle flowrates / [kmol/h]			EtOH conversion	BD Yield
		EtOH	ACH	N_2		
3000	10.904	538.928	5.509	164.238	0.056	0.034
4000	17.843	464.782	5.419	141.764	0.088	0.063
5000	24.011	387.674	4.888	129.392	0.127	0.098
6000	29.811	317.223	4.304	110.408	0.175	0.143
7000	34.422	252.748	3.637	96.865	0.231	0.195
8000	38.423	194.745	3.011	78.347	0.302	0.261
9000	41.278	145.924	2.437	62.132	0.382	0.336
10000	42.839	110.886	1.972	53.386	0.457	0.406
11000	43.682	86.58	1.571	48.016	0.524	0.468
12000	44.236	67.96	1.181	41.512	0.586	0.527
13000	44.455	56.641	0.85	41.512	0.631	0.568
14000	44.69	45.736	0.514	36.221	0.68	0.613
15000	44.775	38.996	0.235	36.221	0.714	0.644
16000	44.901	32.709	0.047	33.69	0.749	0.677
17000	45.033	28.298	0.007	33.69	0.776	0.702
18000	45.172	24.159	0.001	31.837	0.802	0.728
19000	45.297	20.785	0	30.183	0.825	0.75
20000	45.391	18.289	0	30.182	0.843	0.767

Table S3. Economic Potential (EP) values at different levels (inert fraction 0.2)

Cat. weight	BD value	Raw materials cost	EP-1	Reactor Heat transfer area	Reactor cost	Catalyst cost	Reactor utility cost	EP-2	EtOH recycle	EtOH Recycle cost	N_2 recycle cost	EP-3
kg	M$	M$	M$	A2	M$	M$	M$	M$	GJ	M$	M$	M$
3000	7.328	16.56	-9.232	0	0.038	0.18	0.098	-9.55	166852	2.92	0.35	-12.82
4000	11.99	16.56	-4.57	392.8	0.147	0.24	0.16	-5.12	143896.5	2.518	0.3	-7.94
5000	16.135	16.56	-0.425	523.7	0.192	0.3	0.216	-1.13	120024	2.1	0.28	-3.51
6000	20.033	16.56	3.473	654.7	0.24	0.36	0.268	2.61	98212.3	1.719	0.24	0.65
7000	23.132	16.56	6.572	785.6	0.289	0.42	0.309	5.55	78250.8	1.369	0.21	3.98
8000	25.82	16.56	9.26	916.5	0.34	0.48	0.345	8.1	60293.1	1.055	0.17	6.87
9000	27.739	16.56	11.179	1047.5	0.392	0.54	0.371	9.88	45178.1	0.791	0.13	8.95
10000	28.787	16.56	12.227	1178.4	0.446	0.6	0.385	10.8	34330.3	0.601	0.11	10.08
11000	29.354	16.56	12.794	1309.3	0.501	0.66	0.392	11.24	26805.1	0.469	0.1	10.67
12000	29.727	16.56	13.167	1440.3	0.556	0.72	0.397	11.49	21040.3	0.368	0.09	11.04
13000	29.874	16.56	13.314	1571.2	0.614	0.78	0.399	11.52	17536	0.307	0.09	11.12
14000	30.032	16.56	13.472	1702.1	0.671	0.84	0.401	11.56	14160	0.248	0.08	11.23
15000	30.089	16.56	13.529	1833.1	0.73	0.9	0.402	11.5	12073.1	0.211	0.08	11.21
16000	30.174	16.56	13.614	1964	0.79	0.96	0.403	11.46	10126.8	0.177	0.07	11.21
17000	30.262	16.56	13.702	2094.9	0.851	1.02	0.404	11.43	8761.2	0.153	0.07	11.2
18000	30.356	16.56	13.796	2225.9	0.912	1.08	0.406	11.4	7479.5	0.131	0.07	11.2
19000	30.439	16.56	13.879	2356.8	0.974	1.14	0.407	11.36	6435	0.113	0.06	11.18
20000	30.502	16.56	13.942	2487.7	1.037	1.2	0.408	11.3	5662.4	0.099	0.06	11.13

Table S4. Aspen Plus data for evaluating Ep-Aspen economic potential (inert fraction 0.2)

