

Optimization of the direct synthesis of dimethyl ether from CO₂ rich synthesis gas: Closing the loop between experimental investigations and model-based reactor design

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Electronic Supplementary Information

Section 2.1 Experimental setup

The experimental setup depicted in Figure 1 was used to conduct kinetic measurements and the experimental validation of model-based optimization results.

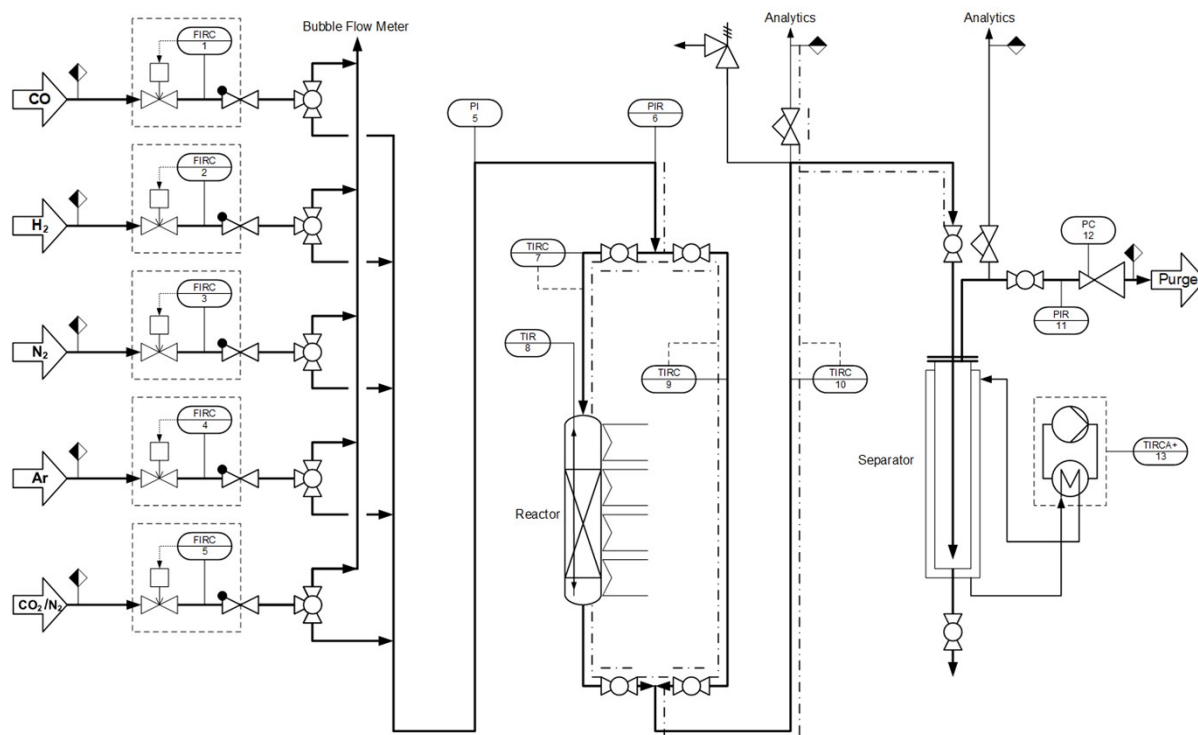
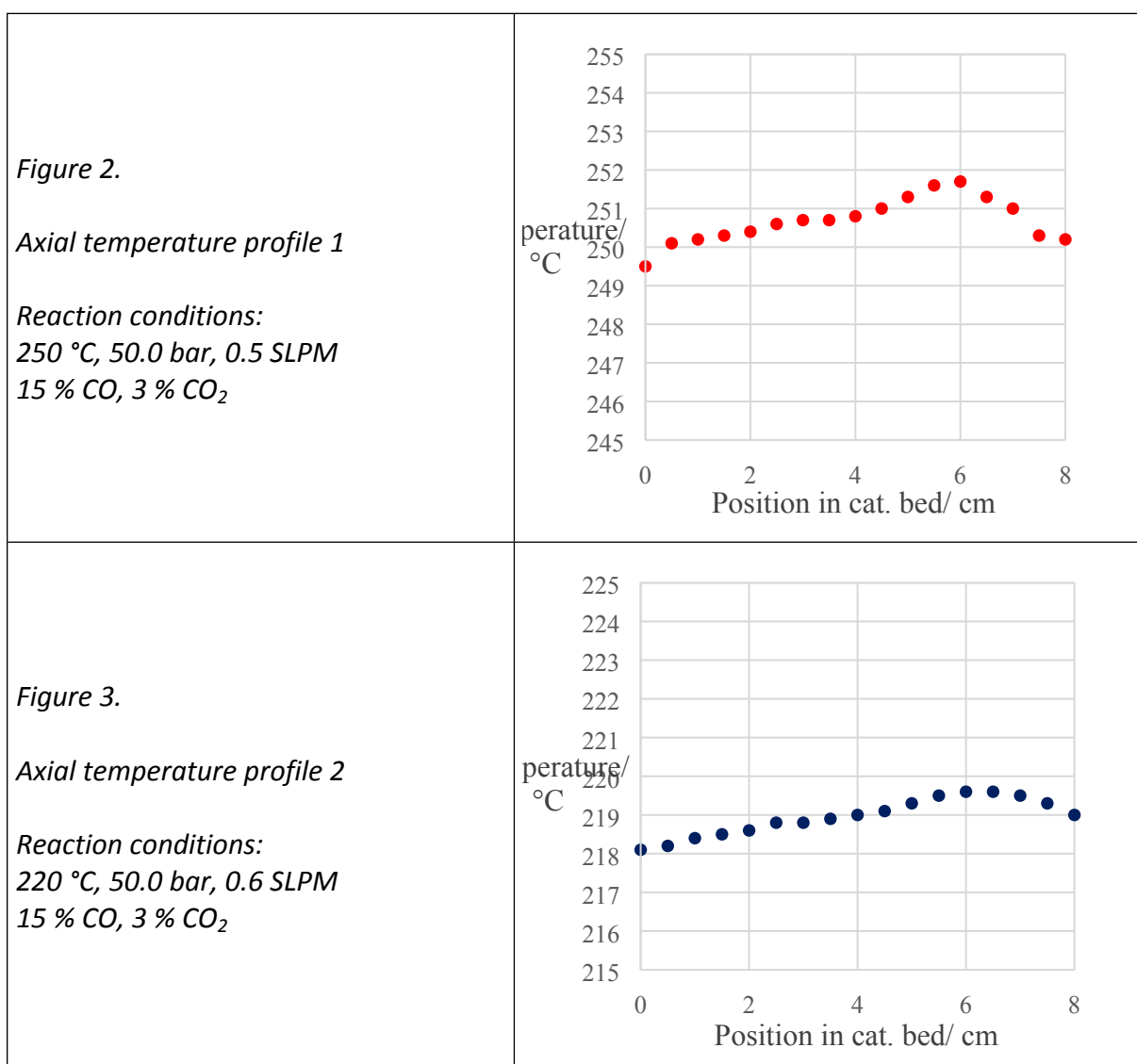


Figure 1: Flow diagram of the experimental setup.

