

# Appendix 1

## Observed plant data (dimensionless) of an industrial tubular reactor startup

- $\sigma$  = dimensionless time, [-]  
 $\phi_V$  = dimensionless fluid velocity, [-]  
 $\psi_B$  = dimensionless reactant *B* concentration at the reactor inlet, [-]  
 $u_\theta$  = dimensionless reactor inlet temperature, [-]  
 $z$  = dimensionless axial reactor length, [-]  
 $\theta(z)$  = dimensionless reactor temperature at position  $z$  and dimensionless time =  $\sigma$  [-]

$\sigma$	$\phi_V$	$\psi_B$	$u_\theta$	$\theta$ <i>0.1714</i>	$\theta$ <i>0.3924</i>	$\theta$ <i>0.4949</i>	$\theta$ <i>0.5957</i>	$\theta$ <i>0.6971</i>	$\theta$ <i>0.7981</i>	$\theta$ <i>0.8992</i>	$\theta$ <i>1.0000</i>
0.0000	0.4022	0.0000	0.9491	0.9030	0.9294	0.9507	0.9663	0.9894	1.0171	1.0283	1.0276
0.0333	0.4050	0.0000	0.9515	0.9033	0.9260	0.9489	0.9645	0.9867	1.0141	1.0277	1.0284
0.0667	0.4110	0.0000	0.9487	0.9084	0.9237	0.9466	0.9629	0.9835	1.0111	1.0268	1.0288
0.1000	0.4097	0.0000	0.9516	0.9131	0.9221	0.9438	0.9612	0.9801	1.0076	1.0254	1.0295
0.1333	0.4690	0.5487	0.9525	0.9164	0.9207	0.9414	0.9595	0.9771	1.0040	1.0240	1.0297
0.1667	0.4774	0.5749	0.9763	0.9191	0.9189	0.9384	0.9572	0.9742	1.0007	1.0220	1.0294
0.2000	0.4849	0.6449	0.9893	0.9222	0.9175	0.9353	0.9546	0.9712	0.9973	1.0202	1.0298
0.2333	0.4933	0.7030	0.9901	0.9264	0.9161	0.9324	0.9525	0.9682	0.9933	1.0176	1.0293
0.2667	0.5006	0.7698	0.9890	0.9301	0.9152	0.9297	0.9501	0.9654	0.9891	1.0141	1.0285
0.3000	0.5133	0.8060	0.9888	0.9351	0.9156	0.9276	0.9473	0.9628	0.9847	1.0105	1.0279
0.3333	0.5222	0.8904	0.9884	0.9411	0.9162	0.9248	0.9444	0.9605	0.9810	1.0070	1.0265
0.3667	0.5239	0.9131	0.9866	0.9472	0.9169	0.9227	0.9412	0.9577	0.9783	1.0031	1.0247
0.4000	0.5316	0.8984	0.9860	0.9525	0.9182	0.9206	0.9387	0.9551	0.9745	0.9992	1.0226
0.4333	0.5301	0.9071	0.9862	0.9587	0.9205	0.9199	0.9357	0.9527	0.9720	0.9957	1.0201
0.4667	0.5328	0.9176	0.9859	0.9636	0.9225	0.9185	0.9326	0.9495	0.9680	0.9910	1.0168
0.5000	0.5348	0.9283	0.9867	0.9683	0.9260	0.9181	0.9304	0.9467	0.9649	0.9874	1.0135
0.5333	0.5326	0.9339	0.9866	0.9719	0.9293	0.9179	0.9277	0.9440	0.9619	0.9839	1.0109
0.5667	0.5310	0.9330	0.9869	0.9758	0.9333	0.9184	0.9255	0.9414	0.9596	0.9794	1.0063
0.6000	0.5334	0.9376	0.9872	0.9790	0.9374	0.9196	0.9242	0.9383	0.9564	0.9761	1.0032
0.6333	0.5340	0.9315	0.9861	0.9819	0.9414	0.9212	0.9226	0.9354	0.9541	0.9733	0.9987
0.6667	0.5563	0.8931	0.9854	0.9854	0.9464	0.9231	0.9222	0.9330	0.9512	0.9703	0.9952
0.7000	0.5562	0.8937	0.9827	0.9876	0.9511	0.9256	0.9215	0.9302	0.9481	0.9667	0.9912
0.7333	0.5548	0.8842	0.9830	0.9897	0.9556	0.9285	0.9217	0.9278	0.9446	0.9629	0.9871
0.7667	0.5584	0.8915	0.9830	0.9915	0.9609	0.9327	0.9221	0.9261	0.9422	0.9602	0.9837
0.8000	0.5552	0.9026	0.9835	0.9937	0.9659	0.9371	0.9233	0.9243	0.9393	0.9571	0.9801
0.8333	0.5617	0.8835	0.9837	0.9949	0.9709	0.9413	0.9251	0.9234	0.9368	0.9546	0.9764
0.8667	0.5552	0.9048	0.9880	0.9963	0.9760	0.9459	0.9270	0.9228	0.9341	0.9512	0.9731
