Non-equilibrium Chemistry in Brown Dwarf Atmospheres

PHY688
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Outline

• What is non-equilibrium chemistry in the context of Brown Dwarfs?
• What is the observational signature of non-equilibrium chemistry?
• What are the relevant timescales?
• Modelling vertical transport and convection
Non-equilibrium Chemistry

• In the context of Brown Dwarf Atmospheres, the relevant chemical processes are

\[ CO + 3H_2 \rightarrow CH_4 + H_2O \]
\[ N_2 + 3H_2 \rightarrow 2NH_3 \]

• Chemical equilibrium sets the relative abundances of each of the molecules above

• If the abundances are observed to be different from expected, then the observed system is not in chemical equilibrium
Observational Signature

• Recall Spectral Type Classification
• M, L, and T dwarfs all have characteristic absorption lines
  - M dwarfs – oxides, i.e. VO, TiO
  - L dwarfs – hydrides, i.e. CaH, FeH
  - T dwarfs – methane and water
• Each spectral type has an associated characteristic temperature
Observational Signature

- In fact, the surface (effective) temperature determines the relative abundances in chemical equilibrium
- Cool M dwarfs (T ~ 2500-2700 K) favor CO and N$_2$
- T dwarfs (T ~ 800 K) favor CH$_4$ and NH$_3$
- The transition temperature is ~ 1100 K
Gl 229B: The Original T Dwarf

- $M_f \approx 16.5$ mag
  - $L_{bol} = 6.4 \times 10^{-6} \ L_{Sun}$
  - $I - J \approx 6.5$ mag
  - $T_{eff} \approx 900$ K
  - Jupiter is 160 K
- $M \approx 0.03 \ M_{Sun}$

(Nakajima et al. 1995)

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(Kirkpatrick et al. 1999)
Figure 6  Spitzer IRS spectra between 5 and 15 μm of an M, an L, and a T dwarf. Features caused by H₂O, CH₄, and NH₃ are marked. Data are taken from Roellig et al. (2004).
Gl 229B CO Detection

- CO abundance is over 3 orders of magnitude greater than expected in thermochemical equilibrium
- What could cause a state of non-equilibrium?

Fig. 1.—UKIRT observations of Gl 229B (squares) from Noll et al. (1997) display the gap between the R- and P-branches of the 1–0 rotational vibrational band. Radiative transfer calculations of CO are shown for $q_{\text{CO}} = 20$ ppm (solid line), $q_{\text{CO}} = 50$ ppm (dotted line), $q_{\text{CO}} = 100$ ppm (dashed line), and a thermochemical equilibrium abundance of CO (dot-dashed line). The absolute flux of the observations is uncertain; therefore, we scale the models using factors of 0.53, 0.72, 0.93, and 0.22, respectively.
How can a system be out of equilibrium?

Let's start by what it means to be in equilibrium...

- The timescale of the chemical reactions considered needs to be fast enough compared to other relevant physical or dynamical processes such that any perturbation in abundances is returned to energetically favored relative abundances.

What timescales are relevant in Brown Dwarf atmospheres?

- Eddy turbulence and convection
CO to CH\textsubscript{4} Timescale

• The reaction rate becomes faster for CO to CH\textsubscript{4} at:
  - Higher pressure
  - Higher temperature

• It's easier to convert CO to CH\textsubscript{4} at high T, P

• i.e. It's hard to convert at low T, P

FIG. 7. Logarithmic time scale (seconds) contours for the chemical conversion of CO to CH\textsubscript{4}. The conversion of CO to CH\textsubscript{4} is favored at high pressures and high temperatures.
Horizontal Mixing Timescale

- \( \tau_{\text{conv}} \sim H_c / v_c \)
- \( H_c \) and \( v_c \) are the convective mixing length and velocity
- Saumon et al. parameterize this using a diffusion timescale in radiative atmospheres
  - \( \tau_{\text{mix}} \sim H^2 / K \)
  - \( H^2 / K = H_c / v_c \)
- \( H \) and \( K \) are the pressure scale height and coefficient of diffusion
Vertical Mixing Timescale

• By setting $H = H_c$, Saumon defines an effective diffusion coefficient $K_c$ for convective mixing
  − This allows for an easy transition between the radiative envelope and convective core
• The diffusion coefficient is essentially a free parameter, but ranges from $10^2 – 10^5$ cm$^2$/s
  − The effective diffusion coefficient for convection ranges from $10^8 – 10^9$ cm$^2$/s
• The timescale for vertical mixing is comparable to chemical reaction timescales relevant in BDs
Comparison

