MASTER

**QIKMIX: A Quick-Turnaround Computer Program for
Computing Opacities of Mixtures**

University of California

LOS ALAMOS SCIENTIFIC LABORATORY

Post Office Box 1663 Los Alamos, New Mexico 87545

LA-7724-M
Manual

Special Distribution
Issued: May 1979

QIKMIX: A Quick-Turnaround Computer Program for Computing Opacities of Mixtures

J. Abdallah, Jr.
W. F. Huebner

NOTICE

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Department of Energy, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

Reg

QIKMIX: A QUICK-TURNAROUND COMPUTER PROGRAM FOR COMPUTING OPACITIES OF MIXTURES

by

J. Abdallah, Jr., and W. F. Huebner

ABSTRACT

QIKMIX is a quick-turnaround computer code developed to compute the radiative Rosseland mean opacity of specified mixtures at specified temperature and density points. The QIKLIB data base, which QIKMIX uses, has been derived from the OPLIB library. For most mixtures, QIKMIX can compute opacities over a temperature range of 50 to 25 000 eV in less than 1 min of CDC 7600 computer time. The purpose of this report is to discuss the QIKLIB data base and the operation of the QIKMIX code.

I. INTRODUCTION

QIKMIX was developed at the Los Alamos Scientific Laboratory (LASL) to provide a method of obtaining approximate values of the radiative Rosseland mean opacity (κ_R) for mixtures of arbitrary composition without using the full OPLIB treatment.¹ Thus the user can experiment with different compositions to get a rough estimate of their effects on the opacity. Users should be aware that the results of QIKMIX are intended to be estimates (within $\pm 20\%$ of OPLIB results); for definitive results, OPLIB should be used. However, QIKMIX will often give results that are within 1% of OPLIB results.

The method for computing the Rosseland mean opacity of a mixture of ions involves combining the reduced group mean extinction coefficients at each value of $u = h\nu/kT^*$ for each component (in proportion to its number fraction) at each temperature (kT) and degeneracy parameter (η) point on a fixed predetermined (u, kT, η) grid. The resulting sets of extinction coefficients are integrated as a function of u to obtain κ_R . This opacity table then may be interpolated to obtain κ_R at the desired temperature and density points.

*Here, $h\nu$ is the photon energy.

Until now, these computations have used the massive OPLIB data files described in Ref. 1. Note that each atomic component on OPLIB exists as a separate file. Although the use of OPLIB gives the best results available, the size and number of these files make data transfer slow and cumbersome even for simple mixtures.

QIKLIB, the data base used by QIKMIX, contains a subset of the OPLIB data plus averaged OPLIB extinction coefficients. QIKLIB is structured in a convenient form for performing the mixture calculation.

Section II gives a detailed description of the data base, Sec. III describes the input required by QIKMIX, and Sec. IV describes the output generated by QIKMIX.

II. DATA BASE DESCRIPTION

QIKLIB consists of four files (QIK1, QIK2, QIK3, and QIK4), each containing data for different temperature regions. Table I shows the temperature points in each file. Note that all extinction coefficients are triple packed, and that more are necessary in the lower temperature regions to yield satisfactory results.

Each QIKn file consists of a file label (see Table I) followed by data records, one for each (kT , η , Z) point,* and then by an end-of-file mark (see Fig. 1). Each data record contains descriptive information and extinction coefficients. The detailed data record format is shown in Table II.

*Here Z is the atomic number of the mixture component.

TABLE I
QIKLIB FILE SUMMARY

Region	File Name	Label	No. Ext. Coeffs.	No. Words per Record [NWR]	File Size in Octal	Temperatures Included (eV)
1	QIK1	680-100EV	680	280	3 554 350	50; 60; 80; 100
2	QIK2	480-300EV	480	213	3 421 111	125; 150; 200; 250; 300
3	QIK3	400-1250EV	400	187	3 563 151	400; 500; 600; 800; 1 000; 1 250
4	QIK4	150-25KEV	150	103	3 616 171	1 500; 2 000; 2 500; 3 000; 4 000; 5 000; 6 000; 8 000; 10 000; 25 000

Fig. 1.
QIKn file structure.

