Exploring Disequilibrium Chemistry in the Atmospheres of Hot Jupiters

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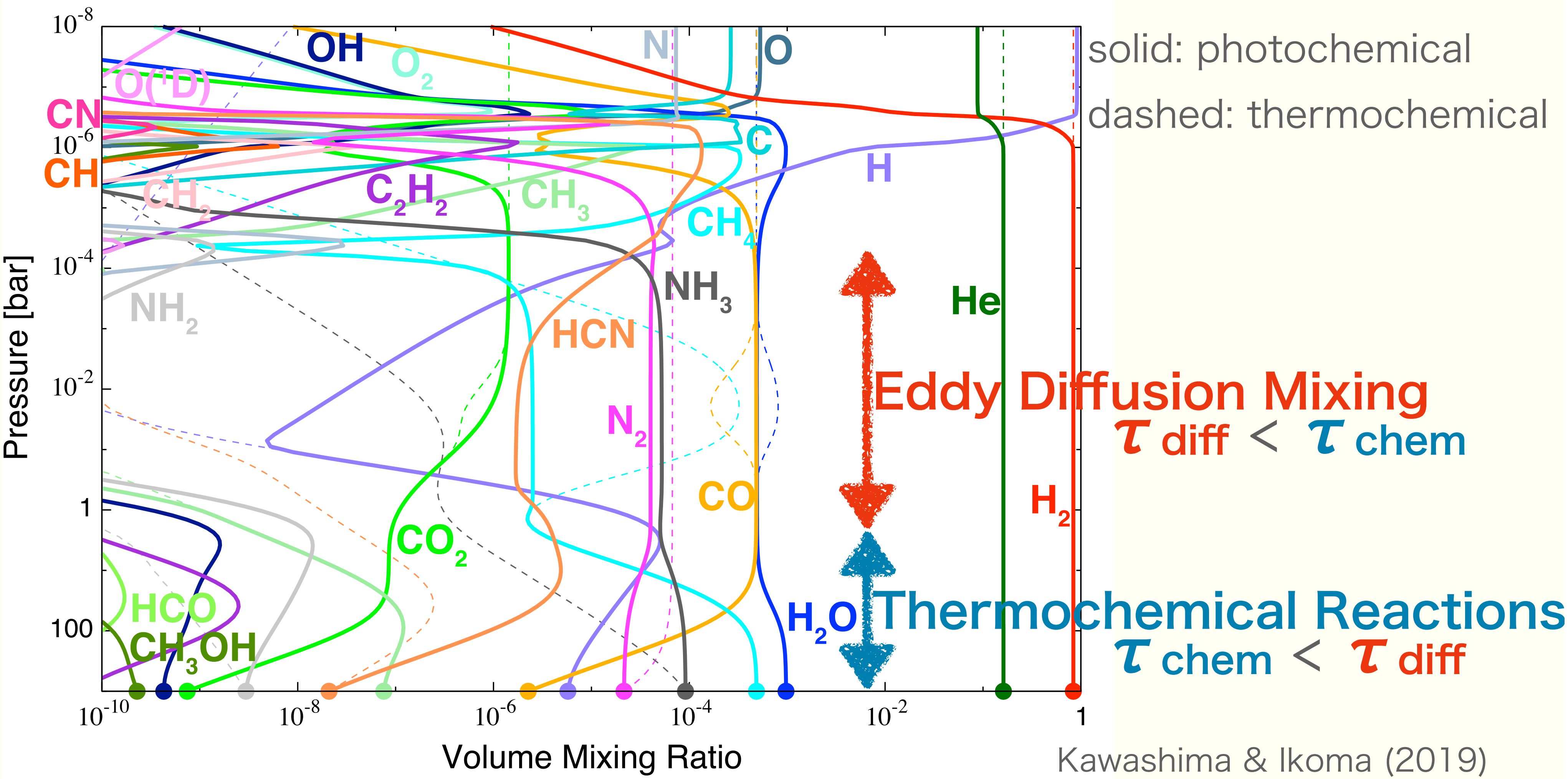
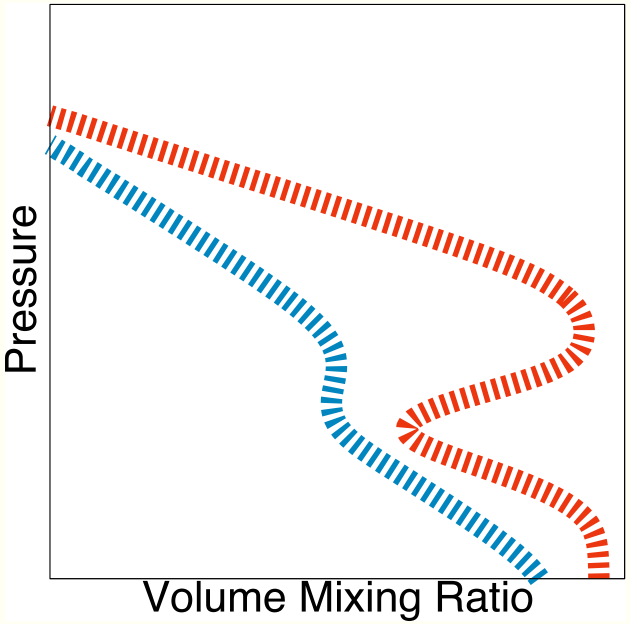
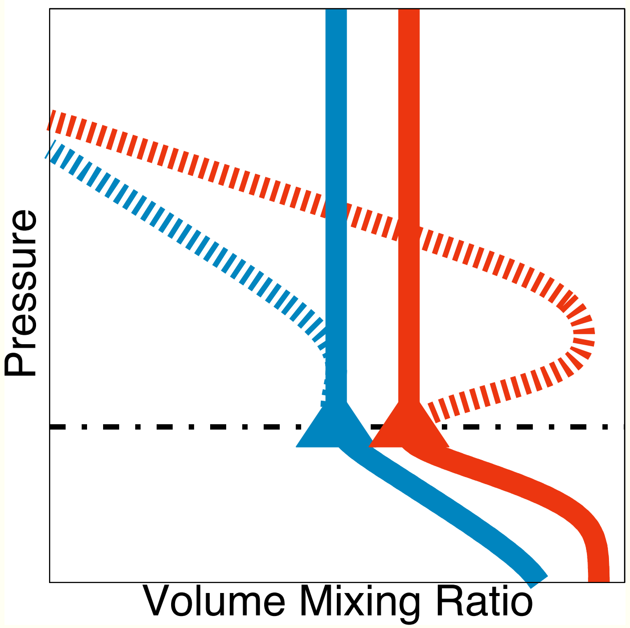
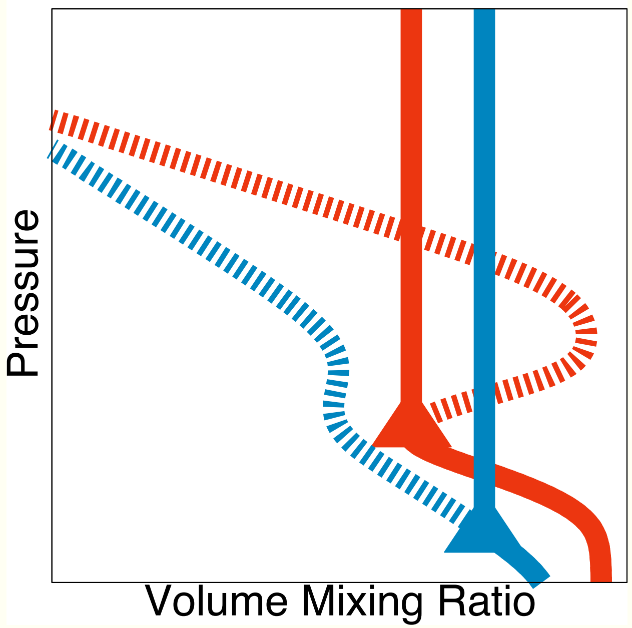
QUENCHING EFFECT

