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TABLES FOR THE EVALUATION OF DECAY CURVES OF A CHEMICAL SPECIES UNDERGOING SIMULTANEOUS FIRST- AND SECOND-ORDER DECAY

by

Klaus H. Schmidt

Chemistry Division

December 1967

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TABLES FOR THE EVALUATION OF DECAY CURVES OF A CHEMICAL SPECIES UNDERGOING SIMULTANEOUS FIRST- AND SECOND-ORDER DECAY

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ABSTRACT

Tables have been computed to facilitate the determination of the first- and second-order components of the decay curve of a chemical species from two measured half-lives.

INTRODUCTION

In pulse-radiolysis studies,[1,2] the formation and decay of transient chemical species are directly observed on the oscilloscope. The oscilloscope traces are often used to calculate the rate constant for a first-* or second-order reaction of the chemical species under investigation.

For a pure first- or second-order reaction, the evaluation is usually carried out by plotting the logarithm or the reciprocal, respectively, of the concentration against time and measuring the slope of the resulting straight line. This procedure still works for a predominantly second-order decay with a small first-order component, or vice versa. One then observes a small deviation from the straight line at one end of the curve.

However, if the first- and second-order components are in the same order of magnitude, a more complicated analysis of the decay curves is required. To facilitate this procedure, the tables described in this paper have been calculated, using an IBM-1620 digital computer. They allow fast calculation of the first- and second-order rate constants from two half-lives and the corresponding initial concentrations, obtained either from one or two different decay curves.

*For the sake of brevity, we shall use the term "first-order reaction" for genuine first-order reactions as well as pseudo first-order reactions.

MATHEMATICAL METHOD

The analysis is based on the assumption that the specie R undergoes the reactions

$$R + R \xrightarrow{k_2} P; \tag{1}$$

and

$$R + S_i \xrightarrow{k_1^{(i)}} Q, \quad i = 1, \ldots, n, \tag{2}$$

where the S_i represent one or more scavengers, $k_1^{(i)}$ and k_2 are second-order rate constants, and P and Q are products with which R does not react.

The decay of R then follows the differential equation

$$\frac{d[R]}{dt} = -\left(\sum_{i=1}^{n} k_1^{(i)}[S_i]\right)[R] - 2k_2[R]^2, \tag{3}$$

or, in abbreviated form,

$$\frac{dc}{dt} = -ac - bc^2, \quad c = c_0 \text{ for } t = 0, \tag{4a}$$

c_0 being the initial concentration, and

$$c = [R], \tag{4b}$$

$$a = \sum_{i=1}^{n} k_1^{(i)}[S_i], \tag{4c}$$

and

$$b = 2k_2. \tag{4d}$$

By integration, we obtain

$$-\int_{c_0}^{c} \frac{dc}{ac + bc^2} = t. \tag{5}$$

The half-life $T_{1/2}$ can now be calculated by setting $c = c_0/2$:

$$T_{1/2} = \int_{c_0/2}^{c_0} \frac{dc}{c(a+bc)} = \frac{1}{a} \log \frac{bc_0 + 2a}{bc_0 + a}. \tag{6}$$

Let $T_{1/2}^{(1)}$ and $T_{1/2}^{(2)}$ be the half-lives obtained from two decay curves or two parts of the same decay curve with the initial concentrations $c_0^{(1)}$ and $c_0^{(2)}$, and let

$$q_1 = \frac{bc_0^{(1)}}{a} \tag{7a}$$

and

$$q_2 = \frac{bc_0^{(2)}}{a} \tag{7b}$$

be the ratios of second- to first-order reaction rates for the two concentrations. Then the ratio of the two half-lives is

$$f_t = \frac{T_{1/2}^{(1)}}{T_{1/2}^{(2)}} = \frac{\log \dfrac{q_1 + 2}{q_1 + 1}}{\log \dfrac{q_2 + 2}{q_2 + 1}}. \tag{8}$$

If we further define

$$f_c = \frac{c_0^{(2)}}{c_0^{(1)}} = \frac{q_2}{q_1} \tag{9}$$

and chose the numbering so that $f_c > 1$, we derive, from Eq. 8;

$$f_t = \frac{\log \dfrac{q_1 + 2}{q_1 + 1}}{\log \dfrac{f_c q_1 + 2}{f_c q_1 + 1}}. \tag{10}$$

For the selected value of f_c, we can now plot f_t against q_1. From this plot, q_1 can be determined for any measured value of f_t. Using Eqs. 6, 7b, and 9, we then obtain

$$a = \frac{\log \dfrac{q_1 + 2}{q_1 + 1}}{T_{1/2}^{(1)}}; \tag{11a}$$

$$q_2 = f_c q_1; \tag{11b}$$

$$bc_0^{(2)} = q_2 \frac{\log \frac{q_2 + 2}{q_2 + 1}}{T_{1/2}^{(2)}}. \tag{11c}$$

With

$$\phi(q_1) = \log \frac{q_1 + 2}{q_1 + 1} \tag{12a}$$

and

$$\Psi(q_2) = \frac{q_2}{2} \log \frac{q_2 + 2}{q_2 + 1}, \tag{12b}$$

we can write

$$a = \frac{\phi(q_1)}{T_{1/2}^{(1)}}; \tag{13a}$$

$$bc_0^{(2)} = \frac{2\Psi(q_2)}{T_{1/2}^{(2)}}. \tag{13b}$$

Here a is the first-order rate constant for the combination of all first-order reactions. The rate constant of the second-order reaction follows from Eqs. 13b and 4d and is

$$k_2 = \frac{\Psi(q_2)}{c_0^{(2)} T_{1/2}^{(2)}}. \tag{14}$$

If the measured quantity is the optical absorption of the solution, absorptions instead of concentrations can be used in Eq. 9 with a good approximation, if the initial absorption is

$$\alpha_0 = \frac{I_0 - I}{I_0} << 1.* \tag{15}$$

In this case,

$$c_0 = \frac{0.4343\alpha_0}{\epsilon x}, \tag{16}$$

*For $\alpha_0 < 0.1$, the relative error of f_c is less than 2%; for $\alpha_0 < 0.05$, it is less than 0.5%.

where ϵ is the molar extinction coefficient, and x is the optical path length in the solution. We then derive, from Eq. 14,

$$k_2 = 2.303 \frac{\epsilon x}{\alpha_0} \frac{\Psi(q_2)}{T_{1/2}^{(2)}}. \tag{17}$$

INSTRUCTIONS FOR USING THE TABLES

For technical reasons, the notation in the tables differs slightly from that in the text.