The gas supply is regulated via mass flow controller (MFC, Bronkhorst High Tech, FIRC 1, 2, 3, 4 and 5) by using proportional-integral-derivative (PID) control.

The tube reactor consists of a vertical cylinder made of the stainless steel 1.4571. The reactor is designed for temperatures up to 350 °C and a maximal pressure of 100 bar. The thermocouple used for the temperature measurement over the reactor length is of the type K, NiCr-Ni. To ensure isothermal operating conditions the catalyst bed was diluted with SiC. Two exemplary temperature profiles measured with thermocouples along the axial direction during the experiments are shown in Figure 2 and 3.



The temperature profiles were measured with a scale division of 0.5 cm for the catalyst bed position. Temperature values were recorded under steady state conditions.

The Gas Chromatograph (GC) G1530A from Agilent Technologies is equipped with a thermal conductivity detector (TCD), a flame ionization detector (FID), an automatic loop filling manager system from Teuner Analysentechnik GmbH (LFM 205) and two capillary columns RT-Msieve 5A and RT-U-BOND from Restek Corporation.

For the kinetic studies, mixtures of a commercially available CuO/ZnO/ α -Al₂O₃ (CZA) catalyst provided by an industrial partner, γ -Al₂O₃ (ALOX, Alfa Aesar) and silicon carbide (SiC, Hausen Mineraliengroßhandel GmbH) were used.

The reactant gases carbon monoxide (CO, 99,97 %), argon (Ar, 99,9999 %), nitrogen (N₂, 99,9999 %), Hydrogen (H₂, 9,9999 %) and mixture carbon dioxide and nitrogen (CO₂/N₂, 50:50 \pm 1.0 vol. %) were provided by Air Liquid Germany GmbH.

Section 3.1 Reaction kinetic measurements

The measured kinetic data used for the parameter estimation of the lumped kinetic model are provided in Table 1.

The reader is advised:

- The feed gas consisted of Hydrogen, Carbon Monoxide, Carbon Dioxide and inert gas (Argon and Nitrogen). Only the concentration of the reactive components is reported here.
- Each operating point was measured under steady state conditions for approx. 90 Minutes. Possible deviations and fluctuations of the reported temperature and inlet volume flow are here neglected.

Table 1: Measured kinetic data

Ex p. ID	Temp.	Inlet Vol. Flow	Mass CZA-Cat.	Mass ALO X-Cat.	Mass SiC	Cat. Bed Length	H ₂ in Feed	CO in Feed	CO ₂ in Feed	H ₂ in Product	CO in Product	CO ₂ in Product	DME in Product
-	°C	SLP M	g	g	g	m	Vol. %	Vol. %	Vol. %	Vol. %	Vol. %	Vol. %	Vol. %
1	220	0.7	1.0002	1.0017	5.0000	0.0545	47.9521	16.0618	2.8835	46.7574	15.2641	2.8206	0.1190
2	220	0.6	1.0002	1.0017	5.0000	0.0545	47.9964	16.1122	2.8830	46.7599	15.2771	2.8282	0.1522
3	220	0.5	1.0002	1.0017	5.0000	0.0545	47.9760	16.0905	2.8811	46.6335	15.0919	2.8310	0.1876
4	220	0.4	1.0002	1.0017	5.0000	0.0545	47.6962	15.7591	2.8476	46.6793	14.9872	2.9265	0.2478
5	220	0.3	1.0002	1.0017	5.0000	0.0545	48.1176	15.9125	2.8534	46.6024	14.8201	3.0040	0.3366
6	220	0.2	1.0002	1.0017	5.0000	0.0545	48.4200	16.0724	2.8148	46.0863	13.8527	3.3271	0.6556
7	230	0.7	1.0002	1.0017	5.0000	0.0545	47.9521	16.0618	2.8835	46.4037	14.7769	2.9888	0.3038
8	230	0.6	1.0002	1.0017	5.0000	0.0545	47.9964	16.1122	2.8830	46.4811	14.7700	2.9967	0.3250
9	230	0.5	1.0002	1.0017	5.0000	0.0545	47.9760	16.0905	2.8811	46.2513	14.5797	3.0496	0.3949
10	230	0.4	1.0002	1.0017	5.0000	0.0545	47.6962	15.7591	2.8476	46.2415	14.3136	3.2145	0.5201
11	230	0.3	1.0002	1.0017	5.0000	0.0545	48.1176	15.9125	2.8534	45.9355	13.9055	3.3430	0.7081

			2	7	0	5	76	25	4	7	8		
12	230	0.2	1.000 2	1.001 7	5.000 0	0.054 5	48.42 00	16.07 24	2.814 8	45.055 8	12.255 2	3.9595	1.3078
13	240	0.7	1.000 2	1.001 7	5.000 0	0.054 5	47.95 21	16.06 18	2.883 5	45.837 3	13.990 8	3.2840	0.6447
14	240	0.6	1.000 2	1.001 7	5.000 0	0.054 5	47.99 64	16.11 22	2.883 0	45.857 1	13.984 4	3.2881	0.6505
15	240	0.5	1.000 2	1.001 7	5.000 0	0.054 5	47.97 60	16.09 05	2.881 1	45.449 0	13.649 0	3.3512	0.7593
16	240	0.4	1.000 2	1.001 7	5.000 0	0.054 5	47.69 62	15.75 91	2.847 6	45.628 3	13.241 2	3.6648	1.0165
17	240	0.3	1.000 2	1.001 7	5.000 0	0.054 5	48.11 76	15.91 25	2.853 4	45.107 8	12.563 2	3.8949	1.2982
18	240	0.2	1.000 2	1.001 7	5.000 0	0.054 5	48.42 00	16.07 24	2.814 8	43.990 3	10.161 2	4.8538	2.2916
19	250	0.7	1.000 2	1.001 7	5.000 0	0.054 5	47.95 21	16.06 18	2.883 5	45.187 0	12.912 6	3.7566	1.1476
20	250	0.6	1.000 2	1.001 7	5.000 0	0.054 5	47.99 64	16.11 22	2.883 0	44.848 5	12.697 2	3.7438	1.1509
21	250	0.5	1.000 2	1.001 7	5.000 0	0.054 5	47.97 60	16.09 05	2.881 1	44.656 7	12.367 3	3.8704	1.3352
22	250	0.4	1.000 2	1.001 7	5.000 0	0.054 5	47.69 62	15.75 91	2.847 6	44.708 9	11.723 2	4.2624	1.7025
23	250	0.3	1.000 2	1.001 7	5.000 0	0.054 5	48.11 76	15.91 25	2.853 4	44.082 4	10.750 4	4.6558	2.1266
24	250	0.2	1.000 2	1.001 7	5.000 0	0.054 5	48.42 00	16.07 24	2.814 8	42.839 3	7.8665	5.8356	3.3782
25	260	0.7	1.000 2	1.001 7	5.000 0	0.054 5	47.95 21	16.06 18	2.883 5	44.578 7	11.665 9	4.2707	1.7367