Each species has constant abundance above a certain altitude, where $\tau_{\mathrm{diff}} = \tau_{\mathrm{chem}}$, due to efficient eddy diffusion mixing



Kawashima & Ikoma (2019)

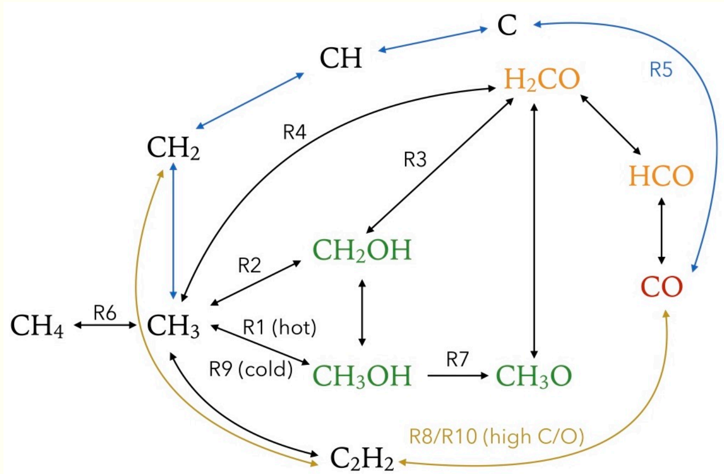
CHEMISTRY IN RETRIEVAL MODELS

Most models	Morley et al. (2017)	Our work
		
Assume constant or chemical equilibrium abundances	Introduced a quenching pressure, but assumed the same altitudes for all species	Calculate quenching pressure for each species as a function of K_{zz}

Chemical Relaxation Method

Chemical timescale:
Slowest reaction along the fastest pathway;
depends on both temperature and pressure

- Tsai et al. (2017)
  Derived chemical timescales;
  valid for currently observable
  exoplanet atmospheres
  (500-3000 K, 0.1 mbar-1000 bar)



$$\tau_{CH_4} = \frac{[CH_4]}{k_1[CH_3][OH][M] + \min(k_2[CH_2OH][H],\, k_3[CH_2OH][M]) + k_9[CH_3OH][H] + \max(k_8[C_2H_2][O],\, k_{10}[C_2H_2][OH])}$$