TABLE II
QIKLIB DATA RECORD FORMAT^a (PURE ELEMENTS ONLY)

Word(s)	Content
1	aaaa b c mm yy ^b
2	Z...atomic number
3	A...atomic weight
4	kT...temperature [eV]
5	η ...degeneracy parameter
6	$I_{1,2}(\eta)$...Fermi integral
7	ρ ...density [g/cm ³]
8	N_f ...number of free electrons per atom
9	P...particle pressure including plasma effect [dyn/cm ²]
10	E...internal energy including plasma effect relative to H ₂ ^c [erg/g]
11	κ_R ...radiative Rosseland opacity (including spectral lines) [cm ² /g]
12	κ_e ...electron conductive opacity [cm ² /g]
13	κ_T ...total Rosseland opacity [cm ² /g]
14	$h\nu_p/kT$...plasma cutoff
15	ϵ ...Coulomb interaction between ions
16	P_e ...electron pressure [dyn/cm ²]
17	P_p ...plasma correction to pressure [dyn/cm ²]
18	P_i ...ion pressure [dyn/cm ²]
19	E_e ...electron kinetic energy [erg/g]
20	E_p ...plasma correction to energy [erg/g]
21	E_i ...ion kinetic energy [erg/g]
22	E_{ix} ...energy of ionization and excitation relative to H ₂ ^c [erg/g]
23	number abundance = 1
24-30	occupation numbers for (n ℓ) levels
31-50	blank
51-NWR ^d	triple-packed extinction coefficients

^aSee Ref. 1 for detailed descriptions of the parameters.

^baaa...number of OPLIB record from which data was extracted

b = 1 or 2...mean ion model

b = 3...explicit ion model

c = 1...electron conduction by Hubbard-Lampe model

c = 2...electron conduction by Mestel model

mm...month of code used to calculate OPLIB opacity

yy...year of code used to calculate OPLIB opacity

^cTo obtain the energy relative to the isolated neutral atom, subtract the dissociation energy of H₂, 2.15×10^{12} erg/g.

^dNWR is defined in Table I.

Note that some parameters such as pressure and energy are included on the data base but not used by QIKMIX. These parameters may be used in future applications as the need arises. A list of the 24 currently available elements is shown in Table III. Space has been reserved for additional elements as they become available. Table IV shows the 36 η values used to generate the QIKLIB grid. If no data exist for a given (kT , η , Z) point, the entire record is zeroed out except for words 2, 4, and 5. The records are sorted in kT , then η , and then Z , all in monotonically increasing order. Therefore, (50, -25, 1) occurs first, (50, -25, 2) occurs next, etc. The multi-element feature of QIKLIB facilitates processing for the QIKMIX code, because records corresponding to elements not in the desired mixture are skipped.

All sets of extinction coefficients in QIKLIB are group averages of those appearing on OPLIB between $u = 0$ and $u = 20$. Because the OPLIB spacing is 0.01, the set of 2000 OPLIB coefficients is reduced to the number of QIKLIB coefficients shown in Table I for each of the temperature regions. QIKLIB averaged coefficients are generated in each region starting at u_A and ending at u_B , in steps of Δu . Thus more coefficients may be retained in frequency ranges that contribute more to the opacity in various temperature ranges. Table V summarizes the u values for which extinction coefficients exist in each of the QIKLIB temperature regions.

