MIXER - A Multi-Species Optical Data and Equation of State Computer Code

R.R. Peterson and G.A. Moses

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MIXER - A Multi-Species Optical Data and
Equation of State Computer Code

R.R. Peterson and G.A. Moses

Fusion Technology Institute
University of Wisconsin
1500 Engineering Drive
Madison, WI 53706

http://fti.neep.wisc.edu

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Robert R. Peterson
Gregory A. Moses

Fusion Engineering Program
Nuclear Engineering Department
University of Wisconsin
Madison, Wisconsin 53706

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I. Introduction

The calculation of opacities and equations of state of gases is important to many areas of applied physics. Specifically, in the design of inertial confinement fusion reactor cavities, one must be able to predict the propagation of the target explosion generated fireball through the cavity gas to the first wall.\(^{(1-5)}\) To do this calculation correctly, one must have optical data, ionization states and internal energy densities for the cavity gas.

We have previously reported work done on the calculation of equations of state and optical data for single species monatomic gases.\(^{(6)}\) However, we have subsequently found that a multiple species gas might better protect the first wall of a light ion beam fusion reactor from the fireball.\(^{(4)}\) Also, target debris and matter evaporated from the reactor chamber\(^{(1)}\) may be dissolved in the cavity gas, making the single species gas an unrealistic case. Thus, it became necessary for us to modify our single species computer code MFP\(^{(6)}\) into a multiple species code which we call MIXER.

In section II of this paper we discuss some differences in the physical model which must be considered when going to a multiple species gas. Section III is a description of the code MIXER including how it differs from MFP. An important sample problem is solved in section IV, where the effects of alkali metal impurities on the opacity of inert gases are considered. Also the optical data, ionization states and internal energy densities are presented for a promising candidate for a light ion beam reactor cavity gas. Section V is a summary and discussion. In Appendix A we provide some sample input and output for MIXER.
II. Physical Model

We have studied the ionization and internal energy of mixtures of monatomic gases and the interaction of radiation with such mixtures. The radiation stopping processes considered are photo-ionization, inverse Bremsstrahlung, Thomson scattering and atomic line absorption. We do not discuss these processes here, because they are the same as in previously reported work. (6) However, the calculation of the ionization state of the gas mixture is somewhat different from that for a single species gas.

We have considered gas mixtures that are assumed to be dense enough to obey the Saha equation, (7)

\[ I_i \left( \bar{m}_i + 1/2 \right) = T_p \ln \left( \frac{A \tau_i^{3/2}}{n_e} \right). \]  

Here, \( I_i \) is the piece-wise linear continuous form of the ionization potential of the \( i \)th gas species and \( \bar{m}_i \) is the average ionization state of that species. \( T_p \) is the temperature of the mixture, \( A = 6.04 \times 10^{21} \text{ eV}^{-3/2} \) and \( n_e \) is the total electron density. Since \( n_e \) is the sum of the electrons ionized from all of the gas species per unit volume, that is

\[ n_e = \sum_{i=1}^{N_i} \bar{m}_i N_i, \]  

where \( N_i \) is the density of atoms of species \( i \), we must solve a set of Saha equations coupled through \( n_e \). Physically, the Saha model assumes that
ionization is balanced with three-body recombination so that when electrons are added from additional ion species, \( \tilde{n}_i \) for the original species decreases. This effect is most important for species that contribute just a small percent to the total number of atoms present because the electron density is much different from density that would be present if the other species were not there. On the other hand, gases that make up a large fraction of the mixture will experience close to the same number of collisions with electrons as they would if there were no other gases present so their ionization states will not change much.

