THE LIMITING EFFECTS OF DUST IN BROWN DWARF MODEL ATMOSPHERES

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ABSTRACT
We present opacity sampling model atmospheres, synthetic spectra, and colors for brown dwarfs and very low mass stars in the following two limiting cases of dust grain formation: (1) Inefficient gravitational settling (i.e., the dust is distributed according to the chemical equilibrium predictions) and (2) efficient gravitational settling (i.e., the dust forms and depletes refractory elements from the gas, but their opacity does not affect the thermal structure). The models include the formation of over 600 gas-phase species and 1000 liquids and crystals and the opacities of 30 different types of grains including corundum (Al₂O₃), the magnesium aluminum spinel MgAl₂O₄, iron, enstatite (MgSiO₃), forsterite (Mg₂SiO₄), amorphous carbon, SiC, and a number of calcium silicates. The models extend from the beginning of the grain formation regime well into the condensation regime of water ice (T_eff = 3000–100 K) and encompass the range of log g = 2.5–6.0 at solar metallicity. We find that silicate dust grains can form abundantly in the outer atmospheric layers of red and brown dwarfs with a spectral type later than M8. The greenhouse effects of dust opacities provide a natural explanation for the peculiarly red spectroscopic distribution of the latest M dwarfs and young brown dwarfs. The grainless (cond) models, on the other hand, correspond closely to methane brown dwarfs such as Gliese 229B. We also discover that the \( \lambda \lambda 5891, 5897 \ Na \ I \ D \) and \( \lambda \lambda 7687, 7701 \ K \ I \) resonance doublets play a critical role in T dwarfs, in which their red wings define the pseudocontinuum from the \( I \) to the \( Z \) bandpass.

Subject headings: stars: atmospheres — stars: fundamental parameters — stars: low-mass, brown dwarfs

On-line material: color figure

1. INTRODUCTION
The discovery of the first unambiguous evolved brown dwarf (Gliese 229B; Oppenheimer et al. 1995; Nakajima et al. 1995), the confirmation of the existence of young brown dwarfs in the Pleiades open cluster (Rebolo et al. 1996; Basri, Marcy, & Graham 1996; Zapatero Osorio et al. 1997a), and the detection of dozens of others from photometric (Delfosse et al. 1997; Kirkpatrick et al. 1999b; Strauss et al. 1999; Tsvetanov et al. 2000) and proper-motion surveys (Ruiz, Leggett, & Allard 1997) have restricted the intriguing gap between stars and planets. In fact, brown dwarfs are bright enough to be easily detected in standard bandpasses (\( ZJHK \)) from ground-based facilities. This is now understood as the natural consequence of strong absorption bands of \( H_2O \) and \( H_2 \) that depress the infrared flux in favor of the near-infrared bandpasses, far from any blackbody distributions. This effect was already apparent from the results of our model atmospheres (Allard & Hauschildt 1995), which were later extended deeper into the temperature regime of evolved brown dwarfs by Allard et al. (1996). As brown dwarf discoveries unfold, however, the following questions arise: Why do brown dwarfs appear to form two distinct subgroups: (1) hotter red objects just below the stellar main sequence and (2) much cooler and blue methane dwarfs? Is the apparent gap between these groups real? Are different physical processes involved in their atmospheres beyond the change of effective temperature?

From previous model atmospheres, it immediately appeared more difficult to explain the behavior of the hotter brown dwarfs than that of the methane dwarfs, in which water vapor and methane bands naturally matched the predictions of models (Allard et al. 1996; Tsuji et al. 1996b; Marley et al. 1996) within the accuracy of available molecular absorption profiles. Even the most detailed model atmospheres had failed to reproduce accurately the spectroscopic and photometric properties of red dwarfs later than about M6: all models were systematically too blue by as much as a magnitude in standard infrared colors \( (V-K, I-K, J-K) \). Allard et al. (1997) have reviewed this situation and the atmosphere modeling at the bottom of the main sequence. The reason for these discrepancies was the onset of dust grain formation. As mass decreases along the main sequence, the latest type red dwarfs bear outer atmospheric layers that reach temperatures well below 1800 K, favoring the formation of dust grains. While it has been long suspected that grains could form under these conditions (Lunine et al. 1989), the inclusion of such a computation to nongray model atmosphere calculations had to wait until—using Gibbs free energies of formation (Burrows et al. 1993) and a simple sphere approximation for the Mie opacity of the grains—Tsuji et al. (1996b) published their exploratory
nongray dusty brown dwarf models. They explored the formation of three dust grain species: Al$_2$O$_3$, Fe, and MgSiO$_3$, and found corundum (Al$_2$O$_3$) to be a very abundant and powerful continuous absorber in red dwarfs with a spectral type later than M8, while cooler methane brown dwarfs appeared comparatively grainless, but their models were based on band models for molecular opacities and could not reproduce the optical spectral distributions and several photometric properties of brown dwarfs.

Recently, Tsuji, Ohnaka, & Aoki (1999) and Ackerman & Marley (2001) have explored models with a finite radial extension of silicate clouds to address the systematic difference between early L- and late T-type brown dwarfs. While it is pertinent to explore such processes, several parameters must inevitably be used to characterize them, and, moreover, these are likely to be time-dependent processes (Bailer-Jones & Mundt 2001; e.g., I-band variability has been recently detected in young brown dwarfs). So, while we do believe that dust diffusion (referred to hereafter as gravitational settling) contributes to reducing the radial extension of clouds in these atmospheres, we feel that, as in all unsolved physical problems, it is important to explore carefully the limiting cases. In this paper we therefore present our model calculations for the following two opposite limiting cases of dust content in brown dwarfs atmospheres: (1) inefficient gravitational settling (i.e., the dust is distributed according to chemical equilibrium predictions, which provides the maximum impact of dust on the brown dwarf properties) and (2) efficient gravitational settling (i.e., the dust forms and depletes refractory elements from the gas, but their opacity does not affect the thermal structure, hence a minimal effect on brown dwarfs properties).

These models bring substantial improvements to the number of grains included both in the chemical equilibrium and in the opacity database as well as with regards to the molecular opacities in the previous similar work of Tsuji, Ohnaka, & Aoki (1996a). In § 2 we describe how hundreds of grain species are now included self-consistently in the chemical equilibrium calculation to allow us to identify the hot condensates that are most abundant in the atmospheres of late-type M dwarfs and brown dwarfs. In § 3 we describe our treatment of the grain opacities. In § 4 we describe the detailed opacity sampling model atmospheres to which these grain formations and opacities are incorporated. Section 6 is reserved for the discussion of the atmospheric structures, while the effects of grains on the spectroscopic and photometric properties of brown dwarfs are discussed in §§ 7 and 8, respectively.

2. CONDENSATION AND THE CHEMICAL EQUILIBRIUM

The chemical equilibrium (CE) of the atmosphere code PHOENIX is solved simultaneously for 40 elements, with usually two to six ionization stages per element and 600 molecular relevant species for oxygen-rich ideal gas compositions. This CE has been gradually updated since Allard & Hauschildt (1995) with additional molecular species using the polynomial partition functions of Irwin (1988) and (Sharp & Huebner 1990, hereafter SH90). The molecular ions TiO$^+$ and ZrO$^+$, which have been found to be important in the balance of TiO and ZrO when departures from the local thermodynamic equilibrium are present (Hauschildt et al. 1997), have been added using the partition functions by Gurvich & Glushko (1982). The ions H$_3^+$ and H$_2^+$, which are important electron donors in low-metallicity subdwarf stars and white dwarfs (see Saumon et al. 1994), have been added to our CE and opacity database by using the partition function of Neale & Tennyson (1995) and a list of 3 × 10$^5$ transitions by Neale, Miller, & Tennyson (1996).