TABLE III

CURRENTLY AVAILABLE MIXTURE COMPONENTS

<u>Component</u>	<u>Z</u>	<u>Component</u>	<u>Z</u>
Hydrogen	1	Silicon	14
Helium	2	Phosphorus	15
Lithium	3	Sulfur	16
Beryllium	4	Chlorine	17
Boron	5	Argon	18
Carbon	6	Potassium	19
Nitrogen	7	Calcium	20
Oxygen	8	Titanium	22
Neon	10	Chromium	24
Sodium	11	Manganese	25
Magnesium	12	Iron	26
Aluminum	13	Nickel	28

TABLE IV

VALUES OF η FOR QIKLIB GRID GENERATION

-25	-16	-7	5
-24	-15	-6	8
-23	-14	-5	12
-22	-13	-4	20
-21	-12	-3	30
-20	-11	-2	50
-19	-10	-1	80
-18	-9	1	120
-17	-8	3	200

TABLE V

VALUES OF u ASSOCIATED WITH STORED EXTINCTION COEFFICIENTS

Temperature Region	u_A	u_B	Δu	Number
1	0.5	1.0	0.5	2
	1.02	2.0	0.02	50
	2.01	6.0	0.01	400
	6.02	10.0	0.02	200
	10.1	12.0	0.1	20
	13.0	20.0	1.0	8
				680 Total
2	0.5	1.0	0.5	2
	1.02	10.0	0.02	450
	10.1	12.0	0.1	20
	13.0	20.0	1.0	8
				480 Total
3	0.5	1.0	0.5	2
	1.02	8.0	0.02	350
	8.1	12.0	0.1	40
	13.0	20.0	1.0	8
				400 Total
4	0.5	1.0	0.5	2
	1.1	3.0	0.1	20
	3.05	8.0	0.05	100
	8.2	12.0	0.2	20
	13.0	20.0	1.0	8
				150 Total

III. QIKMIX INPUT

Core storage requirements for program: 63 064 words (octal) = 26 124 words (decimal)

Disk storage requirements for data: 16 577 023 words (octal) = 3 866 131 words (decimal)

Input to QIKMIX consists of the QIKLIB data base described in the previous section and a control card file QKCTRL. QIK1 and QIK2 exist as a library (LIX) file QIKLB0 on LASL HYDRA photostore under access code T4QIK. Similarly, QIK3 and QIK4 exist as QIKLB1 under the same access code. QIKMIX will automatically retrieve these files from photostore and perform the required LIX operation.

QKCTRL contains control information used by QIKMIX (see Table VI for the QKCTRL format). This control file was introduced to facilitate batch processing and to help the user avoid the repetition of entering the same data on consecutive runs of QIKMIX (which could occur if QIKMIX is used interactively). The data entered into QKCTRL include the composition of the mixture, the density points, and the temperature points for which opacities are to be generated. The mixture composition may be entered as molecular formulas and as individual elements. The number of unique elements in the mixture must not exceed 15 because of dimension statement limitations in the program. The composition information is used to generate internal tables, which include temperatures, densities, and opacities at the fixed (kT , η) grid. Opacities are generated at the requested temperatures and densities by interpolating on this set of internal tables. These tables are output by QIKMIX (as the binary file QKTBL5) and also may be used as input (see Sec. IV). IR1 and IR2 (see Table VI) may be set to nonzero values to obtain a quicker mixture calculation, but the user should be aware that the internal tables generated will not include the full range of temperatures.

Figure 2 shows a sample control card file for a mixture of 1 part aluminum to 100 parts $^6\text{Li } ^2\text{H}$, where ^2H represents a 1-to-1 mixture of deuterium and tritium. Note that two atomic weight override cards are necessary. Also note that QIKMIX will renormalize the number or weight fractions that were specified in the input.

```

      2      1      2
    1.0      3 1 1 1
     .01      13 1
     3.0      6.0
     1.0      2.5
      21
        1.00E-06      3.16E-06      1.00E-05      3.16E-05      1.00E-04
        3.16E-04      1.00E-03      3.16E-03      1.00E-02      3.16E-02
        1.00E-01      3.16E-01      1.00E+00      3.16E+00      1.00E+01
        3.16E+01      1.00E+02      3.16E+02      1.00E+03      3.16E+03
        1.00E+04
      26
        5.00E+01      6.00E+01      8.00E+01      1.00E+02      1.25E+02
        1.50E+02      2.00E+02      2.50E+02      3.00E+02      4.00E+02
        5.00E+02      6.00E+02      8.00E+02      1.00E+03      1.25E+03
        1.50E+03      2.00E+03      2.50E+03      3.00E+03      4.00E+03
        5.00E+03      6.00E+03      8.00E+03      1.00E+04      1.50E+04
        2.50E+04

```

Fig. 2.

