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Computer Calculations of Relaxation Regions and  
Equilibrium Conditions for Shock Waves with  
Tables for  $\text{CO}_2$  and  $\text{N}_2\text{O}$

\* By T. Rees

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# Computer Calculations of Relaxation Regions and Equilibrium Conditions for Shock Waves with Tables for CO<sub>2</sub> and N<sub>2</sub>O

By T. Rees

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Johannesen<sup>2</sup> has discussed a Rayleigh-line method for the analysis of vibrational relaxation regions in shock waves. In this method the flow of the real gas in the relaxation region is treated as the flow of an ideal gas (termed the  $\alpha$ -gas by Johannesen) with heat extraction. The Rayleigh-line method is readily adapted for use on a computer; programs based on this method have been used to deal with experimental data for CO<sub>2</sub>-He mixtures and N<sub>2</sub>O, and also to provide tables of equilibrium conditions for pure CO<sub>2</sub> and N<sub>2</sub>O.

Conditions ( $a$ ) immediately behind the diffusion resisted part of the wave are found using the normal shock relations for the ideal gas and the known conditions (1) in front of the shock wave. The Mach number  $m_1$  of the  $\alpha$ -gas is related to the Mach number  $M_1$  of the real gas by

$$m_1 = M_1 (\gamma_1/\gamma_\alpha)^{\frac{1}{2}}. \quad (1)$$

The total temperature,  $T_{01}$ , which does not vary through the diffusion-resisted part of the shock wave, is given by,

$$T_{01} = T_1(1 + \frac{1}{2}(\gamma_\alpha - 1)m_1^2). \quad (2)$$

The flow variables for the  $\alpha$ -gas can be expressed in terms of the corresponding quantities at sonic conditions, i.e. at  $m = 1$ . This gives the well-known Rayleigh-line relations,

$$\frac{T}{T_b} = \frac{(\gamma_\alpha + 1)^2 m^2}{(1 + \gamma_\alpha m^2)^2}, \quad (3)$$

$$\frac{T_0}{T_{0b}} = \frac{2(\gamma_\alpha + 1)m^2 (1 + \frac{1}{2}(\gamma_\alpha - 1)m^2)}{(1 + \gamma_\alpha m^2)^2}, \quad (4)$$

$$\frac{\rho_b}{\rho} = \frac{v}{v_b} = \frac{(\gamma_\alpha + 1)m^2}{1 + \gamma_\alpha m^2}, \quad (5)$$

$$\frac{p}{p_b} = \frac{\gamma_\alpha + 1}{1 + \gamma_\alpha m^2}. \quad (6)$$

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\*Replaces A.R.C. 27 581.

where suffix (*b*) denotes sonic conditions, and the symbols have their usual meanings. The conditions (*b*) can be found from the known conditions (1) using the relations (3) to (6).

The increase in vibrational energy at any point in the relaxation region is equal to the energy that has been extracted from the  $\alpha$ -gas, i.e.

$$\sigma - \bar{\sigma}_1 = c_{p\alpha} (T_0 - T_{01}) \quad (7)$$

where  $\sigma$  denotes the vibrational energy and  $\bar{\sigma}$  denotes its local equilibrium value.

For the purpose of the computer program it is necessary to obtain an analytic expression for the equilibrium value of the vibrational energy. The simple harmonic oscillator approximation is suitable for most gases. For example, for  $\text{CO}_2$  and  $\text{N}_2\text{O}$  we have

$$\bar{\eta} = \frac{\bar{\sigma}}{c_{p\alpha}} = \frac{Rx}{c_{p\alpha}} \left\{ \frac{2C_1}{\exp(C_1/T) - 1} + \frac{C_2}{\exp(C_2/T) - 1} + \frac{C_3}{\exp(C_3/T) - 1} \right\} \quad (8)$$

where  $x$  is the mole fraction of oscillators present and  $C_1$ ,  $C_2$ , and  $C_3$  are the characteristic temperatures of the various modes. For  $\text{CO}_2$  these are 959, 1920, and 3380 °K respectively, while for  $\text{N}_2\text{O}$  the corresponding values are 847, 1850, and 3200 °K. It was felt that such approximations were sufficiently accurate for evaluating experimental data, the difference between published value (Hilsenrath *et al*<sup>1</sup>, McBride, Heimele, Ehlers and Gordon<sup>4</sup>) of the vibrational energy and the values given by the harmonic oscillator approximation increasing with temperature to 3 per cent at 5000 °K in the cases of  $\text{CO}_2$  and  $\text{N}_2\text{O}$ . However, a correction was applied in the preparation of the Tables of equilibrium conditions. It was found that the difference could be expressed as a linear function of temperature, so that