One important effect of this change in ionization states is the manner in which the radiation mean free paths must be calculated. Two important spectrum averaged radiation mean free paths are the Planck,

\[
\lambda_1 \equiv \frac{U}{\int_0^\infty \kappa_\nu U_\nu \, d\nu}, \tag{3}
\]

and the Rosseland,

\[
\lambda_2 \equiv \frac{\int_0^\infty \frac{1}{\kappa_\nu} (\frac{dU_\nu}{dT_R}) \, d\nu}{\frac{dU}{dT_R}}, \tag{4}
\]

where \( U \) is the integrated radiant energy density, \( U_\nu \) is the Planck spectrum, \( \kappa_\nu \) is the total absorption coefficient, \( \nu \) is the photon frequency and \( T_R \) is
the blackbody radiation temperature. If the ionization states of each of the species were independent, so would be the absorption coefficients for each species, neglecting such effects as additional pressure line broadening. The Planck mean free path could then be found from

$$\frac{1}{\lambda} = \sum \frac{1}{\lambda_{1i}},$$

(5)

where $\lambda_{1i}$ is the Planck mean free path for radiation passing through gas type i alone and $\lambda_1$ is the independently calculated Planck mean free path. The question of interdependence has been tested for a mixture of $1.8 \times 10^{18}$ cm$^{-3}$ argon and $3.6 \times 10^{16}$ cm$^{-3}$ sodium. The results of this test are shown for various equilibrium ($T_R = T_p$) temperatures in Table I. It may be noted that the interdependence is most important at lower temperatures. Because the discrepancy between $\lambda_1$ and $\lambda_{1i}$ is so great at lower temperatures, it is important to solve a set of coupled Saha equations when one is dealing with monatomic gases seeded with small amounts of other gases.

In addition to the total mean free paths, the energy density and ionization must be found for the mixture as a whole. The energy density is the total internal energy divided by the total mass; that is,
Table I

Interdependent and Independent

Planck Mean Free Paths

\[ N_{\text{argon}} = 1.8 \times 10^{18} \text{ cm}^{-3} \]
\[ N_{\text{sodium}} = 3.6 \times 10^{16} \text{ cm}^{-3} \]

<table>
<thead>
<tr>
<th>T (eV)</th>
<th>( \xi_1 ) (cm)</th>
<th>( \xi_1 \text{argon} ) (cm)</th>
<th>( \xi_1 \text{sodium} ) (cm)</th>
<th>( \xi_1^* ) (cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.4</td>
<td>128</td>
<td>6.87 \times 10^4</td>
<td>16.0</td>
<td>16.0</td>
</tr>
<tr>
<td>0.58</td>
<td>34</td>
<td>2.38 \times 10^4</td>
<td>4.79</td>
<td>4.79</td>
</tr>
<tr>
<td>0.85</td>
<td>50.2</td>
<td>243</td>
<td>11.7</td>
<td>11.2</td>
</tr>
<tr>
<td>1.23</td>
<td>44.9</td>
<td>10.5</td>
<td>64.9</td>
<td>9.0</td>
</tr>
</tbody>
</table>

\[ \frac{1}{\xi_1} = \frac{1}{\xi_1 \text{sodium}} + \frac{1}{\xi_1 \text{argon}} \]
\[ \varepsilon = \left[ \sum_i N_i \left( I_i(m_i) + \sum_{j=1}^{j_m} I_i(j) + (1+m_i) T_p \right) \right] / (\sum_i N_i M_i). \]  

Here, \( j_m \) is the largest integer \(< m_i \) and \( M_i \) is the mass of an atom of species \( i \). The ionization state is just the total number of electrons divided by the total number of ions,

\[ m = \sum_i N_i \frac{m_i}{\sum_i N_i}. \]

III. Computer Code

Using the model for ionization outlined in section II, we have converted the single species code MFP(6) into a multiple species gas ionization-optical property code MIXER. MIXER can be used to calculate the radiation mean free paths, ionization states and internal energies of mixtures of up to five species of gas.

This code, which is written in Univac Fortran V, generates disk files containing tables of \( \lambda(T_p, T_R, N_p) \), \( \varepsilon_1(T_p, T_R, N_p) \), \( m(T_p, N_p) \) and \( \varepsilon(T_p, N_p) \) which may be operated on by the data managing programs described previously. When used on the Univac 1180 computer at the Academic Computing Center of the University of Wisconsin-Madison, MIXER requires .75 second of CPU time for each choice of \( T_p \), \( T_R \), and \( N_p \) and 28,000 36-bit words of fast memory.