METHOD

Continuity-transport equation for number density n

$$\frac{\partial n}{\partial t} = \boxed{P - L} - \frac{\partial \Phi}{\partial z}$$

$$\frac{\partial n}{\partial t} = \boxed{-\frac{n - n_{\mathrm{eq}}}{\tau_{\mathrm{chem}}}} - \frac{\partial \Phi}{\partial z}$$

τ_{chem}: chemical timescale

n_{eq}: equilibrium number density

Eddy diffusion flux

$$\Phi = -K_{zz} n_t \frac{\partial}{\partial z}\left(\frac{n}{n_t}\right)$$

K_{zz}: eddy diffusion coefficient

n_t: total number density

Assuming steady-state condition ($\partial/\partial t = 0$)

$$n + \tau_{\mathrm{chem}} \frac{\partial \Phi}{\partial z} = n_{\mathrm{eq}}$$

E: identity matrix

T: matrix for τ_{chem}

M: matrix for eddy diffusion term

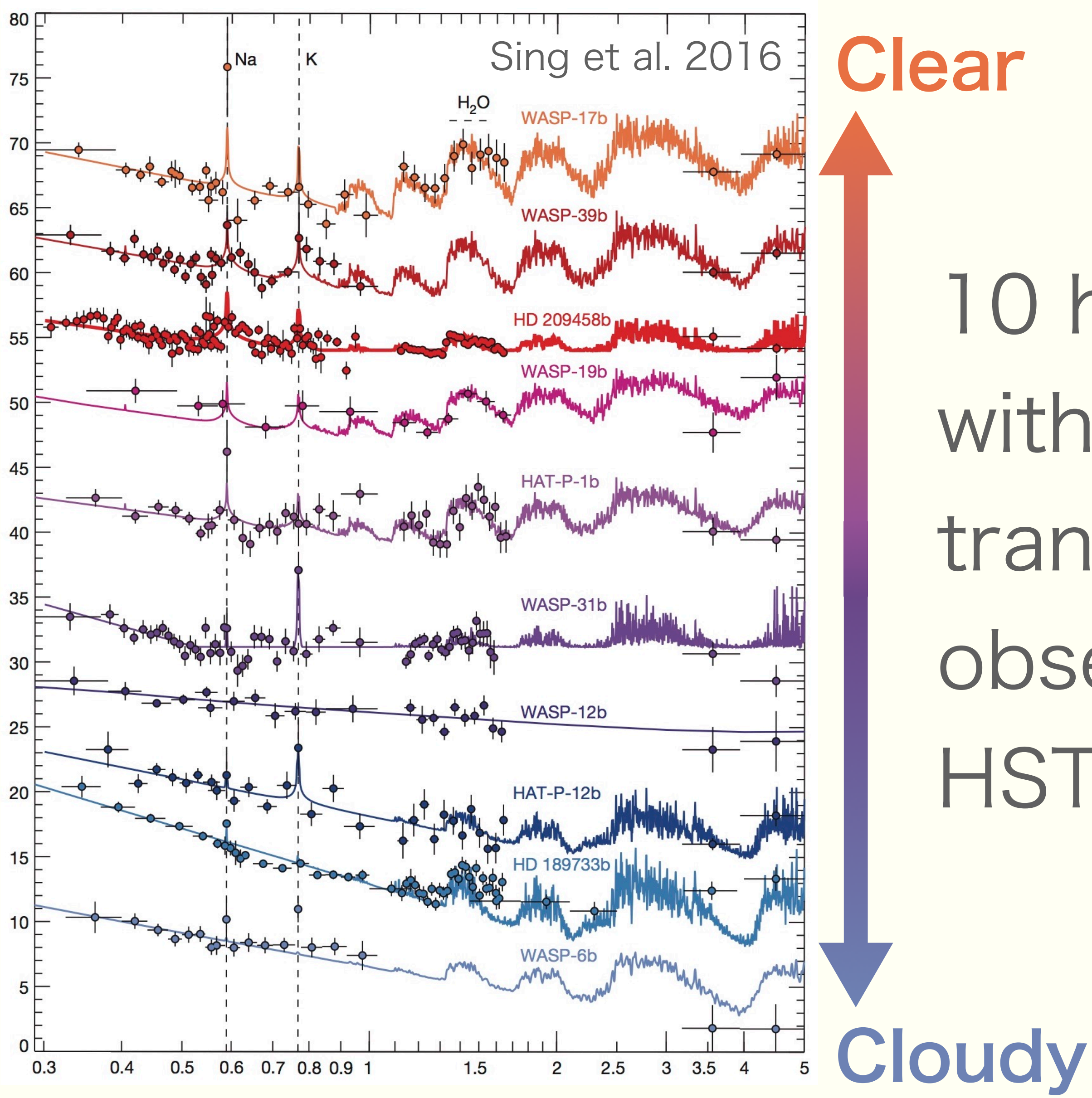
Converting n into matrix N

$$(E + TM)\, N = N_{\mathrm{eq}} \quad \Rightarrow \quad N = (E + TM)^{-1} N_{\mathrm{eq}}$$