26	260	0.6	1.000 2	1.001 7	5.000 0	0.054 5	47.99 64	16.11 22	2.883 0	44.188 8	11.421 1	4.3248	1.7902
27	260	0.5	1.000 2	1.001 7	5.000 0	0.054 5	47.97 60	16.09 05	2.881 1	43.890 9	10.884 8	4.5250	2.0394
28	260	0.4	1.000 2	1.001 7	5.000 0	0.054 5	47.69 62	15.75 91	2.847 6	43.871 4	10.044 2	4.9880	2.4909
29	260	0.3	1.000 2	1.001 7	5.000 0	0.054 5	48.11 76	15.91 25	2.853 4	42.915 6	8.7959	5.4843	3.0326
30	260	0.2	1.000 2	1.001 7	5.000 0	0.054 5	48.42 00	16.07 24	2.814 8	41.749 9	5.9459	6.6015	4.2672
31	220	0.7	1.000 2	1.001 7	10.00 00	0.080 0	30.23 71	8.333 1	2.902 4	29.422 1	8.0958	2.7760	0.0674
32	220	0.6	1.000 2	1.001 7	10.00 00	0.080 0	30.15 34	8.177 9	2.809 6	29.162 4	7.8348	2.8048	0.1366
33	220	0.5	1.000 2	1.001 7	10.00 00	0.080 0	30.28 31	8.287 6	2.854 7	29.252 8	7.7607	2.8760	0.1677
34	220	0.4	1.000 2	1.001 7	10.00 00	0.080 0	30.28 31	8.287 6	2.854 7	29.128 1	7.6512	2.9297	0.2187
35	220	0.3	1.000 2	1.001 7	10.00 00	0.080 0	30.11 09	8.353 2	2.945 1	28.811 7	7.3482	3.0059	0.3170
36	220	0.2	1.000 2	1.001 7	10.00 00	0.080 0	30.25 12	8.373 7	2.880 4	28.574 4	6.7593	3.2333	0.5272
37	230	0.7	1.000 2	1.001 7	10.00 00	0.080 0	30.23 71	8.333 1	2.902 4	29.205 6	7.8803	2.8456	0.1341
38	230	0.6	1.000 2	1.001 7	10.00 00	0.080 0	30.15 34	8.177 9	2.809 6	28.866 0	7.5381	2.9028	0.2479
39	230	0.5	1.000 2	1.001 7	10.00 00	0.080 0	30.28 31	8.287 6	2.854 7	28.957 4	7.4175	2.9850	0.3083
40	230	0.4	1.000	1.001	10.00	0.080	30.28	8.287	2.854	28.750	7.2033	3.0519	0.3946

			2	7	00	0	31	6	7	3			
41	230	0.3	1.000 2	1.001 7	10.00 00	0.080 0	30.11 09	8.353 2	2.945 1	28.432 6	6.7994	3.2084	0.5456
42	230	0.2	1.000 2	1.001 7	10.00 00	0.080 0	30.25 12	8.373 7	2.880 4	28.016 0	5.9863	3.5308	0.8679
43	240	0.7	1.000 2	1.001 7	10.00 00	0.080 0	30.23 71	8.333 1	2.902 4	28.987 3	7.6063	2.9096	0.2493
44	240	0.6	1.000 2	1.001 7	10.00 00	0.080 0	30.15 34	8.177 9	2.809 6	28.623 9	7.1417	3.0868	0.4361
45	240	0.5	1.000 2	1.001 7	10.00 00	0.080 0	30.28 31	8.287 6	2.854 7	28.571 2	6.9478	3.2142	0.5199
46	240	0.4	1.000 2	1.001 7	10.00 00	0.080 0	30.28 31	8.287 6	2.854 7	28.270 3	6.6173	3.2730	0.6452
47	240	0.3	1.000 2	1.001 7	10.00 00	0.080 0	30.11 09	8.353 2	2.945 1	27.836 2	6.0568	3.5481	0.8580
48	240	0.2	1.000 2	1.001 7	10.00 00	0.080 0	30.25 12	8.373 7	2.880 4	27.234 6	5.0335	3.7976	1.2748
49	250	0.7	1.000 2	1.001 7	10.00 00	0.080 0	30.23 71	8.333 1	2.902 4	28.634 0	7.2220	3.0638	0.4168
50	250	0.6	1.000 2	1.001 7	10.00 00	0.080 0	30.15 34	8.177 9	2.809 6	28.302 3	6.5847	3.3296	0.6758
51	250	0.5	1.000 2	1.001 7	10.00 00	0.080 0	30.28 31	8.287 6	2.854 7	28.120 6	6.3270	3.4028	0.7691
52	250	0.4	1.000 2	1.001 7	10.00 00	0.080 0	30.28 31	8.287 6	2.854 7	27.715 5	5.9167	3.5578	0.9363
53	250	0.3	1.000 2	1.001 7	10.00 00	0.080 0	30.11 09	8.353 2	2.945 1	27.281 4	5.2884	3.7935	1.1887
54	250	0.2	1.000 2	1.001 7	10.00 00	0.080 0	30.25 12	8.373 7	2.880 4	26.623 8	4.1922	4.1511	1.6449