Notation in the text:	f_c	f_t	$\phi(q_1)$	$\Psi(q_2)$	q_1	q_1
Notation in the tables:	FC	FT	PHI	PSI	Q1	Q2

The procedure for using the tables is as follows:

1. Find two points on one or two decay curves corresponding to concentrations $c_0^{(1)}$ and $c_0^{(2)}$ with the ratio

$$f_c = \frac{c_0^{(2)}}{c_0^{(1)}} = 2,\ 2.5,\ 3,\ 4,\ 5,\ \text{or } 8.$$

2. Measure the half-lives $T_{1/2}^{(1)}$ and $T_{1/2}^{(2)}$, starting with the above points, and calculate

$$f_t = \frac{T_{1/2}^{(1)}}{T_{1/2}^{(2)}}.$$

3. Select the table for the chosen value f_c, and find the values $\phi(q_1)$ and $\Psi(q_2)$ that belong to the obtained value of f_t.

4. Using Eqs. 13a and 14 or 17, calculate the rate constants a and k_2.

The values q_1 and q_2 also listed in the tables give the ratios of second- to first-order reaction rate for the two concentrations $c_0^{(1)}$ and $c_0^{(2)}$. Values equal to or greater than 100 are printed as 99.999.

TABLES FOR EVALUATION OF DECAY CURVES

FC = 2.0

FT	PHI	PSI	Q1	Q2
1.005	.689	.004	.006	.013
1.010	.686	.009	.014	.028
1.015	.682	.014	.021	.042
1.020	.679	.018	.028	.056
1.025	.675	.023	.035	.071
1.030	.672	.028	.043	.086
1.035	.668	.032	.050	.100
1.040	.665	.037	.058	.116
1.045	.661	.041	.065	.131
1.050	.658	.046	.073	.146
1.055	.654	.050	.081	.162
1.060	.651	.054	.089	.178
1.065	.647	.059	.097	.194
1.070	.644	.063	.105	.210
1.075	.640	.067	.113	.226
1.080	.637	.071	.121	.243
1.085	.633	.075	.130	.260
1.090	.630	.080	.138	.277
1.095	.626	.084	.147	.294
1.100	.623	.088	.155	.311
1.105	.619	.092	.164	.329
1.110	.616	.096	.173	.346
1.115	.612	.100	.182	.364
1.120	.609	.104	.191	.383
1.125	.605	.108	.200	.401
1.130	.602	.112	.210	.420
1.135	.598	.115	.219	.439
1.140	.595	.119	.229	.458
1.145	.591	.123	.238	.477
1.150	.588	.127	.248	.497
1.155	.584	.130	.258	.517
1.160	.581	.134	.268	.537
1.165	.577	.138	.278	.557
1.170	.574	.141	.289	.578
1.175	.570	.145	.299	.599
1.180	.567	.149	.310	.620
1.185	.563	.152	.321	.642
1.190	.560	.156	.331	.663
1.195	.556	.159	.342	.685
1.200	.553	.163	.354	.708
1.205	.549	.166	.365	.730
1.210	.545	.170	.376	.753
1.215	.542	.173	.388	.776
1.220	.538	.176	.400	.800
1.225	.535	.180	.412	.824
1.230	.531	.183	.424	.848
1.235	.528	.186	.436	.872
1.240	.524	.190	.448	.897
1.245	.521	.193	.461	.923
1.250	.517	.196	.474	.948

FC = 2.0

FT	PHI	PSI	Q1	Q2
1.255	.514	.199	.487	.974
1.260	.510	.202	.500	1.000
1.265	.507	.205	.513	1.027
1.270	.503	.209	.527	1.054
1.275	.500	.212	.540	1.081
1.280	.496	.215	.554	1.109
1.285	.493	.218	.568	1.137
1.290	.489	.221	.583	1.166
1.295	.486	.224	.597	1.195
1.300	.482	.227	.612	1.225
1.305	.478	.230	.627	1.255
1.310	.475	.233	.642	1.285
1.315	.471	.236	.658	1.316
1.320	.468	.239	.673	1.347
1.325	.464	.241	.689	1.379
1.330	.461	.244	.705	1.411
1.335	.457	.247	.722	1.444
1.340	.454	.250	.738	1.477
1.345	.450	.253	.755	1.511
1.350	.447	.256	.772	1.545
1.355	.443	.258	.790	1.580
1.360	.440	.261	.808	1.616
1.365	.436	.264	.826	1.652
1.370	.433	.267	.844	1.688
1.375	.429	.269	.863	1.726
1.380	.426	.272	.881	1.763
1.385	.422	.275	.901	1.802
1.390	.419	.277	.920	1.841
1.395	.415	.280	.940	1.881
1.400	.412	.282	.960	1.921
1.405	.408	.285	.981	1.963
1.410	.405	.287	1.002	2.004
1.415	.401	.290	1.023	2.047
1.420	.398	.293	1.045	2.090
1.425	.394	.295	1.067	2.135
1.430	.391	.298	1.089	2.179
1.435	.387	.300	1.112	2.225
1.440	.383	.302	1.136	2.272
1.445	.380	.305	1.159	2.319
1.450	.376	.307	1.183	2.367
1.455	.373	.310	1.208	2.417
1.460	.369	.312	1.233	2.467
1.465	.366	.314	1.259	2.518
1.470	.362	.317	1.285	2.570
1.475	.359	.319	1.311	2.623
1.480	.355	.322	1.338	2.677
1.485	.352	.324	1.366	2.732
1.490	.348	.326	1.394	2.789
1.495	.345	.328	1.423	2.846
1.500	.341	.331	1.452	2.905