A flow chart for MIXER is shown in Fig. 1, where the routines marked with * are those which have been significantly altered from the routine of the same
name in MFP. The unmarked subroutines have been altered only in that they have been kept consistent with the other routines. Because these changes only involve the dimensionality of the variables, we will only discuss the marked routines and refer to descriptions of MFP\(^{(6)}\) for the others. All of the real variables and arrays used in this code are double precision, with the exception of the output arrays, which are single precision.

We now briefly describe the variables, common blocks, output and those routines which have been changed from MFP.

**Basic Variables**

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABSCN(5)</td>
<td>Absorption coef. for each species</td>
</tr>
<tr>
<td>ATMAS(5)</td>
<td>Atomic weight of each species</td>
</tr>
<tr>
<td>D(5)</td>
<td>Density of each species</td>
</tr>
<tr>
<td>DETOT</td>
<td>Total electron density</td>
</tr>
<tr>
<td>ELDEN(5)</td>
<td>Electron density from each species</td>
</tr>
<tr>
<td>EMA(5), EMB(5)</td>
<td>Ionization state of each species</td>
</tr>
<tr>
<td>END(10)</td>
<td>End points of mean free path integrals</td>
</tr>
<tr>
<td>DELEI</td>
<td>Inverse width of bound-bound line</td>
</tr>
<tr>
<td>ERAD</td>
<td>Photon energy</td>
</tr>
<tr>
<td>FNN(20,20)</td>
<td>Oscillator strength</td>
</tr>
<tr>
<td>G</td>
<td>Weighting function in Rosseland mean free path integration</td>
</tr>
<tr>
<td>GBRMS</td>
<td>Gaunt factor for inverse Bremsmstrahlung</td>
</tr>
<tr>
<td>G1</td>
<td>Weighting function in Planck mean free path integration</td>
</tr>
<tr>
<td>H1</td>
<td>Bound-bound line shape</td>
</tr>
<tr>
<td>IM</td>
<td>Largest integer less than (\bar{m})</td>
</tr>
<tr>
<td>IMA(5)</td>
<td>(j_m) for each gas species</td>
</tr>
<tr>
<td>IZGAS(5)</td>
<td>Atomic number of each gas species</td>
</tr>
<tr>
<td>Symbol</td>
<td>Definition</td>
</tr>
<tr>
<td>------------</td>
<td>---------------------------------------------------------------------------</td>
</tr>
<tr>
<td>KAPPA(300)</td>
<td>Absorption coefficient</td>
</tr>
<tr>
<td>LGAS</td>
<td>Gas species number</td>
</tr>
<tr>
<td>LROSS</td>
<td>Rosseland mean free path</td>
</tr>
<tr>
<td>L1</td>
<td>Planck mean free path</td>
</tr>
<tr>
<td>MBAR</td>
<td>Average ionization state, $\bar{m}$</td>
</tr>
<tr>
<td>MINM(5)</td>
<td>One less than the minimum difference between $m$ and $\bar{m}$</td>
</tr>
<tr>
<td>N(LGAS,K)</td>
<td>Density of IM-MINM+K-1 ionized atoms of type LGAS</td>
</tr>
<tr>
<td>NGAST</td>
<td># of gas species</td>
</tr>
<tr>
<td>NSUBN(LGAS,K,NPRIN)</td>
<td>Density of atoms of species LGAS with IM-MINM+K ionization electron in the NPRIN atomic level</td>
</tr>
<tr>
<td>POT(LGAS,M)</td>
<td>Energy needed to ionize the $m^{th}$ electron from atoms of type LGAS</td>
</tr>
<tr>
<td>PHOT(300)</td>
<td>Photon energies</td>
</tr>
<tr>
<td>SIGBR</td>
<td>Free-free (Bremsstrahlung) cross section</td>
</tr>
<tr>
<td>SIGMA</td>
<td>Free-bound (photo-ionization) cross section</td>
</tr>
<tr>
<td>TJOND</td>
<td>Total ion density</td>
</tr>
<tr>
<td>TENER</td>
<td>Total internal energy density</td>
</tr>
<tr>
<td>TP</td>
<td>Gas temperature</td>
</tr>
<tr>
<td>TR</td>
<td>Radiation blackbody temperature</td>
</tr>
</tbody>
</table>