To include dust grains, we have expanded the CE system to include the complete series of over 1000 liquids and crystals also studied by SH90. For each grain or liquid species, we followed the prescriptions of Grossman (1972) and used Gibbs free energy of the formation $\Delta G(T)$, drawn from the JANAF 1986 database (Chase et al. 1985), to compute the so-called equilibrium pressures $P_{eq} = \exp^{-\Delta G(T)/RT}$ of the grains, where $R$ is the gas constant and $T$ is the local gas temperature. $P_{eq}$ was then compared to the pressure $P_c$ obtained from the Guldberg law of mass action (i.e., the product of the pressures of the constituting elements). The abundance of a condensed species was then determined by the condition that this species be in equilibrium with the gas phase $P_c \geq P_{eq}$. For corundum,

$$P(Al_2O_3) = \frac{P(Al_2O_3)^{\text{max}}}{P_{eq}}$$

for $P_{eq} \leq P(Al_2O_3)^{\text{max}}$, where the superscript “max” refers to the maximum concentration of grain cores (one core of corundum equals one Al$_2$O$_3$ unit) given the conservation of the cores of each elements. The complete CE was then solved by the Newton-Raphson iteration of the equation system (Allard 1990; see also Allard & Hauschildt 1995) until the error relative to the gas pressure of all the partial pressures was below −6 dex. The computations were then performed and tabulated in a $[P,T]$-plane largely encompassing the conditions prevailing in low-mass stars and brown dwarfs ($P = −4$ to 12 and $T = 15,000$–10 K) using a solar mix (Grevesse & Noels 1993), except in the case of lithium (meteoritic abundance, same source). The CE tables were then interpolated in the construction of the model atmospheres.

The CE therefore self-consistently accounts for the depletion of refractory elements as a function of the gas temperature and pressure conditions in the model atmospheres. However, it should be clear that thermodynamic equilibrium studies only tell us what can be formed, not what is formed, and the results are only as certain as the JANAF equilibrium constants on which they are based. In favor of CE, note, however, that Lodders & Fegley (1998), who used thermodynamics, were able to explain the abundance patterns of various trace elements dissolved in carbide star dust. We therefore feel confident that our CE calculations allow us at least to reproduce adequately, on average, the limiting thermal and spectroscopic properties of brown dwarfs. However, we do not claim that this CE calculation predicts exactly the distribution of dust species in brown dwarfs atmospheres. Gravitational settling effects would certainly change this distribution. We note in passing that our main results (Allard & Hauschildt 1995 and this paper) concur with both those of SH90 and Tsuji (1973). This consistency between independent CE works is reassuring.

In this paper, contrary to recent calculations by Burrows & Sharp (1999), we have not attempted to handle the effects of gravitational settling (i.e., diffusion of the grains to lower atmospheric layers). We do not account for elemental abundance depletion resulting from dust grain settling. This process is likely to be important in the uppermost layers of brown dwarf atmospheres and would tend to deplete these
layers of their refractory elements and dust grains. However, the error introduced by this omission in the models presented in this paper is small since these represent limiting cases with nonexistent and complete settling, in which the dust opacity has been ignored altogether to recreate the latter case. The available abundance of refractory elements involved in dust formation can, however, be slightly overestimated. The complete treatment of gravitational settling goes beyond a simple parametrization of the problem and involves solving the diffusion of the dust as a function of the characteristic timescale of several important processes such as the sedimentation, coagulation, condensation, and convective mixing of the dust. This paper is, however, under development, and we will present our findings in a separate publication.

Since the predictions of CE calculations have been described in detail by Tsuji (1973) and Lodders (1999), we do not deem it necessary to develop them here again. However, the completeness of the grain species sample included here (within the limits of the CE approximation and JANAF data) provides an opportunity to explore some of the effects of condensation on the composition of late-type dwarf stars and brown dwarf atmospheres. In the atmospheres of brown dwarfs, most of the hydrogen is locked in H₂, most of the oxygen is in CO, H₂O, and SiO, and most of the carbon is in CO and CH₄. The species responsible for the strong optical to near-infrared (0.4–1.1 μm) opacities in M dwarf stars and young brown dwarfs are trace species that are much less abundant than CO or H₂O, which have large opacity cross sections per molecule. The relative abundances of those species are summarized in Figures 1 and 2, which illustrate the nature and progression of the condensation layers into deeper layers of the photosphere as T_eff decreases. At T_eff = 2600 K, which is typical of the young Pleiades brown dwarfs Teide 1 and Calar 3 (see Zapatero Osorio et al. 1997b), the clouds barely touch the top layers of the photosphere, which is located between r₆.2,eff = 10⁻⁴ and 1, depending on the spectral range considered. As can be seen from the inner to outer atmospheric regions (from right to left in the plots), the first species to condense at T ≈ 2000 K is ZrO₂, followed by corundum (Al₂O₃) at T ≈ 1800 K. We clearly identify the perovskite CaTiO₃ as the source of depletion of TiO, which is the principle optical absorber in these atmospheres. However, the depletion occurs in this model only above the photosphere and should leave the spectra relatively unaffected. Other stable species that appear at T < 1600 K are MgAl₂O₄, CaSiO₃, Ca₂SiO₄, Ca₂Al₂SiO₇, Ca₃MgSi₂O₆, and CaMgSi₂O₆, as well as TiO₂ and Ti₂O₃. These grains all compete with the formation of CaTiO₃, and corundum and form an intricate layer of clouds just above the photosphere. Note that contrary to the reports by Tsuji et al. (1996a), corundum is not the most abundant grain species and even disappears in central regions of the clouds.

The situation complicates rapidly as T_eff decreases. Figure 2 shows how the clouds have already invaded most of the photosphere in brown dwarfs of about 1800 K, which is typical of field brown dwarfs such as GD 165B (Becklin & Zuckerman 1988) and Kelu 1 (Ruiz et al. 1997) or the DENIS objects (Delfosse et al. 1997). Dozens of new grain species including iron, enstatite (MgSiO₃), and forsterite (Mg₂SiO₄) are now present. The photospheric gas-phase abundances of TiO, FeH, and CaH (not shown) are now strongly depleted. This is reflected by the gradual disappearance of these features in the latest type M dwarfs and brown dwarfs, a behavior that is already apparent from the observed spectra of brown dwarf candidates BRI 0021, GD 165B, and Kelu 1. The VO abundances seem, on the other hand, much less depleted by the condensation of VO and V₂O₅ occurring only in the upper photosphere, and other compounds of less-reactive elements such as Li, K, Rb, Cs, and CrH are left relatively unaffected, favoring the detection of their features in these objects.

Between T_eff = 1800 and 1000 K, methane (CH₄) gradually forms at the expense of CO. The likelihood of detecting methane lines in the spectra of cool brown dwarfs

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Fig. 1.—Run of the relative abundances of gas phase (solid lines) and crystallized species across a T_eff = 2600 K model atmosphere typical of the young Pleiades brown dwarfs Teide 1 and Calar 3. The condensation of perovskite (CaTiO₃; dashed line) is the principle cause of TiO depletion in the atmospheres of dwarfs later than about M6. The abundance of the condensate Ca₂SiO₄ is drawn at log 10r = −5.0 but is not labeled for sake of clarity.

Fig. 2.—Same as Fig. 1, but for a T_eff = 1800 K model atmosphere typical of the redder known field dwarfs GD 165B and Kelu 1 and the DENIS objects.
therefore depends on the height in the atmosphere where this transition regime occurs and on $T_{\text{eff}}$, gravity, and dust opacity conditions such as gravitational settling, rotation, winds, etc.

