GRAN PHYSICS AND R O S S E L A N D M E A N O P A C I T I E S

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ABSTRACT

Tables of mean opacities are often used to compute the transfer of radiation in a variety of astrophysical simulations, from stellar evolution models to protoplanetary disks. Often these tables, such as those in a recent paper by Ferguson and coworkers, are computed with a predetermined set of physical assumptions that may or may not be valid for a specific application. This paper explores the effects of several assumptions of grain physics on the Rosseland mean opacity in an oxygen-rich environment. We find that changing the distribution of grain sizes, either the power-law exponent or the shape of the distribution, has a marginal effect on the total mean opacity. We also explore the difference in the mean opacity between solid homogenous grains and grains that are porous or conglomerations of several species. Changing the amount of grain opacity included in the mean by assuming a grain-to-gas ratio significantly affects the mean opacity, but in a predictable way.

Subject headings: astronomical data bases: miscellaneous — dust, extinction — equation of state — methods: numerical

1. INTRODUCTION

The opacity of gaseous environments is a topic of interest in many areas of astrophysics, including stellar atmospheres, circumstellar and protoplanetary disks, and the interstellar medium. Often, at least in the case of stellar evolution calculations, opacity tables are needed at many temperature, density, and chemical composition points. For high-temperature opacities, modelers often use either the OPAL opacities (Iglesias & Rogers 1991, 1993, 1996; Rogers & Iglesias 1992a, 1992b; Rogers et al. 1996) or the Opacity Project (OP; Seaton et al. 1994) tables. We have produced low-temperature opacities at Wichita State University (Ferguson et al. 2005, hereafter F05) since 1975. These tables differ from their higher temperature counterparts by including the effects of molecules and dust in the equation of state (EOS) and the opacity.

Typical opacity tables provided by our group include over 1600 temperature and density points with the 155 chemical compositions needed for a complete set. Given the large number of input variables, atomic and molecular physics, grain parameters for grain physics, etc., it is not computationally possible to make a complete set of opacity tables for every astrophysically significant situation. Difficult decisions must be made as to how to choose important physical parameters. For example, in the opacity tables of F05, grains are assumed to have a size distribution like the one described in a classic model (Mathis et al. 1977, hereafter MRN), which is based on grain sizes in the interstellar medium (ISM); however, this choice may not be appropriate for different astrophysical environments. This paper discusses some of the choices made in F05 and how those choices affect the total Rosseland mean opacity.

The calculations discussed here are taken from the same code used to complete the opacity tables described in F05, which includes a summary of the equation of state and opacities. For consistency, we begin with the total Rosseland mean opacity, which is defined as

\[ \frac{1}{\kappa_R} = \frac{\int_0^\infty \left( \frac{1}{\kappa_i} \right) \left( \frac{\partial B_j}{\partial T} \right) d\lambda}{\int_0^\infty \left( \frac{\partial B_j}{\partial T} \right) d\lambda}, \]

where \( \kappa_i \) is the monochromatic opacity and \( \frac{\partial B_j}{\partial T} \) is the derivative of the Planck function with respect to temperature. The monochromatic opacity includes the effects of all contributors,

\[ \kappa_i = \kappa_{\text{cont}} + \kappa_{\text{at}} + \kappa_{\text{mol}} + \kappa_{\text{gr}}, \]

where the terms on the right-hand side are the continuous, atomic, molecular, and grain sources of opacity, respectively. Note that the Rosseland mean is a harmonic mean, one in which individual contributors cannot be added after the mean is taken. This is particularly true of the molecular opacities, which may have a large number of individual lines or bands. If it is desired that an individual source of opacity be modified, it is usually the case that the whole integral must be recomputed. A detailed description of these sources is given in F05. We focus in this paper on the details of the grain contribution to the monochromatic opacity.