0.9000	0.5601	0.8817	1.0005	0.9980	0.9807	0.9515	0.9296	0.9221	0.9318	0.9482	0.9698
0.9333	0.5563	0.8774	1.0089	0.9992	0.9857	0.9572	0.9328	0.9225	0.9298	0.9451	0.9667
0.9667	0.5602	0.8995	1.0124	1.0003	0.9905	0.9632	0.9368	0.9235	0.9280	0.9426	0.9632
1.0000	0.5568	0.8890	1.0129	1.0032	0.9949	0.9689	0.9411	0.9243	0.9266	0.9393	0.9602
1.0333	0.5575	0.8923	1.0133	1.0068	0.9998	0.9749	0.9466	0.9265	0.9260	0.9379	0.9574
1.0667	0.5592	0.8987	1.0128	1.0108	1.0044	0.9805	0.9524	0.9281	0.9255	0.9350	0.9541
1.1000	0.5570	0.8985	1.0111	1.0149	1.0093	0.9871	0.9581	0.9312	0.9250	0.9334	0.9514
1.1333	0.5536	0.8825	1.0098	1.0190	1.0138	0.9934	0.9637	0.9348	0.9257	0.9315	0.9486
1.1667	0.5609	0.8958	1.0075	1.0236	1.0190	0.9994	0.9707	0.9388	0.9267	0.9304	0.9462
1.2000	0.5573	0.8897	1.0073	1.0273	1.0244	1.0064	0.9775	0.9435	0.9278	0.9297	0.9433
1.2333	0.5583	0.8902	1.0050	1.0316	1.0298	1.0127	0.9845	0.9488	0.9293	0.9286	0.9416
1.2667	0.5583	0.8971	1.0028	1.0352	1.0359	1.0200	0.9915	0.9549	0.9319	0.9282	0.9391
1.3000	0.5553	0.8987	1.0025	1.0374	1.0424	1.0269	0.9992	0.9608	0.9343	0.9284	0.9367
1.3333	0.5579	0.9011	1.0007	1.0422	1.0505	1.0354	1.0075	0.9674	0.9387	0.9287	0.9357
1.3667	0.5572	0.9008	0.9999	1.0461	1.0599	1.0449	1.0167	0.9750	0.9419	0.9299	0.9344
1.4000	0.5597	0.8997	0.9993	1.0478	1.0705	1.0558	1.0271	0.9835	0.9472	0.9313	0.9334
1.4333	0.5534	0.8900	0.9980	1.0496	1.0834	1.0686	1.0374	0.9921	0.9530	0.9333	0.9328
1.4667	0.4667	0.0000	0.9957	1.0531	1.1006	1.0840	1.0518	1.0020	0.9604	0.9363	0.9332
1.5000	0.4479	0.0000	0.9644	1.0591	1.1217	1.1031	1.0669	1.0123	0.9670	0.9390	0.9330
1.5333	0.4401	0.0000	0.9587	1.0655	1.1482	1.1284	1.0846	1.0235	0.9733	0.9425	0.9335
1.5667	0.4329	0.0000	0.9620	1.0738	1.1809	1.1609	1.1064	1.0360	0.9806	0.9462	0.9345
1.6000	0.4352	0.0000	0.9647	1.0865	1.2105	1.1958	1.1353	1.0515	0.9898	0.9514	0.9356
1.6333	0.4212	0.0000	0.9663	1.0971	1.2279	1.2185	1.1666	1.0718	0.9993	0.9572	0.9373
1.6667	0.4127	0.0000	0.9670	1.1148	1.2401	1.2287	1.1910	1.0923	1.0103	0.9629	0.9391
1.7000	0.5155	0.9620	0.9784	1.1288	1.2451	1.2335	1.2050	1.1179	1.0228	0.9688	0.9413

$\sigma$	$\phi_V$	$\psi_B$	$u_\theta$	$\theta$ <i>0.1714</i>	$\theta$ <i>0.3924</i>	$\theta$ <i>0.4949</i>	$\theta$ <i>0.5957</i>	$\theta$ <i>0.6971</i>	$\theta$ <i>0.7981</i>	$\theta$ <i>0.8992</i>	$\theta$ <i>1.0000</i>
1.7333	0.5327	0.8850	1.0095	1.1271	1.2468	1.2362	1.2123	1.1440	1.0381	0.9771	0.9450
1.7667	0.5437	0.8743	1.0026	1.1208	1.2473	1.2388	1.2169	1.1642	1.0586	0.9868	0.9495
1.8000	0.5444	0.8675	0.9973	1.1115	1.2466	1.2402	1.2205	1.1778	1.0834	0.9984	0.9546
1.8333	0.5137	0.9220	0.9953	1.1061	1.2454	1.2421	1.2241	1.1868	1.1089	1.0130	0.9612
1.8667	0.5367	0.9019	0.9949	1.0987	1.2411	1.2427	1.2266	1.1932	1.1302	1.0297	0.9684
1.9000	0.5660	0.9235	0.9930	1.0902	1.2339	1.2433	1.2303	1.1986	1.1464	1.0503	0.9767
1.9333	0.6012	0.9269	0.9893	1.0818	1.2240	1.2441	1.2332	1.2041	1.1586	1.0738	0.9879
1.9667	0.5902	0.8973	0.9885	1.0768	1.2111	1.2434	1.2360	1.2081	1.1675	1.0969	1.0023
