Exoplanetary Atmospheres and Habitability
Observatoire de la Côte d'Azur, Nice
October 15th, 2015

Modeling chemical uncertainties in a pale orange dot

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Oak Ridge Associated Universities

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NASA Astrobiology Institute Virtual Planetary Laboratory

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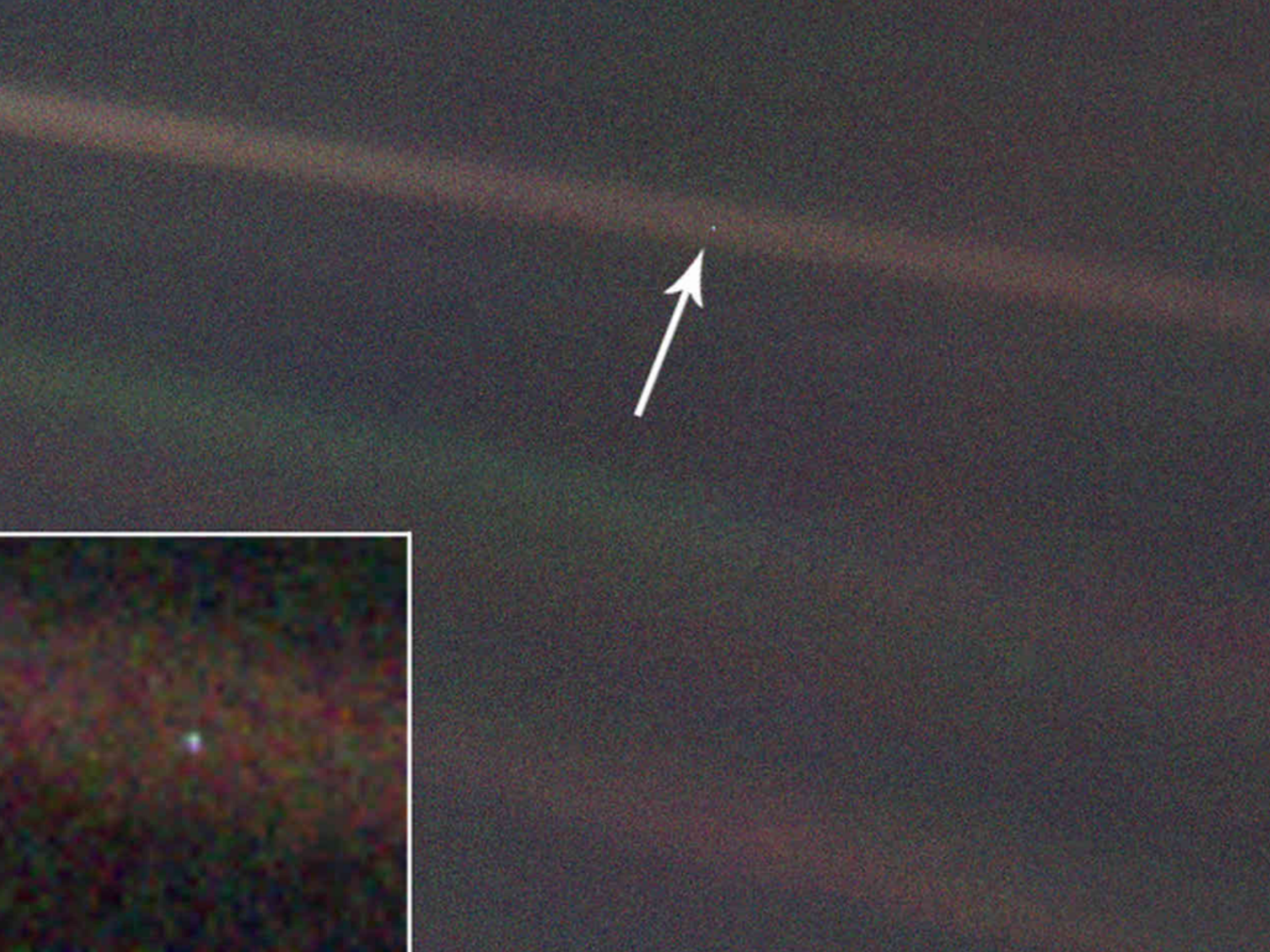
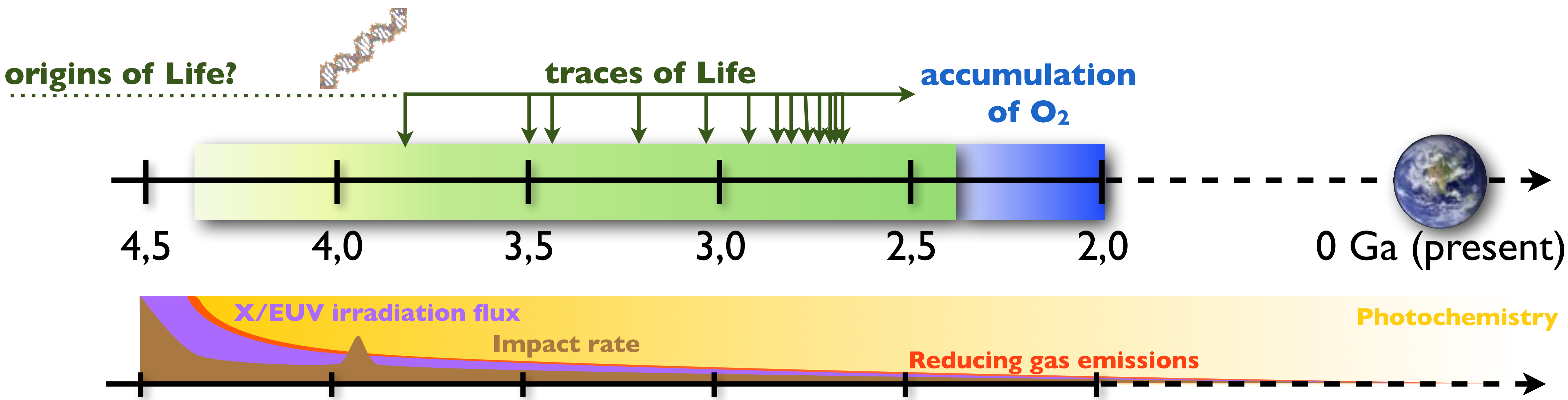
University of Washington - Astronomy Department
NASA Astrobiology Institute Virtual Planetary Laboratory
University of Washington - Astrobiology Program