FC = 2.0

FT	PHI	PSI	Q1	Q2
1.51	.334	.335	1.513	3.026
1.52	.328	.340	1.576	3.152
1.53	.321	.344	1.641	3.283
1.54	.314	.348	1.710	3.420
1.55	.307	.353	1.781	3.563
1.56	.300	.357	1.856	3.713
1.57	.293	.361	1.935	3.870
1.58	.286	.365	2.017	4.035
1.59	.279	.369	2.104	4.208
1.60	.272	.373	2.194	4.389
1.61	.265	.377	2.290	4.580
1.62	.258	.381	2.390	4.781
1.63	.251	.385	2.496	4.993
1.64	.244	.389	2.608	5.216
1.65	.237	.392	2.726	5.453
1.66	.230	.396	2.852	5.704
1.67	.223	.400	2.984	5.969
1.68	.217	.403	3.126	6.252
1.69	.210	.407	3.276	6.553
1.70	.203	.410	3.437	6.874
1.71	.196	.414	3.608	7.217
1.72	.189	.417	3.792	7.585
1.73	.182	.421	3.990	7.981
1.74	.175	.424	4.203	8.407
1.75	.168	.427	4.433	8.867
1.76	.162	.431	4.682	9.365
1.77	.155	.434	4.954	9.908
1.78	.148	.437	5.249	10.499
1.79	.141	.440	5.573	11.147
1.80	.134	.444	5.930	11.860
1.81	.127	.447	6.324	12.648
1.82	.121	.450	6.762	13.524
1.83	.114	.453	7.251	14.503
1.84	.107	.456	7.802	15.604
1.85	.100	.459	8.426	16.853
1.86	.094	.462	9.140	18.280
1.87	.087	.465	9.963	19.926
1.88	.080	.467	10.924	21.849
1.89	.073	.470	12.060	24.120
1.90	.067	.473	13.423	26.846
1.91	.060	.476	15.089	30.178
1.92	.053	.479	17.171	34.343
1.93	.046	.481	19.850	39.700
1.94	.040	.484	23.420	46.841
1.95	.033	.487	28.419	56.838
1.96	.026	.489	35.923	71.847
1.97	.020	.492	48.416	96.833
1.98	.013	.494	73.430	99.999
1.99	.006	.497	99.999	99.999
2.00	0.000	.500	99.999	99.999

FC = 2.5

FT	PHI	PSI	Q1	Q2
1.01	.688	.007	.009	.023
1.02	.683	.015	.018	.046
1.03	.679	.023	.028	.070
1.04	.674	.030	.038	.095
1.05	.669	.038	.048	.120
1.06	.665	.045	.058	.145
1.07	.660	.052	.068	.170
1.08	.656	.059	.078	.196
1.09	.651	.066	.089	.222
1.10	.646	.073	.099	.249
1.11	.642	.080	.110	.276
1.12	.637	.086	.121	.304
1.13	.632	.093	.133	.332
1.14	.627	.099	.144	.361
1.15	.623	.105	.155	.389
1.16	.618	.111	.167	.419
1.17	.613	.117	.179	.449
1.18	.609	.123	.191	.479
1.19	.604	.129	.204	.510
1.20	.599	.135	.216	.542
1.21	.595	.141	.229	.573
1.22	.590	.146	.242	.606
1.23	.585	.152	.255	.639
1.24	.581	.157	.269	.673
1.25	.576	.163	.282	.707
1.26	.571	.168	.296	.741
1.27	.566	.173	.310	.777
1.28	.562	.178	.325	.813
1.29	.557	.183	.339	.849
1.30	.552	.188	.354	.886
1.31	.548	.193	.369	.924
1.32	.543	.198	.385	.963
1.33	.538	.203	.401	1.002
1.34	.533	.207	.417	1.042
1.35	.529	.212	.433	1.083
1.36	.524	.216	.449	1.124
1.37	.519	.221	.466	1.166
1.38	.515	.225	.483	1.209
1.39	.510	.230	.501	1.253
1.40	.505	.234	.519	1.298
1.41	.501	.238	.537	1.343
1.42	.496	.242	.556	1.390
1.43	.491	.247	.574	1.437
1.44	.486	.251	.594	1.485
1.45	.482	.255	.613	1.534
1.46	.477	.259	.633	1.584
1.47	.472	.263	.654	1.636
1.48	.468	.266	.675	1.688
1.49	.463	.270	.696	1.741
1.50	.458	.274	.718	1.795

FC = 2.5

FT	PHI	PSI	Q1	Q2
1.52	.449	.281	.763	1.907
1.54	.439	.289	.809	2.024
1.56	.430	.296	.858	2.146
1.58	.421	.303	.909	2.274
1.60	.411	.309	.962	2.407
1.62	.402	.316	1.018	2.546
1.64	.393	.322	1.077	2.692
1.66	.383	.328	1.138	2.846
1.68	.374	.334	1.202	3.006
1.70	.364	.340	1.270	3.175
1.72	.355	.346	1.341	3.353
1.74	.346	.352	1.416	3.540
1.76	.336	.357	1.495	3.738
1.78	.327	.363	1.578	3.947
1.80	.318	.368	1.667	4.168
1.82	.309	.373	1.760	4.401
1.84	.299	.378	1.860	4.650
1.86	.290	.383	1.965	4.914
1.88	.281	.388	2.078	5.195
1.90	.272	.393	2.198	5.495
1.92	.262	.398	2.326	5.816
1.94	.253	.402	2.464	6.160
1.96	.244	.407	2.612	6.530
1.98	.235	.411	2.771	6.928
2.00	.226	.415	2.943	7.358
2.02	.216	.419	3.130	7.825
2.04	.207	.424	3.333	8.332
2.06	.198	.428	3.554	8.886
2.08	.189	.432	3.797	9.492
2.10	.180	.435	4.064	10.160
2.12	.171	.439	4.359	10.898
2.14	.161	.443	4.687	11.718
2.16	.152	.447	5.054	12.635
2.18	.143	.450	5.466	13.667
2.20	.134	.454	5.934	14.836
2.22	.125	.457	6.469	16.173
2.24	.116	.461	7.086	17.716
2.26	.107	.464	7.807	19.517
2.28	.098	.467	8.658	21.646
2.30	.089	.470	9.680	24.201
2.32	.080	.474	10.929	27.324
2.34	.071	.477	12.491	31.228
2.36	.062	.480	14.498	36.246
2.38	.053	.483	17.176	42.941
2.40	.044	.486	20.924	52.310
2.42	.035	.488	26.548	66.371
2.44	.026	.491	35.916	89.791
2.46	.017	.494	54.641	99.999
2.48	.008	.497	99.999	99.999
2.50	0.000	.500	99.999	99.999