2.0000	0.5805	0.9052	0.9887	1.0701	1.1991	1.2413	1.2378	1.2123	1.1762	1.1165	1.0183
2.0333	0.5588	0.8725	0.9890	1.0648	1.1899	1.2387	1.2396	1.2168	1.1823	1.1312	1.0375
2.0667	0.5575	0.9078	0.9885	1.0624	1.1800	1.2349	1.2409	1.2204	1.1889	1.1420	1.0585
2.1000	0.5571	0.8892	0.9876	1.0611	1.1741	1.2288	1.2410	1.2238	1.1945	1.1524	1.0776
2.1333	0.5551	0.9098	0.9870	1.0614	1.1708	1.2205	1.2403	1.2262	1.1994	1.1598	1.0954
2.1667	0.5600	0.8991	0.9859	1.0714	1.1711	1.2110	1.2396	1.2287	1.2033	1.1674	1.1103
2.2000	0.5610	0.9005	0.9857	1.0772	1.1725	1.2024	1.2370	1.2310	1.2083	1.1749	1.1233
2.2333	0.5595	0.9092	0.9848	1.0803	1.1757	1.1963	1.2344	1.2329	1.2122	1.1815	1.1341
2.2667	0.5641	0.9068	0.9847	1.0801	1.1797	1.1912	1.2300	1.2332	1.2151	1.1870	1.1432
2.3000	0.5580	0.9124	0.9845	1.0827	1.1843	1.1875	1.2238	1.2339	1.2187	1.1918	1.1523
2.3333	0.5591	0.9070	0.9859	1.0839	1.1911	1.1857	1.2165	1.2332	1.2220	1.1971	1.1598
2.3667	0.5605	0.9077	0.9875	1.0870	1.1971	1.1859	1.2098	1.2322	1.2243	1.2018	1.1678
2.4000	0.5594	0.9037	0.9877	1.0909	1.2037	1.1869	1.2036	1.2298	1.2264	1.2061	1.1743
2.4333	0.5597	0.9098	0.9879	1.0937	1.2109	1.1899	1.1991	1.2264	1.2285	1.2104	1.1806
2.4667	0.5246	0.7133	0.9885	1.0952	1.2176	1.1923	1.1953	1.2224	1.2287	1.2140	1.1870
2.5000	0.5548	0.8931	0.9881	1.0976	1.2237	1.1965	1.1932	1.2179	1.2294	1.2167	1.1912
2.5333	0.5592	0.8961	0.9888	1.0976	1.2296	1.2015	1.1919	1.2130	1.2283	1.2194	1.1959
2.5667	0.5547	0.8968	0.9885	1.0997	1.2355	1.2067	1.1925	1.2080	1.2270	1.2219	1.2010
2.6000	0.5587	0.8970	0.9884	1.1036	1.2414	1.2120	1.1935	1.2030	1.2251	1.2238	1.2057
2.6333	0.5566	0.8887	0.9896	1.1060	1.2464	1.2172	1.1963	1.1984	1.2220	1.2256	1.2100
2.6667	0.5873	0.9174	0.9882	1.1094	1.2505	1.2223	1.1987	1.1963	1.2189	1.2264	1.2130
2.7000	0.5875	0.9083	0.9878	1.1101	1.2541	1.2271	1.2022	1.1945	1.2143	1.2255	1.2161
2.7333	0.5688	0.9396	0.9877	1.1128	1.2584	1.2320	1.2069	1.1943	1.2105	1.2253	1.2193
2.7667	0.5673	0.9441	0.9872	1.11079	1.2611	1.2364	1.2121	1.1948	1.2065	1.2232	1.2214
2.8000	0.5484	0.8598	0.9874	1.1164	1.2648	1.2406	1.2163	1.1964	1.2034	1.2218	1.2235
2.8333	0.5570	0.9135	0.9882	1.1184	1.2665	1.2445	1.2206	1.1980	1.2004	1.2188	1.2243
2.8667	0.5611	0.9062	0.9873	1.1229	1.2692	1.2484	1.2249	1.2002	1.1985	1.2164	1.2251
2.9000	0.5413	0.9272	0.9878	1.1206	1.2714	1.2520	1.2294	1.2031	1.1983	1.2135	1.2252
2.9333	0.5375	0.9412	0.9889	1.1285	1.2725	1.2555	1.2340	1.2065	1.1979	1.2096	1.2242
2.9667	0.5466	0.9220	0.9893	1.1301	1.2742	1.2583	1.2379	1.2102	1.1983	1.2080	1.2236
3.0000	0.5569	0.9458	0.9894	1.1307	1.2761	1.2614	1.2417	1.2145	1.1994	1.2055	1.2220
3.0333	0.5556	0.9464	0.9887	1.1320	1.2764	1.2633	1.2460	1.2179	1.2010	1.2032	1.2197
3.0667	0.5662	0.9417	0.9894	1.1285	1.2776	1.2654	1.2492	1.2225	1.2027	1.2018	1.2173
3.1000	0.5653	0.9375	0.9893	1.1348	1.2788	1.2676	1.2528	1.2273	1.2054	1.2015	1.2153
3.1333	0.5714	0.9254	0.9895	1.1391	1.2793	1.2694	1.2563	1.2316	1.2085	1.2018	1.2128
3.1667	0.5722	0.9241	0.9897	1.1405	1.2803	1.2708	1.2589	1.2359	1.2116	1.2022	1.2105