The opacity due to a particular dust species can be computed from

\[ \kappa_{\text{gr}} \rho = \pi \sum_i n_i(a) Q_{\text{ext}}(a, i, \lambda) a^2 da, \]

where \( n_i(a) \) is the number of dust particles (in units of \( \text{cm}^{-3} \)) of species \( i \) of size \( a \) and \( Q_{\text{ext}}(a, i, \lambda) \) is the total extinction (absorption plus scattering) efficiency of the particle. The size distribution \( n_i(a) \) depends on both the number abundance of species \( i \) and on the size distribution of the dust particles. Ordinarily, in
our opacity tables the size distribution is taken from MRN, the
classic distribution of dust sizes in the ISM, which is given by

\[ n_i(a) = ka^q, \quad (4) \]

where \( k \) is a normalization constant of the distribution and \( q \) is the
exponent of the power law. In F05 the value of \( q \) is taken to be the
classical MRN value of \(-3.5\).

Additional work by many other groups has resulted in other
“favored” size distributions; however, none of them have fully
superseded the work of MRN (Clayton et al. 2003). Other
distributions, such as those of Kim et al. (1994, hereafter KMH94)
and Weingartner & Draine (2001, hereafter WD01), use power
laws as their basis, but they include transitions for large grains
so that the distribution behaves smoothly. For carbon grains,
WD01, using the work of Draine & Li (2001) and Li & Draine (2001),
go a step further and include multiple distributions for
different sizes of grains. While this is not an exhaustive list of
size distribution used in the astrophysical community to-
day, it is representative of the types of grain models available.
Each of the distributions listed have been inserted into our code
for comparison with the MRN distribution.

In equation (3), the grain extinction efficiency is computed
with Mie theory, assuming that grains are solid. This may not
be the case in all, or any, astrophysical environments. Many
researchers argue that interstellar grains are likely to be porous or
“fluffy” in nature (see, for example, Mathis & Whifin 1989;
Mathis 1996; Chiar & Tielens 2006). Having grains that are part
vacuum can significantly affect the opacity (see Wolff et al. 1994,
1998; Voshchinnikov et al. 2005). However, in astrophysical
grains the amount of porosity, generally defined as the volume
fraction of vacuum, is not well constrained; Chiar & Tielens
(2006) interpret observations to constrain the porosity of dust in
the ISM to be in the 25%–50% range, whereas Mathis (1996)
indicates that dust may be up to 80% vacuum.

Related to the porosity of grains is the question of whether
gains are composed of aggregates or are homogeneous. It is likely
that astrophysical grains are not homogeneous, as is assumed
in the opacity tables of F05, but rather are an aggregate of two,
three, or more different species. The effect of heterogeneous
grains on the mean opacity, using the utilities of Ossenkopf
(1991), will be discussed below.

The opacity tables of F05 assume that gas and dust are in
equilibrium, but this may not be the case in real environments
due to dynamical effects such as winds or gravitational settling
of gains. One simple way to mimic the effects of grains either
setting or being blown out of an environment is by changing the
gain-to-gas ratio by assuming that certain percentages of grain
material have been removed from the gas.

This work is an exploration of the effects of grain physics on
the total Rosseland mean opacity of a gas at cool temperatures
(below \( \sim 3200 \) K). Opacities calculated here are for solar abun-
dances from Grevesse & Noels (1993), scaled to \( X = 0.7 \) and
\( Z = 0.02 \) (where \( X \) is the mass fraction of hydrogen and \( Z \) is the
mass fraction of metals), for \( 2.7 \leq \log T \leq 3.30 \) and a constant
value of \( \log R = -3.0 \) (see F05). The value of \( \log R = -3.0 \)
best models the atmosphere of an AGB-type star and was arbit-
trarily chosen here as a convenient way to demonstrate grain
physics effects. All comparisons are done in an oxygen-rich chem-
istry and include only silicate grains; future work will emphasize
carbon grains. We will discuss five important aspects of grain
physics in the following sections: (1) the size distribution expo-
nent (see eq. [4]), (2) the size distribution itself, (3) grain po-
| porosity, (4) aggregate grains, (5) and the relative grain-to-gas ratio.