FC = 3.0

FT	PHI	PSI	Q1	Q2
1.02	.686	.014	.014	.042
1.04	.679	.027	.028	.085
1.06	.672	.040	.043	.129
1.08	.665	.053	.058	.174
1.10	.658	.065	.073	.220
1.12	.651	.077	.089	.267
1.14	.644	.089	.105	.316
1.16	.637	.100	.121	.365
1.18	.630	.111	.138	.416
1.20	.623	.121	.156	.468
1.22	.616	.131	.173	.521
1.24	.609	.141	.192	.576
1.26	.602	.151	.210	.632
1.28	.595	.160	.229	.689
1.30	.587	.169	.249	.748
1.32	.580	.177	.269	.808
1.34	.573	.186	.290	.870
1.36	.566	.194	.311	.934
1.38	.559	.202	.333	.999
1.40	.552	.210	.355	1.066
1.42	.545	.217	.378	1.134
1.44	.538	.225	.401	1.205
1.46	.531	.232	.425	1.277
1.48	.524	.239	.450	1.352
1.50	.517	.246	.476	1.428
1.52	.510	.252	.502	1.507
1.54	.503	.259	.529	1.588
1.56	.496	.265	.557	1.671
1.58	.488	.271	.585	1.756
1.60	.481	.277	.615	1.845
1.62	.474	.283	.645	1.935
1.64	.467	.289	.676	2.029
1.66	.460	.295	.708	2.125
1.68	.453	.300	.741	2.225
1.70	.446	.305	.776	2.328
1.72	.439	.311	.811	2.433
1.74	.432	.316	.847	2.543
1.76	.425	.321	.885	2.656
1.78	.418	.325	.924	2.772
1.80	.411	.330	.964	2.893
1.82	.404	.335	1.006	3.018
1.84	.397	.339	1.049	3.147
1.86	.390	.344	1.093	3.281
1.88	.383	.348	1.140	3.420
1.90	.376	.353	1.188	3.564
1.92	.369	.357	1.238	3.714
1.94	.362	.361	1.289	3.869
1.96	.355	.365	1.343	4.030
1.98	.348	.369	1.399	4.197
2.00	.341	.373	1.457	4.372

FC = 3.0

FT	PHI	PSI	Q1	Q2
2.02	.334	.376	1.517	4.553
2.04	.327	.380	1.581	4.743
2.06	.320	.384	1.646	4.940
2.08	.313	.387	1.715	5.146
2.10	.306	.391	1.787	5.361
2.12	.299	.394	1.862	5.587
2.14	.292	.398	1.941	5.823
2.16	.285	.401	2.023	6.070
2.18	.278	.404	2.109	6.329
2.20	.271	.407	2.200	6.601
2.22	.264	.411	2.296	6.888
2.24	.258	.414	2.396	7.190
2.26	.251	.417	2.502	7.508
2.28	.244	.420	2.614	7.843
2.30	.237	.423	2.733	8.199
2.32	.230	.425	2.858	8.575
2.34	.223	.428	2.991	8.974
2.36	.216	.431	3.132	9.398
2.38	.209	.434	3.283	9.850
2.40	.202	.436	3.444	10.332
2.42	.196	.439	3.615	10.847
2.44	.189	.442	3.800	11.400
2.46	.182	.444	3.997	11.993
2.48	.175	.447	4.210	12.632
2.50	.168	.449	4.440	13.322
2.52	.161	.451	4.690	14.071
2.54	.155	.454	4.961	14.884
2.56	.148	.456	5.257	15.771
2.58	.141	.459	5.581	16.743
2.60	.134	.461	5.937	17.813
2.62	.127	.463	6.331	18.995
2.64	.121	.465	6.770	20.310
2.66	.114	.467	7.259	21.778
2.68	.107	.469	7.810	23.431
2.70	.100	.472	8.434	25.304
2.72	.093	.474	9.148	27.445
2.74	.087	.476	9.971	29.915
2.76	.080	.478	10.933	32.799
2.78	.073	.480	12.068	36.205
2.80	.066	.482	13.431	40.294
2.82	.060	.483	15.097	45.291
2.84	.053	.485	17.180	51.540
2.86	.046	.487	19.858	59.576
2.88	.040	.489	23.429	70.287
2.90	.033	.491	28.423	85.269
2.92	.026	.493	35.933	99.999
2.94	.020	.494	48.414	99.999
2.96	.013	.496	73.351	99.999
2.98	.006	.498	99.999	99.999
3.00	0.000	.500	99.999	99.999