55	260	0.7	1.000 2	1.001 7	10.00 00	0.080 0	30.23 71	8.333 1	2.902 4	28.274 2	6.7380	3.2400	0.6188
56	260	0.6	1.000 2	1.001 7	10.00 00	0.080 0	30.15 34	8.177 9	2.809 6	27.837 7	6.0005	3.4991	0.9141
57	260	0.5	1.000 2	1.001 7	10.00 00	0.080 0	30.28 31	8.287 6	2.854 7	27.614 2	5.7184	3.5971	1.0343
58	260	0.4	1.000 2	1.001 7	10.00 00	0.080 0	30.28 31	8.287 6	2.854 7	27.246 9	5.2907	3.7708	1.2109
59	260	0.3	1.000 2	1.001 7	10.00 00	0.080 0	30.11 09	8.353 2	2.945 1	26.669 7	4.5852	3.9625	1.4868
60	260	0.2	1.000 2	1.001 7	10.00 00	0.080 0	30.25 12	8.373 7	2.880 4	26.018 0	3.6080	4.3567	1.9090
61	220	0.7	1.000 2	1.001 7	10.00 00	0.080 0	20.37 39	4.118 0	2.859 5	19.808 7	3.9426	2.7458	0.0657
62	220	0.6	1.000 2	1.001 7	10.00 00	0.080 0	20.37 39	4.118 0	2.859 5	19.671 0	3.9061	2.7453	0.0744
63	220	0.5	1.000 2	1.001 7	10.00 00	0.080 0	20.17 65	4.045 8	2.883 0	19.519 7	3.8318	2.7799	0.0923
64	220	0.4	1.000 2	1.001 7	10.00 00	0.080 0	20.17 65	4.045 8	2.883 0	19.442 6	3.7183	2.8087	0.1229
65	220	0.3	1.000 2	1.001 7	10.00 00	0.080 0	20.22 29	4.008 5	2.849 6	19.477 8	3.5695	2.8672	0.1724
66	220	0.2	1.000 2	1.001 7	10.00 00	0.080 0	20.33 01	4.050 7	2.862 6	19.497 4	3.2875	2.9309	0.2794
67	230	0.7	1.000 2	1.001 7	10.00 00	0.080 0	20.37 39	4.118 0	2.859 5	19.637 6	3.8179	2.7495	0.1114
68	230	0.6	1.000 2	1.001 7	10.00 00	0.080 0	20.37 39	4.118 0	2.859 5	19.489 3	3.7667	2.7689	0.1285
69	230	0.5	1.000	1.001	10.00	0.080	20.17	4.045	2.883	19.322	3.6605	2.8114	0.1559

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70	230	0.4	1.000 2	1.001 7	10.00 00	0.080 0	20.17 65	4.045 8	2.883 0	19.240 7	3.5196	2.8461	0.2020
71	230	0.3	1.000 2	1.001 7	10.00 00	0.080 0	20.22 29	4.008 5	2.849 6	19.321 3	3.3273	2.9407	0.2775
72	230	0.2	1.000 2	1.001 7	10.00 00	0.080 0	20.33 01	4.050 7	2.862 6	19.174 0	2.9323	3.0258	0.4218
73	240	0.7	1.000 2	1.001 7	10.00 00	0.080 0	20.37 39	4.118 0	2.859 5	19.499 7	3.6736	2.8073	0.1765
74	240	0.6	1.000 2	1.001 7	10.00 00	0.080 0	20.37 39	4.118 0	2.859 5	19.279 7	3.5911	2.8033	0.2030
75	240	0.5	1.000 2	1.001 7	10.00 00	0.080 0	20.17 65	4.045 8	2.883 0	19.183 2	3.4863	2.8768	0.2415
76	240	0.4	1.000 2	1.001 7	10.00 00	0.080 0	20.17 65	4.045 8	2.883 0	19.036 3	3.3077	2.9388	0.2992
77	240	0.3	1.000 2	1.001 7	10.00 00	0.080 0	20.22 29	4.008 5	2.849 6	19.110 6	3.0527	3.0197	0.3999
78	240	0.2	1.000 2	1.001 7	10.00 00	0.080 0	20.33 01	4.050 7	2.862 6	18.783 4	2.5695	3.1438	0.5700
79	250	0.7	1.000 2	1.001 7	10.00 00	0.080 0	20.37 39	4.118 0	2.859 5	19.320 0	3.5212	2.8476	0.2505
80	250	0.6	1.000 2	1.001 7	10.00 00	0.080 0	20.37 39	4.118 0	2.859 5	19.109 0	3.4051	2.8903	0.2851
81	250	0.5	1.000 2	1.001 7	10.00 00	0.080 0	20.17 65	4.045 8	2.883 0	19.005 5	3.2768	2.9561	0.3314
82	250	0.4	1.000 2	1.001 7	10.00 00	0.080 0	20.17 65	4.045 8	2.883 0	18.781 7	3.0787	2.9893	0.4006
83	250	0.3	1.000 2	1.001 7	10.00 00	0.080 0	20.22 29	4.008 5	2.849 6	18.860 3	2.7960	3.0871	0.5085

84	250	0.2	1.000 2	1.001 7	10.00 00	0.080 0	20.33 01	4.050 7	2.862 6	18.598 3	2.3130	3.1967	0.6835
85	260	0.7	1.000 2	1.001 7	10.00 00	0.080 0	20.37 39	4.118 0	2.859 5	19.149 0	3.3891	2.8903	0.3131
86	260	0.6	1.000 2	1.001 7	10.00 00	0.080 0	20.37 39	4.118 0	2.859 5	19.002 9	3.2503	2.9465	0.3527
87	260	0.5	1.000 2	1.001 7	10.00 00	0.080 0	20.17 65	4.045 8	2.883 0	18.816 7	3.1226	2.9831	0.4013
88	260	0.4	1.000 2	1.001 7	10.00 00	0.080 0	20.17 65	4.045 8	2.883 0	18.576 2	2.9056	3.0461	0.4704
89	260	0.3	1.000 2	1.001 7	10.00 00	0.080 0	20.22 29	4.008 5	2.849 6	18.650 2	2.6586	3.1209	0.5726
90	260	0.2	1.000 2	1.001 7	10.00 00	0.080 0	20.33 01	4.050 7	2.862 6	18.440 7	2.2483	3.2382	0.7175
91	220	0.7	1.000 2	1.001 7	10.00 00	0.080 0	41.28 34	15.81 43	0.909 3	40.898 2	15.465 2	0.9273	0.1296
92	220	0.6	1.000 2	1.001 7	10.00 00	0.080 0	41.28 34	15.81 43	0.909 3	41.083 0	15.536 4	0.9760	0.1850
93	220	0.5	1.000 2	1.001 7	10.00 00	0.080 0	41.67 09	15.98 54	0.911 3	41.039 9	15.470 7	1.0148	0.2462
94	220	0.4	1.000 2	1.001 7	10.00 00	0.080 0	41.67 09	15.98 54	0.911 3	40.865 9	15.262 5	1.0735	0.3395
95	220	0.3	1.000 2	1.001 7	10.00 00	0.080 0	41.84 97	16.06 62	0.894 7	40.619 9	14.943 1	1.1611	0.4713
96	220	0.2	1.000 2	1.001 7	10.00 00	0.080 0	42.32 76	16.13 62	0.819 2	39.733 9	14.157 8	1.4173	0.8071
97	230	0.7	1.000 2	1.001 7	10.00 00	0.080 0	41.28 34	15.81 43	0.909 3	40.771 4	15.242 9	1.0121	0.2388
98	230	0.6	1.000	1.001	10.00	0.080	41.28	15.81	0.909	40.911	15.231	1.1026	0.3269