**Output Variables**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>DENS</td>
<td>Density of gas species 1</td>
</tr>
<tr>
<td>DENS(2)</td>
<td>Density of gas species 2</td>
</tr>
<tr>
<td>DENS(3)</td>
<td>Density of gas species 3</td>
</tr>
<tr>
<td>DENS(4)</td>
<td>Density of gas species 4</td>
</tr>
<tr>
<td>DENS(5)</td>
<td>Density of gas species 5</td>
</tr>
</tbody>
</table>
EEM(20) Ionization state
EEN(20) Internal energy
GL1(20,20) Planck mean free path
GROSS(20,20) Rosseland mean free path
TMPR(20) Radiation blackbody temperature
TMPP(20) Gas temperature

Common Blocks

ABSORP KAPPA(300), PHOT(300)
COMEND END(10), HIPT
CONTR IPRT(20), JPO, JRO, IO, DELEI, EPSL, IMAX, JMAX, JRMAS, DLOW, TLOW, DELTR, DELTP, DELD, UNFAC, IDEN(5), DEN(5)
POPU IMA(5), NSUBN(5,6,20), N(5,6), MINM(5), ELDEN(5), D(5), MBAR, NGAST, EMA(5), EMB(5), TIOND, TION1, DETOT
RITE GROSS(20,20), GL1(20,20), DENS(5), TMPP(20), EEM(20), EEN(20)
SAHDT POT(5,55), STATE(55), IZGAS(5), ATMAS(5)
TEMP TR, TP, TRINV, TPINV

Main Program

The routine MAIN is the main program for MIXER. It does no calculation itself but leads the code from accepting input through calculations to printing and storing the results. Information controlling the operation of the code is passed into MAIN through common block CONTR. From this information MAIN calculates for each output mesh point the radiation temperature, the gas temperature and, for each gas species, the density. IDEN(2), IDEN(3), IDEN(4) and IDEN(5) determine how the densities of the gas species #2, 3, 4 and 5, respectively, are calculated. If, for example,
IDEN(2) = 1, then the density of species 2 is DEN(2) times the density of species 1. If, on the other hand, IDEN(2) ≠ 1, then the density of species 2 is DEN(2). The results are passed to subroutine OUT2 in common block RITE, where they are printed and stored.

COMMON BLOCKS: CONTR, POPU, RITE, TEMP.

SUBROUTINES CALLED: INPUT, EMBAR, POPUL, ENDP, ABSCON, INTEG, OUT2.

Altered Subroutines

ABSCON: This subroutine calculates the absorption coefficient for values of photon energy between 0 and HIPT. The values of photon energy are determined by end points received in common block COMEND from subroutine ENDP, where they are chosen to optimize the integrations in subroutine INTEG. Each of the eleven subintervals, given by the end points, are separated by EPSL and contain IPRT(2) points, except for the final subinterval which contains 2 times IPRT(2) points. These two parameters, as well as HIPT, are passed from subroutine INPUT in common block CONTR. Photo-ionization, inverse Bremsstrahlung, atomic line absorption and Thomson scattering have been adopted as absorption mechanisms. Ion and electron densities are passed from POPUL through common block POPU. The absorption coefficient is stored in KAPPA(300) and is passed in common block ABSORP for use in INTEG.

COMMON BLOCKS: ABSORP, COMEND, CONTR, POPU, SAHDT, TEMP.

CALLED FROM: MAIN.