Calculation Setup

- Spectral retrieval code: **ARCiS** (Min et al. submitted)
- Chemistry: equilibrium VS **disequilibrium**
- T-P profile: Analytical solution of Guillot (2010)
- Clouds: Ormel & Min (2019)
  $(NaAl)_xMg_ySiO_3$, SiO_2, Fe, FeS, Al_2O_3, C, SiC, TiO_2, VO
- 12 parameters:
  - **Chemistry K_{zz}**
  - R_{ref}
  - C/O, Si/O, N/O, metallicity
  - T_{int}, f_{irr}, γ $(=\kappa_{vis}/\kappa_{IR})$, κ_{vis}
  - **Cloud K_{zz}** and nucleation rate

PLANET SAMPLES

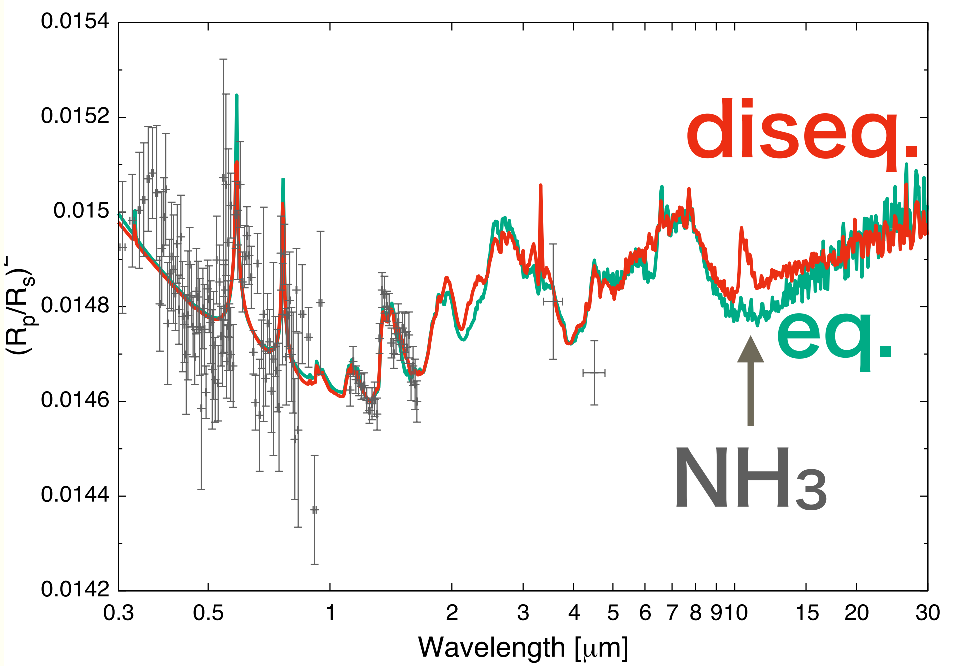


10 hot Jupiters with high-quality transmission spectra observed with HST and Spitzer