3.2000	0.5712	0.9320	0.9898	1.1397	1.2811	1.2725	1.2623	1.2395	1.2161	1.2035	1.2092
3.2333	0.5792	0.9186	0.9900	1.1457	1.2824	1.2741	1.2651	1.2435	1.2198	1.2055	1.2080
3.2667	0.5841	0.9601	0.9896	1.1512	1.2830	1.2754	1.2670	1.2471	1.2239	1.2075	1.2073
3.3000	0.5943	0.9473	0.9885	1.1508	1.2839	1.2762	1.2692	1.2506	1.2277	1.2100	1.2071
3.3333	0.5966	0.9441	0.9885	1.1497	1.2851	1.2776	1.2710	1.2533	1.2323	1.2131	1.2074
3.3667	0.5921	0.9616	0.9884	1.1521	1.2861	1.2781	1.2723	1.2565	1.2362	1.2158	1.2077
3.4000	0.6014	0.9318	0.9877	1.1571	1.2871	1.2789	1.2733	1.2593	1.2396	1.2203	1.2090
3.4333	0.6020	0.9441	0.9882	1.1573	1.2885	1.2801	1.2752	1.2620	1.2435	1.2232	1.2109
3.4667	0.6023	0.9436	0.9877	1.1559	1.2898	1.2811	1.2763	1.2644	1.2468	1.2274	1.2135
3.5000	0.6092	0.9737	0.9872	1.1566	1.2905	1.2821	1.2774	1.2663	1.2506	1.2314	1.2157
3.5333	0.6223	0.9521	0.9875	1.1603	1.2919	1.2832	1.2790	1.2681	1.2536	1.2359	1.2187
3.5667	0.6239	0.9526	0.9869	1.1608	1.2930	1.2845	1.2797	1.2697	1.2571	1.2395	1.2215
3.6000	0.6261	0.9622	0.9864	1.1597	1.2946	1.2861	1.2807	1.2715	1.2594	1.2433	1.2254
3.6333	0.6293	0.9621	0.9862	1.1572	1.2956	1.2870	1.2822	1.2725	1.2620	1.2474	1.2297
3.6667	0.6366	0.9510	0.9859	1.1605	1.2962	1.2883	1.2831	1.2741	1.2643	1.2506	1.2332
3.7000	0.6407	0.9449	0.9857	1.1620	1.2970	1.2894	1.2848	1.2754	1.2661	1.2540	1.2372
3.7333	0.6412	0.9455	0.9853	1.1603	1.2976	1.2902	1.2854	1.2761	1.2686	1.2565	1.2410
3.7667	0.6468	0.9487	0.9854	1.1588	1.2987	1.2913	1.2869	1.2779	1.2701	1.2598	1.2452
3.8000	0.6542	0.9424	0.9850	1.1587	1.2995	1.2922	1.2881	1.2791	1.2713	1.2624	1.2496
3.8333	0.6516	0.9409	0.9846	1.1592	1.3002	1.2936	1.2894	1.2805	1.2735	1.2649	1.2529
3.8667	0.6635	0.9616	0.9845	1.1559	1.3003	1.2942	1.2897	1.2814	1.2744	1.2668	1.2560

$\sigma$	$\phi_V$	$\psi_B$	$u_\theta$	$\theta$ <i>0.1714</i>	$\theta$ <i>0.3924</i>	$\theta$ <i>0.4949</i>	$\theta$ <i>0.5957</i>	$\theta$ <i>0.6971</i>	$\theta$ <i>0.7981</i>	$\theta$ <i>0.8992</i>	$\theta$ <i>1.0000</i>
3.9000	0.6668	0.9575	0.9840	1.1572	1.3009	1.2949	1.2915	1.2832	1.2758	1.2692	1.2594
3.9333	0.6670	0.9674	0.9839	1.1535	1.3018	1.2959	1.2927	1.2841	1.2774	1.2709	1.2624
3.9667	0.6747	0.9551	0.9832	1.1530	1.3023	1.2970	1.2943	1.2858	1.2791	1.2722	1.2650
4.0000	0.6790	0.9787	0.9818	1.1502	1.3023	1.2972	1.2943	1.2863	1.2798	1.2736	1.2675
4.0333	0.6812	0.9815	0.9821	1.1470	1.3028	1.2982	1.2956	1.2875	1.2808	1.2754	1.2693
4.0667	0.7050	0.9438	0.9812	1.1440	1.3032	1.2987	1.2969	1.2891	1.2831	1.2770	1.2714
4.1000	0.6983	0.9607	0.9807	1.1421	1.3029	1.2991	1.2973	1.2901	1.2838	1.2785	1.2735
4.1333	0.7182	0.9383	0.9807	1.1412	1.3034	1.2994	1.2984	1.2912	1.2853	1.2801	1.2752
4.1667	0.7242	0.9186	0.9794	1.1349	1.3032	1.2996	1.2986	1.2921	1.2863	1.2812	1.2770
4.2000	0.7244	0.9203	0.9786	1.1359	1.3034	1.3001	1.2996	1.2929	1.2880	1.2827	1.2785
4.2333	0.7209	0.9280	0.9776	1.1321	1.3037	1.3005	1.3001	1.2942	1.2892	1.2845	1.2805
4.2667	0.7265	0.9217	0.9774	1.1259	1.3032	1.3007	1.3005	1.2950	1.2902	1.2858	1.2821