			2	7	00	0	34	43	3	1	5		
99	230	0.5	1.000 2	1.001 7	10.00 00	0.080 0	41.67 09	15.98 54	0.911 3	40.755 2	15.027 0	1.1637	0.4242
100	230	0.4	1.000 2	1.001 7	10.00 00	0.080 0	41.67 09	15.98 54	0.911 3	40.429 4	14.714 8	1.2708	0.5729
101	230	0.3	1.000 2	1.001 7	10.00 00	0.080 0	41.84 97	16.06 62	0.894 7	40.010 3	14.188 1	1.4312	0.7828
102	230	0.2	1.000 2	1.001 7	10.00 00	0.080 0	42.32 76	16.13 62	0.819 2	38.944 2	12.969 8	1.8464	1.3010
103	240	0.7	1.000 2	1.001 7	10.00 00	0.080 0	41.28 34	15.81 43	0.909 3	40.425 9	14.807 2	1.1584	0.4117
104	240	0.6	1.000 2	1.001 7	10.00 00	0.080 0	41.28 34	15.81 43	0.909 3	40.610 5	14.781 5	1.2878	0.5467
105	240	0.5	1.000 2	1.001 7	10.00 00	0.080 0	41.67 09	15.98 54	0.911 3	40.208 6	14.350 8	1.4003	0.6977
106	240	0.4	1.000 2	1.001 7	10.00 00	0.080 0	41.67 09	15.98 54	0.911 3	39.921 6	13.934 2	1.5756	0.9266
107	240	0.3	1.000 2	1.001 7	10.00 00	0.080 0	41.84 97	16.06 62	0.894 7	39.133 9	13.048 3	1.8323	1.2556
108	240	0.2	1.000 2	1.001 7	10.00 00	0.080 0	42.32 76	16.13 62	0.819 2	37.873 6	11.374 2	2.4964	2.0382
109	250	0.7	1.000 2	1.001 7	10.00 00	0.080 0	41.28 34	15.81 43	0.909 3	40.006 1	14.199 0	1.3890	0.6812
110	250	0.6	1.000 2	1.001 7	10.00 00	0.080 0	41.28 34	15.81 43	0.909 3	40.055 8	14.011 4	1.5600	0.8783
111	250	0.5	1.000 2	1.001 7	10.00 00	0.080 0	41.67 09	15.98 54	0.911 3	39.641 1	13.467 7	1.7418	1.1102
112	250	0.4	1.000 2	1.001 7	10.00 00	0.080 0	41.67 09	15.98 54	0.911 3	39.006 9	12.721 7	2.0205	1.4307

113	250	0.3	1.000 2	1.001 7	10.00 00	0.080 0	41.84 97	16.06 62	0.894 7	38.086 7	11.517 1	2.4156	1.9394
114	250	0.2	1.000 2	1.001 7	10.00 00	0.080 0	42.32 76	16.13 62	0.819 2	36.338 2	9.1713	3.2742	2.9509
115	260	0.7	1.000 2	1.001 7	10.00 00	0.080 0	41.28 34	15.81 43	0.909 3	39.421 3	13.333 8	1.7268	1.0742
116	260	0.6	1.000 2	1.001 7	10.00 00	0.080 0	41.28 34	15.81 43	0.909 3	39.291 3	12.929 5	1.9652	1.3370
117	260	0.5	1.000 2	1.001 7	10.00 00	0.080 0	41.67 09	15.98 54	0.911 3	38.630 2	12.173 4	2.2193	1.6576
118	260	0.4	1.000 2	1.001 7	10.00 00	0.080 0	41.67 09	15.98 54	0.911 3	37.968 8	11.206 4	2.5730	2.0891
119	260	0.3	1.000 2	1.001 7	10.00 00	0.080 0	41.84 97	16.06 62	0.894 7	36.699 3	9.6157	3.1148	2.7614
120	260	0.2	1.000 2	1.001 7	10.00 00	0.080 0	42.32 76	16.13 62	0.819 2	35.047 0	7.0272	4.1437	3.9770
121	220	0.7	1.000 2	1.001 7	10.00 00	0.080 0	23.95 62	8.481 4	0.885 9	23.217 0	8.0966	0.9005	0.1232
122	220	0.6	1.000 2	1.001 7	10.00 00	0.080 0	23.89 21	8.474 5	0.878 5	23.314 4	8.1380	0.9153	0.1322
123	220	0.5	1.000 2	1.001 7	10.00 00	0.080 0	23.81 56	8.555 2	0.852 3	23.149 0	8.0504	0.9519	0.1787
124	220	0.4	1.000 2	1.001 7	10.00 00	0.080 0	23.81 56	8.555 2	0.852 3	23.608 5	7.9027	0.9906	0.2340
125	220	0.3	1.000 2	1.001 7	10.00 00	0.080 0	23.85 91	8.588 6	0.825 9	22.868 1	7.6531	1.0384	0.3368
126	220	0.2	1.000 2	1.001 7	10.00 00	0.080 0	24.02 15	8.569 7	0.764 0	22.664 7	7.2701	1.1547	0.5221
127	230	0.7	1.000	1.001	10.00	0.080	23.95	8.481	0.885	23.047	7.9275	0.9889	0.1977