- Timescales comparable for CO, N$_2$ and mixing

Figure 1. Chemistry inside a $T_{\text{eff}} = 1200$ K, $g = 10^5$ cm/s$^2$ cloudless atmosphere. Dashed lines show the equilibrium abundances of molecules of interest and solid lines show the abundances that result from non-equilibrium chemistry driven by vertical transport. In the radiative zone, the eddy diffusion coefficient is set to $K = 100$ cm$^2$/s. The extent of the convection zone is indicated in the upper right corner.
Comparable Timescales

• When the timescale for mixing is fast enough, then CO does not have enough time to convert to CH$_4$
  – A parcel of fluid containing CO is hot in the core and stable as CO
  – Convection pushes the fluid out to the cool atmosphere where it is further mixed by turbulent eddies in the radiative zone
  – The time the parcel of fluid spends in this cool region is short compared to the time it needs to convert to CH$_4$, therefore it remains CO.
Non-equilibrium Abundances

- Non-equilibrium abundances are set to the equilibrium abundance at a layer in the brown dwarf where the mixing timescale and chemical reaction timescale are the same.

- The result:
  - We see CO abundance in the cool BD atmosphere that is characteristic of the hotter interior.
  - Explains the CO overabundance in GL 229B.
Comparison

- Dashed lines are equilibrium abundances
- Solid lines are non-equilibrium abundances
- CO is orders of mag. different

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The transition temperature in which chemical equilibrium favors CO vs CH$_4$ occurs around $T \sim 1100$K for a pressure of $\sim 1$ bar.

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**Figure 2.** A comparison of spectra computed with abundances from chemical equilibrium and with the non-equilibrium abundances resulting from vertical transport. All models have $g = 10^5$ cm/s$^2$ and $K = 10^4$ cm$^2$/s. $T_{\text{eff}}$ decreases from 1600 K (top) to 800 K (bottom) in steps of 200 K. The spectra are plotted at a resolution of $R = 200$ and are offset vertically for clarity. The main bands of CO and CH$_4$ and the bandpass of the $M'$ filter are indicated.
Modeling Gl 229B

• All brown dwarfs have log g ~ 5
• The surface temperature is fairly well known to be T ~ 1000K
• The only other parameter that significantly effects the outcome of the model is the coefficient of diffusivity, K
• This parameter can be adjusted to fit the CO feature in Gl 229B
Model Fit

- The best fit occurs when $K = 10^2$ cm$^2$/s
- Not great due to noisy signal, but clearly in non-eq. (top line)

Figure 3. Carbon monoxide in Gl 229B. The spectrum of Gl 229B is shown as a thick solid line (Oppenheimer et al. 1998; Leggett et al. 1999). The 4.5 – 5 µm spectrum is flux-calibrated using the \( M' \) photometry of Golimowski et al. (2002). Thin curves are models with \( T_{\text{eff}} = 1000 \) K, \( g = 10^5 \) cm/s$^2$ and \( K = 0, 10^2 \) and \( 10^4 \) cm$^2$/s, from top to bottom, respectively. \( K = 0 \) corresponds to the chemical equilibrium case. The absolute flux level of the models has not been adjusted to fit the data. The models are plotted at a resolution of \( R = 200 \).
M' Band

- M' narrow band centered at 4.6 μm
  - Probes the strength of the CO band
  - Data is available for multiple brown dwarfs
  - Can use this to test whether other BDs are out of thermochemical equilibrium
M' Band Analysis

- All Brown Dwarfs appear to be out of thermo-equilibrium with $K = 10^2 \text{ cm}^2/\text{s}$

Figure 4. Absolute $M'$ (MKO) magnitude versus effective temperature for L and T dwarfs. The data are from Leggett et al. (2002) and Golimowski et al. (2002). Open squares show 2MASS 0559−14 as a single star (upper point) and as an equal pair binary (lower point). Curves show sequences of models with $g = 10^5 \text{ cm/s}^2$ for different values of the eddy diffusion coefficient. From top to bottom, $K = 0$, $10^2$, $10^4$, and $10^6 \text{ cm}^2/\text{s}$, respectively. $K = 0$ corresponds to the equilibrium case.
References


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• S. Metchev, Class Notes PHY688 (2009)