4.3000	0.7279	0.9184	0.9776	1.1256	1.3038	1.3005	1.3010	1.2953	1.2911	1.2866	1.2836
4.3333	0.7299	0.9170	0.9763	1.1221	1.3031	1.3006	1.3009	1.2961	1.2916	1.2876	1.2845
4.3667	0.7337	0.9516	0.9763	1.1198	1.3039	1.3012	1.3015	1.2972	1.2932	1.2895	1.2865
4.4000	0.7421	0.9433	0.9751	1.1174	1.3033	1.3010	1.3019	1.2972	1.2936	1.2904	1.2877
4.4333	0.7491	0.9386	0.9744	1.1143	1.3033	1.3009	1.3019	1.2978	1.2947	1.2915	1.2890
4.4667	0.7497	0.9382	0.9727	1.1085	1.3031	1.3011	1.3021	1.2983	1.2953	1.2929	1.2907
4.5000	0.7588	0.9199	0.9715	1.1047	1.3024	1.3009	1.3019	1.2982	1.2954	1.2931	1.2914
4.5333	0.7548	0.9501	0.9713	1.1043	1.3017	1.3007	1.3022	1.2985	1.2962	1.2941	1.2927
4.5667	0.7611	0.9563	0.9707	1.1024	1.3009	1.3007	1.3023	1.2987	1.2967	1.2951	1.2940
4.6000	0.7707	0.9470	0.9704	1.0967	1.3001	1.3008	1.3025	1.2993	1.2975	1.2965	1.2953
4.6333	0.7718	0.9519	0.9704	1.0972	1.2988	1.2995	1.3021	1.2990	1.2976	1.2967	1.2959
4.6667	0.7841	0.9297	0.9723	1.0878	1.2982	1.2993	1.3020	1.2994	1.2981	1.2973	1.2970
4.7000	0.7795	0.9477	0.9729	1.0893	1.2972	1.2984	1.3020	1.2996	1.2993	1.2981	1.2980
4.7333	0.7877	0.9373	0.9731	1.0817	1.2961	1.2975	1.3012	1.2997	1.2985	1.2982	1.2987
4.7667	0.7927	0.9345	0.9735	1.0813	1.2949	1.2968	1.3012	1.2995	1.2987	1.2987	1.2995
4.8000	0.7925	0.9418	0.9734	1.0780	1.2949	1.2959	1.3006	1.2993	1.2989	1.2991	1.3002
4.8333	0.8012	0.9181	0.9736	1.0747	1.2951	1.2956	1.2999	1.2989	1.2989	1.2994	1.3012
4.8667	0.8055	0.9500	0.9743	1.0703	1.2944	1.2946	1.2989	1.2989	1.2992	1.2994	1.3016
4.9000	0.8103	0.9413	0.9738	1.0646	1.2943	1.2943	1.2984	1.2985	1.2990	1.3000	1.3017
4.9333	0.8157	0.9462	0.9736	1.0530	1.2940	1.2936	1.2974	1.2980	1.2990	1.3002	1.3021
4.9667	0.8148	0.9524	0.9739	1.0470	1.2939	1.2925	1.2963	1.2968	1.2984	1.2998	1.3022
5.0000	0.8208	0.9349	0.9742	1.0428	1.2936	1.2926	1.2962	1.2967	1.2984	1.3004	1.3029
5.0333	0.8265	0.9295	0.9741	1.0325	1.2930	1.2928	1.2956	1.2956	1.2975	1.3001	1.3028
5.0667	0.8334	0.9517	0.9743	1.0233	1.2903	1.2924	1.2950	1.2947	1.2974	1.3000	1.3033
5.1000	0.8289	0.9627	0.9740	1.0208	1.2907	1.2918	1.2948	1.2942	1.2966	1.2995	1.3033
5.1333	0.8343	0.9560	0.9736	1.0197	1.2899	1.2921	1.2945	1.2935	1.2964	1.2993	1.3030
5.1667	0.8527	0.9260	0.9740	1.0120	1.2891	1.2921	1.2940	1.2931	1.2955	1.2989	1.3034
5.2000	0.8494	0.9442	0.9742	1.0115	1.2882	1.2918	1.2937	1.2927	1.2947	1.2985	1.3032
5.2333	0.8521	0.9405	0.9742	1.0082	1.2868	1.2911	1.2938	1.2923	1.2940	1.2977	1.3028
5.2667	0.8595	0.9280	0.9745	1.0055	1.2853	1.2912	1.2937	1.2921	1.2938	1.2972	1.3022
5.3000	0.8562	0.9551	0.9740	1.0064	1.2831	1.2911	1.2931	1.2918	1.2932	1.2964	1.3020
5.3333	0.8668	0.9454	0.9736	1.0020	1.2789	1.2904	1.2923	1.2914	1.2924	1.2958	1.3012
5.3667	0.8733	0.9417	0.9742	1.0022	1.2747	1.2902	1.2923	1.2912	1.2922	1.2953	1.3009
5.4000	0.8723	0.9458	0.9751	1.0013	1.2713	1.2903	1.2928	1.2915	1.2920	1.2950	1.3005
5.4333	0.8804	0.9307	0.9748	1.0000	1.2637	1.2903	1.2924	1.2906	1.2917	1.2947	1.2996