Although the clouds appear to persist in Figures 1 and 2 out to the outer edge of the photosphere in our coolest models, this only reflects the omission, mentioned above, of the gravitational settling of the grains. Clouds more likely form in thin decks above the deepest condensation layer in brown dwarfs (see, e.g., Tsuji et al. 1999; Ackerman & Marley 2001).

The principle impact of condensation on the photospheres and spectra of cool dwarfs is a gradual depletion of their refractory elements, especially zirconium, titanium, silicon, calcium, magnesium, aluminum, iron, and nickel. Clearly, it is crucial for the balance of the opacities in the models to account for the leading grain species in the CE. Partially accounting for condensation leads to errors of several orders of magnitudes in the model opacities and predicted fluxes (see Allard 1998 for a comparison between existing dusty models). To understand fully the spectroscopic and photometric properties of brown dwarfs, one must also consider the optical and radiative properties of dust grains.

3. DUST CLOUD CONSTRUCTION AND OPACITIES

In this paper we account for the dust opacity only in the limiting case of the AMES-dusty models, in which gravitational settling is neglected and which are relevant for the analysis of hot red dwarfs. In these models, cloud layers build up automatically following the condensation equilibrium that determines the atmospheric layers occupied by the grains. The study of the Jovian planets suggests that cloud layers are not generally distributed homogeneously over the atmospheric surface, but if the nucleation process of dust grains is favored by a combination of high gas densities and low gas temperatures, hotter red dwarfs could be expected to retain more easily smaller grains in their photosphere and have them more uniformly distributed over the stellar surface. In this paper we account for the average effect of the presence of clouds on the model structures and emitted spectra. We therefore assume a plane-parallel symmetry, i.e., an homogeneous distribution of clouds across the surface of the brown dwarfs. The spectral distribution of a brown dwarf with a more complex ring pattern of clouds familiar to Jovian planets could, in the end, be reconstructed from a mosaic of the present models until a full three-dimensional calculation becomes possible.

Early attempts to compute the opacities of grains were made by Cameron & Pine (1973) and Alexander (1975). More detailed calculations, including the effects of CE calculations and grain-size distributions, were reported by Alexander, Johnson, & Rypma (1983) and Pollack, McKay, & Christofferson (1985). Alexander & Ferguson (1994) have described the computation of the opacity of grains with the inclusion of equilibrium condensation abundances, the effects of the distribution of grain sizes, and the effect of grain shape through the continuous distribution of ellipsoid (CDE) model of Bohren & Huffman (1983, p. 82). These calculations included the absorption and scattering due to magnesium silicates, iron, carbon, and silicon carbide grains for a wide range of chemical compositions down to 700 K. We have explored the CDE method employed by Alexander & Ferguson but have retained a purely spherical shape of the grains in the present study for simplicity. Another difference with Alexander & Ferguson is that instead of approximating the number density of grains indirectly, these quantities are now provided by our CE, as described in § 2. Twenty-six new condensates have been added to the original list of Fe, C, SiC, and magnesium silicates for a total of 30, among which are MgSiO$_3$, Mg$_2$SiO$_4$, Al$_2$O$_3$, and MgAlO$_2$, using polarizability constants from laboratory studies by Tropf & Thomas (1990), Koike et al. (1995), Begemann et al. (1997), and Dorschner et al. (1995). Figures 1 and 2 suggest that the calcium silicates can also play an important role in the opacity of brown dwarf atmospheres. In fact, complex calcium silicates (here Ca$_2$Al$_2$SiO$_7$, Ca$_2$MgSi$_2$O$_7$, and CaMgSi$_2$O$_4$) are among the most abundant species in the layers where these grains are present. Since for the latter two species no data were available to construct their opacity profiles, we have simulated their opacity using the profile of Ca$_2$Al$_2$SiO$_7$. We include, in general, more accurate number densities and better and more complete cross sections of dust grains than those included in Alexander & Ferguson (1994). Updated Rosseland and Planck opacities computed with these updated opacities will be published separately in more detail (D. R. Alexander et al. 2001, in preparation).

The opacity profiles of these grains are shown in Figure 3. Most spectral distributions seen in this plot are pure absorption profiles. Scattering contributes only at UV to optical wavelengths for the grain sizes adopted. Corundum, enstatite, forsterite, hematite, magnetite, and Ca$_2$Al$_2$SiO$_7$ have absorption cross sections exceeding those of water vapor. In a brown dwarf atmosphere, however, water is at least 2 orders of magnitude more abundant than most of these grain species, so water vapor remains the leading opacity source between 1 and 8 µm and beyond 20 µm. In other words, grains do not contribute significantly to the opacities in the near-infrared, where water bands still dominate the brown dwarf spectra from J to K (1.0–3 µm).
have demonstrated in § 2 that grain species have concentrations similar to those of TiO, VO, and most other optical absorbers. The impact of the grain opacities is, therefore, to enhance and gradually replace the optical opacities as these gas-phase species disappear via condensation.

The extinction caused by grains in a stellar atmosphere also depends on the rate of grain formation and the resulting size distribution. For all grains included, we have assumed, as in Alexander & Ferguson, an interstellar size distribution of the grains with diameters ranging from 0.00625 to 0.24 μm. For comparison, Tsuji et al. (1996a, 1996b) assumed grains with a fixed diameter of 0.1 μm in their model atmosphere calculations. Although those choices are purely arbitrary, the consequences are minimal since the grain diameter cancels out in the opacity calculations as long as (1) abundance conservatism is assumed (i.e., larger grains must lock more particles, reducing the number of grains per gram of stellar plasma) and (2) that the cross sections behave in the Rayleigh limit (i.e., the wavelength is larger than the size of the grains). Our tests, shown in Figure 4, confirm that this is the case for 1–10 μm size grains, but they also indicate that the scattering increases rapidly for grain sizes larger than 10 μm, i.e., when the Rayleigh limit breaks down over the wavelengths carrying the flux in these objects. Even if the opacities are sensitive to the grain sizes beyond the Rayleigh regime, the enormous scattering effects seen for 100 μm grains in Figure 4 seem to exclude the presence of such grains in brown dwarfs. We therefore believe that such large grains tend to rapidly become larger by coagulation and to be eliminated by sedimentation in these high-gravity atmospheres. An accurate answer to this question can only come from time-dependent grain growth calculations incorporating the effects of sedimentation, diffusion, coagulation, and coalescence for the conditions prevailing in brown dwarf atmospheres. See D. R. Alexander et al. (2001, in preparation) for a detailed description of the dust opacities used in the present models.

4. MOLECULAR OPACITIES

Molecules dominate the spectral distribution of brown dwarfs. Young brown dwarfs hotter than 2000 K emit flux principally in the near-infrared ZJHK bandpasses from 0.9 to 2.5 μm, with bands of water steam in the infrared and TiO and VO bands in the optical shaping each side of this spectral distribution. Below 2000 K, TiO, VO, and CaH bands vanish as a result of the condensation of these refractory elements, and the collision-induced opacities of H₂ and the growth of CH₄ bands become increasingly important in the H, K, and L bandpasses at 1.6, 2.0, and 3.5 μm, respectively. It is this situation that causes the radiation to remain forced to emerge principally from the near-infrared bandpasses rather than emerging redward, as blackbodies would do. Several other molecules are also present in brown dwarf spectra; overtones of CO at 2.3 and 4.7 μm are strong Teff indicators and play an important cooling role on the upper atmospheric structure, vibrational bands of SiO and hydrides such as OH, SiH, and MgH determine the ultraviolet and visual radiation, and the Wing-Ford system of FeH at 0.98 μm is one of the most prominent features in the spectra of late-type stars and young and/or massive brown dwarfs.