Sample QKCTRL file for 1 part aluminum to 100 parts $^6\text{Li } ^2\text{H}$.

TABLE VI
QKCTRL FORMAT

Card	Format	Parameter	Description
1	(1X, I4, 4I5)	NMOL	NMOL equals the number of molecules and individual atoms input. If NMOL < 0, previously generated internal tables are read in from file QKTBL5 (see Sec. IV) and interpolation is performed.
		NORWTF	If NORWTF = 0, input is in weight fractions. If NORWTF = 1, input is in number fractions.
		NI	Number of atomic weight overrides. Atomic weight overrides are included to allow the user to input atomic weights other than those on QIKLIB. Thus, different isotopes can be accounted for.
		IR1, IR2	If IR1 and IR2 are other than 0, QIKMIX is forced to use only temperature regions IR1 to IR2 ($IR1 \leq IR2$) in the mixture calculation. If both are 0 omitted, all four regions are used.
Next NMOL cards	(1X, E11.0, 16F2.0)	ALFABET	Number or weight fraction depending on value of NORWTF for the molecule.
		(Z, S) repeating group	Atomic number of molecular constituent and its associated subscript (stoichiometric coefficient). A maximum of eight elements may appear in each molecular formula.
Next NI cards (if any)	(1X, F9.5, F10.5)	ZI, AI	Atomic weight override cards. ZI is the atomic number of the element whose atomic weight is to be overridden, and AI is the atomic weight override (weight of isotope).
Next card	(1X, I4)	NRU	Number of densities requested. The maximum value of NRU is 21.
Next cards	(5E15.8)	RHOTBL	Densities requested (g/cm^3); as many cards as required by NRU.
Next card	(1X, I4)	NTU	Number of temperatures requested. The maximum value of NTU is 26.
Next cards	(5E15.8)	TEVR	Temperatures requested (eV); as many cards as required by NTU.

IV. QIKMIX OUTPUT

Output from QIKMIX consists of a file of internal tables of mixture opacities at the fixed (kT , η) grid points (QKTBLs) and an output file listing the mixture opacities at the desired temperature-density grid points (QKLIST).

QKTBLs can be used as input to QIKMIX when the user wants to generate more points for a previously processed mixture. To initiate this, set NMOL negative (see Table VI), set the new temperature-density grid, and execute QIKMIX. The internal tables will be read from QKTBLs by QIKMIX to avoid repeating the time-consuming mixture calculation.

Figure 3 shows the output file (QKLIST) generated by the execution of QIKMIX using QKCTRL as shown in Fig. 2. It includes a listing of the control cards, a summary of the contents of QIKLIB, a summary of the molecular and atomic fractions input, and a listing of κ_R at the requested grid points. Note that blanks appear at grid points for which no κ_R could be computed.

REFERENCE

1. W. F. Huebner, A. L. Merts, N. H. Magee, Jr., and M. F. Argo, "Astrophysical Opacity Library," Los Alamos Scientific Laboratory report LA-6760-M (August 1977).

QIKMIX CONTROL CARDS

```

      2      1      2      0      0
1.0      3 1 1 1
.01      13 1
3.00000 6.00000
1.00000 2.50000
21
.10000000E-05 .31600000E-05 .10000000E-04 .31600000E-04 .10000000E-03
.31600000E-03 .10000000E-02 .31600000E-02 .10000000E-01 .31600000E-01
.10000000E+00 .31600000E+00 .10000000E+01 .31600000E+01 .10000000E+02
.31600000E+02 .10000000E+03 .31600000E+03 .10000000E+04 .31600000E+04
.10000000E+05
26
.50000000E+02 .60000000E+02 .80000000E+02 .10000000E+03 .12500000E+03
.15000000E+03 .20000000E+03 .25000000E+03 .30000000E+03 .40000000E+03
.50000000E+03 .60000000E+03 .80000000E+03 .10000000E+04 .12500000E+04
.15000000E+04 .20000000E+04 .25000000E+04 .30000000E+04 .40000000E+04
.50000000E+04 .60000000E+04 .80000000E+04 .10000000E+05 .15000000E+05
.25000000E+05