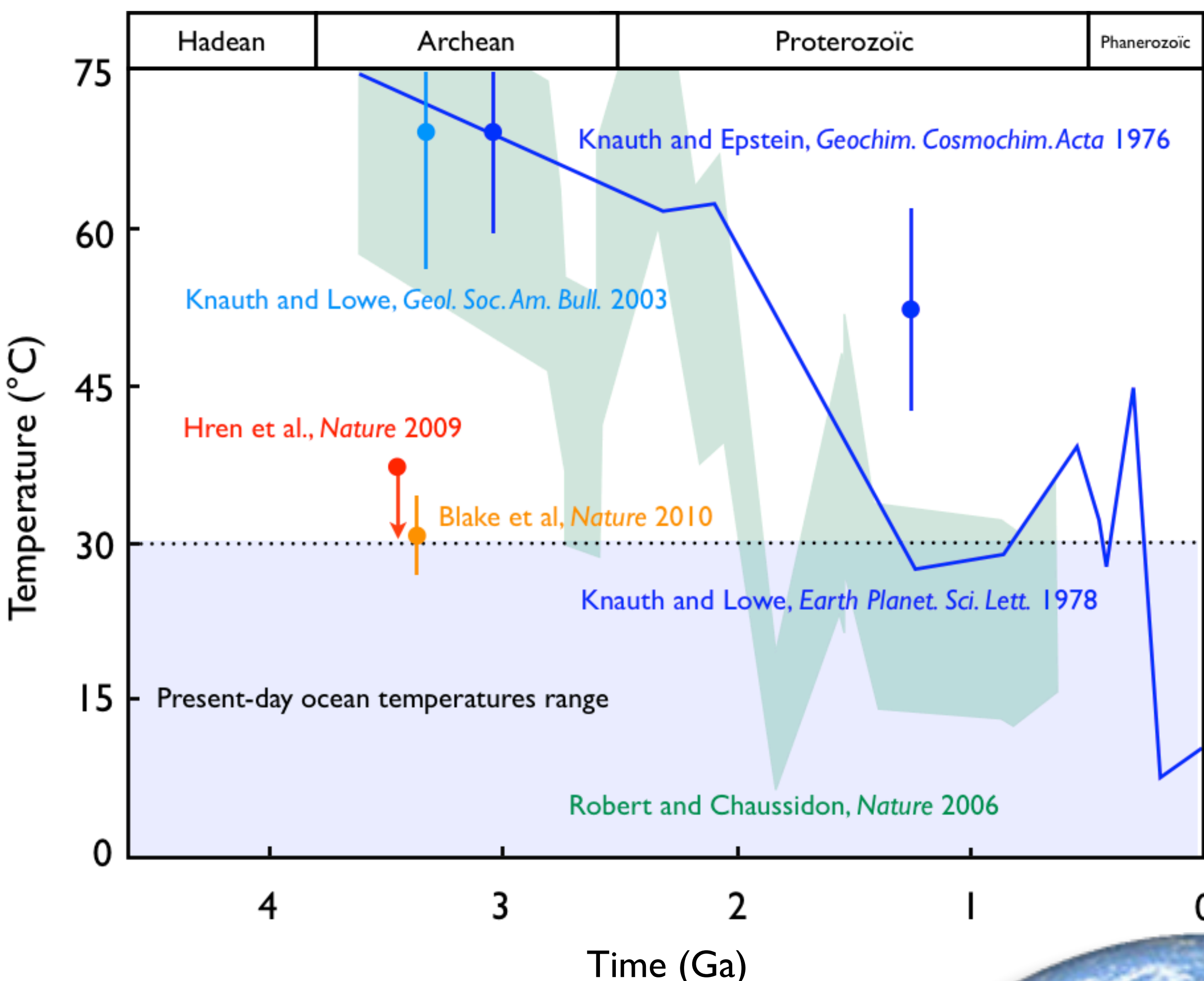
EARTH THROUGH TIME