TRANSMISSION SPECTRA

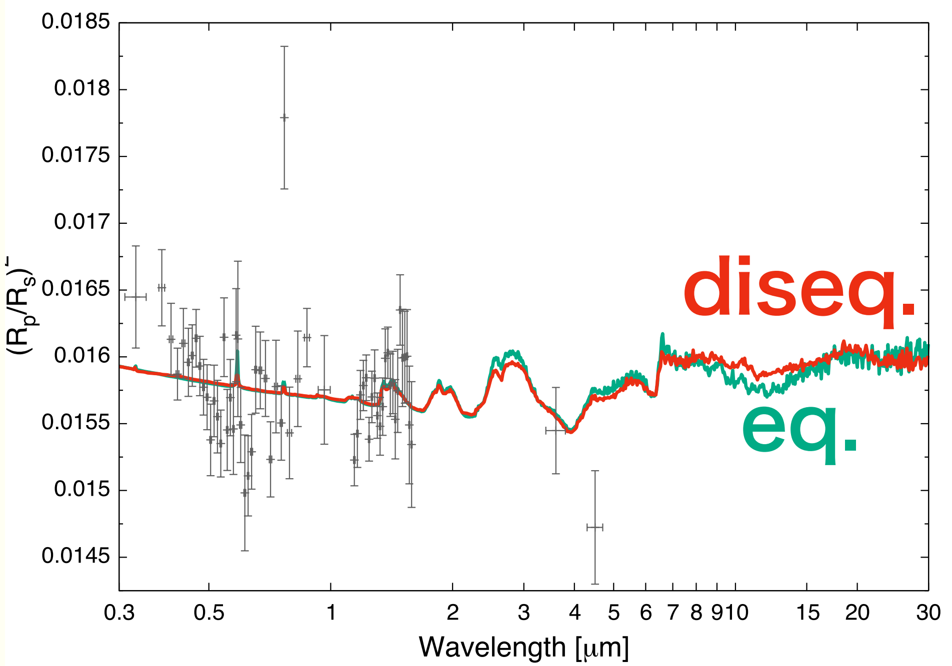
HD 209458b

K_{zz} = 1.1 x 10^{11} cm^2/s



WASP-31b

K_{zz} = 2.7 x 10^2 cm^2/s



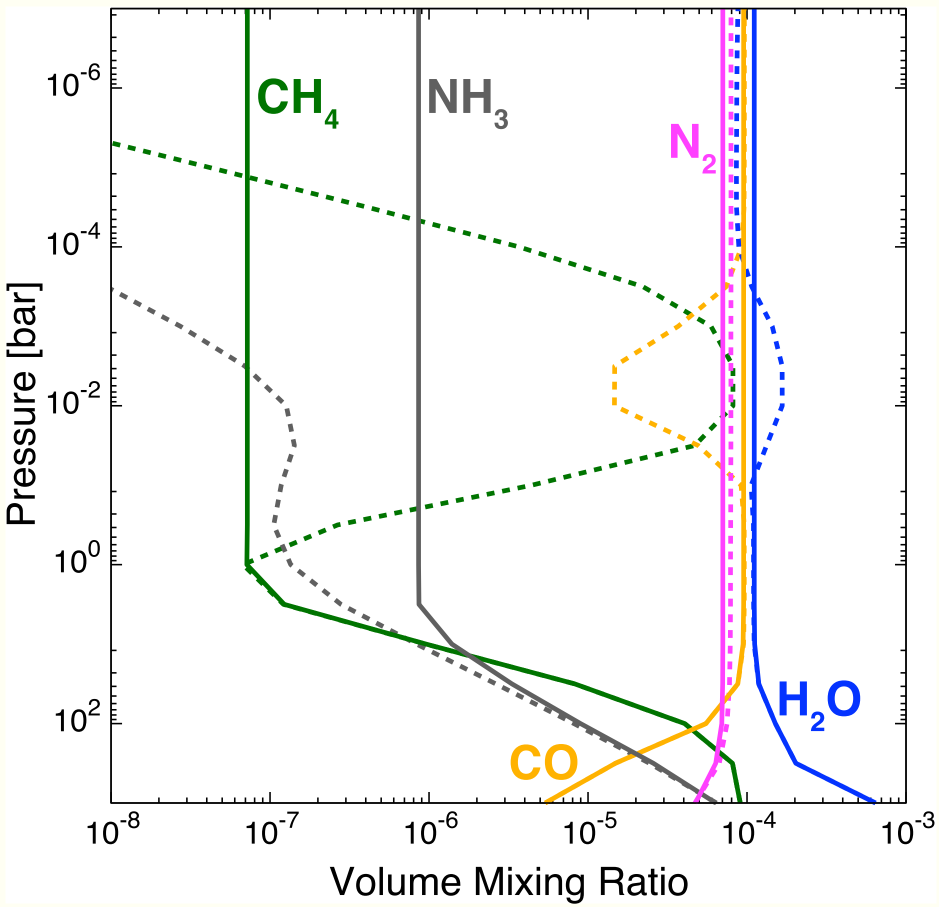
Large differences in NH_3 features

Almost similar

Molecular Distributions

HD 209458b

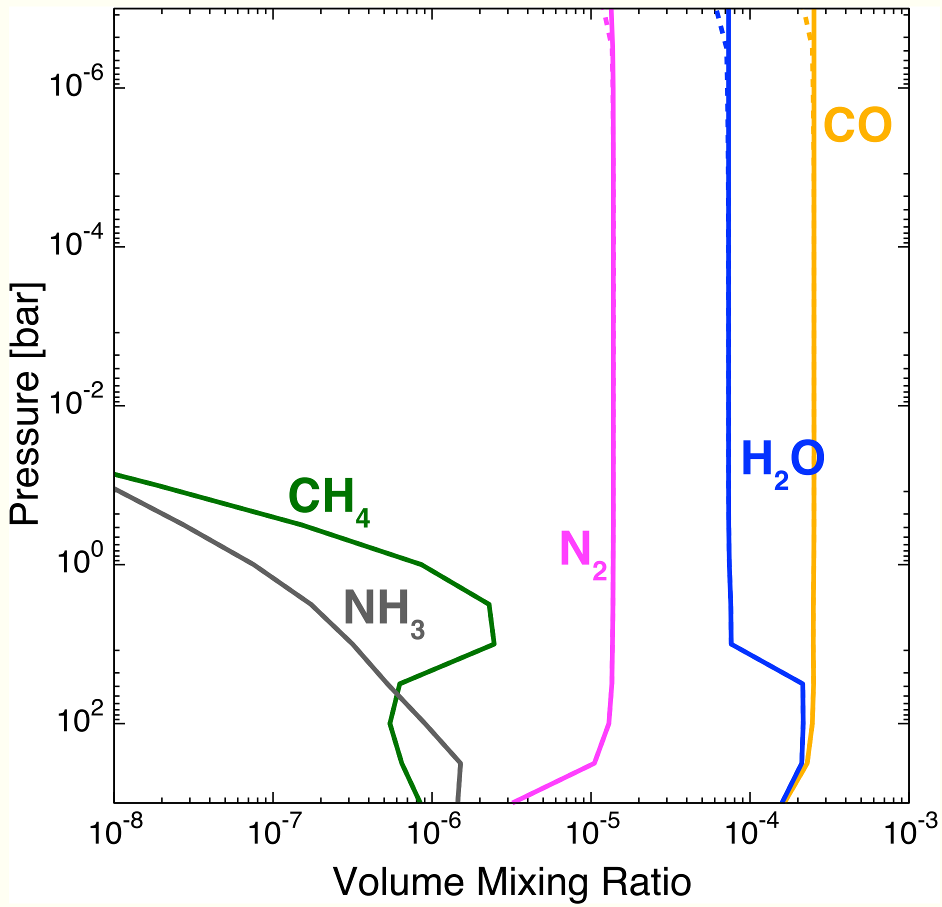
K_{zz} = 1.1 x 10^{11} cm^2/s



Disequilibrium

WASP-31b

K_{zz} = 2.7 x 10^{2} cm^2/s

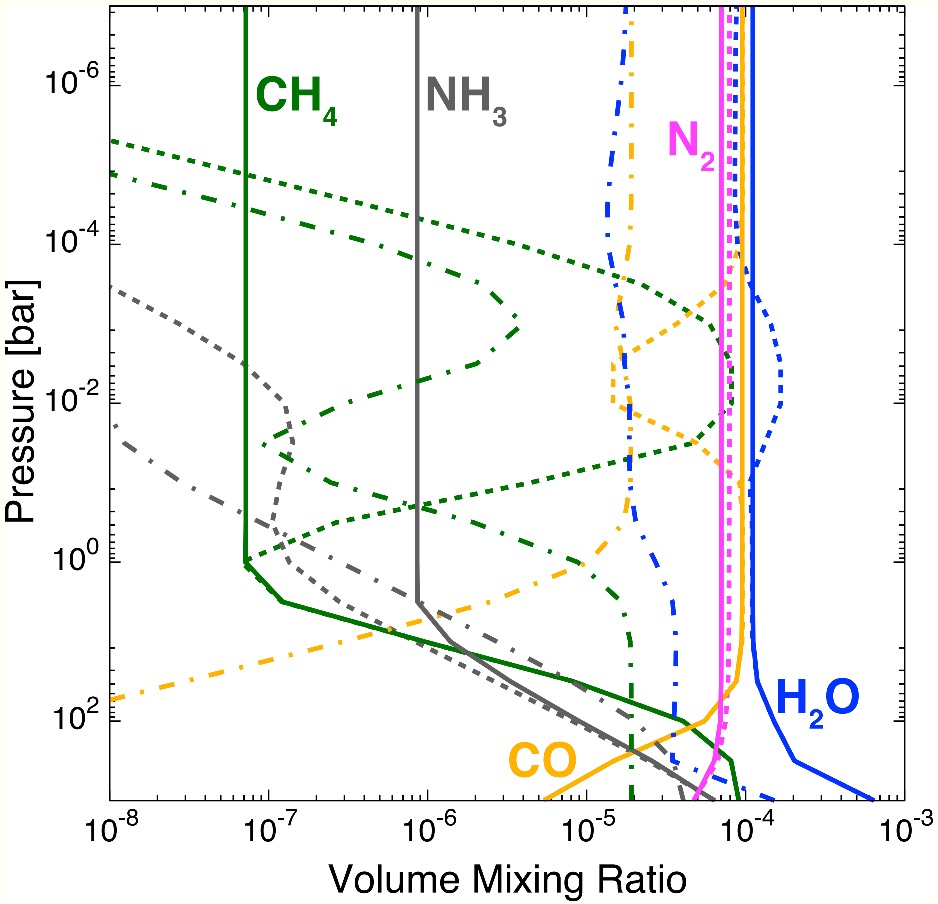