2. GRAIN PHYSICS

In gas at high temperatures, above \( \sim 5000 \) K, neutral and ion-
ized atoms (including lines) are the dominant opacity sources. As
the temperature decreases, molecular effects become significant
and begin to dominate the opacity (see F05). Below \( \sim 1600 \) K,
at \( \log R = -3.0 \), grains begin to appear in the equation of state
and quickly become the strongest source of opacity. For pur-
poses of illustration, a plot similar to one from F05 is given in
Figure 1, with the regions of dominant opacity marked. The fea-
tures below \( \log T = 3.2 \) are caused by various grain species ap-
ppearing or disappearing from the equation of state. At \( \log T =
3.2 \), solid \( Al_2O_3 \) appears in the EOS and causes a sudden rise
in total opacity as the temperature decreases. Silicate grains
begin to appear at \( \log T \sim 3.08 \). The opacity has another bump at
\( \log T = 3.02 \), where solid Fe appears and becomes the dominant
source of opacity. At temperatures below \( \log T = 3.0 \), iron and
silicates are the predominant opacity sources (F05); no addi-
tional significant species appear or disappear, and the mean opac-
ity is fairly featureless, gradually lessening as the temperature
decreases.

The opacity tables computed in F05 assumed spherical, solid,
homogeneous grains with sizes that obeyed the MRN size dis-
tribution and with absorption and scattering cross sections that
could be simulated with Mie theory. We further assume in F05
that the grains form in equilibrium with, and remain with, the gas
in which they form. We will relax a few of these assumptions in
the following subsections to explore how the Rosseland mean
opacity is affected.

2.1. Size Distribution Exponent

Equation (4) is a normalized power-law distribution. As the
value of the exponent, \( q \), is varied—i.e., as the power law steep-
ens or flattens—the size distribution will vary. As \( q \) increases,
the function will become steeper; that is, there are more small gains
than large gains. The distribution is normalized for each grain
species so that the volume of grain material is constant for the
different values of \( q \). The normalizations and summations are
performed in terms of \( \log a \), where \( a \) is the grain size.

As an illustration, we include a plot of the “guts” of equa-
tion (3) in Figure 2. The figure shows how \( Q(a)n(a)a^2 \) behaves
for a single grain species (Al$_2$O$_3$) and a single wavelength (1 $\mu$m). As the exponent of the size distribution increases from $-2.5$ to $-5.5$, the size distribution, $n(a)$, steepens, but $Q(a)n(a)a^2$ flattens out. This flattening is due to the combination of the $a^2$ factor and the extinction efficiency $Q$ increasing with size (as the grains are smaller than the Rayleigh limit) for the species shown.

What happens to the mean opacity if the value of the power-law exponent, $q$, is varied from $-2.5$ to $-5.5$? Figure 3 shows that the mean opacity in the dust region ($\log T < 3.2$) increases as the power law flattens out. Considering Figure 2, this result is not surprising. As the grain size distribution, $Q$, flattens out, the extinction efficiency, which is a function of grain size but not of the distribution, rises for larger grains. Thus, a flatter grain size distribution contains more large grains, and those larger grains contribute more to the total opacity.

The overall result for the mean opacity is that a flatter grain size distribution results in more opacity by as much as a factor of 3 when the power-law exponent changes from $-4.5$ to $-2.5$. It is easy to see the difference that results from changing the exponent, $q$, to the mean opacity in the bottom panel of Figure 3. In the bottom panel, the logarithm of the ratio of the mean opacity computed with a certain $q$-value compared with the baseline value of $-3.5$ is shown. This type of plot easily allows us to see the change in the mean opacity.

There are several features in the bottom panel of Figure 3 that deserve discussion, such as the stair-step behavior seen in the comparison of the $q = -5.5$ computation with the baseline. We include in our computations of the total mean opacity several species of grains with their different optical constants and extinction efficiencies. As different species appear or disappear from the EOS, the mean opacity is affected in a variety of ways based on the dominant species. More particularly, there is a large dip in the mean opacity is the range $3.04 \leq \log T \leq 3.08$. This feature, and the much smaller one seen in the $q = -4.5$ computation, is due to the differing effects on changing the size distribution for different species. In the bottom panel of Figure 3, at $\log T = 3.08$ the difference between the baseline and the $q = -5.5$ computation begins to move downward as the Mg silicates begin to dominate the opacity. The difference then moves upward at the Mg silicates become the dominant source of opacity (see F05). Changing the size distribution in the same way for every species in our EOS has a different effect on that species’ contribution to the total mean opacity.