SUBROUTINES CALLED: NONE.

EMBAR(TENER): This subroutine calculates the average ionization state of the gas mixture by solving a system of continuous forms of the Saha equation. Each Saha, which is a transcendental equation, is solved iteratively. Since each Saha equation is affected by ionization states of the other species, the whole system is then solved iteratively. This subroutine
also calculates the total internal energy density of the mixture of gases and returns it in the variable TENER.

COMMON BLOCKS: POPU, SAHD1, TEMP.

CALLED FROM: MAIN.

SUBROUTINES CALLED: LHSF.

INPUT: This subroutine reads atomic ionization potentials, sets the parameters necessary for computation and output and prints a heading which lists the initial parameter used. The ionization potentials are read from units 12 through 16 for gas species number 1 through 5 respectively. There must be NGAST files provided starting consequently in unit 12. The ionization potentials for species LGAS are stored in POT(LGAS,55), which is passed in common block SAHD1 for use in other subroutines. The parameters needed for output and computation are passed to the other subroutines in common block CONTR. A sample output heading with the listed parameters is shown in Appendix A. A more complete description of the manner in which data may be read and parameters may be specified is given in the section on INPUT/OUTPUT.

COMMON BLOCKS: COMEND, CONTR, SAHD1.

CALLED FROM: MAIN.

SUBROUTINES CALLED: None.

INPUT/OUTPUT: There are two types of input for this code: atomic ionization potentials and changes to the parameters which control the operation of the code. Both modes of input occur in subroutine INPUT.

Atomic ionization potentials are read into the matrix POT from units 12 through 16. The ionization potentials are read, one piece of data per record, under a D 12.6 format. The number of records read is IZGAS(LGAS)+1, which must be at least six, but under no circumstances will more than 55 records be read. There must be at least IZEE+1 or 55, whichever is smaller, records in
these files. There must also be NGAST files, starting with unit 12. This data must be written in double precision real.

The controlling parameters are first set to the default values in Table II. Parameters having no default values are DEN(LGAS), IZGAS(LGAS), and ATMAS(LGAS), the atomic masses in grams. These must be set and any desired changes to the other parameters may be made through a namelist read from unit 5. On a Univac 1110 unit 5 is the input buffer. The namelist contains all of the parameters listed in Table II and IZEE, POT, DEN. POT is included so that specific changes to the ionization potentials may be made without changing the data files. IZEE must be chosen so that the data files meet the conditions described in the previous paragraph. As noted in the section describing MAIN, the values of DEN(LGAS) depend upon the values of IDEN(LGAS). Values for DEN(LGAS) must be chosen for LGAS between 2 and NGAST. The file containing these changes must be in unit 5 and must be named INIT. An example of such a file is given in Appendix A.

There are also two types of output from this code: printed results and storage of the results on disk files. The output is achieved in subroutine OUT2. The results include Rosseland and Planck mean free paths, ionization states, and internal energies per unit mass. The mean free paths are in units of centimeters, the ionization states in units of electronic charge and the internal energies in units of MJ per gram times UNFAC. For each combination of density, radiation temperature and plasma temperature there is one set of these results where the density is tabulated in cm$^{-3}$ and the temperatures are in electron volts. The printed output is exemplified in Appendix A. To be useful in other computer codes, the results are also written onto disk files. These are all written in single precision real with a 4E12.6 format, so that there are up to four numbers per record. The Rosseland mean free path
is written onto unit 20, the Planck onto unit 21, the ionization state onto unit 22, and the internal energy per unit mass onto unit 23.