FC = 4.0

FT	PHI	PSI	Q1	Q2
1.02	.688	.012	.009	.037
1.04	.683	.024	.018	.075
1.06	.679	.036	.028	.113
1.08	.674	.047	.038	.152
1.10	.669	.058	.048	.192
1.12	.665	.069	.058	.232
1.14	.660	.079	.068	.273
1.16	.655	.089	.078	.315
1.18	.651	.098	.089	.357
1.20	.646	.107	.100	.400
1.22	.641	.116	.111	.444
1.24	.637	.125	.122	.488
1.26	.632	.133	.133	.533
1.28	.627	.142	.144	.579
1.30	.623	.150	.156	.626
1.32	.618	.157	.168	.673
1.34	.613	.165	.180	.721
1.36	.608	.172	.192	.770
1.38	.604	.179	.205	.820
1.40	.599	.186	.217	.870
1.42	.594	.193	.230	.922
1.44	.590	.199	.243	.974
1.46	.585	.205	.256	1.027
1.48	.580	.212	.270	1.081
1.50	.575	.218	.284	1.136
1.52	.571	.224	.298	1.192
1.54	.566	.229	.312	1.249
1.56	.561	.235	.326	1.307
1.58	.557	.240	.341	1.365
1.60	.552	.246	.356	1.425
1.62	.547	.251	.371	1.486
1.64	.542	.256	.387	1.548
1.66	.538	.261	.402	1.611
1.68	.533	.266	.419	1.676
1.70	.528	.270	.435	1.741
1.72	.523	.275	.452	1.808
1.74	.519	.279	.468	1.875
1.76	.514	.284	.486	1.944
1.78	.509	.288	.503	2.015
1.80	.505	.292	.521	2.087
1.82	.500	.296	.540	2.160
1.84	.495	.300	.558	2.234
1.86	.490	.304	.577	2.310
1.88	.486	.308	.597	2.388
1.90	.481	.312	.616	2.466
1.92	.476	.316	.636	2.547
1.94	.472	.319	.657	2.629
1.96	.467	.323	.678	2.713
1.98	.462	.327	.699	2.798
2.00	.457	.330	.721	2.886

FC = 4.0

FT	PHI	PSI	Q1	Q2
2.02	.453	.333	.743	2.975
2.04	.448	.337	.766	3.065
2.06	.443	.340	.789	3.158
2.08	.439	.343	.813	3.253
2.10	.434	.346	.837	3.350
2.12	.429	.349	.862	3.449
2.14	.425	.352	.887	3.550
2.16	.420	.355	.913	3.653
2.18	.415	.358	.939	3.759
2.20	.411	.361	.966	3.867
2.22	.406	.364	.994	3.978
2.24	.401	.366	1.022	4.091
2.26	.397	.369	1.051	4.207
2.28	.392	.372	1.081	4.325
2.30	.387	.374	1.111	4.446
2.32	.383	.377	1.142	4.571
2.34	.378	.379	1.174	4.698
2.36	.373	.382	1.207	4.828
2.38	.369	.384	1.240	4.962
2.40	.364	.387	1.274	5.099
2.42	.359	.389	1.310	5.240
2.44	.355	.391	1.346	5.384
2.46	.350	.394	1.383	5.532
2.48	.345	.396	1.421	5.685
2.50	.341	.398	1.460	5.841
2.52	.336	.400	1.500	6.001
2.54	.331	.402	1.541	6.166
2.56	.327	.404	1.584	6.336
2.58	.322	.406	1.627	6.510
2.60	.317	.408	1.672	6.689
2.62	.313	.410	1.718	6.874
2.64	.308	.412	1.766	7.064
2.66	.303	.414	1.815	7.260
2.68	.299	.416	1.865	7.462
2.70	.294	.418	1.917	7.670
2.72	.290	.420	1.971	7.885
2.74	.285	.422	2.026	8.106
2.76	.280	.424	2.083	8.335
2.78	.276	.425	2.142	8.571
2.80	.271	.427	2.203	8.815
2.82	.267	.429	2.267	9.068
2.84	.262	.431	2.332	9.329
2.86	.257	.432	2.400	9.600
2.88	.253	.434	2.470	9.880
2.90	.248	.436	2.542	10.171
2.92	.244	.437	2.618	10.472
2.94	.239	.439	2.696	10.785
2.96	.234	.440	2.777	11.110
2.98	.230	.442	2.862	11.448
3.00	.225	.443	2.949	11.799

FC = 4.0

FT	PHI	PSI	Q1	Q2
3.02	.221	.445	3.041	12.165
3.04	.216	.446	3.136	12.546
3.06	.211	.448	3.235	12.943
3.08	.207	.449	3.339	13.358
3.10	.202	.451	3.447	13.791
3.12	.198	.452	3.561	14.244
3.14	.193	.453	3.679	14.718
3.16	.189	.455	3.803	15.215
3.18	.184	.456	3.934	15.736
3.20	.179	.457	4.070	16.283
3.22	.175	.459	4.214	16.858
3.24	.170	.460	4.366	17.464
3.26	.166	.461	4.525	18.103
3.28	.161	.463	4.694	18.777
3.30	.157	.464	4.872	19.490
3.32	.152	.465	5.061	20.244
3.34	.148	.466	5.261	21.045
3.36	.143	.468	5.473	21.895
3.38	.139	.469	5.700	22.801
3.40	.134	.470	5.941	23.767
3.42	.130	.471	6.200	24.800
3.44	.125	.472	6.476	25.907
3.46	.121	.473	6.774	27.096
3.48	.116	.474	7.094	28.376
3.50	.111	.476	7.440	29.760
3.52	.107	.477	7.814	31.258
3.54	.102	.478	8.221	32.887
3.56	.098	.479	8.666	34.664
3.58	.093	.480	9.152	36.610
3.60	.089	.481	9.687	38.751
3.62	.084	.482	10.279	41.118
3.64	.080	.483	10.937	43.748
3.66	.075	.484	11.671	46.687
3.68	.071	.485	12.498	49.995
3.70	.066	.486	13.435	53.742
3.72	.062	.487	14.507	58.028
3.74	.058	.488	15.743	62.972
3.76	.053	.489	17.184	68.738
3.78	.049	.490	18.887	75.550
3.80	.044	.491	20.932	83.731
3.82	.040	.492	23.431	93.725
3.84	.035	.493	26.555	99.999
3.86	.031	.493	30.574	99.999
3.88	.026	.494	35.928	99.999
3.90	.022	.495	43.413	99.999
3.92	.017	.496	54.651	99.999
3.94	.013	.497	73.432	99.999
3.96	.008	.498	99.999	99.999
3.98	.004	.499	99.999	99.999
4.00	0.000	.500	99.999	99.999