5.4667	0.8738	0.9453	0.9752	0.9984	1.2565	1.2903	1.2923	1.2903	1.2915	1.2937	1.2990
5.5000	0.8825	0.9356	0.9755	0.9985	1.2461	1.2911	1.2929	1.2906	1.2914	1.2936	1.2986
5.5333	0.8764	0.9379	0.9753	0.9979	1.2319	1.2909	1.2921	1.2902	1.2909	1.2931	1.2981
5.5667	0.8690	0.9523	0.9756	0.9977	1.2162	1.2912	1.2917	1.2897	1.2904	1.2928	1.2973
5.6000	0.8845	0.9352	0.9757	0.9960	1.1991	1.2914	1.2919	1.2898	1.2901	1.2920	1.2970
5.6333	0.8799	0.9359	0.9761	0.9967	1.1816	1.2921	1.2924	1.2895	1.2901	1.2920	1.2965
5.6667	0.8870	0.9304	0.9763	0.9958	1.1631	1.2927	1.2925	1.2898	1.2897	1.2915	1.2961
5.7000	0.8836	0.9414	0.9760	0.9957	1.1444	1.2928	1.2934	1.2899	1.2894	1.2918	1.2959
5.7333	0.8816	0.9420	0.9765	0.9971	1.1219	1.2935	1.2941	1.2903	1.2900	1.2919	1.2958
5.7667	0.8773	0.9486	0.9761	0.9957	1.1077	1.2938	1.2946	1.2904	1.2898	1.2913	1.2952
5.8000	0.8755	0.9425	0.9764	0.9964	1.0968	1.2944	1.2953	1.2911	1.2895	1.2915	1.2953
5.8333	0.8801	0.9399	0.9759	0.9957	1.0862	1.2944	1.2955	1.2909	1.2899	1.2910	1.2951
5.8667	0.8794	0.9458	0.9755	0.9959	1.0786	1.2932	1.2960	1.2918	1.2901	1.2911	1.2942
5.9000	0.8834	0.9382	0.9754	0.9962	1.0778	1.2910	1.2970	1.2924	1.2907	1.2913	1.2950
5.9333	0.8784	0.9511	0.9749	0.9959	1.0702	1.2887	1.2972	1.2930	1.2909	1.2913	1.2946
5.9667	0.8742	0.9519	0.9744	0.9946	1.0663	1.2815	1.2974	1.2931	1.2910	1.2914	1.2944
6.0000	0.8867	0.9417	0.9736	0.9946	1.0639	1.2710	1.2976	1.2937	1.2915	1.2913	1.2943

## Appendix 2. Initial Reactor Temperature Profile Estimate

$z$  = dimensionless axial reactor length, [-]

$\theta(z,0)$  = dimensionless reactor temperature at axial position  $z$  and at time  $\sigma = 0.0$ , [-]

The initial temperature profile has been estimated using an equidistant grid of 501 points for the axial reactor length  $z$ .

$z$	$\theta(z,0)$	$z$	$\theta(z,0)$	$z$	$\theta(z,0)$	$z$	$\theta(z,0)$	$z$	$\theta(z,0)$
0.0000	0.9491	0.1100	0.9087	0.2200	0.9060	0.3300	0.9186	0.4400	0.9395
0.0020	0.9481	0.1120	0.9083	0.2220	0.9062	0.3320	0.9189	0.4420	0.9400
0.0040	0.9472	0.1140	0.9079	0.2240	0.9063	0.3340	0.9192	0.4440	0.9404
0.0060	0.9463	0.1160	0.9075	0.2260	0.9065	0.3360	0.9195	0.4460	0.9408
0.0080	0.9454	0.1180	0.9071	0.2280	0.9067	0.3380	0.9198	0.4480	0.9413
0.0100	0.9445	0.1200	0.9067	0.2300	0.9068	0.3400	0.9201	0.4500	0.9417
0.0120	0.9436	0.1220	0.9063	0.2320	0.9070	0.3420	0.9204	0.4520	0.9421
0.0140	0.9427	0.1240	0.9060	0.2340	0.9072	0.3440	0.9208	0.4540	0.9426
0.0160	0.9418	0.1260	0.9057	0.2360	0.9073	0.3460	0.9211	0.4560	0.9430
0.0180	0.9409	0.1280	0.9054	0.2380	0.9075	0.3480	0.9214	0.4580	0.9434
0.0200	0.9400	0.1300	0.9051	0.2400	0.9077	0.3500	0.9217	0.4600	0.9438
0.0220	0.9391	0.1320	0.9048	0.2420	0.9079	0.3520	0.9221	0.4620	0.9443
0.0240	0.9382	0.1340	0.9045	0.2440	0.9081	0.3540	0.9224	0.4640	0.9447
0.0260	0.9374	0.1360	0.9043	0.2460	0.9083	0.3560	0.9228	0.4660	0.9451
0.0280	0.9365	0.1380	0.9041	0.2480	0.9085	0.3580	0.9231	0.4680	0.9455
0.0300	0.9357	0.1400	0.9039	0.2500	0.9086	0.3600	0.9234	0.4700	0.9459
