Disequilibrium in planetary atmospheres:

*a new physical method coupled with new computational tool*

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Atmospheric Chemical Disequilibrium and Life

Earth
The extent of chemical disequilibrium

\[ \frac{d_i S}{dt} = J \cdot X = \frac{d \xi}{dt} \cdot \frac{\alpha}{T} \]

Extent of reaction:
\[ \xi(t) = \frac{[A]_0 - [A](t)}{\nu_A} \]

Chemical Affinity
\[ \alpha(t) = -\left( \frac{\partial \Delta_r G(t)}{\partial \xi} \right)_{T,p} \]

It can be also written as:
\[ \frac{d_i S}{dt} = R \cdot (R_f - R_r) \cdot ln \left( \frac{R_f}{R_r} \right) \]

\[ R_f = \text{forward rate} \]
\[ R_r = \text{backward rate} \]

Simoncini E., Extent of chemical disequilibrium and planetary habitability, \textit{in prep.}
[ The chemical potential and the reaction kinetics ]

\[ k_r = k_f \cdot \exp \left( \frac{\Delta_R G^0}{R \cdot T_0} + K_R(T) \right) \]

\[ \text{CO} + \text{NO}_2 \rightleftharpoons \text{CO}_2 + \text{NO} \]

KROME

- Python Pre-processor provides Fortran routines
- Creates modules from chemical network
- Dust evolution, Cooling, Heating, Photoionization
- Large test suite (MC, 1D SNe, planet, stellar, 3D wrappers, …)
- Highly optimized, fast solvers
- Open source, bitbucket community
- Grassi et al. 2013


www.kromepackage.org
Earth Atmospheric Chemical Disequilibrium

Our first calculation:


* 64 layers (~1km each); no eddy diffusion, only chemistry.

* Entropy production and the power dissipation

\[ \sigma = \frac{d_i S}{dt} \]

\[ \frac{\sigma \times T}{A_{Earth}} \sim W m^{-2} \]
Earth Power dissipation in atmosphere

Thermal or mechanical powers in the Earth’s atmosphere:

\[ \sim 10/100 \text{ W m}^{-2} \]
Perspectives

• Comparison of entropy production between planets (=> habitability?)
• Comparison between different power sources
• Application to any typology of exoplanet
Thanks for your attention!

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