Our molecular opacity database includes (1) a list of 43 × 10⁶ atomic transitions by Kurucz (1994), (2) collision-induced absorption opacities for H₂, He, H₂, Ar, CH₄, and CO₂ by Borysow, Jørgensen, & Zheng (1997a, 1997b), Borysow & Frommhold (1986a, 1986b, 1986c, 1987a, 1987b), Borysow & Tang (1993), Samuelson, Nath, & Borysow (1997), and Gruszka & Borysow (1997 and references therein), (3) ab initio line lists for H₂O and TiO by Partridge & Schwenke (1997) and Schwenke (1998), (4) CO from the line list by Goorvitch & Chackerian (1994a, 1994b) and Goorvitch (1994), (5) most other molecular systems such as MgH and OH are included from the list by Kurucz (1993), (5) VO and CrH lines have been calculated by R. D. Freedman (1999, private communication) for this paper, while (6) FeH lines from Phillips & Davis (1993) has been also included. For the remaining molecular band systems for which no line lists were available to us (CaH), we apply the just overlapping line approximation (JOLA) as described and utilized by Tsuji (1995) and Tsuji et al. (1996a, 1996b, and references therein).

We have also included a combination of the HITRAN92 and GEISA databases (Rothman et al. 1992; Hudson et al. 1992), summing up to about 700,000 lines of 31 molecules with a total of 74 isotopes. The molecules with the largest number of lines that are included in our models are O₃ (168,881 lines), CO₂ (60,790 lines), and CH₄ (47,415 lines). This database only includes the strongest lines of these molecules. However, the gf-values and positions of the lines have a comparatively high accuracy and allow us to diagnose their importance in brown dwarf atmospheres. A comparison of models computed with these opacities to the NEXTGEN models (Hauschildt, Allard, & Baron 1999; Allard et al. 1997) can be found in Allard, Hauschildt, & Schwenke (2000).

5. THE MODEL ATMOSPHERE

We use the model atmosphere code PHOENIX, Version 10.8. The original versions of PHOENIX were developed
for the modeling of novae and supernovae ejecta described by Hauschildt & Baron (1999 and references therein) and includes a detailed radiative transfer (Hauschildt 1992) that allows for spherical symmetry. Its more recent application to cool dwarfs is described in detail by Allard & Hauschildt (1995) and Hauschildt et al. (1999) and has served to generate grids of stellar model atmospheres that successfully described low-mass stars in globular clusters (Baraffe et al. 1995, 1997) and the Galactic disk main sequence (Baraffe et al. 1998). These former model grids are known to the stellar community as the 1995 EXTENDED and the 1996–1999 NEXTGEN models, and allowed a preliminary incursion into the regime of evolved brown dwarfs down to \( T_{\text{eff}} = 1600 \) K (EXTENDED models) and 900 K (Allard et al. 1996). These models successfully predicted the general spectroscopic properties of evolved brown dwarfs prior to the discovery of Gliese 229B, which then helped confirm its very cool brown dwarf nature (Allard 1995). Yet the lack, in these essentially stellar models, of dust condensation in the CE made them inadequate for modeling in detail such cool objects.

The addition to PHOENIX of the treatment of condensation in the CE and of dust clouds, as described in §§ 2 and 3, was completed in 1996 (Allard 1998; Allard et al. 1998b; Allard, Alexander, & Hauschildt 1998a) and served to compute M dwarfs and brown dwarfs model atmospheres, synthetic spectra, and broadband colors for specific analysis (Leggett et al. 1996, 2000; Ruiz, Leggett, & Allard 1997; Tinney et al. 1998; Leggett, Allard, & Hauschildt 1998; Martin et al. 1998; Kirkpatrick et al. 1999a; Leinert et al. 2000; Basri et al. 2000) and interior models (Chabrier et al. 2000). In this paper we present the final version of these models in the following two limiting cases: (1) “AMES-dusty,” which includes both the dust formation in the CE and opacities, and (2) “AMES-cond,” which includes the effects of condensation in the CE but ignores the effects of dust opacities altogether. This latter case is computed to explore the case where dust grains have formed but have disappeared completely (e.g., by sedimentation, i.e., settling below the photosphere). These two model sets also distinguish themselves from the standard NEXTGEN models by the use of the NASA AMES H₂O and TiO line lists, while the NEXTGEN models were computed using the Jørgensen (1994) and Schryber, Miller, & Tennyson (1995) line lists. This choice is motivated by the incompleteness of the 1994 lists to high gas temperatures (\( T_{\text{gas}} > 2000 \) K), as discussed in Allard et al. (2000).

For the purpose of this analysis, we use the radiative transfer in plane-parallel mode. The convective mixing is treated according to the mixing-length theory (MLT). We consider a pressure-dependent line-by-line opacity sampling treatment for both atomic and molecular lines in all models. We do not pretable or remanipulate the opacities in any way; PHOENIX includes typically \( \approx 15 \times 10^6 \) molecular and atomic transitions, which are reselected at each model iteration and each atmospheric depth point from our database described above. The lines are selected from three representative layers of the atmosphere at each model iteration to ensure the consistency of the calculation. Van der Waals pressure broadening of the atomic and molecular lines is applied as described by Schweitzer et al. (1996). We neglect the effects of convective motion on line formation since the velocities of the convection cells are too small to be detected in low-resolution spectra and will have a negligible influence on the transfer of line radiation.

A trial atmospheric profile is applied, the equations of hydrostatic and radiative transfer are solved, and the solution is tested until convergence is reached. The model is considered converged when the energy is conserved within 0.1% from layer to layer. At each of the model iterations, a spectrum with typically over 30,000 points is generated that samples the bolometric flux from 0.001 to 500 \( \mu \)m with a step of 2 Å in the region where most of the flux is emitted (i.e., 0.1–10 \( \mu \)m). The final spectrum must generally be degraded to the instrumental resolution before being compared to low-resolution observations of stars and brown dwarfs. The model atmospheres are characterized by the following parameters: (1) the surface gravity \( g \), (2) the effective temperature \( T_{\text{eff}} \), (3) the mixing length—scale height ratio \( \alpha \), here taken to be unity, (4) the microturbulent velocity \( \xi \), here set to 2 km s\(^{-1}\), and (5) the element abundances taken from Grevesse & Noels (1993).

For this paper, we have calculated a uniform grid of AMES-cond models ranging from \( T_{\text{eff}} = 3000 \) to 100 K in 100 K steps and with gravities ranging from log \( g = 2.5 \) to 6.0 in steps of 0.5 dex at solar metallicity. The AMES-dusty grid was calculated from \( T_{\text{eff}} = 3000 \) to 1400 K in steps of 100 K, with gravity ranging from log \( g = 3.5 \) to 6.0 in steps of 0.5 dex. All models were fully converged.

Although PHOENIX can treat the effects of external radiation fields on the model atmosphere and the synthetic spectrum (Baron et al. 1993), we assume here a negligible external radiation field for simplicity. It is clear, however, that UV radiation impinging on the brown dwarf from a hotter companion will change the structure of the atmosphere and the corresponding spectra. We are investigating these effects in a separate publication (Barman, Hauschildt, & Allard 2001).