Catalyst weight	Electricity amount	Electricity cost	Thermal utility amount	Thermal utility price	Utility price	Equipment cost	Annual capital cost	Total cost	EP-Aspen
kg	MW	M$	GJ/h	M$	M$	M$	M$	M$	M$
3000	1.053	0.674	32.62	2.61	3.663	8.295	0.83	4.49	-17.31
4000	1.014	0.649	29.74	2.379	3.393	8.234	0.823	4.22	-12.16
5000	0.984	0.63	26.88	2.15	3.134	8.07	0.807	3.94	-7.45
6000	0.932	0.596	24.1	1.928	2.86	7.901	0.79	3.65	-3
7000	0.858	0.549	21.45	1.716	2.574	7.829	0.783	3.36	0.62
8000	0.785	0.502	18.97	1.518	2.303	7.577	0.758	3.06	3.81
9000	0.73	0.467	16.93	1.354	2.084	7.212	0.721	2.81	6.15
10000	0.707	0.452	15.38	1.23	1.937	7.131	0.713	2.65	7.43
11000	0.686	0.439	14.33	1.146	1.832	7.08	0.708	2.54	8.13
12000	0.614	0.393	13.49	1.079	1.693	6.638	0.664	2.36	8.68
13000	0.614	0.393	12.98	1.038	1.652	6.415	0.642	2.29	8.83
14000	0.599	0.383	12.59	1.007	1.606	6.341	0.634	2.24	8.99
15000	0.598	0.383	12.31	0.985	1.583	6.294	0.629	2.21	9
16000	0.597	0.382	12.09	0.967	1.564	6.284	0.628	2.19	9.02
17000	0.582	0.372	11.89	0.951	1.533	6.262	0.626	2.16	9.04
18000	0.582	0.372	11.73	0.938	1.52	6.5	0.65	2.17	9.03
19000	0.582	0.372	11.58	0.926	1.508	6.49	0.649	2.16	9.02
20000	0.567	0.363	11.48	0.918	1.485	6.48	0.648	2.13	9

3. Data for calculating Economic Potential values (inert fraction 0.4)

Table S5. Flowrates, EtOH conversion and BD Yield (inert fraction 0.4)

Catalyst weight/ [kg]	BD flowrate/ [kmol/h]	Recycle flowrates / [kmol/h]			EtOH conversion	BD Yield
		EtOH	ACH	N_2		
3000	6.197	432.474	3.345	345.446	0.047	0.023
4000	10.802	386.766	3.458	326.332	0.072	0.044
5000	15.907	343.547	3.394	298.502	0.102	0.072
6000	20.718	299.862	3.167	274.331	0.137	0.104
7000	25.05	258.629	2.874	252.5	0.176	0.14
8000	29.865	220.338	2.632	214.321	0.225	0.186
9000	32.746	186.56	2.299	202.191	0.27	0.229
10000	35.762	155.864	2.017	179.725	0.325	0.28
11000	38.261	128.866	1.746	158.352	0.383	0.334
12000	39.818	107.48	1.445	145.706	0.435	0.384
13000	41.09	89.546	1.163	132.929	0.488	0.434
14000	42.158	74.224	0.895	119.483	0.542	0.484
15000	42.942	61.764	0.636	108.011	0.592	0.531
16000	43.219	54.258	0.434	108.012	0.624	0.56
17000	43.761	45.313	0.202	97.114	0.669	0.602
18000	43.95	40.132	0.08	97.115	0.695	0.627
19000	44.373	33.654	0.014	87.508	0.734	0.664
20000	44.536	29.979	0.004	87.508	0.756	0.685

Table S6. Economic Potential (EP) values at different levels (inert fraction 0.4)