0.0320	0.9348	0.1420	0.9037	0.2520	0.9088	0.3620	0.9238	0.4720	0.9463
0.0340	0.9340	0.1440	0.9035	0.2540	0.9090	0.3640	0.9241	0.4740	0.9467
0.0360	0.9331	0.1460	0.9033	0.2560	0.9092	0.3660	0.9245	0.4760	0.9471
0.0380	0.9323	0.1480	0.9032	0.2580	0.9094	0.3680	0.9248	0.4780	0.9475
0.0400	0.9315	0.1500	0.9031	0.2600	0.9097	0.3700	0.9252	0.4800	0.9479
0.0420	0.9307	0.1520	0.9030	0.2620	0.9099	0.3720	0.9256	0.4820	0.9483
0.0440	0.9298	0.1540	0.9029	0.2640	0.9101	0.3740	0.9259	0.4840	0.9487
0.0460	0.9290	0.1560	0.9028	0.2660	0.9103	0.3760	0.9263	0.4860	0.9491
0.0480	0.9283	0.1580	0.9028	0.2680	0.9105	0.3780	0.9267	0.4880	0.9495
0.0500	0.9275	0.1600	0.9027	0.2700	0.9107	0.3800	0.9270	0.4900	0.9498
0.0520	0.9267	0.1620	0.9027	0.2720	0.9109	0.3820	0.9274	0.4920	0.9502
0.0540	0.9259	0.1640	0.9027	0.2740	0.9112	0.3840	0.9278	0.4940	0.9506
0.0560	0.9252	0.1660	0.9028	0.2760	0.9114	0.3860	0.9282	0.4960	0.9509
0.0580	0.9244	0.1680	0.9028	0.2780	0.9116	0.3880	0.9286	0.4980	0.9513
0.0600	0.9237	0.1700	0.9029	0.2800	0.9119	0.3900	0.9290	0.5000	0.9516
0.0620	0.9229	0.1720	0.9030	0.2820	0.9121	0.3920	0.9294	0.5020	0.9520
0.0640	0.9222	0.1740	0.9031	0.2840	0.9123	0.3940	0.9298	0.5040	0.9523
0.0660	0.9215	0.1760	0.9032	0.2860	0.9126	0.3960	0.9302	0.5060	0.9526
0.0680	0.9208	0.1780	0.9033	0.2880	0.9128	0.3980	0.9306	0.5080	0.9529
0.0700	0.9201	0.1800	0.9034	0.2900	0.9131	0.4000	0.9310	0.5100	0.9532
0.0720	0.9194	0.1820	0.9035	0.2920	0.9133	0.4020	0.9314	0.5120	0.9536
0.0740	0.9188	0.1840	0.9036	0.2940	0.9136	0.4040	0.9318	0.5140	0.9539
0.0760	0.9181	0.1860	0.9037	0.2960	0.9138	0.4060	0.9322	0.5160	0.9542
0.0780	0.9175	0.1880	0.9038	0.2980	0.9141	0.4080	0.9326	0.5180	0.9545
0.0800	0.9168	0.1900	0.9040	0.3000	0.9143	0.4100	0.9330	0.5200	0.9548
0.0820	0.9162	0.1920	0.9041	0.3020	0.9146	0.4120	0.9335	0.5220	0.9550
0.0840	0.9156	0.1940	0.9042	0.3040	0.9149	0.4140	0.9339	0.5240	0.9553
0.0860	0.9150	0.1960	0.9043	0.3060	0.9151	0.4160	0.9343	0.5260	0.9556
0.0880	0.9144	0.1980	0.9045	0.3080	0.9154	0.4180	0.9347	0.5280	0.9559
0.0900	0.9138	0.2000	0.9046	0.3100	0.9157	0.4200	0.9352	0.5300	0.9562
0.0920	0.9132	0.2020	0.9047	0.3120	0.9160	0.4220	0.9356	0.5320	0.9565
0.0940	0.9127	0.2040	0.9049	0.3140	0.9162	0.4240	0.9360	0.5340	0.9567
0.0960	0.9121	0.2060	0.9050	0.3160	0.9165	0.4260	0.9365	0.5360	0.9570
0.0980	0.9116	0.2080	0.9051	0.3180	0.9168	0.4280	0.9369	0.5380	0.9573
0.1000	0.9111	0.2100	0.9053	0.3200	0.9171	0.4300	0.9373	0.5400	0.9576
0.1020	0.9106	0.2120	0.9054	0.3220	0.9174	0.4320	0.9378	0.5420	0.9578
0.1040	0.9101	0.2140	0.9056	0.3240	0.9177	0.4340	0.9382	0.5440	0.9581
0.1060	0.9096	0.2160	0.9057	0.3260	0.9180	0.4360	0.9386	0.5460	0.9584
0.1080	0.9092	0.2180	0.9059	0.3280	0.9183	0.4380	0.9391	0.5480	0.9587

$z$	$\theta(z,0)$	$z$	$\theta(z,0)$	$z$	$\theta(z,0)$	$z$	$\theta(z,0)$	$z$	$\theta(z,0)$
0.5500	0.9589	0.6440	0.9767	0.7380	1.0006	0.8320	1.0232	0.9260	1.0291
0.5520	0.9592	0.6460	0.9771	0.7400	1.0012	0.8340	1.0234	0.9280	1.0292
0.5540	0.9595	0.6480	0.9776	0.7420	1.0018	0.8360	1.0237	0.9300	1.0292