6. Atmospheric Structures and Convection

The photospheric thermal structures of the AMES-cond models with \( T_{\text{eff}} \) ranging from 3000 to 100 K are displayed in Figure 5. The convection zones are labeled with crosses. As \( T_{\text{eff}} \) decreases, the photosphere becomes progressively more isothermal. While the convection zone retreats to deeper layers down to \( T_{\text{eff}} = 1000 \) K, an outer convection zone begins to form in the clouds until it detaches itself from the inner convection regime in models cooler than 500 K. Meanwhile, the inner convection continues to retreat inward. This appears to confirm qualitatively earlier work by Guillot et al. (1994) and Burrows et al. (1997). Yet even in our coolest models, the inner convection zone always reaches at least up to an optical depth of \( \tau_{1.2 \mu m} = 10 \). For \( T_{\text{eff}} = 1000 \) K, for example, the convection zone seems to be much deeper in the Burrows et al. (1997) models (roughly \( P_{\text{gas}} > 100 \) bars as seen from their Fig. 5) than in our models. Note that we treat the convection according to the MLT from the onset of the Schwarzschild criterion, while Burrows et al. (1997) assumed a pure adiabatic mixing throughout the convective unstable zones. This appears to be a valid approximation, however, since our calculations indicate that the true temperature gradient as predicted by the MLT remains within 0.05% of the adiabatic gradient value at each layer. So the difference appears to lie in the opacities included in the construction of the respective models: their models would be more transparent to radiation than ours.

The optical resonance lines of K I and Na I D also con-
decreases, the photosphere becomes progressively more isothermal. If the thermal structure of a K, log $g$ = 5.0, solar metallicity. The convection zones are marked by solid lines, while the convective region is shown as dotted lines. The location of the photosphere is also indicated, and uncertainties in the applicability of Lorentz profiles (estimated from models computed with restricted coverage of the line wing opacity contributions) produce a corresponding uncertainty of less than 40 K in the photosphere and 150 K in the internal layers. These uncertainties are therefore of little importance for the synthetic spectra and evolution models compared to those tied to the treatment of the dust (cond vs. dusty) and incomplete molecular opacities (e.g., the H$_2$O opacity profile; see Allard et al. 2000). However, neglecting the K I and Na I D doublet opacities altogether in the construction of the thermal structures has a greater impact and fully explains the difference between our models and those of Burrows et al. (1997). Indeed, while our model at $T_{\text{eff}}$ = 500 K and log $g$ = 5.0 does not present detached convection zones, we reproduce exactly the several detached convection zones found by these authors when neglecting atomic line opacity in the model construction. We must conclude from this that these opacities were neglected in their work. The reality of the occurrence of a detached convection zone is therefore likely to be closer to our predictions.

The thermal structures of the fully dusty AMES-dusty models over the $T_{\text{eff}}$ range in which dust begins to form (2500–1500 K) are displayed in Figure 6 at a constant gravity. The convection zone, marked by dotted lines, extends out to $T_{\text{gas}}$ = 2500 K in all these models. This corresponds to optically thin layers in models hotter than 1600 K. Even down to 500 K, these dusty atmospheres never become fully radiative, but the interesting part is what happens to photospheric regions as grain opacities begin to heat up the outer layers. Within the photosphere (filled circles and triangles), the temperature normally decrease smoothly with decreasing $T_{\text{eff}}$, and the thermal structures are parallel for grainless models. Here, the greenhouse effect of the dust tends to raise the temperature of the outer layers increasingly with decreasing $T_{\text{eff}}$. This has the effect that the outer structures level off between $T_{\text{eff}}$ = 2600 and 1800 K to a $T_{\text{gas}}$ value in a narrow range between 1280 and 1350 K. The slope of the thermal structure in the line-forming region therefore becomes increasingly flatter in that $T_{\text{eff}}$ range. Below 1800 K, the greenhouse effect saturates, and the outer thermal structure resumes its decrease in temperature with decreasing $T_{\text{eff}}$. It is interesting to note that 1800 K is also the break-up temperature at which full dusty atmospheres become unrealistic in modeling brown dwarfs. This can be seen from Figure 6 of Chabrier et al. (2000) and from § 8. We believe that grain sedimentation has certainly started at these temperatures, as is also concluded by Lunine et al. (1989), Burrows & Sharp (1999), and Ackerman & Marley (2001).

7. SYNTHETIC SPECTRA

In Figure 7 we display the spectral sequence of brown dwarfs to extrasolar giant planets (EGPs) model atmospheres from $T_{\text{eff}}$ = 3000 to 200 K in the total gravitational settling (AMES-cond) approximation. All dust opacity is neglected, but also all the optical molecular opacity sources disappear because of the condensation of species involving Ti, V, Ca, and Fe (TiO, VO, CaH, FeH, etc.), making these models transparent to the emergent radiation blueward of 1.0 μm. Because of the absence of dust opacity, the photospheric layers are very cool compared to nondepleted atm-
spheres. The formation of optical atomic resonance lines and infrared molecular bands is then favored. We observe that water vapor bands (0.93, 0.95, 1.2, 1.4, 1.8, 2.5, and 5–10 µm in the window shown by this plot) increase rapidly in strength. Another striking consequence of the cool photospheric temperatures is the formation of CH$_4$ bands (3.5 and 6–10 µm, with weaker bands at 1.6 and 2.2 µm appearing in cooler models) already at 2000 K. Methane gradually replaces water vapor bands while H$_2$O condenses to ice below 300 K.

One major feature of the AMES-cond model spectra is the extraordinary growth of atomic resonance absorption lines at short wavelengths. Burrows, Marley, & Sharp (2000) have explored grainless models of methane dwarfs and found that van der Waals broadening of K and Na resonance optical lines can extend to several thousands of angstroms on each side of the line cores. Our models behave similarly. Figure 8 shows how the van der Waals wings of the Na D and K resonance optical lines at 5891 and 5897 Å and 7687 and 7701 Å completely depress the optical flux of cool brown dwarfs. In this case ($T_{\text{eff}} = 1000$ K, log $g = 5.0$), the wings extend far over 7000 Å on each side of the line center. This is as large as hydrogen Balmer line wings in cool white dwarfs! However, to our knowledge, it is the first case of such behavior in metal lines encountered in stellar astronomy. While the van der Waals collisional C$_6$ damping constant may be sufficiently accurate for the treatment of alkali element lines in the hydrogenic approximation in low-mass stars and red dwarfs, where these lines rarely exceed a width of 50 Å, this treatment becomes questionable under these unprecedented conditions, as was also concluded by Burrows et al. (2000). Here, we observe, for example, that the red wings of these transitions prevent even a fraction of the flux from escaping in the J-band window around 1.25 µm, while observed spectral distributions of methane dwarfs tend to carry more flux in this window. The reason for such large line broadening is not the decreasing $T_{\text{eff}}$ of the photospheric gas pressure. It is rather, as also observed by Allard (1990), Allard & Hauschildt (1995), and Tinney et al. (1998) for metal-depleted atmospheres, the result of the increasing transparency of the atmosphere, which allows us to see deeper into the structure to inner high pressure depths. The line wing flux therefore integrates over an increasingly large column density of the atmosphere as optical molecular opacities vanish via condensation.

Figures 9 and 10 display the change of the optical to red spectra as a function of temperature, where the gradual disappearance of TiO, VO, FeH, and CaH bands (by condensation of related species) and the gradual strengthening of optical Na D and K lines becomes obvious. The TiO band systems (0.545, 0.616, 0.639, 0.665, 0.757, 0.774, and 0.886 µm) become undetectable below 2000 K, while the MgH (0.513 µm), CaH (0.694 and 0.706 µm), VO (0.829, 0.848, and 0.961 µm), and FeH (0.990 µm) bands persist down to 1500 K. The CrH bands at 0.861 µm, already visible at 2500 K in these AMES-cond models, grow in strength as $T_{\text{eff}}$ decreases until they disappear because of the condensation of Cr$_2$O$_3$ below 900 K. However, we must point out that red dwarfs are heavily reddened by dust opacities at least down to $T_{\text{eff}} = 2000$ K, so that the cond models overpredict the strength of CrH bands over that temperature range. Still, clearly the CrH bands become one of the strongest molecular system to be observed in the red spectra of cooler brown dwarfs.