$$\bar{\eta}_T = \bar{\eta}_{HO} (1 + aT + b). \quad (10)$$

Here suffix *T* denotes values obtained from tables and *HO* those given by the harmonic oscillator expression. Values of *a* and *b* were found for  $\text{CO}_2$  and  $\text{N}_2\text{O}$  in the interval 300 to 5000 °K by the method of least squares, and these values are given with the corresponding tables of equilibrium conditions. Where it is necessary to calculate the ratio of the specific heats of the real gas, the contribution,  $c_{\text{vib}}$ , of the vibrational modes to the specific heats was obtained by differentiating equation (10) with respect to *T*.

In the program *m* is decreased in steps of 0.01 from  $m_a$ . At each value of *m*, *T* and  $T_0$  are found from (3) and (4) and hence  $\bar{\eta}$  and  $\eta$  from (10) and (7). This process is continued until a value of *m*,  $m(n)$ , is reached where  $(\bar{\eta} - \eta)$  becomes negative. A linear interpolation using  $m(n)$  and the previous value  $m(n-1)$  gives an approximate value of  $m_2$  for which  $\eta = \bar{\eta}$ . Station (2) is the point at which equilibrium is reached. Values of  $\eta$  and  $\bar{\eta}$  corresponding to this value of  $m_2$  are calculated and a second interpolation, or extrapolation as the case may be, with  $m(n-1)$  yields a better value for  $m(2)$ . This is repeated until successive values of  $m_2$  differ by less than 0.0001. Equilibrium values of the pressure, temperature, and density are then obtained by substituting  $m_2$  into the Rayleigh-line relations. Examples of Tables prepared in this way are given together with *h* flow diagram of the calculation. Also included in the Tables are values of  $M_2^*$  the equilibrium Mach number of the flow of the real gas produced by a shock moving into a gas at rest. It should be noted that the method does not make any use of the relaxation equation.

The program was also used to calculate relaxation frequencies at points in the relaxation region from experimental data using the method due to Johannesen, Zienkiewicz, Blythe and Gerrard<sup>3</sup>. The simple relaxation equation

$$\frac{d\sigma}{dt} = \rho \Phi (\bar{\sigma} - \sigma) \quad (11)$$

was used, where  $\Phi$  is the relaxation frequency. It was shown that  $\Phi$  may be written

$$\Phi = \frac{v_b T_b}{\rho_b} c_{p\alpha} L(m) \frac{A(\rho_2 - \rho)}{\rho_b(\bar{\sigma} - \sigma)}. \quad (12)$$

Here it is assumed that a logarithmic plot of the difference between final and local values of the density against distance,  $x$ , behind the shock-wave is a straight line, i.e.

$$\log(\rho_2 - \rho) = -Ax + B. \quad (13)$$

The function  $L(m)$  is defined by

$$L(m) = \frac{T}{T_b} \left\{ \frac{v}{v_b} \right\}^3 (1 - m^2). \quad (14)$$

Thus, for a given value of  $m_1$ , all the quantities on the right-hand side of equation (12) can be found, except for the value of  $A$  which is provided by experiment. Usually  $\Phi$  was calculated for five values of  $m$  in the interval  $m_a$  to  $m_2$ , and hence a plot of  $\Phi$  versus local temperature was obtained instead of a single overall value.

*Acknowledgement.*

The author is indebted to Professor N. H. Johannesen and Dr. H. K. Zienkiewicz for many helpful discussions.