FC = 5.0

FT	PHI	PSI	Q1	Q2
1.02	.689	.011	.006	.034
1.04	.686	.023	.014	.070
1.06	.682	.034	.021	.105
1.08	.679	.044	.028	.142
1.10	.675	.054	.035	.178
1.12	.672	.064	.043	.215
1.14	.668	.074	.050	.253
1.16	.665	.083	.058	.291
1.18	.661	.092	.065	.329
1.20	.658	.101	.073	.368
1.22	.654	.109	.081	.407
1.24	.651	.117	.089	.447
1.26	.647	.125	.097	.488
1.28	.644	.133	.105	.528
1.30	.640	.140	.114	.570
1.32	.637	.147	.122	.612
1.34	.633	.154	.130	.654
1.36	.630	.161	.139	.697
1.38	.626	.168	.148	.740
1.40	.622	.174	.156	.784
1.42	.619	.180	.165	.828
1.44	.615	.186	.174	.873
1.46	.612	.192	.183	.919
1.48	.608	.198	.193	.965
1.50	.605	.204	.202	1.011
1.52	.601	.209	.211	1.059
1.54	.598	.214	.221	1.106
1.56	.594	.220	.231	1.155
1.58	.591	.225	.240	1.204
1.60	.587	.230	.250	1.253
1.62	.583	.235	.260	1.304
1.64	.580	.239	.270	1.354
1.66	.576	.244	.281	1.406
1.68	.573	.248	.291	1.458
1.70	.569	.253	.302	1.511
1.72	.566	.257	.313	1.565
1.74	.562	.261	.323	1.619
1.76	.559	.265	.334	1.674
1.78	.555	.269	.345	1.729
1.80	.552	.273	.357	1.786
1.82	.548	.277	.368	1.843
1.84	.544	.281	.380	1.901
1.86	.541	.285	.391	1.959
1.88	.537	.288	.403	2.019
1.90	.534	.292	.415	2.079
1.92	.530	.295	.428	2.140
1.94	.527	.299	.440	2.202
1.96	.523	.302	.452	2.264
1.98	.520	.305	.465	2.328
2.00	.516	.309	.478	2.392

FC = 5.0

FT	PHI	PSI	Q1	Q2
2.02	.513	.312	.491	2.458
2.04	.509	.315	.504	2.524
2.06	.505	.318	.518	2.591
2.08	.502	.321	.531	2.659
2.10	.498	.324	.545	2.729
2.12	.495	.327	.559	2.799
2.14	.491	.329	.574	2.870
2.16	.488	.332	.588	2.942
2.18	.484	.335	.603	3.015
2.20	.481	.337	.617	3.089
2.22	.477	.340	.633	3.165
2.24	.474	.343	.648	3.241
2.26	.470	.345	.663	3.319
2.28	.467	.348	.679	3.398
2.30	.463	.350	.695	3.478
2.32	.460	.352	.711	3.559
2.34	.456	.355	.728	3.641
2.36	.452	.357	.745	3.725
2.38	.449	.359	.762	3.810
2.40	.445	.362	.779	3.897
2.42	.442	.364	.797	3.985
2.44	.438	.366	.814	4.074
2.46	.435	.368	.832	4.164
2.48	.431	.370	.851	4.256
2.50	.428	.372	.870	4.350
2.52	.424	.374	.889	4.445
2.54	.421	.376	.908	4.542
2.56	.417	.378	.928	4.640
2.58	.414	.380	.948	4.740
2.60	.410	.382	.968	4.842
2.62	.407	.384	.989	4.945
2.64	.403	.386	1.010	5.051
2.66	.400	.388	1.031	5.158
2.68	.396	.389	1.053	5.267
2.70	.393	.391	1.075	5.377
2.72	.389	.393	1.098	5.490
2.74	.386	.395	1.121	5.605
2.76	.382	.396	1.144	5.722
2.78	.379	.398	1.168	5.841
2.80	.375	.400	1.192	5.962
2.82	.372	.401	1.217	6.086
2.84	.368	.403	1.242	6.212
2.86	.365	.404	1.268	6.340
2.88	.361	.406	1.294	6.471
2.90	.358	.407	1.320	6.604
2.92	.354	.409	1.348	6.740
2.94	.351	.410	1.375	6.878
2.96	.347	.412	1.404	7.020
2.98	.344	.413	1.432	7.164
3.00	.340	.415	1.462	7.311

FC = 5.0

FT	PHI	PSI	Q1	Q2
3.02	.337	.416	1.492	7.461
3.04	.333	.418	1.522	7.614
3.06	.330	.419	1.554	7.770
3.08	.326	.420	1.585	7.929
3.10	.323	.422	1.618	8.092
3.12	.319	.423	1.651	8.259
3.14	.316	.424	1.685	8.429
3.16	.313	.426	1.720	8.603
3.18	.309	.427	1.756	8.780
3.20	.306	.428	1.792	8.962
3.22	.302	.429	1.829	9.148
3.24	.299	.431	1.867	9.338
3.26	.295	.432	1.906	9.532
3.28	.292	.433	1.946	9.731
3.30	.288	.434	1.987	9.935
3.32	.285	.435	2.028	10.143
3.34	.281	.437	2.071	10.357
3.36	.278	.438	2.115	10.576
3.38	.274	.439	2.160	10.800
3.40	.271	.440	2.206	11.030
3.42	.268	.441	2.253	11.266
3.44	.264	.442	2.301	11.508
3.46	.261	.443	2.351	11.756
3.48	.257	.444	2.402	12.011
3.50	.254	.445	2.454	12.273
3.52	.250	.446	2.508	12.542
3.54	.247	.447	2.563	12.818
3.56	.243	.448	2.620	13.102
3.58	.240	.449	2.678	13.394
3.60	.237	.450	2.738	13.694
3.62	.233	.451	2.800	14.003
3.64	.230	.452	2.864	14.321
3.66	.226	.453	2.929	14.649
3.68	.223	.454	2.997	14.987
3.70	.219	.455	3.067	15.335
3.72	.216	.456	3.138	15.694
3.74	.212	.457	3.213	16.065
3.76	.209	.458	3.289	16.447
3.78	.206	.459	3.368	16.842
3.80	.202	.460	3.450	17.251
3.82	.199	.460	3.534	17.673
3.84	.195	.461	3.622	18.110
3.86	.192	.462	3.712	18.562
3.88	.189	.463	3.806	19.031
3.90	.185	.464	3.903	19.516
3.92	.182	.465	4.004	20.020
3.94	.178	.466	4.108	20.542
3.96	.175	.466	4.217	21.085
3.98	.171	.467	4.329	21.649
4.00	.168	.468	4.447	22.236