From 2000 K, we also see the H$_2$O band system at 0.927 µm becoming increasingly stronger. The Na D resonance doublet remains visible down to 400 K, and K I already begins to get locked into dust below about 900 K, a temperature typical of currently known methane dwarfs such as...
GL 229B. Other features growing in strength as $T_{\text{eff}}$ decreases are the lines of alkali elements such as Li i at 6708 Å, Rb i at 7802 and 7949 Å, Cs i at 8523 and 8946 Å, and Na i at 8185 Å. We also note the presence of diagnostic lines farther in the near-infrared such as the K i doublet at 11693 and 11776 Å and 12436 and 12525 Å and an Na i line at 11409 Å.

The $\lambda$6708 Li line, normally used to determine the substellar nature of brown dwarfs (Rebolo, Martín, & Magazzù 1992), remains detectable down to 700 K. The Na i, Rb i, and Cs i lines keep increasing in strength, but this is likely to be an artifact of the inevitable incompleteness of thermochemical databases in the construction of the chemical composition at these temperatures.

Thanks to R. D. Freedman (1999, private communication; NASA-Ames), we were able to replace the band model approximation with a detailed line list for VO besides also being able to include CrH lines for which we had no previous counterparts. The result is that the present models show weaker VO band strengths, relative to TiO, than in previous models. A detailed comparison to high-resolution observations of M and brown dwarfs is being published separately (Schweitzer et al. 2001). However, note that the VO line list does not include the C-X system at 0.75 μm. Our current models, therefore, overestimate the flux in the 0.75 μm region.

In Figure 11 we explore the behavior of the 4.55 μm CH$_3$O band system between $T_{\text{eff}} = 2000$ and 400 K. At these wavelengths, H$_2$O provides the pseudocontinuum absorption. In the limit of the cond models, CH$_3$O is practically undetectable until it begins to grow from 1000 K to lower effective temperatures. The ammonia band at around 11 μm behaves similarly, as can be seen from Figure 12. This is a result of the growing transparency of the atmosphere while water begins to condense in the uppermost layers of these cond models. Note that although CO bands at 4.67 μm are not visible in cond models with $T_{\text{eff}} \geq 1800$ K, these bands do appear in corresponding brown dwarfs and stars.
This is because the cond limit does not apply for those dusty dwarfs.

In Figure 13 we present the full dusty (AMES-dusty) limiting case from 2500 to 1500 K. Here the strong heating effects of dust opacities prevent the formation of methane bands, and H$_2$O is dissociated while producing a hotter water vapor opacity profile, which is much weaker and more transparent to radiation. From 1700 K, the grain opacity profiles rapidly dominate the UV to red spectral region, smoothing out the emergent flux into a continuum. Only the cores of the strongest atomic resonance lines (Na I D and K I) can be seen. The result is a spectral distribution getting closer to the equivalent blackbody distribution of same effective temperature (see also Fig. 19). Note, however, that dusty models can never be approximated by blackbodies because of the important optical-to-red dust veiling and the strong near-IR water vapor bands. We have explored the effects of grain sizes on these models and found that for grains with sizes in the submicron to micron range, the increased cross sections are compensated for by the corresponding reduction in the number density of these grains given the conservation of the elemental abundance. For grains with sizes beyond 10 $\mu$m, an increased global opacity is found that produces even redder models, but grains are likely to be distributed in a spectrum of sizes where the balance between coagulation, sedimentation, and condensation decides the upper limit of the masses reached. Preliminary calculations (T. Guillot 2000, private communication), which will be published separately, show that when accounting for all the relevant processes, the grain sizes remain in the submicron range. We are therefore confident that the current models with grain sizes in the submicron range do constitute an adequate full dusty limit for these dwarfs.

7.1. Gravity

In Figures 14 and 15, we explore the effects of surface gravity on the AMES-cond models with $T_{\text{eff}} = 2500$ and 500 K. At 2500 K, gravity sensitivity is essentially noticeable in hydride bands (CaH at 0.624 and 0.639 $\mu$m and FeH at 0.98 $\mu$m), while the oxide bands (TiO and VO) form too high in the atmosphere ($\tau_{\text{rad}} = 10^{-4}$) to be affected except in the interband pseudocontinuum regions. Effects of gravity are, however, more extensive in the strength of atomic lines (essentially K I and Ti I) at the peak of the spectral distribution (1.05–1.3 $\mu$m) and in the red wing of the water vapor bands as well as in the CO bands at 2.3–2.4 $\mu$m. In the 500 K case, H$_2$O bands are only moderately affected by the gravity change, while the optical continuum opacity, provided by the van der Waals wings of the Na I D and K I resonance doublets, is reduced by nearly a factor of 10 in the 500 K model in the low-gravity case in response to the drop in pressure. The most interesting feature is the enhanced sensitivity of the K-band flux at 2.2 $\mu$m to gravity. As already pointed out by Allard et al. (1996), this feature can be used to disentangle the temperature, age, and mass of a brown dwarf or planet independently. This trend is observed in the entire regime from 1500 to 300 K and provides a useful tool in the analysis of free floating methane dwarfs such as those discovered recently by Strauss et al. (1999) and Tsvetanov et al. (2000). The CH$_4$ and CO bands are also sensitive to gravity in this regime. One more gravity indicator should be the slope and height of the $Z$-band flux between the core of the K I resonance doublet at 7687, 7701 Å and 1.1 $\mu$m compared to the height of the J-band flux peak. However, for the reasons mentioned above, it is difficult to quantify this effect on the basis of the present models.

Surface gravity effects have also been explored for the fully dusty case (AMES-dusty models) at $T_{\text{eff}} = 2000$ and 1500 K (see Figs. 16 and 17). In the 2000 K case, the pseudocontinuum formed by saturated bands of TiO blueward of 0.75 $\mu$m is fainter and flatter at reduced gravity. This is a result of the cooler temperatures prevailing in the outskirts of the photosphere at reduced gravity. This explains and supports the conclusions of Martin, Rebolo, & Zapatero Osorio (1996), who noticed a similar trend comparing young red dwarfs of the Pleiades cluster to presumably older field M dwarfs. Previous M dwarf model atmospheres (Allard & Hauschildt 1995) did not show such a sensitivity
Fig. 15.—Same as Fig. 14, but for the $T_{\text{eff}} = 500$ K AMES-cond models. Solid line: $\log g = 4.0$; dotted line: $\log g = 2.5$. Here the spectral resolution has been reduced to 30 Å by boxcar smoothing. In the inset we show a zoom of the optical to red spectral regime, where we distinguish water vapor bands at 0.93, 0.95, and 1.12 µm, Cs I resonance transitions at 0.86 and 0.89 µm, the K I resonance doublet at 0.77, 0.79 µm, and the cores of a few other lines such as the Na I D doublet blueward of 0.75 µm. While molecular bands are moderately affected by the gravity change, the optical background opacity due to the wings of the Na I D and K I doublets is reduced by nearly a factor of 10 in the low-gravity model. The latter model is more typical of low-mass brown dwarfs and Jovian planets.