Note also that the comparisons with the $q = -2.5$ and $q = -4.5$ computations are not symmetrical about the reference line at 0.0. This shows that changing the value of the exponent does not lead to a linear or clearly defined change in the mean opacity. This fact is not surprising, as we note in Figure 2 that the extinction efficiency, which is a function of grain size, rises with $a$, but not in a linear way.

It would be convenient to have a scaling factor with which to convert the baseline opacities to a set of mean opacities with a different grain size distribution, and this may be possible away from transition zones. However, at those temperatures where the dominant grain species are changing, a simple scaling factor is not possible.

### 2.2. Grain Size Distributions

The size distributions discussed in §1 have been added to our opacity code, and to be complete, we include a short summary of the KMH94 and WD01 grain size distributions. The size distribution from KMH94 is given by

$$n_i(a) = ka^q \exp(-a/a_i),$$

where $a_i$ is the transition size for the exponential decay. The values chosen for our computations are discussed below.

A more sophisticated grain distribution, which includes a smoother transition from the power law to the exponential decay, is given by WD01 for silicate dust and has the form

$$\frac{dn_i}{da} = \frac{k}{a} \left( \frac{a}{a_i} \right)^q F(a; \beta, a_i)$$

$$\times \left\{ \begin{array}{ll}
1, & 3.5 \text{ Å} < a < a_i, \\
\exp\left\{-[(a - a_i)/a_i]^{3}\right\}, & a > a_i,
\end{array} \right.$$
Similar distributions are assumed by WD01 for carbon or graphitic grains, which include a lognormal distribution for the grain sizes to account for the very small grains thought to emit the “unidentified infrared” (UIR) bands seen in the diffuse ISM. The comparisons in the present paper focus on oxygen-rich mixtures, and carbon grains do not exist under these conditions.

For our comparisons, we use the values given by WD01 for silicate dust in the ISM; that is, \( a_i = 0.17 \) \( \mu m \) and \( a_e = 0.1 \) \( \mu m \), with a value of \( \beta = 0.3 \) and a power-law exponent of \( -2.1 \) for all grain types. The computations using the KMH94 distribution use their stated parameters as well. That is, \( a_i \) is taken to be 0.14 \( \mu m \), and a value of \( -3.06 \) for \( q \) is used for silicate dust.

Figure 4 shows the comparison between the Rosseland mean opacities computed with grain size distributions from MRN, WD01, and KMH94. In the figure, the mean opacities are shown in the top panel and the differences in the logarithm of the opacities is shown in the bottom panel. The results show that the mean opacities are somewhat similar, with MRN having the lowest values, WD01 having higher values, and KMH94 having the highest values of mean opacity. It is interesting to note that the KMH94 distribution, with a very simple exponential transition for large grains, tends to tail upward at the lowest temperatures. At log \( T = 2.7 \) (500 K), silicate grains are the dominant source of grain opacity, with solid iron grains falling in abundance in favor of FeS (see Fig. 1 of F05).

There is also a strange series of bumps in the bottom panel of Figure 4 at intermediate temperatures, \( 3.00 < \text{log} \ T < 3.15 \). As discussed in the previous section (§ 2.1), these temperatures constitute a transition region in which the strongest opacity source is passing from minor grain species to the silicates to solid Fe. Different grain species have different contributions to the opacity based on which form of the size distribution is used, due to different optical constants and extinction efficiencies. The feature seen in the bottom panel of Figure 4, centered at log \( T = 3.08 \), in the computations with KMH94 compared with the baseline, is much more pronounced than in the computations with WD01. The difference between the KMH94 and WD01 grain distributions is in how the size transition to large grains is treated. The minor grain species are much more sensitive to the KMH94 distribution than the solid Fe grains are, since when solid Fe dominates the opacity, both the KMH94 and WD01 computations appear to be a simple scaling factor greater in the mean opacity.

As discussed in the previous section, there does appear to be a simple scaling factor that might apply to the grain distributions, but only for a limited range in temperature, \( 2.80 < \text{log} \ T < 3.02 \). At other temperatures, where the strongest opacity source is changing from one grain species to another, no such simple scaling factor is evident.