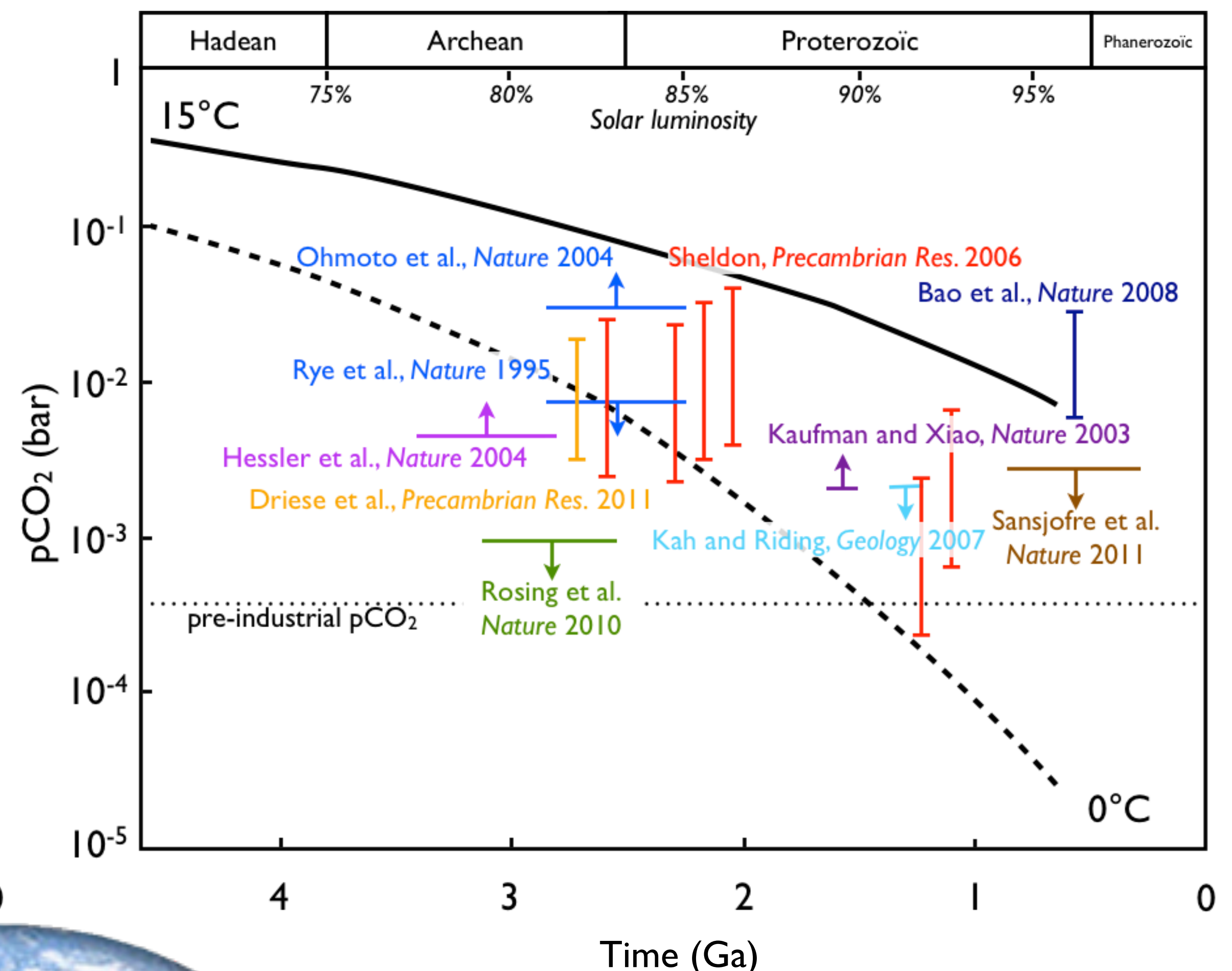
From an atmospheric evolution...