			2	7	00	0	62	4	9	3			
128	230	0.6	1.000 2	1.001 7	10.00 00	0.080 0	23.89 21	8.474 5	0.878 5	23.128 2	7.9371	1.0048	0.2192
129	230	0.5	1.000 2	1.001 7	10.00 00	0.080 0	23.81 56	8.555 2	0.852 3	22.934 0	7.7698	1.0501	0.2845
130	230	0.4	1.000 2	1.001 7	10.00 00	0.080 0	23.81 56	8.555 2	0.852 3	23.436 8	7.5664	1.1161	0.3714
131	230	0.3	1.000 2	1.001 7	10.00 00	0.080 0	23.85 91	8.588 6	0.825 9	22.540 9	7.2095	1.1883	0.5121
132	230	0.2	1.000 2	1.001 7	10.00 00	0.080 0	24.02 15	8.569 7	0.764 0	22.032 9	6.5939	1.3721	0.7841
133	240	0.7	1.000 2	1.001 7	10.00 00	0.080 0	23.95 62	8.481 4	0.885 9	22.829 7	7.6373	1.0866	0.3090
134	240	0.6	1.000 2	1.001 7	10.00 00	0.080 0	23.89 21	8.474 5	0.878 5	22.859 7	7.6164	1.1075	0.3449
135	240	0.5	1.000 2	1.001 7	10.00 00	0.080 0	23.81 56	8.555 2	0.852 3	22.663 5	7.4010	1.1844	0.4359
136	240	0.4	1.000 2	1.001 7	10.00 00	0.080 0	23.81 56	8.555 2	0.852 3	22.517 5	7.1155	1.2804	0.5525
137	240	0.3	1.000 2	1.001 7	10.00 00	0.080 0	23.85 91	8.588 6	0.825 9	22.012 6	6.5926	1.3919	0.7542
138	240	0.2	1.000 2	1.001 7	10.00 00	0.080 0	24.02 15	8.569 7	0.764 0	21.281 0	5.7053	1.6789	1.1271
139	250	0.7	1.000 2	1.001 7	10.00 00	0.080 0	23.95 62	8.481 4	0.885 9	22.449 2	7.2782	1.1941	0.4486
140	250	0.6	1.000 2	1.001 7	10.00 00	0.080 0	23.89 21	8.474 5	0.878 5	22.527 8	7.2016	1.2531	0.5126
141	250	0.5	1.000 2	1.001 7	10.00 00	0.080 0	23.81 56	8.555 2	0.852 3	22.186 6	6.8944	1.3496	0.6280

142	250	0.4	1.000 2	1.001 7	10.00 00	0.080 0	23.81 56	8.555 2	0.852 3	21.990 5	6.5179	1.4779	0.7940
143	250	0.3	1.000 2	1.001 7	10.00 00	0.080 0	23.85 91	8.588 6	0.825 9	21.364 8	5.8472	1.6505	1.0493
144	250	0.2	1.000 2	1.001 7	10.00 00	0.080 0	24.02 15	8.569 7	0.764 0	20.391 8	4.7508	1.9806	1.4958
145	260	0.7	1.000 2	1.001 7	10.00 00	0.080 0	23.95 62	8.481 4	0.885 9	22.280 4	6.9234	1.3520	0.6173
146	260	0.6	1.000 2	1.001 7	10.00 00	0.080 0	23.89 21	8.474 5	0.878 5	22.044 7	6.7020	1.4120	0.7052
147	260	0.5	1.000 2	1.001 7	10.00 00	0.080 0	23.81 56	8.555 2	0.852 3	21.762 4	6.3559	1.5370	0.8444
148	260	0.4	1.000 2	1.001 7	10.00 00	0.080 0	23.81 56	8.555 2	0.852 3	21.432 2	5.8775	1.6871	1.0413
149	260	0.3	1.000 2	1.001 7	10.00 00	0.080 0	23.85 91	8.588 6	0.825 9	20.710 2	5.1354	1.8776	1.3149
150	260	0.2	1.000 2	1.001 7	10.00 00	0.080 0	24.02 15	8.569 7	0.764 0	19.765 7	4.0504	2.2075	1.7679
151	220	0.7	1.000 2	1.001 7	10.00 00	0.080 0	13.04 99	4.102 6	0.864 6	12.368 7	3.9014	0.8990	0.0984
152	220	0.6	1.000 2	1.001 7	10.00 00	0.080 0	13.04 99	4.102 6	0.864 6	12.292 4	3.8293	0.9214	0.1266
153	220	0.5	1.000 2	1.001 7	10.00 00	0.080 0	12.79 18	4.174 9	0.853 7	12.245 2	3.7663	0.9342	0.1627
154	220	0.4	1.000 2	1.001 7	10.00 00	0.080 0	12.79 18	4.174 9	0.853 7	12.452 8	3.7700	0.9477	0.1751
155	220	0.3	1.000 2	1.001 7	10.00 00	0.080 0	12.91 64	4.228 4	0.807 0	12.253 5	3.5891	0.9668	0.2487
156	220	0.2	1.000	1.001	10.00	0.080	13.09	4.264	0.757	11.927	3.3229	1.0013	0.3578

			2	7	00	0	45	2	4	9			
157	230	0.7	1.000 2	1.001 7	10.00 00	0.080 0	13.04 99	4.102 6	0.864 6	12.219 6	3.7518	0.9408	0.1499
158	230	0.6	1.000 2	1.001 7	10.00 00	0.080 0	13.04 99	4.102 6	0.864 6	12.206 8	3.6770	0.9636	0.1875
159	230	0.5	1.000 2	1.001 7	10.00 00	0.080 0	12.79 18	4.174 9	0.853 7	12.160 0	3.6261	0.9911	0.2225
160	230	0.4	1.000 2	1.001 7	10.00 00	0.080 0	12.79 18	4.174 9	0.853 7	12.157 8	3.5197	1.0093	0.2578
161	230	0.3	1.000 2	1.001 7	10.00 00	0.080 0	12.91 64	4.228 4	0.807 0	11.995 9	3.3062	1.0493	0.3463
162	230	0.2	1.000 2	1.001 7	10.00 00	0.080 0	13.09 45	4.264 2	0.757 4	11.645 6	2.9711	1.1019	0.4865
163	240	0.7	1.000 2	1.001 7	10.00 00	0.080 0	13.04 99	4.102 6	0.864 6	12.058 3	3.5966	0.9945	0.2151
164	240	0.6	1.000 2	1.001 7	10.00 00	0.080 0	13.04 99	4.102 6	0.864 6	12.016 3	3.5149	1.0288	0.2558
165	240	0.5	1.000 2	1.001 7	10.00 00	0.080 0	12.79 18	4.174 9	0.853 7	11.963 4	3.4135	1.0653	0.3061
166	240	0.4	1.000 2	1.001 7	10.00 00	0.080 0	12.79 18	4.174 9	0.853 7	11.870 5	3.2864	1.0971	0.3538
167	240	0.3	1.000 2	1.001 7	10.00 00	0.080 0	12.91 64	4.228 4	0.807 0	11.720 5	2.9828	1.1561	0.4609
168	240	0.2	1.000 2	1.001 7	10.00 00	0.080 0	13.09 45	4.264 2	0.757 4	11.296 7	2.5965	1.2235	0.6183
169	250	0.7	1.000 2	1.001 7	10.00 00	0.080 0	13.04 99	4.102 6	0.864 6	11.895 5	3.4241	1.0450	0.2816
170	250	0.6	1.000 2	1.001 7	10.00 00	0.080 0	13.04 99	4.102 6	0.864 6	11.837 1	3.3364	1.0909	0.3265