Table II
Code Controlling Parameters and Default Values

<table>
<thead>
<tr>
<th>Name</th>
<th>Default Value</th>
<th>Use</th>
</tr>
</thead>
<tbody>
<tr>
<td>IPRT(1)</td>
<td>0</td>
<td>If ≠ 0, print absorption coefficient</td>
</tr>
<tr>
<td>IPRT(2)</td>
<td>20</td>
<td># of steps per sub-integrand</td>
</tr>
<tr>
<td>IPRT(3)</td>
<td>0</td>
<td>If ≠ 0, print end points of subintegrations after they are sorted in numerical order</td>
</tr>
<tr>
<td>IPRT(4)</td>
<td>0</td>
<td>If ≠ 0, print end points before they are sorted</td>
</tr>
<tr>
<td>IPRT(5)</td>
<td>0</td>
<td>If ≠ 0, print ionization states</td>
</tr>
<tr>
<td>IPRT(6)</td>
<td>0</td>
<td>If ≠ 0, skip opacity calculation</td>
</tr>
<tr>
<td>IPRT(7)</td>
<td>0</td>
<td>If ≠ 0, ( T_r = T_p )</td>
</tr>
<tr>
<td>DELEI</td>
<td>2.00</td>
<td>Inverse of width of absorption line in eV</td>
</tr>
<tr>
<td>EPSL</td>
<td>1.0-4</td>
<td>Spacing between sub-integrals</td>
</tr>
<tr>
<td>DELD</td>
<td>.500</td>
<td>Log of the incremental ratio of densities</td>
</tr>
<tr>
<td>DELTR</td>
<td>.16299500</td>
<td>Log of the incremental ratio of radiation temperatures</td>
</tr>
<tr>
<td>DELTP</td>
<td>.16299500</td>
<td>Log of the incremental ratio of plasma temperatures</td>
</tr>
<tr>
<td>DLOW</td>
<td>14.431400</td>
<td>Log of lowest density in result mesh in ( \text{cm}^{-3} )</td>
</tr>
</tbody>
</table>
TLOW
---
-3.9794D0

Log of lowest radiation and plasma temperatures in result mesh in eV

IO
---
1

Log of ratio of density of adjacent mesh points
=DELDxIO

JRO
---
1

Log of ratio of radiation temperatures of adjacent mesh points
=DELTRxJRO

JPO
---
1

Log of ratio of plasma temperatures of adjacent mesh points=DELPxJPO

IMAX
---
17

# of densities in mesh

JRXAX
---
20

# of radiation temperatures in mesh

JPMAX
---
20

# of plasma temperatures in mesh

HIPT
---
2.04

Largest photon energy in integration

HIPOT
---
1.010

Value of POT(I) when IZEE+1<1<55

UNFAC
---
1

The output energies are written on the disk files in units of MJ times UNFAC

NGAST
---
1

# of gas species

IDEN(2,3,4,5)
---
0

If IDEN(LGAS)=0, D(LGAS)=DEN(LGAS);
if IDEN(LGAS)≠0, D(LGAS)=DEN(LGAS)>D(1)

Utility Programs

The utility programs used for MFP are applicable to MIXER so that we will not describe these routines here.
IV. Results for Sodium-Argon Mixtures

As an example of the use of MIXER, we have done a series of calculations for mixtures of sodium and argon. This example was chosen to test the hypothesis that the opacity of an inert light ion beam reactor cavity gas could be manipulated with the addition of small amounts of alkali metal vapor.(5) In such a reactor the $1.8 \times 10^{18}$ cm$^{-3}$ argon is found to be transparent to target generated fireball radiation.(4) Here we show that the addition of less than 2% by volume of sodium will make the cavity gas opaque to this radiation. We will also show ionization states, internal energy densities, Rosseland and Planck mean free paths for an important case.

In Fig. 2, we show the Planck mean free path for $1.8 \times 10^{18}$ cm$^{-3}$ argon for concentrations of sodium ranging from 0% to 2% by volume. The densities are expressed in terms of the partial pressure in torr the gas would have at room temperature. From this graph, where the gas temperature equals the radiation temperature, it is clear that low temperature radiation passes through the gas very easily compared to high temperature radiation. This occurs because photo-ionization, the strongest mechanism of photo-absorption, cannot occur with photons less energetic than the ionization potential of the gas. Since the ionization potential of argon is higher than that of sodium, higher energy photons will pass through argon than through sodium so that the addition of sodium to argon should decrease the low temperature mean free paths. This effect is clearly shown in Fig. 2.