Fig. 16.—Comparison of two $T_{\text{eff}} = 2000$ K AMES-dusty models of different surface gravity. Solid line: $\log g = 6.0$; dotted line: $\log g = 3.5$. The spectral resolution has been reduced to 10 Å by boxcar smoothing.

because of the overestimated blocking caused by straight mean and JOLA opacities. To longer wavelengths, an important veiling provided by the dust covers the 0.7–1.3 µm region in the high-gravity model. Atomic lines and molecular bands are generally quite sensitive to gravity changes in this range, while the near-infrared water vapor bands are also affected markedly (much more than in the grainless 2500 K case discussed above). Collision-induced H$_2$ absorption cutting the flux in a negative slope at 2.2–2.3 µm as well as the CO bands redward of this again make the shape of the K-band spectrum an especially excellent gravity indicator. A similar behavior is observed at 1500 K (Fig. 17), where, however, the dust is now so strong that most features, except H$_2$O band troughs, are no longer seen.

7.2. Comparing Limits

Figures 18 and 19 compare the full settling and full dusty limits for $T_{\text{eff}} = 2000$ and 1500 K, respectively. In the 2000 K case, the presence of dust opacities simply has the effect of veiling the optical to red spectral region, while the addi-
Fig. 17.—Same as Fig. 16, but for the $T_{\text{eff}} = 1500$ K AMES-dusty models. While gravity effects are quasi-nonexistent redward of 2.5 $\mu$m, they are quite large in the optical to red spectral region, mainly as a result of enhanced efficiency of dust grain formation at the higher pressures and densities of high-gravity atmospheres. A log $g$ value of 5.5 is typical of most field brown dwarfs discovered since 1996.

Fig. 18.—Two $T_{\text{eff}} = 2000$ K models with log $g = 5.5$ compared to illustrate the difference between our two limiting cases: solid line: AMES-dusty with full dust opacity; dotted line: AMES-cond with full gravitational settling (no dust opacity).

Fig. 19.—Same as Fig. 18, but for the $T_{\text{eff}} = 1500$ K models with log $g = 5.0$. A 1500 K blackbody (dashed line) is overplotted for comparison.

dwarfs (1800 K). In the former case, the cloud layers form above the photosphere, as can be seen from Figure 1, such that heating takes place above the line-forming region, leaving the thermal structure little affected by the dust. At 1800 K, on the other hand, the clouds form deep into the photosphere (see Fig. 2). The line-forming region is therefore heated up by as much as 500 K, while the internal layers only warm up by less than 80 K. This effect is enough to dissociate water vapor by nearly 50% in the outer layers, leaving a far shallower structure over most of the photosphere. It is interesting to note that cond models cooler than about $T_{\text{eff}} = 1800$ K have similar thermal structures than the corresponding NEXTGEN models.

This similarity of the thermal structures translates into similar synthetic spectra. We compare the present AMES-
cond models to the earlier brown dwarfs models (NEXTGEN) of Allard et al. (1996) in Figure 21 for the $T_{\text{eff}} = 1000$ K case. Although the NEXTGEN models used in our 1996 publication were constructed without dust condensation, the molecular bands of TiO, VO, and FeH were completely crushed by the wings of the alkali lines, and the results are quasi-independent of condensation. The models remain sensitive to the physics mainly in the interband regions at 1.0, 1.25, 1.6, and 2.2 $\mu$m, which probe, by their relative brightness, the thermal structure of the atmosphere at various depths.

8. COLORS

The models are most readily compared to large samples of stars and brown dwarfs in color-magnitude diagrams. The standard system of broadband colors is sufficiently constraining when evaluating the accuracy of the models. This is because most spectral features are several thousands of angstroms wide, and the remaining emission windows are well sampled by each bandpass: $Z$ at 1.0 $\mu$m, $J$ at 1.3 $\mu$m, $H$ at 1.6 $\mu$m, $K$ at 2.2 $\mu$m, $M$ at 4.5 $\mu$m, and $N$ at 10 $\mu$m. Methane bands appear in brown dwarfs cooler than about 1700 K at 1.7, 2.4, and 3.3 $\mu$m, reducing the flux sampled by the $H$, $K$, and $L$ bandpasses, respectively. The pressure-induced H$_2$ opacity, on the other hand, depresses the flux in the $K$ bandpass in the coolest brown dwarfs and low-metallicity dwarf stars.

We have computed synthetic $UBVRIJHKL$ magnitudes by integrating our model spectra according to the photon count prescription at a wavelength step of 1 Å. We have adopted the filter responses by Bessell & Brett (1988) and Bessell (1990), bringing our synthetic photometry on to the Cousins and Johnson-Glass system. Transformations to the CIT or other systems are readily obtained from Leggett (1992). As in previous papers, we used the energy distribution of Vega as observed by Hayes & Latham (1975), Hayes (1985), and Mountain et al. (1985) to provide an absolute calibration. Zero magnitudes and colors are assumed for Vega. The grainless NEXTGEN models of Allard et al. (1996, 1997), Hauschildt et al. (1999), Baraffe et al. (1997, 1998), as well as the AMES-cond and AMES-dusty models from this paper are compared to the observed stellar and brown dwarfs samples of Leggett (1992), Tinney (1993), Kirkpatrick & McCarthy (1994), Ianna & Fredrick (1995), Delfosse et al. (1997), and Zapatero Osorio, Martin, & Rebolo (1997a) in Figure 22. Please note that we have applied here a +0.18 dex shift in $J-K$ to the current models to match the position of the NEXTGEN models in the nondusty regime in order to isolate the dust effects. This offset of the current models to the blue of the earlier NEXTGEN models is due to some inaccuracies of the NASA-Ames H$_2$O opacity database in describing these relatively hot atmospheres (see Allard et al. 2000 for details).

These colors are interesting since they have helped distinguish interesting brown dwarf candidates from the databases of large-scale surveys such as DENIS and 2MASS and have helped us to obtain an appreciation of the spectral sensitivity needed to detect new brown dwarfs. The methane bands cause the $J-K$ colors of brown dwarfs to get progressively bluer with decreasing mass and as they cool over time. Yet their $I-J$ colors remain very red, which allows us to distinguish them from hotter low-mass stars, redshifted galaxies, red giant stars, and even from low-metallicity brown dwarfs that are also blue because of pressure-induced H$_2$ opacities in the $K$ bandpasses. Fortunately,
grain formation and uncertainties in molecular opacities are greatly reduced under low-metallicity conditions ([M/H] $< -0.5$). Therefore, model atmospheres of metal-poor subdwarf stars and halo brown dwarfs are free of uncertainties on the dust compared to their metal-rich counterparts. This has been nicely demonstrated by Baraffe et al. (1997), who reproduced closely the main sequences of globular clusters ranging in metallicities from [M/H] $= -2.0$ to $-1.0$ as well as the sequence of the Monet et al. (1992) halo subdwarfs in color-magnitude diagrams.

As can be seen from Figure 22, the AMES-dusty models reproduce well the locus of the coolest dwarfs that deviate from that of main-sequence star red values of $J - K$ as dust effects grow in their atmospheres with decreasing effective temperature (see also Leggett et al. 1998 for more such color comparisons). It appears, therefore, that this full dusty limit at which grain settling is negligible is adequate to reproduce the global properties of late-type low-mass stars and young or massive brown dwarfs with $T_{\text{eff}} \leq 1800$ K. Below this temperature, the AMES-dusty models keep getting redder and do not correspond to the properties of known T dwarfs illustrated in this diagram by the position of Gl 229B and SDSS 1624.