## LIST OF SYMBOLS

$M_1$	Mach number of the shock in the real gas
$m_1$	Mach number of the shock in the $\alpha$ -gas
$T_1$	Temperature in front of the shock
$p_1$	Pressure in front of the shock
$\rho_1$	Density in front of the shock
$m_2$	Value of the equilibrium Mach number relative to the shock in the $\alpha$ -gas
$M_2$	Equilibrium Mach number in the real gas of the flow produced by a shock wave moving into a gas at rest
$T_2$	Equilibrium temperature
$p_2$	Equilibrium pressure
$\rho_2$	Equilibrium density

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*Equilibrium Values for Normal Shocks in*

*Carbon Dioxide for  $T_1 = 295$  °K.*

$$a = 7.8 \times 10^{-6} (\text{°K})^{-1}$$

$$b = -6.042 \times 10^{-3}$$

$M_1$	$m_1$	$m_2$	$T_2$	$p_2/p_1$	$\rho_2/\rho_1$	$\rho_1/\rho_2$	$M_2^*$
1.1	1.056	0.8726	309.6	1.240	1.181	0.8465	0.1653
1.2	1.152	0.8025	323.3	1.503	1.371	0.7294	0.3117
1.3	1.248	0.7455	336.8	1.789	1.567	0.6383	0.4431
1.4	1.344	0.6980	350.2	2.098	1.767	0.5659	0.5628
1.5	1.440	0.6579	363.7	2.430	1.971	0.5073	0.6727
1.6	1.536	0.6236	377.4	2.786	2.178	0.4592	0.7745
1.7	1.632	0.5939	391.5	3.165	2.385	0.4193	0.8692
1.8	1.728	0.5680	405.9	3.568	2.593	0.3856	0.9577
1.9	1.824	0.5453	420.7	3.994	2.801	0.3570	1.0408
2.0	1.920	0.5251	435.9	4.444	3.007	0.3325	1.1190
2.1	2.016	0.5072	451.6	4.918	3.212	0.3113	1.1928
2.2	2.112	0.4910	467.8	5.416	3.415	0.2928	1.2626
2.3	2.208	0.4765	484.4	5.937	3.616	0.2765	1.3288
2.4	2.304	0.4633	501.4	6.482	3.814	0.2622	1.3917
2.5	2.400	0.4514	518.9	7.051	4.009	0.2494	1.4515
2.6	2.496	0.4404	536.9	7.645	4.201	0.2381	1.5085
2.7	2.592	0.4304	555.3	8.262	4.389	0.2278	1.5629
2.8	2.688	0.4212	574.1	8.903	4.574	0.2186	1.6149
2.9	2.784	0.4127	593.4	9.568	4.756	0.2102	1.6646
3.0	2.880	0.4048	613.2	10.257	4.935	0.2027	1.7122
3.1	2.976	0.3975	633.4	10.971	5.110	0.1957	1.7578
3.2	3.072	0.3906	654.0	11.708	5.281	0.1894	1.8015
3.3	3.168	0.3843	675.1	12.470	5.449	0.1835	1.8435
3.4	3.264	0.3783	696.6	13.256	5.614	0.1781	1.8839
3.5	3.360	0.3728	718.6	14.066	5.775	0.1732	1.9228
3.6	3.456	0.3675	740.9	14.901	5.933	0.1686	1.9601
3.7	3.552	0.3626	763.7	15.759	6.087	0.1643	1.9962
3.8	3.648	0.3580	786.9	16.642	6.239	0.1603	2.0309
3.9	3.744	0.3536	810.6	17.549	6.387	0.1566	2.0644
4.0	3.840	0.3495	834.6	18.481	6.532	0.1531	2.0967