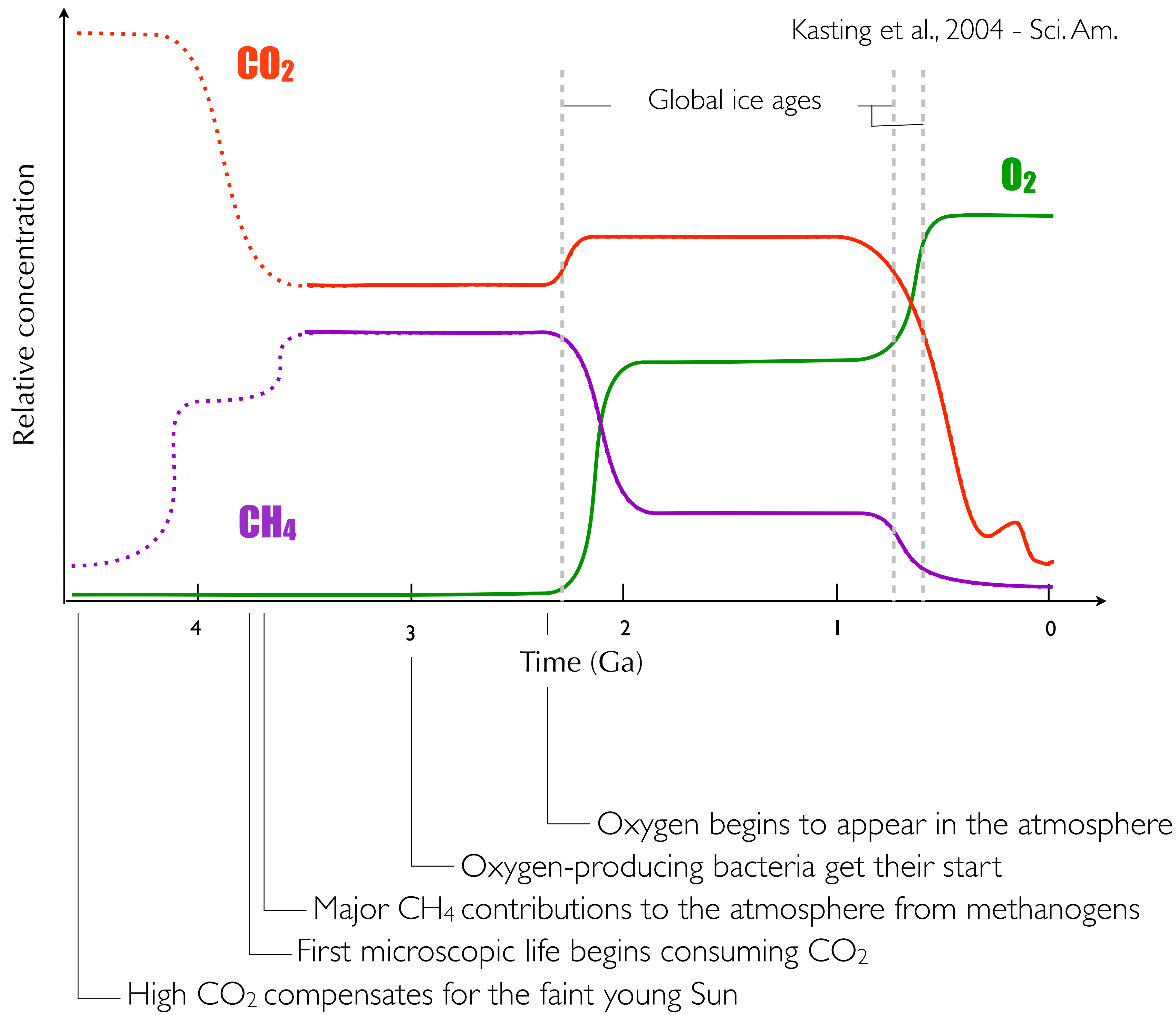
... to observable features evolution

EARTH THROUGH TIME

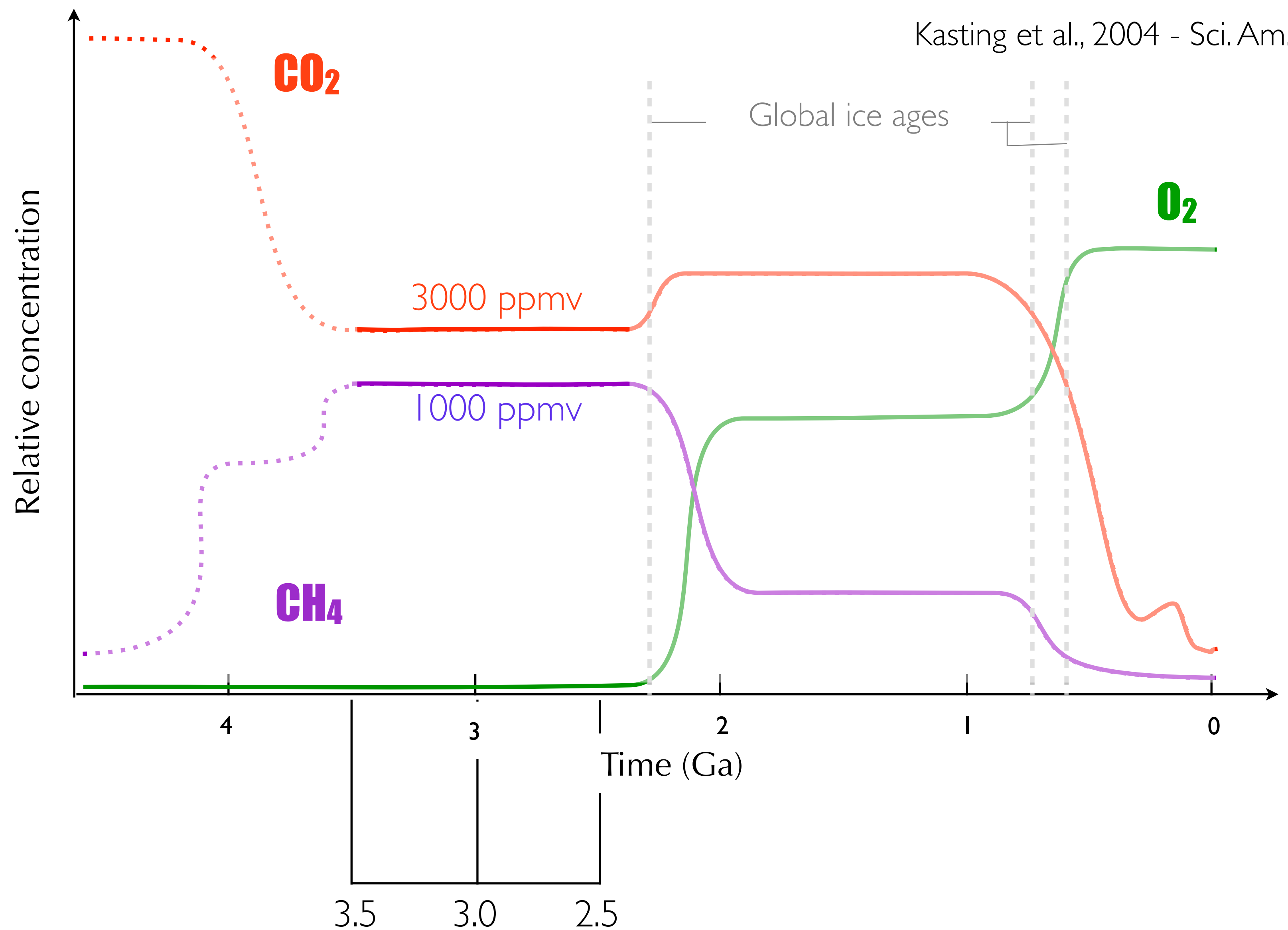