171	250	0.5	1.000 2	1.001 7	10.00 00	0.080 0	12.79 18	4.174 9	0.853 7	11.762 0	3.2227	1.1239	0.3808
172	250	0.4	1.000 2	1.001 7	10.00 00	0.080 0	12.79 18	4.174 9	0.853 7	11.654 2	3.0664	1.1553	0.4371
173	250	0.3	1.000 2	1.001 7	10.00 00	0.080 0	12.91 64	4.228 4	0.807 0	11.380 2	2.7695	1.2195	0.5468
174	250	0.2	1.000 2	1.001 7	10.00 00	0.080 0	13.09 45	4.264 2	0.757 4	11.048 0	2.3576	1.2899	0.7073
175	260	0.7	1.000 2	1.001 7	10.00 00	0.080 0	13.04 99	4.102 6	0.864 6	11.739 6	3.2848	1.0866	0.3308
176	260	0.6	1.000 2	1.001 7	10.00 00	0.080 0	13.04 99	4.102 6	0.864 6	11.727 1	3.2006	1.1217	0.3722
177	260	0.5	1.000 2	1.001 7	10.00 00	0.080 0	12.79 18	4.174 9	0.853 7	11.627 5	3.0665	1.1568	0.4239
178	260	0.4	1.000 2	1.001 7	10.00 00	0.080 0	12.79 18	4.174 9	0.853 7	11.594 0	2.9437	1.2055	0.4800
179	260	0.3	1.000 2	1.001 7	10.00 00	0.080 0	12.91 64	4.228 4	0.807 0	11.396 0	2.6932	1.2454	0.5787
180	260	0.2	1.000 2	1.001 7	10.00 00	0.080 0	13.09 45	4.264 2	0.757 4	11.000 3	2.3508	1.2939	0.7097
181	220	0.6	1.000 0	0.000 0	5.000 0	0.035 0	47.05 51	15.40 21	2.879 5	44.841 9	14.200 1	2.7966	0.0001
182	220	0.5	1.000 0	0.000 0	5.000 0	0.035 0	46.17 78	15.34 84	2.851 2	44.532 6	13.969 1	2.8062	0.0002
183	220	0.4	1.000 0	0.000 0	5.000 0	0.035 0	48.98 91	16.06 47	2.939 0	46.938 7	15.025 0	2.8546	0.0003
184	230	0.6	1.000 0	0.000 0	5.000 0	0.035 0	47.05 51	15.40 21	2.879 5	43.977 3	13.819 7	2.8461	0.0006
185	230	0.5	1.000	0.000	5.000	0.035	46.17	15.34	2.851	43.052	13.519	2.8316	0.0009

			0	0	0	0	78	84	2	3	6		
186	230	0.4	1.000 0	0.000 0	5.000 0	0.035 0	48.98 91	16.06 47	2.939 0	45.818 3	14.355 0	2.8908	0.0007
187	240	0.6	1.000 0	0.000 0	5.000 0	0.035 0	47.05 51	15.40 21	2.879 5	43.001 2	13.187 8	2.9384	0.0019
188	240	0.5	1.000 0	0.000 0	5.000 0	0.035 0	46.17 78	15.34 84	2.851 2	42.036 8	12.817 3	2.9077	0.0023
189	240	0.4	1.000 0	0.000 0	5.000 0	0.035 0	48.98 91	16.06 47	2.939 0	44.645 4	13.638 9	2.9838	0.0022
190	250	0.6	1.000 0	0.000 0	5.000 0	0.035 0	47.05 51	15.40 21	2.879 5	42.493 6	12.756 0	3.0240	0.0046
191	250	0.5	1.000 0	0.000 0	5.000 0	0.035 0	46.17 78	15.34 84	2.851 2	41.502 4	12.368 9	2.9719	0.0047
192	250	0.4	1.000 0	0.000 0	5.000 0	0.035 0	48.98 91	16.06 47	2.939 0	43.984 8	13.123 8	3.0763	0.0048
193	260	0.6	1.000 0	0.000 0	5.000 0	0.035 0	47.05 51	15.40 21	2.879 5	42.337 7	12.666 5	3.0152	0.0079
194	260	0.5	1.000 0	0.000 0	5.000 0	0.035 0	46.17 78	15.34 84	2.851 2	41.692 5	12.472 9	3.0318	0.0110
195	260	0.4	1.000 0	0.000 0	5.000 0	0.035 0	48.98 91	16.06 47	2.939 0	43.583 2	12.868 9	3.0323	0.0105
196	220	0.6	1.000 0	0.000 0	5.000 0	0.035 0	28.90 52	8.083 7	2.804 9	28.474 0	7.7887	2.7664	0.0003
197	220	0.5	1.000 0	0.000 0	5.000 0	0.035 0	30.54 46	8.450 3	2.946 4	28.890 5	7.7596	2.8427	0.0003
198	220	0.4	1.000 0	0.000 0	5.000 0	0.035 0	30.46 74	8.530 7	2.946 0	28.482 3	7.5844	2.8395	0.0003
199	230	0.6	1.000 0	0.000 0	5.000 0	0.035 0	28.90 52	8.083 7	2.804 9	28.153 0	7.5237	2.8023	0.0004