Cat. weight	BD value	Raw materials cost	EP-1	Reactor Heat transfer area	Reactor cost	Catalyst cost	Reactor utility cost	EP-2	EtOH recycle	EtOH Recycle cost	N_2 recycle cost	EP-3
kg	M$	M$	M$	A2	M$	M$	M$	M$	GJ	M$	M$	M$
3000	4.165	16.56	-12.4	0	0.038	0.18	0.056	-12.67	133894	2.343	0.743	-15.76
4000	7.259	16.56	-9.3	392.8	0.147	0.24	0.097	-9.79	119742.8	2.095	0.702	-12.58
5000	10.689	16.56	-5.87	523.7	0.192	0.3	0.143	-6.51	106362.1	1.861	0.642	-9.01
6000	13.923	16.56	-2.64	654.7	0.24	0.36	0.186	-3.42	92837.4	1.625	0.59	-5.64
7000	16.834	16.56	0.27	785.6	0.289	0.42	0.225	-0.66	80071.5	1.401	0.543	-2.6
8000	20.07	16.56	3.51	916.5	0.34	0.48	0.268	2.42	68216.8	1.194	0.461	0.77
9000	22.006	16.56	5.45	1047.5	0.392	0.54	0.294	4.22	57758.9	1.011	0.435	2.77
10000	24.032	16.56	7.47	1178.4	0.446	0.6	0.321	6.11	48255.4	0.844	0.386	4.87
11000	25.711	16.56	9.15	1309.3	0.501	0.66	0.344	7.65	39896.9	0.698	0.341	6.61
12000	26.758	16.56	10.2	1440.3	0.556	0.72	0.358	8.56	33275.7	0.582	0.313	7.67
13000	27.612	16.56	11.05	1571.2	0.614	0.78	0.369	9.29	27723.3	0.485	0.286	8.52
14000	28.33	16.56	11.77	1702.1	0.671	0.84	0.379	9.88	22979.9	0.402	0.257	9.22
15000	28.857	16.56	12.3	1833.1	0.73	0.9	0.386	10.28	19122.1	0.335	0.232	9.71
16000	29.043	16.56	12.48	1964	0.79	0.96	0.388	10.35	16798.4	0.294	0.232	9.82
17000	29.407	16.56	12.85	2094.9	0.851	1.02	0.393	10.58	14028.8	0.246	0.209	10.13
18000	29.534	16.56	12.97	2225.9	0.912	1.08	0.395	10.59	12424.7	0.217	0.209	10.16
19000	29.819	16.56	13.26	2356.8	0.974	1.14	0.398	10.75	10419.4	0.182	0.188	10.38
20000	29.928	16.56	13.37	2487.7	1.037	1.2	0.4	10.73	9281.4	0.162	0.188	10.38

Table S7. Aspen Plus data for evaluating Ep-Aspen economic potential (inert fraction 0.4)

Catalyst weight	Electricity amount	Electricity cost	Thermal utility amount	Thermal utility price	Utility price	Equipment cost	Annual capital cost	Total cost	EP-Aspen
kg	MW	M$	GJ/h	M$	M$	M$	M$	M$	M$
3000	1.795	1.149	27.46	2.197	3.992	8.835	0.884	4.88	-20.63
4000	1.745	1.117	26.21	2.097	3.842	8.819	0.882	4.72	-17.31
5000	1.639	1.049	24.55	1.964	3.603	8.343	0.834	4.44	-13.45
6000	1.509	0.966	22.85	1.828	3.337	8.234	0.823	4.16	-9.8
7000	1.466	0.938	21.24	1.699	3.165	8.156	0.816	3.98	-6.58
8000	1.311	0.839	19.72	1.578	2.889	8.048	0.805	3.69	-2.93
9000	1.281	0.82	18.26	1.461	2.742	7.963	0.796	3.54	-0.76
10000	1.168	0.748	16.99	1.359	2.527	7.649	0.765	3.29	1.58
11000	1.105	0.707	15.89	1.271	2.376	7.583	0.758	3.13	3.47
12000	1.025	0.656	14.95	1.196	2.221	7.461	0.746	2.97	4.7
13000	0.975	0.624	14.23	1.138	2.113	7.405	0.741	2.85	5.67
14000	0.922	0.59	13.61	1.089	2.011	7.313	0.731	2.74	6.48
15000	0.922	0.59	13.18	1.054	1.976	7.36	0.736	2.71	7
16000	0.872	0.558	12.81	1.025	1.897	7.302	0.73	2.63	7.19
17000	0.872	0.558	12.53	1.002	1.874	7.299	0.73	2.6	7.53
18000	0.845	0.541	12.27	0.982	1.827	7.216	0.722	2.55	7.61
19000	0.819	0.524	12.06	0.965	1.784	7.196	0.72	2.5	7.87
20000	0.799	0.511	11.89	0.951	1.75	7.192	0.719	2.47	7.91