EARTH THROUGH TIME

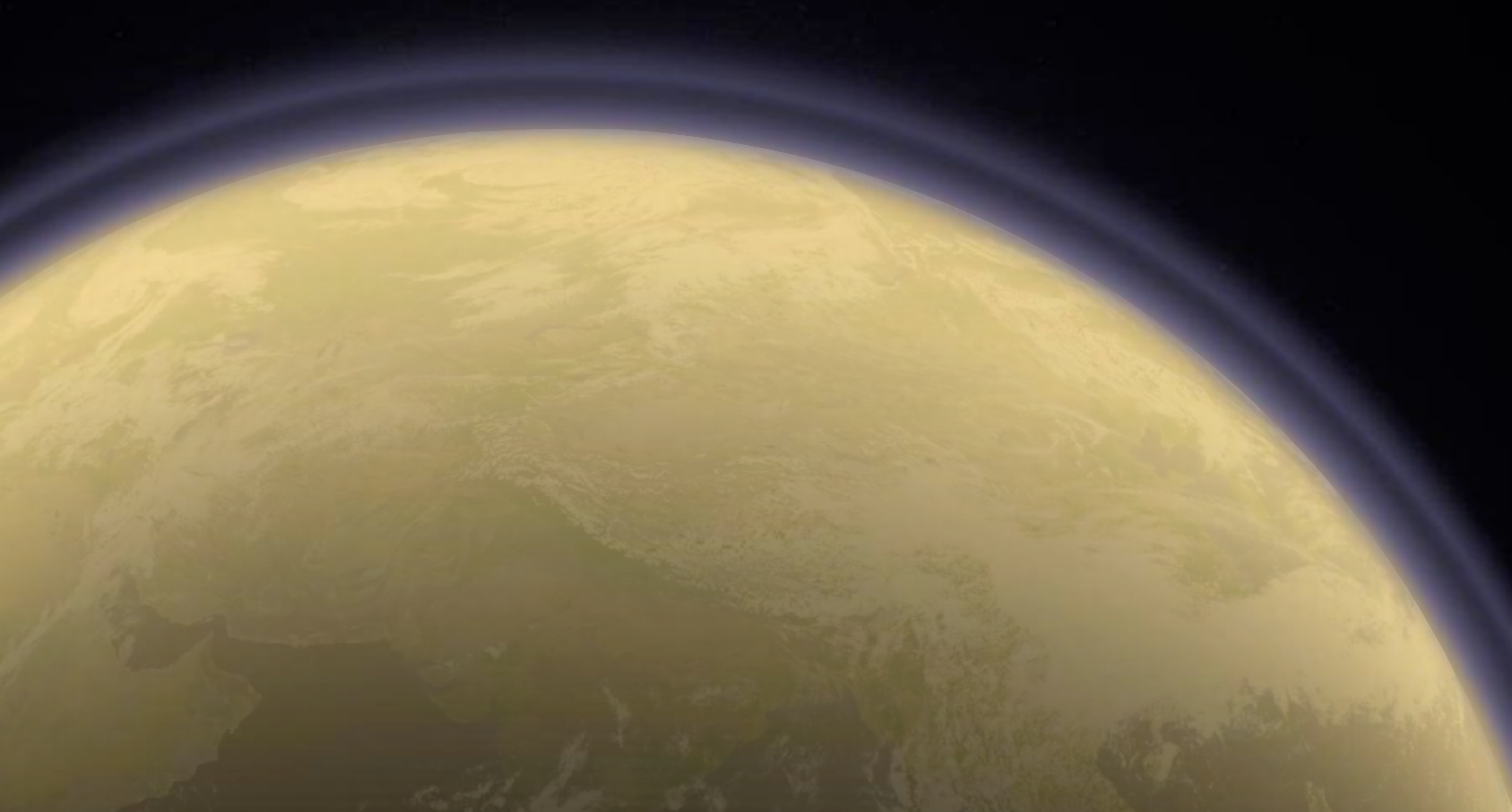


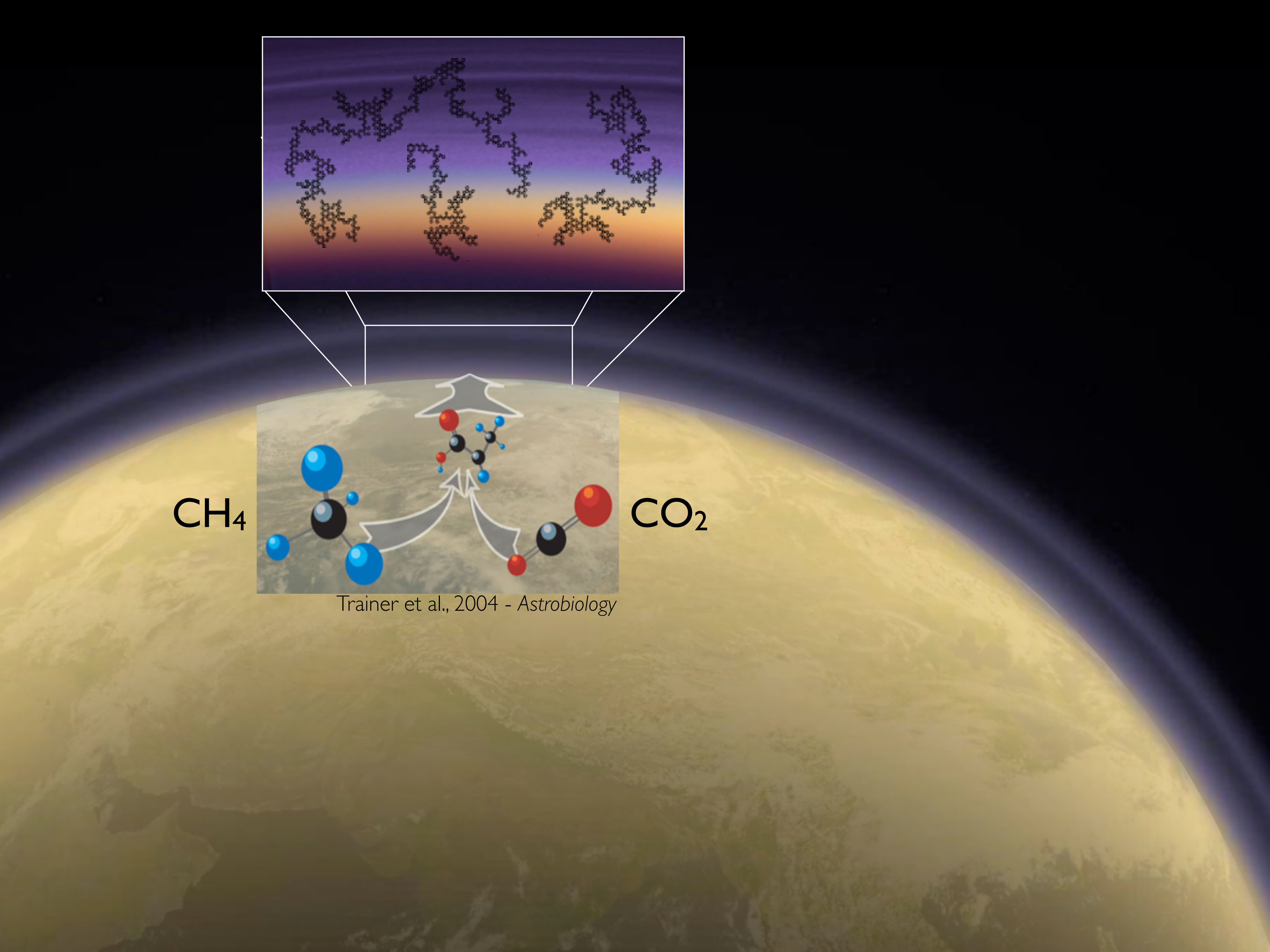