```

OPACITY FILE 680-100EV CONTAINS 24 ELEMENTS

ATOMIC NO	ATOMIC WT
1.00000	1.00800
2.00000	4.00300
3.00000	6.94000
4.00000	9.01300
5.00000	10.82000
6.00000	12.01100
7.00000	14.00800
8.00000	16.00000
10.00000	20.18300
11.00000	22.99100
12.00000	24.32000
13.00000	26.98000
14.00000	28.09000
15.00000	30.97500
16.00000	32.06600
17.00000	35.45700
18.00000	39.94400
19.00000	39.10000
20.00000	40.08000
22.00000	47.90000
24.00000	52.01000
25.00000	54.94000
26.00000	55.85000
28.00000	58.71000

Fig. 3.

QKLIST file listing generated by executing *QIKMIX* with the *QKCTRL* control cards shown in Fig. 2.

INPUT DATA MOLECULAR FRACTIONS

Z	A	ZSUB	Z	A	ZSUB	Z	A	ZSUB	Z	A	ZSUB	Z	A	ZSUB	Z	A	ZSUB	Z	A	ZSUB	Z	A	ZSUB	Z	A	ZSUB	Z	A	ZSUB	NO. FRCT.	WT. FRCT.
3.	6.00	1.	1.	2.50	1.	0.	0.00	0.	0.	0.00	0.	0.	0.00	0.	0.	0.00	0.	0.	0.00	0.	0.	0.00	0.	0.	0.00	0.	0.	0.00	0.	9.90E-01	9.69E-01
13.	26.98	1.	0.	0.00	0.	0.	0.00	0.	0.	0.00	0.	0.	0.00	0.	0.	0.00	0.	0.	0.00	0.	0.	0.00	0.	0.	0.00	0.	0.	0.00	0.	9.90E-03	3.08E-02

ATOMIC FRACTIONS

Z	AWT	NO. FRCT.	WT. FRCT.
1.	2.500	4.975124E-01	2.850692E-01
3.	6.000	4.975124E-01	6.841661E-01
13.	26.980	4.975124E-03	3.076467E-02

SUMA= 1.00000000E+00 SUMAZ= 2.05472637E+00 SUMAM= 4.36308458E+00

DENSITY GRID (G/CC)

.1000E-05	.3160E-05	.1000E-04	.3160E-04	.1000E-03	.3160E-03	.1000E-02	.3160E-02	.1000E-01	.3160E-01
.1000E+00	.3160E+00	.1000E+01	.3160E+01	.1000E+02	.3160E+02	.1000E+03	.3160E+03	.1000E+04	.3160E+04
.1000E+05									

T(EV) ROSSELAND MEAN OPACITIES OF MIXTURE AT REQUESTED GRID

50.00	.2457E+00	.3384E+00	.6046E+00	.1449E+01	.4453E+01	.1530E+02	.5291E+02	.1632E+03	.4010E+03	.7627E+03
	.1271E+04	.2204E+04	.3383E+04	.5570E+04						
60.00	.2138E+00	.2590E+00	.3786E+00	.7207E+00	.1850E+01	.5882E+01	.1982E+02	.6317E+02	.1582E+03	.3237E+03
	.5584E+03	.9949E+03	.1651E+04	.2660E+04						
80.00	.1965E+00	.2098E+00	.2456E+00	.3361E+00	.5974E+00	.1390E+01	.3852E+01	.1114E+02	.2978E+02	.6881E+02
	.1363E+03	.2702E+03	.5047E+03	.8555E+03						
100.00	.1914E+00	.1962E+00	.2093E+00	.2436E+00	.3294E+00	.5564E+00	.1176E+01	.2872E+01	.7407E+01	.1890E+02
	.4311E+02	.9186E+02	.1935E+03	.3560E+03						
125.00	.1913E+00	.1932E+00	.1984E+00	.2118E+00	.2464E+00	.3247E+00	.5110E+00	.9781E+00	.2197E+01	.5384E+01
	.1325E+02	.3041E+02	.7465E+02	.1601E+03	.3008E+03					