0.5560	0.9598	0.6500	0.9781	0.7440	1.0024	0.8380	1.0239	0.9320	1.0292
0.5580	0.9601	0.6520	0.9785	0.7460	1.0030	0.8400	1.0242	0.9340	1.0293
0.5600	0.9604	0.6540	0.9790	0.7480	1.0036	0.8420	1.0244	0.9360	1.0293
0.5620	0.9607	0.6560	0.9795	0.7500	1.0042	0.8440	1.0246	0.9380	1.0293
0.5640	0.9609	0.6580	0.9799	0.7520	1.0047	0.8460	1.0248	0.9400	1.0293
0.5660	0.9612	0.6600	0.9804	0.7540	1.0053	0.8480	1.0250	0.9420	1.0293
0.5680	0.9615	0.6620	0.9809	0.7560	1.0059	0.8500	1.0252	0.9440	1.0293
0.5700	0.9618	0.6640	0.9814	0.7580	1.0065	0.8520	1.0254	0.9460	1.0293
0.5720	0.9622	0.6660	0.9819	0.7600	1.0071	0.8540	1.0256	0.9480	1.0293
0.5740	0.9625	0.6680	0.9823	0.7620	1.0077	0.8560	1.0257	0.9500	1.0293
0.5760	0.9628	0.6700	0.9828	0.7640	1.0082	0.8580	1.0259	0.9520	1.0293
0.5780	0.9631	0.6720	0.9833	0.7660	1.0088	0.8600	1.0261	0.9540	1.0293
0.5800	0.9634	0.6740	0.9838	0.7680	1.0094	0.8620	1.0262	0.9560	1.0293
0.5820	0.9638	0.6760	0.9843	0.7700	1.0099	0.8640	1.0264	0.9580	1.0292
0.5840	0.9641	0.6780	0.9848	0.7720	1.0105	0.8660	1.0265	0.9600	1.0292
0.5860	0.9645	0.6800	0.9852	0.7740	1.0110	0.8680	1.0267	0.9620	1.0292
0.5880	0.9648	0.6820	0.9857	0.7760	1.0116	0.8700	1.0268	0.9640	1.0291
0.5900	0.9652	0.6840	0.9862	0.7780	1.0121	0.8720	1.0269	0.9660	1.0291
0.5920	0.9656	0.6860	0.9867	0.7800	1.0127	0.8740	1.0270	0.9680	1.0291
0.5940	0.9659	0.6880	0.9872	0.7820	1.0132	0.8760	1.0272	0.9700	1.0290
0.5960	0.9663	0.6900	0.9877	0.7840	1.0137	0.8780	1.0273	0.9720	1.0289
0.5980	0.9667	0.6920	0.9882	0.7860	1.0142	0.8800	1.0274	0.9740	1.0289
0.6000	0.9671	0.6940	0.9886	0.7880	1.0147	0.8820	1.0275	0.9760	1.0288
0.6020	0.9675	0.6960	0.9891	0.7900	1.0152	0.8840	1.0276	0.9780	1.0287
0.6040	0.9679	0.6980	0.9896	0.7920	1.0157	0.8860	1.0277	0.9800	1.0287
0.6060	0.9683	0.7000	0.9901	0.7940	1.0162	0.8880	1.0278	0.9820	1.0286
0.6080	0.9687	0.7020	0.9906	0.7960	1.0167	0.8900	1.0279	0.9840	1.0285
0.6100	0.9691	0.7040	0.9911	0.7980	1.0171	0.8920	1.0280	0.9860	1.0284
0.6120	0.9696	0.7060	0.9916	0.8000	1.0176	0.8940	1.0281	0.9880	1.0283
0.6140	0.9700	0.7080	0.9922	0.8020	1.0180	0.8960	1.0282	0.9900	1.0282
0.6160	0.9704	0.7100	0.9927	0.8040	1.0184	0.8980	1.0283	0.9920	1.0281
0.6180	0.9708	0.7120	0.9932	0.8060	1.0188	0.9000	1.0283	0.9940	1.0280
0.6200	0.9713	0.7140	0.9938	0.8080	1.0192	0.9020	1.0284	0.9960	1.0279
0.6220	0.9717	0.7160	0.9943	0.8100	1.0196	0.9040	1.0285	0.9980	1.0278
0.6240	0.9721	0.7180	0.9949	0.8120	1.0200	0.9060	1.0286	1.0000	1.0276
0.6260	0.9726	0.7200	0.9954	0.8140	1.0204	0.9080	1.0286		
0.6280	0.9730	0.7220	0.9960	0.8160	1.0207	0.9100	1.0287		
0.6300	0.9735	0.7240	0.9966	0.8180	1.0211	0.9120	1.0288		
0.6320	0.9739	0.7260	0.9971	0.8200	1.0214	0.9140	1.0288		
0.6340	0.9744	0.7280	0.9977	0.8220	1.0217	0.9160	1.0289		
0.6360	0.9748	0.7300	0.9983	0.8240	1.0220	0.9180	1.0290		
0.6380	0.9753	0.7320	0.9989	0.8260	1.0223	0.9200	1.0290		
0.6400	0.9757	0.7340	0.9995	0.8280	1.0226	0.9220	1.0291		
0.6420	0.9762	0.7360	1.0000	0.8300	1.0229	0.9240	1.0291		