200	230	0.5	1.000 0	0.000 0	5.000 0	0.035 0	30.54 46	8.450 3	2.946 4	28.349 1	7.4634	2.8762	0.0008
201	230	0.4	1.000 0	0.000 0	5.000 0	0.035 0	30.46 74	8.530 7	2.946 0	27.940 0	7.2329	2.8746	0.0010
202	240	0.6	1.000 0	0.000 0	5.000 0	0.035 0	28.90 52	8.083 7	2.804 9	27.909 3	7.3213	2.8626	0.0011
203	240	0.5	1.000 0	0.000 0	5.000 0	0.035 0	30.54 46	8.450 3	2.946 4	27.906 0	7.2056	2.9005	0.0013
204	240	0.4	1.000 0	0.000 0	5.000 0	0.035 0	30.46 74	8.530 7	2.946 0	27.459 2	6.9622	2.8912	0.0021
205	250	0.6	1.000 0	0.000 0	5.000 0	0.035 0	28.90 52	8.083 7	2.804 9	27.717 8	7.1975	2.8495	0.0019
206	250	0.5	1.000 0	0.000 0	5.000 0	0.035 0	30.54 46	8.450 3	2.946 4	27.784 6	7.1309	2.8957	0.0028
207	250	0.4	1.000 0	0.000 0	5.000 0	0.035 0	30.46 74	8.530 7	2.946 0	27.440 9	6.9693	2.9172	0.0036
208	260	0.6	1.000 0	0.000 0	5.000 0	0.035 0	28.90 52	8.083 7	2.804 9	28.044 0	7.2673	2.8757	0.0042
209	260	0.5	1.000 0	0.000 0	5.000 0	0.035 0	30.54 46	8.450 3	2.946 4	28.046 1	7.2726	2.8987	0.0046
210	260	0.4	1.000 0	0.000 0	5.000 0	0.035 0	30.46 74	8.530 7	2.946 0	27.748 3	7.1680	2.8900	0.0061
211	220	0.6	1.000 0	0.000 0	5.000 0	0.035 0	20.35 88	4.086 5	2.926 2	19.381 1	3.8319	2.7550	0.0000
212	220	0.5	1.000 0	0.000 0	5.000 0	0.035 0	20.39 61	4.048 9	2.885 5	19.451 1	3.7850	2.7645	0.0000
213	220	0.4	1.000 0	0.000 0	5.000 0	0.035 0	20.45 05	4.081 4	2.744 2	19.272 2	3.6935	2.6407	0.0000
214	230	0.6	1.000	0.000	5.000	0.035	20.35	4.086	2.926	19.240	3.7343	2.7535	0.0000

			0	0	0	0	88	5	2	1			
215	230	0.5	1.000 0	0.000 0	5.000 0	0.035 0	20.39 61	4.048 9	2.885 5	19.307 9	3.7063	2.7876	0.0001
216	230	0.4	1.000 0	0.000 0	5.000 0	0.035 0	20.45 05	4.081 4	2.744 2	19.095 7	3.5794	2.6585	0.0002
217	240	0.6	1.000 0	0.000 0	5.000 0	0.035 0	20.35 88	4.086 5	2.926 2	19.176 3	3.6972	2.7619	0.0002
218	240	0.5	1.000 0	0.000 0	5.000 0	0.035 0	20.39 61	4.048 9	2.885 5	19.193 9	3.6563	2.7724	0.0004
219	240	0.4	1.000 0	0.000 0	5.000 0	0.035 0	20.45 05	4.081 4	2.744 2	19.037 2	3.5557	2.6410	0.0007
220	250	0.6	1.000 0	0.000 0	5.000 0	0.035 0	20.35 88	4.086 5	2.926 2	19.201 3	3.7195	2.7526	0.0007
221	250	0.5	1.000 0	0.000 0	5.000 0	0.035 0	20.39 61	4.048 9	2.885 5	19.315 4	3.7010	2.7806	0.0009
222	250	0.4	1.000 0	0.000 0	5.000 0	0.035 0	20.45 05	4.081 4	2.744 2	19.164 6	3.6435	2.6339	0.0013
223	260	0.6	1.000 0	0.000 0	5.000 0	0.035 0	20.35 88	4.086 5	2.926 2	19.363 0	3.8358	2.7351	0.0011
224	260	0.5	1.000 0	0.000 0	5.000 0	0.035 0	20.39 61	4.048 9	2.885 5	19.454 5	3.8211	2.7394	0.0014
225	260	0.4	1.000 0	0.000 0	5.000 0	0.035 0	20.45 05	4.081 4	2.744 2	19.404 3	3.7903	2.6187	0.0019
226	220	0.6	1.000 0	0.000 0	5.000 0	0.035 0	41.49 47	15.87 93	0.901 6	40.380 8	15.304 9	0.8354	0.0001
227	220	0.5	1.000 0	0.000 0	5.000 0	0.035 0	41.58 78	15.96 64	0.918 4	40.117 6	15.096 2	0.8783	0.0003
228	220	0.4	1.000 0	0.000 0	5.000 0	0.035 0	42.02 74	16.16 33	0.933 9	40.272 1	15.150 0	0.8998	0.0007

229	230	0.6	1.000 0	0.000 0	5.000 0	0.035 0	41.49 47	15.87 93	0.901 6	39.922 4	15.044 9	0.8529	0.0006
230	230	0.5	1.000 0	0.000 0	5.000 0	0.035 0	41.58 78	15.96 64	0.918 4	39.452 1	14.780 5	0.8975	0.0011
231	230	0.4	1.000 0	0.000 0	5.000 0	0.035 0	42.02 74	16.16 33	0.933 9	39.502 1	14.689 2	0.9109	0.0022
232	240	0.6	1.000 0	0.000 0	5.000 0	0.035 0	41.49 47	15.87 93	0.901 6	39.146 1	14.580 1	0.8706	0.0017
233	240	0.5	1.000 0	0.000 0	5.000 0	0.035 0	41.58 78	15.96 64	0.918 4	38.648 6	14.328 1	0.9101	0.0026
234	240	0.4	1.000 0	0.000 0	5.000 0	0.035 0	42.02 74	16.16 33	0.933 9	38.842 8	14.242 1	0.9441	0.0045
235	250	0.6	1.000 0	0.000 0	5.000 0	0.035 0	41.49 47	15.87 93	0.901 6	38.425 8	14.200 2	0.8956	0.0039
236	250	0.5	1.000 0	0.000 0	5.000 0	0.035 0	41.58 78	15.96 64	0.918 4	38.067 6	13.984 0	0.9377	0.0051
237	250	0.4	1.000 0	0.000 0	5.000 0	0.035 0	42.02 74	16.16 33	0.933 9	38.483 5	13.980 6	0.9656	0.0075
238	260	0.6	1.000 0	0.000 0	5.000 0	0.035 0	41.49 47	15.87 93	0.901 6	38.111 8	13.956 2	0.9152	0.0058
239	260	0.5	1.000 0	0.000 0	5.000 0	0.035 0	41.58 78	15.96 64	0.918 4	37.726 1	13.781 3	0.9699	0.0093
240	260	0.4	1.000 0	0.000 0	5.000 0	0.035 0	42.02 74	16.16 33	0.933 9	38.454 8	13.879 8	0.9923	0.0136

Section 4.4 Optimization results

The reaction rate profiles for optimization cases A2, B1 and B2, along with the respective reference cases are presented here (Figures 4 to 6) complementary to the results in Section 4.4. At optimal conditions, increased reaction rates along the reactor coordinate can be observed in each case. These results resemble the ones obtained for optimization case A1, which were previously discussed in Section 4.4.1.1.