4. Data for calculating Economic Potential values (inert fraction 0.6)

Table S8. Flowrates, EtOH conversion and BD Yield (inert fraction 0.6)

Catalyst weight/ [kg]	BD flowrate/ [kmol/h]	Recycle flowrates / [kmol/h]			EtOH conversion	BD Yield
		EtOH	ACH	N_2		
3000	1	342.997	1.926	500.001	0.041	0.015
4000	6.006	308.989	1.994	500	0.059	0.029
5000	8.735	276.898	1.924	500	0.08	0.046
6000	11.347	248.047	1.798	500	0.102	0.065
7000	13.75	222.669	1.654	500	0.125	0.085
8000	17.34	205.971	1.655	465.768	0.155	0.113
9000	20.825	188.558	1.618	432.463	0.187	0.144
10000	23.374	170.477	1.511	415.955	0.217	0.173
11000	26.4	153.992	1.437	385.119	0.254	0.208
12000	28.948	138.099	1.331	360.218	0.291	0.243
13000	31.146	123.212	1.205	337.97	0.329	0.279
14000	32.568	110.429	1.062	328.085	0.361	0.31
15000	34.838	96.874	0.929	296.523	0.407	0.354
16000	35.835	87.008	0.795	289.341	0.439	0.383
17000	37.188	76.953	0.658	271.629	0.477	0.42
18000	38.059	68.931	0.53	262.686	0.509	0.451
19000	39.566	59.162	0.37	234.583	0.558	0.497
20000	39.915	54.014	0.264	234.648	0.581	0.518

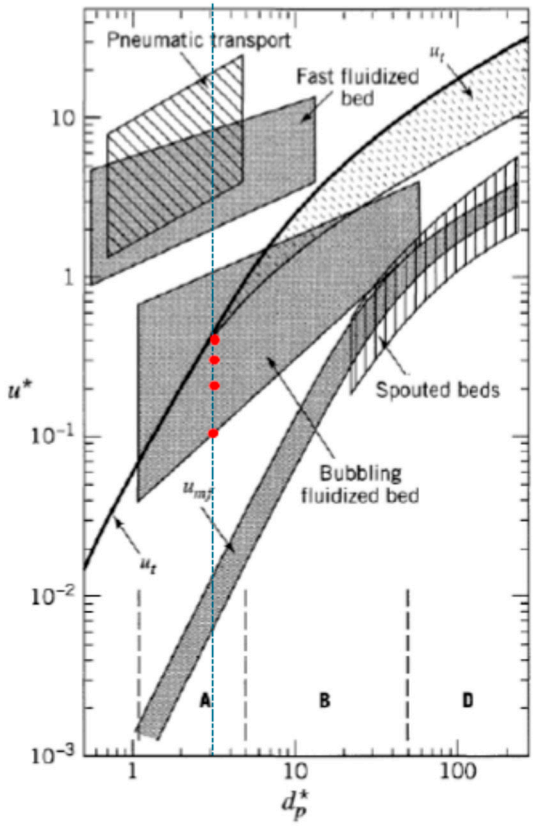
Table S9. Economic Potential (EP) values at different levels (inert fraction 0.6)