The locus of the AMES-cond models for their part depends on two major uncertainties. The first, likely tied to the second, is a hump of flux excess between 0.8 and 0.93 $\mu$m, i.e., in the $I$ bandpass, which prevents the cond models from becoming redder than $I - J = 4.2$. The second is the description of the far wings of the absorption lines of K I and Na I D as discussed above and illustrated in Figure 8. In Figure 22 we show two grids of cond models, one computed with a coverage of the line wings opacity contributions of 5000 Å on each side of each atomic line core (long-dashed line) and the other computed with a maximum coverage of 15,000 Å (short-dashed line). Both grids use Lorentz profiles for the atomic lines. Obviously, the profiles of the optical Na I D and K I doublets are no longer Lorentzian beyond 5000 Å from the line cores, as has also been found by Burrows et al. (2000). Since T dwarfs appear in the cone defined by these cond models, an adequate theory of line broadening could be sufficient to reproduce their properties. Yet no theory exists for the treatment of the far wings of alkali elements broadened by collisions with H$_2$ and helium species to this date (Burrows et al. 2000). Until these become available, the present grid with a line wing coverage of 5000 Å seems to provide an acceptable compromise and limiting case (with the dusty models) for the spectroscopic properties of brown dwarfs.

9. DISCUSSION AND CONCLUSIONS

We have investigated the two limiting cases of dust in low-mass stars and brown dwarfs atmospheres by comparing the following two sets of models: (1) AMES-cond models ranging from $T_{\text{eff}} = 3000$ to 100 K in 100 K steps and with gravities ranging from log $g = 2.5$ to 6.0 in steps of 0.5 dex at solar metallicity and (2) AMES-dusty models from $T_{\text{eff}} = 3000$ to 1400 K in steps of 100 K with gravity ranging from log $g = 3.5$ to 6.0 in steps of 0.5 dex. The AMES-cond grid corresponds to the case where all dust has disappeared from the atmosphere by gravitational settling, while the AMES-dusty grid describes the case of negligible settling throughout the atmosphere. The two sets of models rely on the assumption that dust forms in equilibrium with the gas phase. (See also Chabrier et al. (2000) for the corresponding evolution models of late type stars and brown dwarfs and a more detailed description of their photometric properties.)

From the comparison of the two limits described here and their comparisons to observations (see § 8), we find that dwarfs with $T_{\text{eff}} \geq 1800$ K are successfully described by the full dusty limit and conclude that dust must be in close equilibrium with the gas phase with little sedimentation or compensated sedimentation effects. This would be the case if, for example, convective mixing was efficient in returning material to the line-forming regions. We are exploring these issue by modeling hydrodynamically the convection in three-dimensional models (H. G. Ludwig et al. 2001, in preparation).

Observations of T dwarfs such as Gliese 229B indicate that brown dwarfs with $T_{\text{eff}} \leq 1300$ K are, on the other hand, more closely following the full-settling limiting case, as has also been shown by Tsuji et al. (1996a, 1996b), Allard et al. (1996), and Marley et al. (1996). However, there has been a history of failure to explain the optical spectra of these cool brown dwarfs since the discovery of Gl 229B. For example, Griffith, Yelle, & Marley (1998) claimed a veiling due to photodissociation by the parent starlight in the upper brown dwarf atmosphere, but this suggestion did not pass the acid test, and free-floating T dwarfs were discovered (Tsvetanov et al. 2000). Finally, Tinney et al. (1998), Kirkpatrick et al. (1999a), Burrows et al. (2000), and Liebert et al. (2000) have stressed the importance of the $\lambda\lambda$5891, 5897 Na I D and $\lambda\lambda$7687, 7701 K I resonance doublets. Our analysis recovers the latter results in predicting that the red wings of these lines heat up the photospheric thermal structure by as much as 100 K, and it defines the pseudocontinuum out to at least 1.1 $\mu$m in T dwarfs. This indicates that red flux out to 1.1 $\mu$m must be sensitive to gravity. We also find that the traditional Lorentz profile does not describe adequately their red wings beyond 5000 Å from the line center; it overestimates the wing opacity contribution. While this overestimation has negligible effects on the thermal structure as long as the lines are included in the calculation, it is important to realize that an adequate handling of the collisional broadening of alkali lines by H$_2$ and He must be developed in order to model successfully the optical to 1.1 $\mu$m flux and $VRI$ colors of T dwarfs (Burrows et al. 2000). Nevertheless, we believe that our AMES-cond models, limited in the coverage of the atomic line wings contributions, can provide the full-settling limit that they were intended to define.

Based on the cond models, we also find that currently known T dwarfs with effective temperatures around 1000 K are in a special regime in which several of their important spectral features start to reverse their behavior with decreasing $T_{\text{eff}}$: Cs I lines weaken as Cs begins to lock into CsCl, and CO and NH$_3$ bands begin to grow in strength as a result of decreasing background opacities. While Noll, Geballe, & Marley (1997), Griffith & Yelle (2000), and Saumon et al. (2000) all fail to reproduce these features in Gl 229B with solar composition models in thermodynamic equilibrium, it is perhaps due to the fact that each of these spectral synthesis analyses were based on thermal structures exempt of atomic line opacities. Indeed, in the fit to the overall spectrum, a subsolar composition could compensate (via an increased pressure) for the neglect of atomic line opacities in the thermal structure calculations. To clarify the issue of the metallicity of Gl 229B, we need to explore
the composition of the parent star Gl 229A. This paper is in progress and will be published shortly. However, we feel that it is unlikely, though not impossible, that the first known T dwarfs are metal-deficient, while more massive brown dwarfs are only found in metal-rich environments.

There remains a regime between 1300 and 1800 K where brown dwarfs should behave between these limits. We hope that our two sets of models can help bracket brown dwarf’s properties and identify objects. They can also be used to evaluate the effects of intrinsic variability as weathering effects that cause clouds to form and vanish. The full dusty models give the aspect of a cloudy atmosphere while the cond models resemble a cloud-free sky.

In the atmospheres of brown dwarfs and late-type M dwarfs, the dust likely forms in clouds distributed more or less evenly across the dwarf’s surface, as we observe on planets. These cloud layers should be well confined close to the deepest/hottest location where the grain type can condense (see, e.g., Lunine et al. 1989; Tsuji et al. 1999; Ackerman & Marley 2001), but the physical process that defines this confinement of the cloud layers are not known. It could either be (1) an inefficient condensation of the dust in the upper atmosphere or (2) an efficient gravitational settling (sedimentation) of the dust in those upper layers. Time-dependent grain growth analysis must be done to determine the first point. This paper is under progress at Berlin University, but our CE calculations indicate that the local [T, P] conditions favor dust formation. The second can be understood by opposing sedimentation and convective mixing, one pushing the grains down and the other bringing upward material to condense. Since the convection zone retreats progressively from the photosphere with decreasing T_{eff}, it seems to be a natural explanation of the fact that dust also retreats from the photosphere as T_{eff} decreases. This is why we mention the potential importance of gravitational settling throughout this paper.

The cond models represent a limiting case in which these cloud layers are all sitting below the photosphere independently of the cause for the cloud confinement. The dusty models, on the other hand, represent a case where confinement does not occur. So it is clear that nature is likely between the cond and dusty limits, with partial gravitational settling occurring with a fraction that varies with the depth in the atmosphere. The detailed modeling of this process relies on characteristic diffusion timescales for several processes such as condensation, sedimentation, coagulation, and convective mixing to name a few that are not known accurately for the type of grains important under the conditions prevailing in brown dwarf atmospheres. Models incorporating these effects can therefore only be exploratory. The two limits described here will remain useful until the physics of these processes become solidly mastered.

All the models discussed in this paper are available on request. We will also provide, as we have in the past, colors computed from these spectra on any requested color system. Please send requests to France Allard and consult the CRAL anonymous ftp site.2

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