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$M_1$	$m_1$	$m_2$	$T_2$	$p_2/p_1$	$\rho_2/\rho_1$	$\rho_1/\rho_2$	$M_2^*$
4.1	3.936	0.3456	859.1	19.436	6.674	0.1498	2.1279
4.2	4.032	0.3418	884.0	20.416	6.813	0.1468	2.1581
4.3	4.128	0.3383	909.3	21.420	6.949	0.1439	2.1872
4.4	4.224	0.3350	935.0	22.449	7.082	0.1412	2.2154
4.5	4.320	0.3318	961.2	23.501	7.213	0.1386	2.2427
4.6	4.416	0.3287	987.8	24.578	7.340	0.1362	2.2690
4.7	4.512	0.3258	1014.7	25.680	7.465	0.1340	2.2946
4.8	4.608	0.3231	1042.1	26.805	7.588	0.1318	2.3194
4.9	4.704	0.3204	1070.0	27.955	7.707	0.1297	2.3434
5.0	4.800	0.3179	1098.2	29.129	7.825	0.1278	2.3666
5.1	4.896	0.3155	1126.9	30.327	7.939	0.1260	2.3892
5.2	4.992	0.3132	1155.9	31.550	8.052	0.1242	2.4110
5.3	5.088	0.3110	1185.4	32.797	8.162	0.1225	2.4323
5.4	5.184	0.3088	1215.4	34.068	8.269	0.1209	2.4529
5.5	5.280	0.3068	1245.7	35.364	8.375	0.1194	2.4729
5.6	5.376	0.3048	1276.5	36.683	8.478	0.1180	2.4923
5.7	5.472	0.3029	1307.7	38.027	8.579	0.1166	2.5112
5.8	5.568	0.3011	1339.3	39.395	8.677	0.1152	2.5295
5.9	5.664	0.2994	1371.3	40.788	8.774	0.1140	2.5473
6.0	5.760	0.2977	1403.8	42.205	8.869	0.1128	2.5646
6.1	5.856	0.2961	1436.7	43.645	8.962	0.1116	2.5815
6.2	5.952	0.2945	1470.1	45.111	9.052	0.1105	2.5978
6.3	6.047	0.2930	1503.8	46.600	9.141	0.1094	2.6138
6.4	6.143	0.2916	1538.0	48.114	9.228	0.1084	2.6293
6.5	6.239	0.2902	1572.7	49.651	9.313	0.1074	2.6444
6.6	6.335	0.2888	1607.8	51.214	9.397	0.1064	2.6591
6.7	6.431	0.2875	1643.3	52.800	9.479	0.1055	2.6734
6.8	6.527	0.2862	1679.2	54.410	9.559	0.1046	2.6873
6.9	6.623	0.2850	1715.6	56.045	9.637	0.1038	2.7009
7.0	6.719	0.2838	1752.4	57.704	9.714	0.1029	2.7141
7.1	6.815	0.2827	1789.7	59.387	9.789	0.1022	2.7270
7.2	6.911	0.2816	1827.4	61.094	9.863	0.1014	2.7395
7.3	7.007	0.2805	1865.5	62.826	9.935	0.1007	2.7518
7.4	7.103	0.2794	1904.1	64.581	10.005	0.0999	2.7637
7.5	7.199	0.2784	1943.2	66.361	10.075	0.0993	2.7753

*Equilibrium Values for Normal Shocks in  
Nitrous Oxide for  $T_1 = 295$  °K.*

$$a = 15 \times 10^{-6} (\text{°K})^{-1}$$

$$b = -6.493 \times 10^{-3}$$

$M_1$	$m_1$	$m_2$	$T_2$	$p_2/p_1$	$\rho_2/\rho_1$	$\rho_1/\rho_2$	$M_2^*$
1.1	1.050	0.8680	308.9	1.238	1.182	0.8458	0.1661
1.2	1.146	0.7984	322.1	1.499	1.373	0.7282	0.3134
1.3	1.241	0.7416	335.0	1.783	1.570	0.6367	0.4458
1.4	1.336	0.6943	347.8	2.090	1.773	0.5640	0.5664
1.5	1.432	0.6543	360.7	2.420	1.979	0.5053	0.6773
1.6	1.527	0.6201	373.9	2.773	2.188	0.4571	0.7799
1.7	1.623	0.5905	387.4	3.150	2.398	0.4170	0.8755
1.8	1.718	0.5646	401.3	3.549	2.609	0.3833	0.9648
1.9	1.814	0.5419	415.6	3.972	2.820	0.3546	1.0487
2.0	1.909	0.5218	430.3	4.419	3.030	0.3301	1.1277
2.1	2.005	0.5039	445.4	4.889	3.238	0.3088	1.2022
2.2	2.100	0.4878	461.0	5.382	3.444	0.2903	1.2728
2.3	2.196	0.4733	477.0	5.899	3.648	0.2741	1.3396
2.4	2.291	0.4602	493.5	6.440	3.849	0.2598	1.4032
2.5	2.387	0.4482	510.4	7.004	4.048	0.2470	1.4636
2.6	2.482	0.4373	527.8	7.592	4.243	0.2357	1.5211
2.7	2.577	0.4273	545.7	8.204	4.435	0.2255	1.5761
2.8	2.673	0.4181	564.0	8.839	4.623	0.2163	1.6285
2.9	2.768	0.4096	582.7	9.498	4.808	0.2080	1.6787
3.0	2.864	0.4018	601.9	10.181	4.990	0.2004	1.7267
3.1	2.959	0.3945	621.6	10.888	5.168	0.1935	1.7727
3.2	3.055	0.3877	641.6	11.619	5.342	0.1872	1.8169
3.3	3.150	0.3814	662.1	12.374	5.513	0.1814	1.8593
3.4	3.246	0.3755	683.0	13.152	5.680	0.1760	1.9000
3.5	3.341	0.3700	704.4	13.955	5.844	0.1711	1.9392
3.6	3.437	0.3648	726.2	14.781	6.005	0.1665	1.9769
3.7	3.532	0.3599	748.4	15.632	6.162	0.1623	2.0132
3.8	3.628	0.3553	771.0	16.506	6.316	0.1583	2.0482
3.9	3.723	0.3509	794.0	17.404	6.466	0.1546	2.0820
4.0	3.819	0.3468	817.4	18.327	6.614	0.1512	2.1145