Almost equilibrium

Molecular Distributions

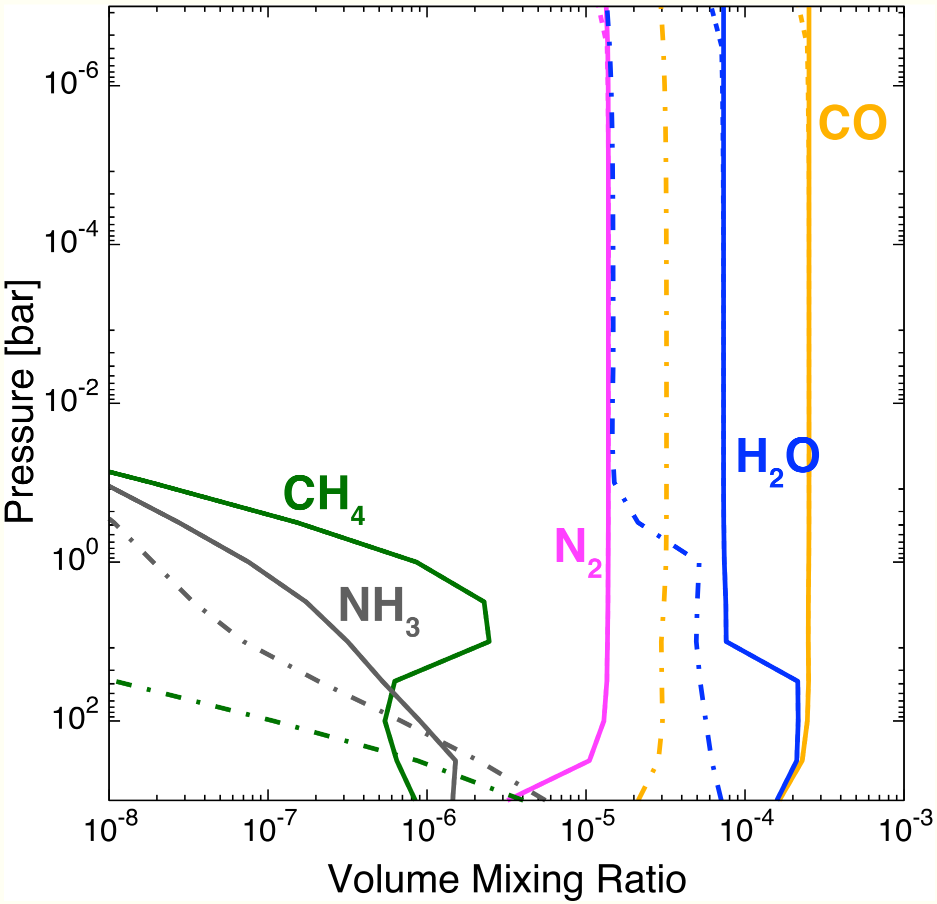
HD 209458b

K_{zz} = 1.1 x 10^{11} cm^2/s



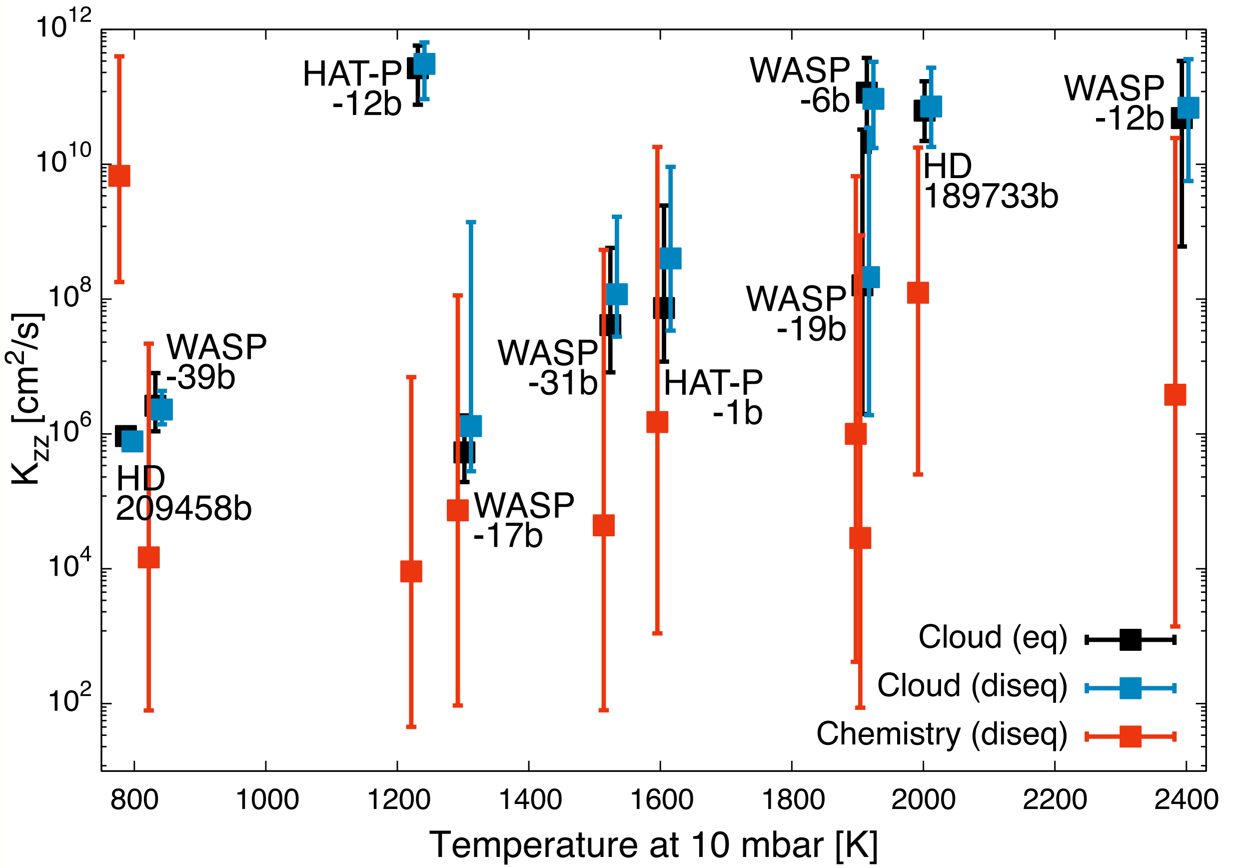
WASP-31b

K_{zz} = 2.7 x 10^{2} cm^2/s



Ignoring chemical disequilibrium process can result in incorrect abundances

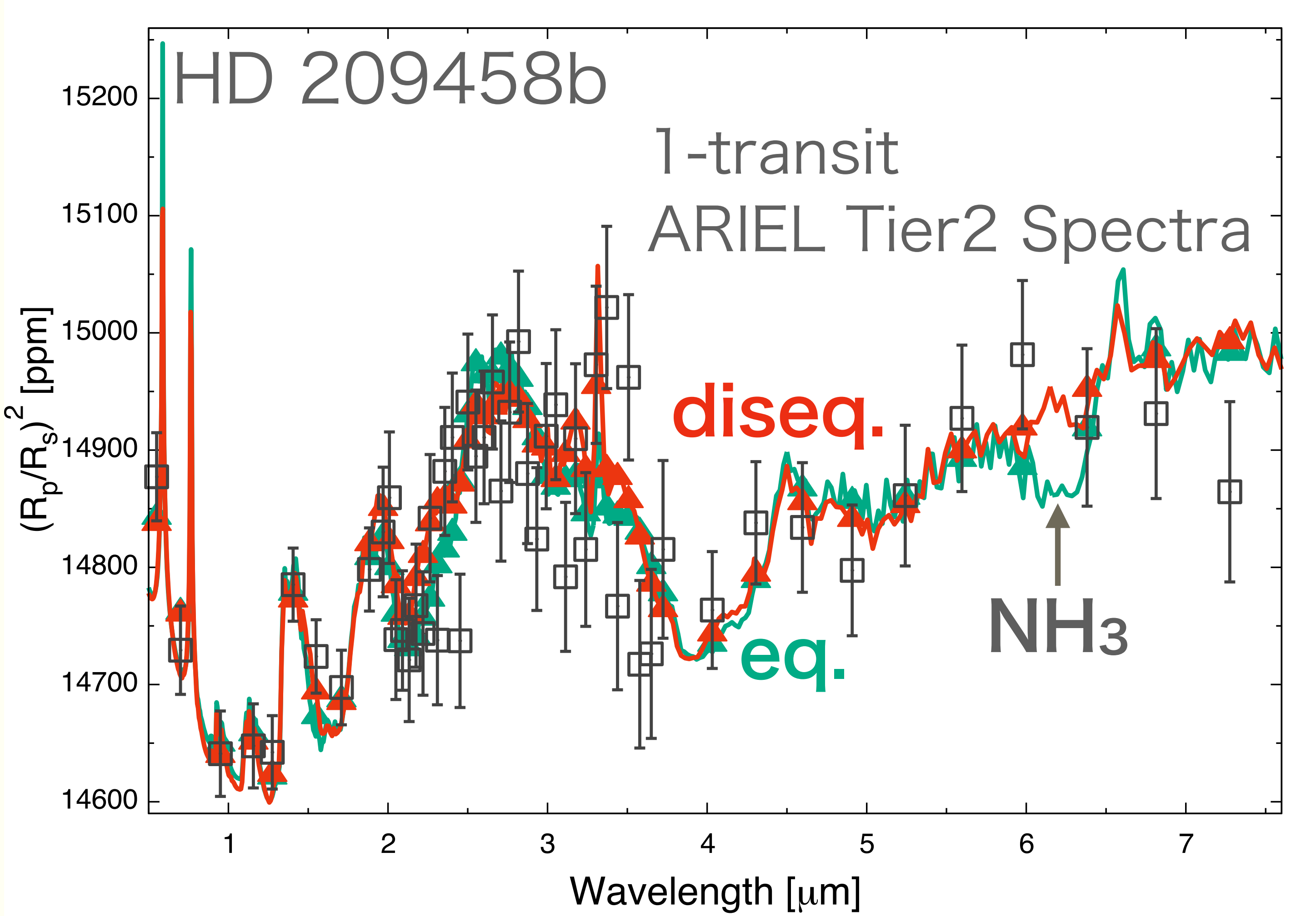
Cloud and Chemistry Kzz



We can retrieve profile of Kzz and explore its trend

- **Cloud Kzz** is almost similar
- **Chemistry Kzz** is lower than **cloud Kzz**: lower Kzz in the lower atmosphere?
- Tentative trend of higher **chemistry Kzz** for hotter atmospheres?

CAN WE EXPLORE DISEQUILIBRIUM EFFECT BY ARIEL?



noises simulated by Edwards+ 2019

Multiple transit observations by ARIEL enable us to explore disequilibrium effect

SUMMARY

- We have developed a model to compute the quenching pressure for each species as a function of the eddy diffusion coefficient using the chemical timescales as derived by Tsai et al. (2018)
- We have implemented this module to the spectral retrieval code ARCiS (Min et al. submitted)
- We have found evidence for disequilibrium chemistry for some planets such as HD 209458b while almost equilibrium chemistry for planets such as WASP-31b
- **ARIEL provides us the opportunity to explore disequilibrium chemistry through NH_3 absorption features for good targets such as HD 209458b**