It has been found in a related study that the optimum cavity gas in a light ion beam fusion cavity reactor is $1.8 \times 10^{18}$ cm$^{-3}$ argon with a 0.2% sodium impurity.(5) This mixture is advantageous because it allows the formation of laser initiated plasma channels for beam propagation and protects the first wall of a fusion reactor cavity. The opacity of such a gas is just large enough to protect the wall from large fluxes of thermal radiation while allowing enough radiation out to cool the cavity gas.
The ionization state and internal energy density of this optimal cavity gas are shown in Figs. 3 and 4, respectively. The rapid rise in the ionization state at high gas temperature causes the very non-ideal behavior of the internal energy density. This clearly shows that it is very important, when considering the equation of state, to include the effects of ionization on the energy density.

The Rosseland and Planck mean free paths of this gas mixture are shown in Figs. 5 and 6. The main feature of both of these plots is the sharp increase in mean free paths at low gas and radiation temperatures.

V. Summary and Conclusions

In this paper, we have shown the need for a multi-species gas equation of state computer code. We have presented such a code, MIXER, which we produced by modifying the single species code MFP.\(^6\) Using MIXER, we have shown that small concentrations of alkali metals can greatly change the low temperature opacity of inert gases. Finally, we have presented the optical and equation of state data for a promising choice of a light ion beam fusion reactor cavity gas.

There are several improvements to MIXER which could be made; some of these were mentioned in our description of MFP.\(^6\) One of the most serious causes of inaccuracy in our model is the unsophisticated treatment of the atomic line widths. This could be done much better in the impact approximation.\(^6,8-10\) The range of validity of MIXER could be extended by including the Madelung energy in the high density equation of state\(^11\) and by using the coronal ionization model for the low density equation of state.\(^12\) Molecular gases could be treated if vibrational and rotational transition were included in the calculation of the absorption coefficient.
Acknowledgement

This work was supported by Sandia Laboratory under contract #13-9838.
References


Appendix A

We now present an example of the use of MIXER. The problem shown is for an argon density of $1.8 \times 10^{18}$, a sodium concentration of 0.2% and gas temperatures of .4 eV and .58 eV. Only the first ten default radiation temperatures are used so that the input namelist, which is held in element MIXER INIT and is called INIT, becomes

```
&INIT I2GAS=18,11,
   NGAST=2,
   DEN(2)=2.0D-3,
   IDEN(2)=1,
   ATMAS=6.666D-23,3.176D-23,
   JPMA=2,
   JRM=10,
   IMAX=1,
   DLOW=1.82553D1,
   DELEI=.2D0,
   DNAV=1,D16,
   INOM=9,
&END
```

The first page of output is the heading shown in the next page. This page is printed by subroutine INPUT and it lists all of the parameters used in MFP. The energies, EPSL, HIPT, HIPOT and 1/DELEI as well as the temperatures TLOW, DELTR and DELTP are all in units of eV. The densities DLOW and DELD are in cm$^{-3}$ and the mass ATMAS is in grams.

The remaining page of output is generated by the subroutine OUT2 and is shown below for this example. The units are clearly marked - the density is in cm$^{-3}$, the temperatures are in eV, the mean free paths are in cm, the ionization state is in units of electronic charge and the energy density is in MJ/gm. Even though the energy densities written on the disk files are in MJ/gm times UNFAC, the printed results remain in MJ/gm.
MIXER - A CODE TO CALCULATE THE
EQUATIONS OF STATE AND OPACITIES
OF MIXTURES OF GASES

WRITTEN BY ROBERT R. PETERSON

IPRT(1)
IPRT(1) = 0 PRINT ABSORPTION COEF?
IPRT(2) = 20 # STEPS / SUBINTEGRAND
IPRT(3) = 0 PRINT ENDPOINTS AFTER SORT?
IPRT(4) = 0 PRINT ENDPOINTS BEFORE SORT?
IPRT(5) = 0 PRINT OUT IONIZATION CALC?
IPRT(6) = 0 SKIP MFP CALCULATIONS?
IPRT(7) = 0 TR = TP ?