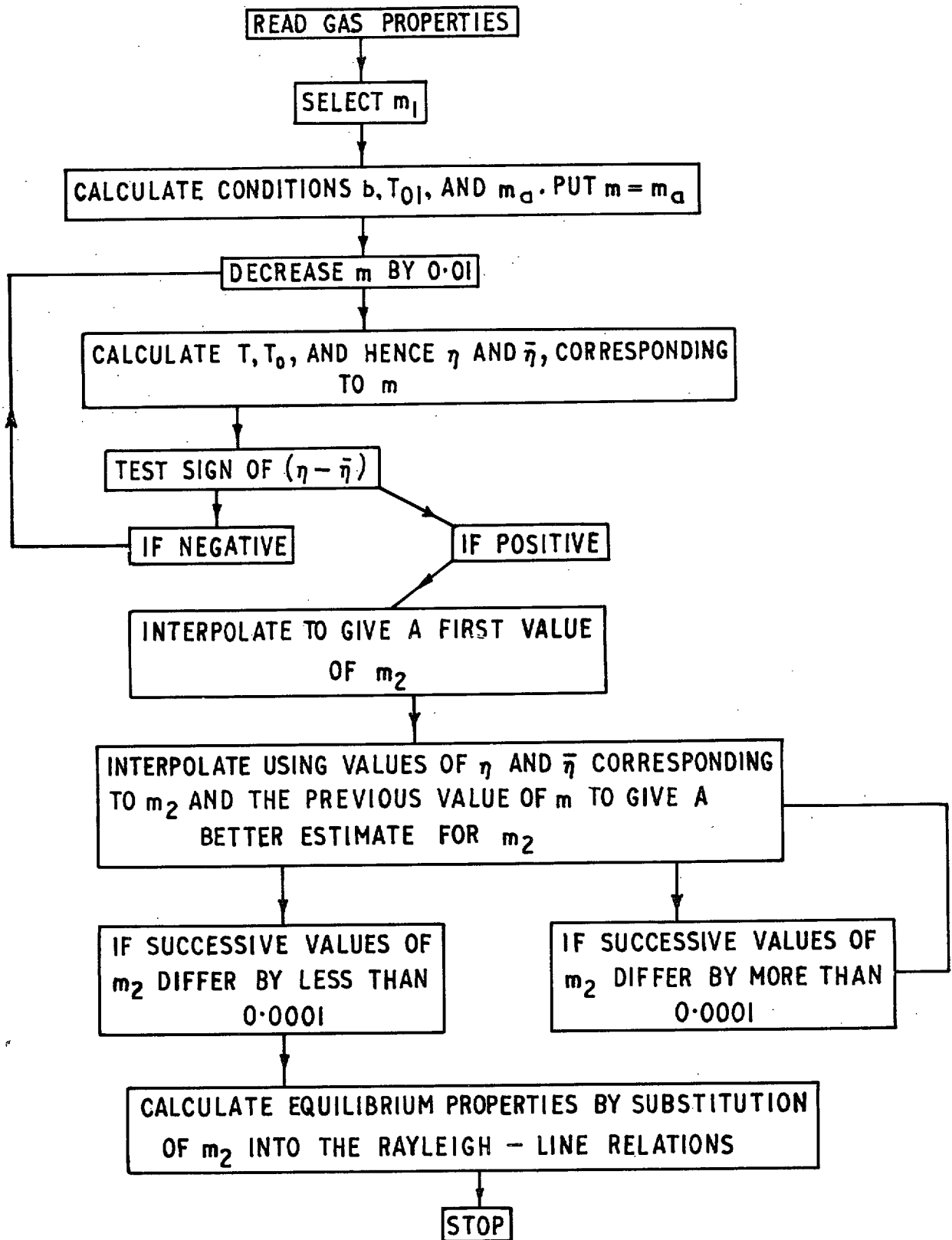
*Equilibrium Values for Normal Shocks in  
Nitrous Oxide for  $T_1 = 295 \text{ }^\circ\text{K}$ .*