FC = 5.0

FT	PHI	PSI	Q1	Q2
4.02	.165	.469	4.569	22.847
4.04	.161	.470	4.696	23.483
4.06	.158	.470	4.829	24.147
4.08	.154	.471	4.967	24.839
4.10	.151	.472	5.112	25.562
4.12	.148	.473	5.263	26.319
4.14	.144	.473	5.422	27.110
4.16	.141	.474	5.587	27.939
4.18	.137	.475	5.761	28.809
4.20	.134	.476	5.944	29.722
4.22	.131	.476	6.136	30.682
4.24	.127	.477	6.338	31.693
4.26	.124	.478	6.551	32.758
4.28	.120	.478	6.776	33.883
4.30	.117	.479	7.014	35.072
4.32	.114	.480	7.266	36.331
4.34	.110	.480	7.533	37.667
4.36	.107	.481	7.817	39.086
4.38	.104	.482	8.119	40.596
4.40	.100	.482	8.441	42.208
4.42	.097	.483	8.786	43.931
4.44	.093	.484	9.155	45.776
4.46	.090	.484	9.551	47.758
4.48	.087	.485	9.978	49.894
4.50	.083	.486	10.439	52.199
4.52	.080	.486	10.939	54.698
4.54	.077	.487	11.483	57.416
4.56	.073	.487	12.075	60.379
4.58	.070	.488	12.724	63.623
4.60	.066	.489	13.438	67.190
4.62	.063	.489	14.226	71.134
4.64	.060	.490	15.103	75.519
4.66	.056	.490	16.085	80.427
4.68	.053	.491	17.186	85.931
4.70	.050	.491	18.437	92.186
4.72	.046	.492	19.863	99.316
4.74	.043	.493	21.514	99.999
4.76	.040	.493	23.434	99.999
4.78	.036	.494	25.703	99.999
4.80	.033	.494	28.433	99.999
4.82	.030	.495	31.757	99.999
4.84	.026	.495	35.935	99.999
4.86	.023	.496	41.283	99.999
4.88	.020	.496	48.439	99.999
4.90	.016	.497	58.385	99.999
4.92	.013	.497	73.443	99.999
4.94	.010	.498	98.300	99.999
4.96	.006	.498	99.999	99.999
4.98	.003	.499	99.999	99.999
5.00	0.000	.500	99.999	99.999

FC = 8.0

FT	PHI	PSI	Q1	Q2
1.02	.691	.010	.003	.031
1.04	.689	.021	.007	.063
1.06	.687	.031	.012	.096
1.08	.685	.040	.016	.128
1.10	.683	.050	.020	.161
1.12	.681	.059	.024	.194
1.14	.679	.067	.028	.227
1.16	.677	.076	.032	.261
1.18	.675	.084	.036	.295
1.20	.673	.092	.041	.329
1.22	.671	.099	.045	.363
1.24	.669	.107	.049	.397
1.26	.667	.114	.054	.432
1.28	.665	.121	.058	.467
1.30	.663	.128	.062	.502
1.32	.661	.134	.067	.538
1.34	.659	.141	.071	.573
1.36	.657	.147	.076	.609
1.38	.655	.153	.080	.646
1.40	.653	.159	.085	.682
1.42	.651	.164	.089	.719
1.44	.649	.170	.094	.756
1.46	.646	.175	.099	.793
1.48	.644	.181	.103	.830
1.50	.642	.186	.108	.868
1.52	.640	.191	.113	.906
1.54	.638	.196	.118	.944
1.56	.636	.200	.122	.983
1.58	.634	.205	.127	1.022
1.60	.632	.209	.132	1.061
1.62	.630	.214	.137	1.100
1.64	.628	.218	.142	1.140
1.66	.626	.222	.147	1.180
1.68	.624	.226	.152	1.220
1.70	.622	.230	.157	1.260
1.72	.620	.234	.162	1.301
1.74	.618	.238	.167	1.342
1.76	.616	.242	.172	1.383
1.78	.614	.246	.178	1.425
1.80	.612	.249	.183	1.467
1.82	.610	.253	.188	1.509
1.84	.608	.256	.193	1.551
1.86	.606	.259	.199	1.594
1.88	.604	.263	.204	1.637
1.90	.602	.266	.210	1.680
1.92	.600	.269	.215	1.724
1.94	.598	.272	.221	1.768
1.96	.596	.275	.226	1.812
1.98	.594	.278	.232	1.857
2.00	.592	.281	.237	1.902