CONSTANTS USED
DELEI = .200000*000 WIDTH OF ABS. LINE
EPSL = .100000-003 SPACE BETWEEN INTEGRALS
HIPT = .200000+005 HIGHEST PHOTON ENERGY
HIPOT = .100000+011 DEFAULT IONIZATION POT
IZGAS(1) = 18 ATOMIC # OF GAS # 1
IZGAS(2) = 11 ATOMIC # OF GAS # 2
IZGAS(3) = 3 ATOMIC # OF GAS # 3
IZGAS(4) = 0 ATOMIC # OF GAS # 4
IZGAS(5) = 0 ATOMIC # OF GAS # 5
ATMAS(1) = .666600-022 MASS OF ATOM # 1
ATMAS(2) = .361700-022 MASS OF ATOM # 2
ATMAS(3) = .000000+000 MASS OF ATOM # 3
ATMAS(4) = .000000+000 MASS OF ATOM # 4
ATMAS(5) = .000000+000 MASS OF ATOM # 5
UNFAC = .100000+001 JOULES PER ENERGY UNIT

CONSTANTS FOR RESULT MESH
IMAX = 1 # OF DENSITIES
JRMAX = 10 # OF RAD TEMPS
JPMAX = 2 # OF GAS TEMPS
DLLOW = .162553+002 LOG OF LOWEST DENSITY
TLLOW = .397940+000 LOG OF LOWEST TEMPS
DELTR = .162995+000 LOG OF RATIO OF SUCCESSING RAD TEMPS
DELTG = .162995+000 LOG OF RATIO OF SUCCESSING GAS TEMPS
DELGD = .500000+000 LOG OF RATIO OF SUCCESSING DENSITIES
ID = 1 DENSITY SKIP FACTOR
JRD = 1 RAD TEMP SKIP FACTOR
JPG = 1 GAS TEMP SKIP FACTOR
| DENSITY OF FIRST GAS = | \(1.6 \times 10^{11} \text{+19} \) / CM ** 3 |
| DENSITY OF SECOND GAS= | \(3.6 \times 10^{23} \text{+16} \) / CM ** 3 |
| DENSITY OF THIRD GAS = | \(0.0 \times 0.0 \) / CM ** 3 |
| DENSITY OF FOURTH GAS = | \(0.0 \times 0.0 \) / CM ** 3 |
| DENSITY OF FIFTH GAS = | \(0.0 \times 0.0 \) / CM ** 3 |

<table>
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<tr>
<th>DENSITY / CM**3</th>
<th>RAD TEMP E.V.</th>
<th>GAS TEMP E.V.</th>
<th>ROSS MFP CM</th>
<th>THIN MFP CM</th>
<th>CHARGE E</th>
<th>ENERGY DENS J/GM</th>
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Figure 1

Schematic flow chart of MIXER.
Planck mean free paths of argon mixed with various amounts of sodium vs. temperature. The radiation temperature is assumed to be equal to the plasma temperature.
SAHA CHARGE STATE
ARGON - 0.2% SODIUM

Figure 3
Ionization state of argon mixed with 0.2% sodium by volume.
TOTAL INTERNAL ENERGY DENSITY
ARGON - 0.2% SODIUM

Figure 4

Internal energy density of argon mixed with 0.2% sodium by volume.
PLANCK MFP
ARGON - 0.2% SODIUM

Figure 5
Planck mean free path of argon mixed with 0.2% sodium by volume. The argon density is $2.7 \times 10^{18}$ cm$^{-3}$. 
ROSSELAND MFP
ARGON - 0.2% SODIUM

Figure 6
Rosseland mean free path of argon mixed with 0.2% sodium by volume. The argon density is $2.7 \times 10^{18} \text{ cm}^{-3}$. 