$$a = 15 \times 10^{-6} (\text{ }^\circ\text{K})^{-1}$$

$$b = -6.493 \times 10^{-3}$$

$M_1$	$m_1$	$m_2$	$T_2$	$p_2/p_1$	$\rho_2/\rho_1$	$\rho_1/\rho_2$	$M_2^*$
4.1	3.914	0.3429	841.3	19.273	6.758	0.1480	2.1460
4.2	4.009	0.3393	865.6	20.244	6.899	0.1449	2.1764
4.3	4.105	0.3358	890.3	21.238	7.037	0.1421	2.2057
4.4	4.200	0.3324	915.4	22.256	7.173	0.1394	2.2341
4.5	4.296	0.3293	940.9	23.299	7.305	0.1369	2.2616
4.6	4.391	0.3263	966.8	24.365	7.435	0.1345	2.2882
4.7	4.487	0.3234	993.1	25.456	7.561	0.1323	2.3139
4.8	4.582	0.3207	1019.9	26.570	7.685	0.1301	2.3388
4.9	4.678	0.3180	1047.1	27.709	7.807	0.1281	2.3630
5.0	4.773	0.3155	1074.6	28.871	7.926	0.1262	2.3864
5.1	4.869	0.3131	1102.6	30.058	8.042	0.1243	2.4091
5.2	4.964	0.3108	1131.0	31.269	8.156	0.1226	2.4311
5.3	5.060	0.3086	1159.8	32.503	8.267	0.1210	2.4525
5.4	5.155	0.3065	1189.0	33.762	8.376	0.1194	2.4733
5.5	5.250	0.3045	1218.7	35.045	8.483	0.1179	2.4934
5.6	5.346	0.3026	1248.7	36.351	8.588	0.1164	2.5130
5.7	5.441	0.3007	1279.2	37.682	8.690	0.1151	2.5320
5.8	5.537	0.2989	1310.1	39.036	8.790	0.1138	2.5504
5.9	5.632	0.2972	1341.4	40.415	8.888	0.1125	2.5684
6.0	5.728	0.2955	1373.1	41.818	8.984	0.1113	2.5859
6.1	5.823	0.2939	1405.2	43.245	9.078	0.1102	2.6028
6.2	5.919	0.2923	1437.8	44.695	9.171	0.1090	2.6194
6.3	6.014	0.2909	1470.7	46.170	9.261	0.1080	2.6354
6.4	6.110	0.2894	1504.1	47.668	9.349	0.1070	2.6511
6.5	6.205	0.2880	1537.9	49.191	9.436	0.1060	2.6663
6.6	6.301	0.2867	1572.2	50.738	9.520	0.1050	2.6812
6.7	6.396	0.2854	1606.8	52.308	9.603	0.1041	2.6956
6.8	6.491	0.2841	1641.9	53.903	9.685	0.1033	2.7097
6.9	6.587	0.2829	1677.4	55.522	9.764	0.1024	2.7234
7.0	6.682	0.2817	1713.4	57.164	9.842	0.1016	2.7368
7.1	6.778	0.2806	1749.7	58.831	9.919	0.1008	2.7498
7.2	6.873	0.2795	1786.5	60.521	9.994	0.1001	2.7626
7.3	6.969	0.2784	1823.7	62.236	10.067	0.0993	2.7750
7.4	7.064	0.2774	1861.4	63.974	10.139	0.0986	2.7871
7.5	7.160	0.2764	1899.4	65.736	10.210	0.0979	2.7989

Flow Diagram for Calculation of Equilibrium Values.



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