FC = 8.0

FT	PHI	PSI	Q1	Q2
2.02	.590	.284	.243	1.947
2.04	.588	.287	.249	1.992
2.06	.586	.289	.254	2.038
2.08	.584	.292	.260	2.084
2.10	.582	.295	.266	2.131
2.12	.579	.297	.272	2.178
2.14	.577	.300	.278	2.225
2.16	.575	.302	.284	2.272
2.18	.573	.305	.290	2.320
2.20	.571	.307	.296	2.368
2.22	.569	.310	.302	2.417
2.24	.567	.312	.308	2.466
2.26	.565	.314	.314	2.515
2.28	.563	.317	.320	2.565
2.30	.561	.319	.326	2.615
2.32	.559	.321	.333	2.665
2.34	.557	.323	.339	2.716
2.36	.555	.325	.345	2.767
2.38	.553	.327	.352	2.818
2.40	.551	.329	.358	2.870
2.42	.549	.331	.365	2.922
2.44	.547	.333	.371	2.975
2.46	.545	.335	.378	3.028
2.48	.543	.337	.385	3.081
2.50	.541	.339	.391	3.135
2.52	.539	.341	.398	3.189
2.54	.537	.343	.405	3.244
2.56	.535	.344	.412	3.299
2.58	.533	.346	.419	3.355
2.60	.531	.348	.426	3.411
2.62	.529	.350	.433	3.467
2.64	.527	.351	.440	3.524
2.66	.525	.353	.447	3.581
2.68	.523	.355	.454	3.639
2.70	.521	.356	.462	3.697
2.72	.519	.358	.469	3.755
2.74	.517	.359	.476	3.814
2.76	.515	.361	.484	3.874
2.78	.513	.363	.491	3.934
2.80	.511	.364	.499	3.994
2.82	.508	.365	.506	4.055
2.84	.506	.367	.514	4.116
2.86	.504	.368	.522	4.178
2.88	.502	.370	.530	4.241
2.90	.500	.371	.538	4.304
2.92	.498	.373	.545	4.367
2.94	.496	.374	.553	4.431
2.96	.494	.375	.561	4.495
2.98	.492	.377	.570	4.560
3.00	.490	.378	.578	4.626

FC = 8.0

FT	PHI	PSI	Q1	Q2
3.05	.485	.381	.599	4.792
3.10	.480	.384	.620	4.961
3.15	.475	.387	.641	5.135
3.20	.470	.390	.664	5.312
3.25	.465	.393	.686	5.492
3.30	.460	.396	.709	5.677
3.35	.455	.398	.733	5.865
3.40	.450	.401	.757	6.058
3.45	.445	.403	.782	6.256
3.50	.440	.406	.807	6.457
3.55	.435	.408	.832	6.663
3.60	.430	.410	.859	6.874
3.65	.425	.413	.886	7.090
3.70	.420	.415	.914	7.312
3.75	.415	.417	.942	7.538
3.80	.410	.419	.971	7.770
3.85	.405	.421	1.000	8.007
3.90	.400	.423	1.031	8.251
3.95	.395	.425	1.062	8.500
4.00	.390	.427	1.094	8.756
4.05	.385	.429	1.127	9.019
4.10	.380	.430	1.161	9.288
4.15	.375	.432	1.195	9.564
4.20	.370	.434	1.231	9.848
4.25	.365	.435	1.267	10.139
4.30	.360	.437	1.304	10.439
4.35	.355	.439	1.343	10.746
4.40	.350	.440	1.382	11.063
4.45	.345	.442	1.423	11.388
4.50	.340	.443	1.465	11.723
4.55	.335	.444	1.508	12.067
4.60	.330	.446	1.552	12.422
4.65	.325	.447	1.598	12.787
4.70	.320	.449	1.645	13.164
4.75	.315	.450	1.694	13.552
4.80	.310	.451	1.744	13.953
4.85	.305	.452	1.795	14.366
4.90	.300	.454	1.849	14.793
4.95	.295	.455	1.904	15.234
5.00	.290	.456	1.961	15.690
5.05	.286	.457	2.020	16.161
5.10	.281	.458	2.081	16.649
5.15	.276	.459	2.144	17.153
5.20	.271	.460	2.209	17.677
5.25	.266	.462	2.277	18.219
5.30	.261	.463	2.347	18.781
5.35	.256	.464	2.420	19.365
5.40	.251	.465	2.496	19.971
5.45	.246	.466	2.575	20.601
5.50	.241	.467	2.657	21.257

FC = 8.0

FT	PHI	PSI	Q1	Q2
5.55	.236	.468	2.742	21.940
5.60	.231	.469	2.831	22.651
5.65	.227	.469	2.924	23.392
5.70	.222	.470	3.020	24.166
5.75	.217	.471	3.121	24.974
5.80	.212	.472	3.227	25.819
5.85	.207	.473	3.338	26.704
5.90	.202	.474	3.453	27.631
5.95	.197	.475	3.575	28.603
6.00	.192	.475	3.703	29.625
6.05	.187	.476	3.837	30.699
6.10	.183	.477	3.978	31.829
6.15	.178	.478	4.127	33.020
6.20	.173	.479	4.284	34.278
6.25	.168	.479	4.451	35.608
6.30	.163	.480	4.627	37.017
6.35	.158	.481	4.813	38.511
6.40	.153	.481	5.012	40.099
6.45	.149	.482	5.223	41.789
6.50	.144	.483	5.449	43.593
6.55	.139	.484	5.690	45.520
6.60	.134	.484	5.948	47.586
6.65	.129	.485	6.225	49.804
6.70	.124	.486	6.524	52.194
6.75	.119	.486	6.847	54.776
6.80	.115	.487	7.196	57.574
6.85	.110	.487	7.576	60.614
6.90	.105	.488	7.991	63.929
6.95	.100	.489	8.445	67.562
7.00	.095	.489	8.944	71.559
7.05	.090	.490	9.496	75.975
7.10	.086	.490	10.110	80.883
7.15	.081	.491	10.796	86.372
7.20	.076	.492	11.568	92.549
7.25	.071	.492	12.442	99.539
7.30	.066	.493	13.441	99.999
7.35	.062	.493	14.595	99.999
7.40	.057	.494	15.940	99.999
7.45	.052	.494	17.532	99.999
7.50	.047	.495	19.441	99.999
7.55	.042	.495	21.769	99.999
7.60	.038	.496	24.689	99.999
7.65	.033	.496	28.436	99.999
7.70	.028	.497	33.433	99.999
7.75	.023	.497	40.415	99.999
7.80	.019	.498	50.893	99.999
7.85	.014	.498	68.342	99.999
7.90	.009	.499	99.999	99.999
7.95	.004	.499	99.999	99.999
8.00	0.000	.500	99.999	99.999

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