The next step of modelling disequilibrium chemistry in exoplanet atmospheres

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Outline

• A brief overview of chemical Models

• Chemical relaxation — a simplified chemical scheme that can be implemented in 3D circulation models

• 2D photochemical kinetics model — including the horizontal transport
Why are chemical models useful?

- Determining the atmospheric composition
- Interpreting observations
- Sanity checks on spectral retrievals
- False-positives of biosignatures
VULCAN 1D thermo-photochemical kinetics

Open source: https://github.com/exoclime/VULCAN

-HD189733b model comparison-
-photolysis
-vertical mixing ($\tau_{\text{chem}} > \tau_{\text{dyn}}$)
equilibrium ($\tau_{\text{chem}} < \tau_{\text{dyn}}$)

Tsai et al. in prep
Transport-induced quenching

Equilibrium: \[ \tau_{\text{chem}} < \tau_{\text{dyn}} \]

Disequilibrium: (depending on where it starts to quench)

- \( \tau_{\text{chem}} > \tau_{\text{dyn}} \)
- \( \tau_{\text{chem}} = \tau_{\text{dyn}} \) (quench point)
- \( \tau_{\text{chem}} < \tau_{\text{dyn}} \)
Vertical mixing brings molecules aloft and leads to more absorption.
Challenges of characterising atmospheres

- Uncertainty in rate coefficients
- Sparse observational data
- Chemistry in 3D simulations is over-simplified
- Atmospheric dynamics in 1D chemical models ($K_{zz}$) is over-simplified

(See also Zhang & Showman 2018. Poster: #51)
But planets are 3D!

Examples of 3D circulation models of hot Jupiters

Heng & Showman Annu. Rev. Earth Planet. Sci. 2015. 43
Beyond 1D models

Pseudo 2D (spinning 1D)

Chemical relaxation (for CO) in a GCM


Agundez et al 2017 AA

Drummond et al. 2018 ApJL
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Finding the shortest path is so “relaxing”

Relaxation method:

\[ \sum_{n} \frac{\partial n_i}{\partial t} = Q(n_1, n_2, \ldots) \]

N\_species \times N\_levels matrix

\( T_{\text{chem}} \) is determined by the slowest reaction along the fastest pathway

Finding the fastest path using Dijkstra’s algorithm
Validation of chemical relaxation with T-P dependent timescales

“Rate-limiting reactions” for CH4—CO

$\tau_{\text{chem}} (P, T)$ for CH4, CO, H2O, CO2, NH3 and N2

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2D chemical kinetics

y: current step  
y': the next step

1:  \[ y'_1 = C_1 - \nabla \phi_z - \nabla \phi_h(y_1, y_4) \]

2:  \[ y'_2 = C_2 - \nabla \phi_z - \nabla \phi_h(y'_1, y_3) \]

3:  \[ y'_3 = C_3 - \nabla \phi_z - \nabla \phi_h(y'_2, y_4) \]

4:  \[ y'_4 = C_4 - \nabla \phi_z - \nabla \phi_h(y'_3, y'_1) \]
Applying to WASP-43 b
—GCM output

Applying to WASP-43 b
—Taking the GCM output as the input for the 2D chemical model
2D evolution

Wasp 43-b

10 steps and $1.74 \times 10^{-10}$ s

Tsai et al. in prep

Pressure (bar)

$10^{-6}$

$10^{-4}$

$10^{-2}$

$10^0$

$10^2$

$10^4$

$10^6$

Mixing Ratios

$10^{-16}$

$10^{-14}$

$10^{-12}$

$10^{-10}$

$10^{-8}$

$10^{-6}$

$10^{-4}$

$10^{-2}$

$10^0$

Day

Night

Morning

Evening

Tsai et al. in prep
T-P and wind input

Graph showing temperature (K) vs. pressure (bar) with wind velocities (m/s) on the x-axis. Lines represent different times of day:
- Red line: day, $U_{peak} = 1000$ (m/s)
- Purple line: evening/morning, $U_{peak} = 1000$ (m/s)
- Blue line: night, $U_{peak} = 5000$ (m/s)
Sensitivity of CH$_4$ to horizontal transport

constant $K_{zz} = 10^9$ cm$^2$s$^{-1}$

$\tau_{\text{day}}^{\text{CH}_4} < \tau_h < \tau_{\text{day}}^{\text{z}} < \tau_{\text{night}}^{\text{CH}_4}$

$\tau_h$: horizontal transport
$\tau_z$: vertical mixing
Sensitivity of HCN to horizontal transport

Equilibrium Kinetics

constant $K_{zz} = 10^{10}$ cm$^2$s$^{-1}$

0.01 X H$_2$O observable

(MacDonald & Madhusudhan 2018, ApJL, 850)
Observational consequences — synthetic transit spectra

sensitivity to vertical mixing

sensitivity to horizontal wind
Summary

- Chemical relaxation scheme is validated and fast enough to be implemented in a 3D GCM

- 2D photochemical kinetics models allow us to include horizontal transport

- The compositions on the morning/evening limbs are sensitive to horizontal transport

- Transmission spectra hints the circulation regime

- Some hot/warm Jupiters might smell like almonds on the nightside (photochemically generated species quenched)
Thanks to

Transit spectra
Equilibrium chemistry
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Radiative transfer
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(Poster: 114)

GCM
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(Poster: 115)

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https://github.com/exoclime/VULCAN/tree/vulcan_photo