Cat. weight	BD value	Raw materials cost	EP-1	Reactor Heat transfer area	Reactor cost	Catalyst cost	Reactor utility cost	EP-2	EtOH recycle	EtOH Recycle cost	N_2 recycle cost	EP-3
kg	M$	M$	M$	A2	M$	M$	M$	M$	GJ	M$	M$	M$
3000	2.291	16.56	-14.27	0	0.038	0.18	0.031	-14.52	106191.8	1.858	1.075	-17.45
4000	4.036	16.56	-12.52	392.8	0.147	0.24	0.054	-12.97	95662.9	1.674	1.075	-15.71
5000	5.87	16.56	-10.69	523.7	0.192	0.3	0.078	-11.26	85727.7	1.5	1.075	-13.84
6000	7.625	16.56	-8.93	654.7	0.24	0.36	0.102	-9.64	76795.5	1.344	1.075	-12.06
7000	9.24	16.56	-7.32	785.6	0.289	0.42	0.123	-8.15	68938.4	1.206	1.075	-10.43
8000	11.653	16.56	-4.91	916.5	0.34	0.48	0.156	-5.88	63768.6	1.116	1.002	-8
9000	13.994	16.56	-2.57	1047.5	0.392	0.54	0.187	-3.68	58377.6	1.022	0.93	-5.64
10000	15.707	16.56	-0.85	1178.4	0.446	0.6	0.21	-2.11	52779.8	0.924	0.894	-3.93
11000	17.741	16.56	1.18	1309.3	0.501	0.66	0.237	-0.22	47676	0.834	0.828	-1.88
12000	19.453	16.56	2.89	1440.3	0.556	0.72	0.26	1.36	42755.5	0.748	0.775	-0.17
13000	20.93	16.56	4.37	1571.2	0.614	0.78	0.28	2.7	38146.3	0.668	0.727	1.3
14000	21.886	16.56	5.33	1702.1	0.671	0.84	0.292	3.52	34188.8	0.598	0.706	2.22
15000	23.411	16.56	6.85	1833.1	0.73	0.9	0.313	4.91	29992.3	0.525	0.638	3.75
16000	24.081	16.56	7.52	1964	0.79	0.96	0.322	5.45	26937.7	0.471	0.622	4.36
17000	24.991	16.56	8.43	2094.9	0.851	1.02	0.334	6.23	23824.7	0.417	0.584	5.22
18000	25.576	16.56	9.02	2225.9	0.912	1.08	0.342	6.68	21341.2	0.373	0.565	5.74
19000	26.588	16.56	10.03	2356.8	0.974	1.14	0.355	7.56	18316.6	0.321	0.504	6.73
20000	26.823	16.56	10.26	2487.7	1.037	1.2	0.358	7.67	16722.7	0.293	0.505	6.87

Table S10. Aspen Plus data for evaluating Ep-Aspen economic potential (inert fraction 0.6)

Catalyst weight	Electricity amount	Electricity cost	Thermal utility amount	Thermal utility price	Utility price	Equipment cost	Annual capital cost	Total cost	EP-Aspen
kg	MW	M$	GJ/h	M$	M$	M$	M$	M$	M$
3000	2.337	1.496	24.13	1.93	4.267	9.484	0.948	5.22	-22.67
4000	2.336	1.495	22.82	1.826	4.162	9.44	0.944	5.11	-20.82
5000	2.333	1.493	21.57	1.726	4.059	9.44	0.944	5	-18.84
6000	2.331	1.492	20.43	1.634	3.965	9.38	0.938	4.9	-16.96
7000	2.331	1.492	19.42	1.554	3.885	9.35	0.935	4.82	-15.25
8000	2.331	1.492	18.84	1.507	3.838	9.29	0.929	4.77	-12.77
9000	2.091	1.338	18.11	1.449	3.54	8.63	0.863	4.4	-10.04
10000	2.09	1.338	17.4	1.392	3.482	8.59	0.859	4.34	-8.27
11000	2.09	1.338	16.73	1.338	3.428	8.6	0.86	4.29	-6.17
12000	1.884	1.206	16.11	1.289	3.173	8.55	0.855	4.03	-4.19
13000	1.884	1.206	15.51	1.241	3.125	8.5	0.85	3.98	-2.67
14000	1.68	1.075	14.99	1.199	2.879	7.97	0.797	3.68	-1.46
15000	1.68	1.075	14.52	1.162	2.842	7.92	0.792	3.63	0.11
16000	1.58	1.011	14.08	1.126	2.706	7.9	0.79	3.5	0.86
17000	1.54	0.986	13.68	1.094	2.634	7.85	0.785	3.42	1.81
18000	1.5	0.96	13.33	1.066	2.566	7.83	0.783	3.35	2.39
19000	1.42	0.909	13.06	1.045	2.465	7.83	0.783	3.25	3.49
20000	1.38	0.883	12.77	1.022	2.402	7.89	0.789	3.19	3.68

5. **Working regime for fluidized bed reactor**



$$d_p^* = d_p\left[\frac{\rho_g(\rho_p-\rho_g)g}{\eta^2}\right]^{1/3} \quad ; \quad u^* = u_0\left[\frac{\rho_g^2}{\eta(\rho_p-\rho_g)g}\right]^{1/3}$$

Figure S1. Working regime for the fluidized bed reactor in Levenspiel [60] diagram (red points corresponding to Table 6 in main manuscript, lower value u_0=10 u_{mf}, upper value u_0=40 u_{mf})