Fig. 3. (cont)

150.00	.1910E+00	.1924E+00	.1956E+00	.2031E+00	.2201E+00	.2602E+00	.3469E+00	.5409E+00	.1033E+01	.2320E+01
	.5746E+01	.1430E+02	.3452E+02	.8080E+02	.1633E+03					
200.00	.1900E+00	.1912E+00	.1932E+00	.1971E+00	.2055E+00	.2243E+00	.2654E+00	.3479E+00	.5341E+00	.9881E+00
	.2220E+01	.5642E+01	.1479E+02	.3620E+02	.7769E+02	.1270E+03				
250.00	.1892E+00	.1899E+00	.1915E+00	.1949E+00	.2012E+00	.2129E+00	.2378E+00	.2926E+00	.4132E+00	.7110E+00
	.1518E+01	.3653E+01	.9909E+01	.2417E+02	.5421E+02	.8899E+02	.1550E+03			
300.00	.1887E+00	.1890E+00	.1898E+00	.1919E+00	.1973E+00	.2084E+00	.2287E+00	.2679E+00	.3547E+00	.5806E+00
	.1232E+01	.3064E+01	.8171E+01	.2006E+02	.3984E+02	.6990E+02	.1151E+03			
400.00	.1883E+00	.1886E+00	.1889E+00	.1895E+00	.1910E+00	.1957E+00	.2084E+00	.2387E+00	.3027E+00	.4404E+00
	.8331E+00	.2151E+01	.5698E+01	.1407E+02	.2661E+02	.4041E+02	.5940E+02	.8575E+02		
500.00	.1876E+00	.1877E+00	.1877E+00	.1880E+00	.1887E+00	.1906E+00	.1959E+00	.2098E+00	.2470E+00	.3386E+00
	.5734E+00	.1269E+01	.3433E+01	.7595E+01	.1536E+02	.2160E+02	.3131E+02	.4557E+02	.7110E+02	
600.00	.1871E+00	.1872E+00	.1872E+00	.1872E+00	.1874E+00	.1881E+00	.1901E+00	.1960E+00	.2136E+00	.2609E+00
	.3863E+00	.7260E+00	.1655E+01	.3845E+01	.7293E+01	.1212E+02	.1728E+02	.2582E+02	.4217E+02	
800.00	.1862E+00	.1862E+00	.1862E+00	.1862E+00	.1863E+00	.1864E+00	.1870E+00	.1886E+00	.1931E+00	.2064E+00
	.2426E+00	.3340E+00	.5498E+00	.1043E+01	.2038E+01	.3521E+01	.6053E+01	.1014E+02	.1752E+02	.2940E+02
1000.00	.1852E+00	.1852E+00	.1852E+00	.1852E+00	.1853E+00	.1853E+00	.1855E+00	.1862E+00	.1880E+00	.1932E+00
	.2063E+00	.2413E+00	.3203E+00	.4905E+00	.8450E+00	.1545E+01	.2783E+01	.4674E+01	.8623E+01	.1560E+02
1250.00	.1840E+00	.1840E+00	.1840E+00	.1840E+00	.1841E+00	.1841E+00	.1842E+00	.1844E+00	.1851E+00	.1870E+00
	.1925E+00	.2063E+00	.2387E+00	.3077E+00	.4468E+00	.7323E+00	.1296E+01	.2353E+01	.4273E+01	.8183E+01
	.1261E+02									

Fig. 3. (cont)

[illegible]