Overall, the effect on the mean opacity is fairly significant, with the KMH94 calculation differing from the baseline (MRN) by 0.27 dex at log \( T = 2.9 \) (800 K), or nearly a factor of 3. As Figure 4 shows, the difference from the baseline is not constant with temperature, especially in the regions in which the significant contributors to the opacity are from different grain species (with different extinction efficiencies). For example, at around log \( T \sim 3.15 \) the differences between the computations are smaller than those at cooler temperatures. This implies that arbitrarily adding a factor of 3 to the mean opacity tables of F05 to mimic the effects of different size distributions is not a good approximation. This is particularly true when combined with the mean opacity changes with differing size distribution exponents, as described above.

### 2.3. Grain Porosity

Calculations of grain efficiencies due to grain porosity are taken from Bohren & Huffman (1983). To initially probe the effect of porosity on the mean opacity, we assume that the vacuum inclusions are spherical, and we use either the Maxwell-Garnett or the Bruggeman average dielectric constant for the grain/vacuum composite. The Maxwell-Garnett constant is more appropriate for a mixture in which the matrix and inclusions are well defined.

The Bruggeman approximation is more symmetric and is valid for a two-component mixture in which the matrix and inclusions are indistinguishable. As Bohren & Huffman (1983) discuss, both the Maxwell-Garnett and Bruggeman approximations are equally valid, but either one or the other will be more valid in a particular circumstance.

In our computations we find that certain grain species misbehave when we use the Bruggeman approximation. Most particularly troubling is solid Fe. At certain wavelengths, the \( k \) portion of the optical constant will be unphysically negative, causing the mean opacity to increase discontinuously by large factors. To test our method, we have utilized the publicly available average dielectric routines of Ossenkopf (1991) and found that this program fails to compute porous Fe grains without either blowing up with a fatal error or producing negative parts of the optical constants. We have decided to remove Fe from the porosity computation and let it remain solid and not porous. We assume that the other grain species are valid under the Bruggeman assumption, in which the EOS is mostly dominated by MgSiO3 and Mg2SiO4 at 1000 K and below (see Fig. 1 of F05).

Results for a range of grain porosities, denoted by the volume fraction \( f \), are shown in Figure 5, with the mean opacities shown in the top panel. The baseline value is \( f = 0.0 \) (solid grains), and
the tested values include \( f = 0.1, 0.25, 0.5, \) and 0.8. Recent work by Chiar & Tielens (2006) reports porosities of grains in the ISM as being between 25% and 50% vacuum by volume, in line with previous studies by Wolff et al. (1993). The bottom panel shows the opacity differences compared with the baseline of \( f = 0 \).

As the porosity of grains is increased, the total mean opacity is mostly unaffected, except for the largest f-value. This is somewhat intuitive in that since the mean opacity is already dominated by small particles, making those small particles slightly larger does not change the mean opacity greatly. At the largest value of porosity, \( f = 0.8 \), the mean opacity does change by as much as 50% at the lowest temperature shown. Note that at "intermediate" temperatures, \( 3.05 < \log T < 3.13 \), the bottom panel of Figure 5 clearly shows that the mean opacity decreases with increasing porosity. The materials responsible for most of the mean opacity at these temperatures are \( \text{SiO}_2 \), calcium silicates, and \( \text{MgAl}_2\text{O}_4 \) for the most part (see Fig. 1 of F05). As these types of grains become larger and more porous, they also become more transparent, unlike the silicates at cooler temperatures, where the mean opacity slightly increases with porosity.

### 2.4. Aggregate Grains

To explore the use of aggregate grains and their effects on the Rosseland mean opacity, we compute the average dielectric function as outlined by Bohren & Huffman (1983), using effective medium theory (EMT). More specifically, we assume the Maxwell-Garnett theory for aggregates, which is valid as long as the inclusions obey the Rayleigh limit, as illustrated by Wolff et al. (1998). We use this simple EMT approximation rather than a more formal solution such as a discrete dipole approximation (DDA) due to limits on computational time. In addition, many of the features of a DDA are not needed for mean opacities computations, such as the scattering and polarization phase functions.

To make a comparison with the baseline runs as outlined above, we assume an aggregate grain that is similar in composition to the silicate species computed in our EOS at \( \log T = 2.9 \) (800 K) and that has ratios similar to the silicates found in the inclusions of a typical meteorite such as Semarkona, as discussed in Hewins et al. (1996). While our EOS did not ideally produce the Semarkona results, qualitatively it was fairly close; we compared our EOS with that of Semarkona and chose a median value. The ratios of enstatite, forsterite, fayalite, and silicon dioxide were assumed to be 42%, 36%, 12%, and 10%, respectively. We computed the average dielectric functions using the routines of Ossenkopf (1991) with the stated ratios. Solid iron grains were kept separate from the aggregate, as is found in meteoritic inclusions. The mean opacity was then computed at a single temperature and density (\( \log R \)) point and was compared with the baseline. Repeating this numerical experiment at lower temperatures did not dramatically change the results.

The comparisons show that aggregate grains have a lower mean opacity, on the order of 0.05 dex (12%) below the baseline, which is a smaller change than that shown in Figure 3 for changes in the grain size exponent \( q \) from \(-3.5\) to \(-4.5\). The amount of change in the mean opacity for aggregate grains from the baseline is very modest and is near the estimated range of error in the grain thermodynamic and optical data of 0.02 dex (5%) based on comparisons with other opacity databases (see F05). This result implies that including or not including aggregate grains in the computation of the mean opacity is not an important decision when computing mean opacity tables.

### 2.5. Grain-to-Gas Ratio

The opacities of F05 were not intended to be used in non-equilibrium conditions. However, we can mimic such environments, such as conditions of gravitational "rainout." If the gas/dust environment is under a gravitational influence with insignificant radiation pressure, then grains that should appear in the equation of state will settle down into the gravitational potential and "disappear" from view. This will leave behind the appearance of a grain-depleted, or a gas-rich, environment. This is best simulated by letting the grains appear in the equation of state, but not counting their opacities. Figure 6 shows such simulations. The baseline amount from F05 includes 100% of the grain
opacity for each species. The top panel of Figure 6 shows the effects of including 50%, 10%, and 1% of the total grain opacity.

The effect on the mean opacity is roughly equivalent to the amount of grains removed from the grain opacity term. That is, if the grain opacity is cut in half, then the total mean opacity is also roughly half of the baseline value because the grain opacity usually completely dominates the total opacity whenever grains are present. This is easy to see in the bottom panel of Figure 6. Note that this effect is not true for all temperatures, however. At higher temperatures, the differences in the opacities (between the baseline and the test cases) are not smooth. Just below the grain appearance temperature at \( \log T \sim 3.2 \), there is still a modest molecular opacity present. If a small amount of grain opacity, say, 1%, is added to the (now) larger molecular opacity, the roughly linear scaling does not apply. As the molecular opacity drops at lower temperatures, there is a roughly linear relationship between the amount of dust included in the monochromatic opacity and the total mean opacity. This result means that, to a reasonable approximation, the opacity tables of F05 could, in principle, be modified to account for the effect of a grainless gas by multiplying by the desired factor, but only at the coolest temperatures. It would not be advisable to do so near the transitions between molecules and grains dominating the opacity.

3. DISCUSSION

This work implies that caution should be taken when requesting or downloading prefabricated opacity tables and using them in environments in which grain condensation is significant. It is important to include the physical effects that are desired in order to have accurate opacities; most notably, changes in the size distribution can greatly affect the Rosseland mean.

Opacity tables for the F05 base set are available for download at our Web site. Custom opacity tables for nonstandard compositions or for different physical assumptions are available upon request, as are tables in gas density or gas pressure space instead of in \( \log R \). Note that a full set of opacity tables as outlined in Ferguson et al. (2005), with (now) 155 values of hydrogen (\( X \)) and metal (\( Z \)) abundances, takes approximately a week of computer time to complete, due to our full treatment of the molecular opacity sampling.

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6 See http://webs.wichita.edu/physics/opacity.