EARTH THROUGH TIME

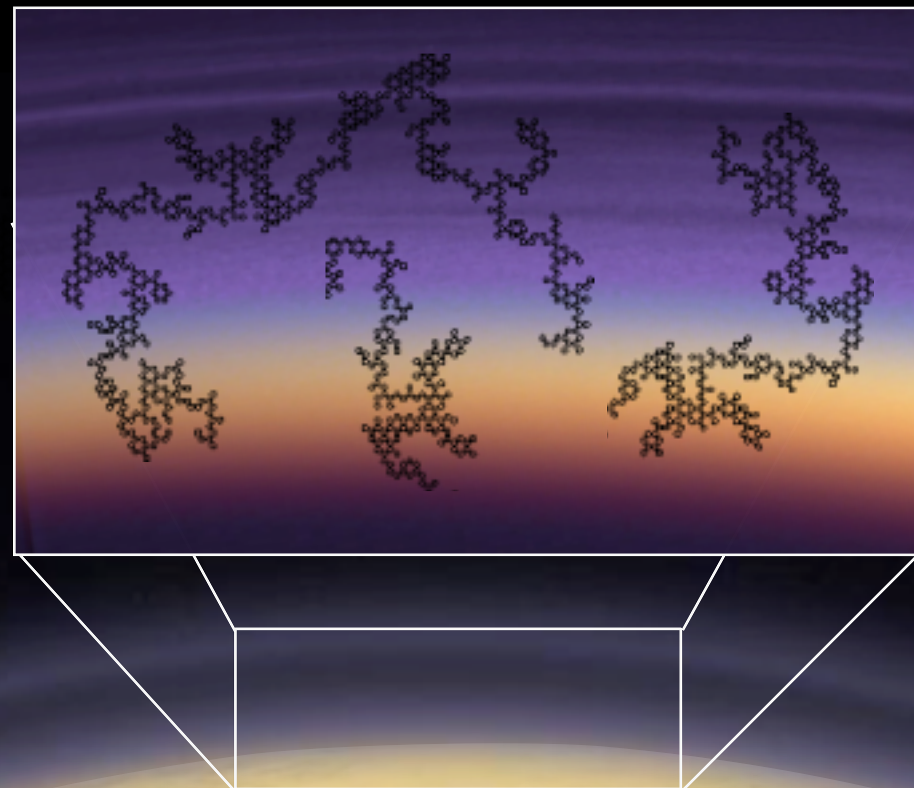


Pavlov et al., 2001a
Pavlov et al., 2001b
Trainer et al., 2004
Trainer et al., 2006
Haqq-Misra et al., 2008
Domagal-Goldman et al., 2008
Zerkle et al., 2012
Kurzweil et al., 2013

ARCHEAN EARTH



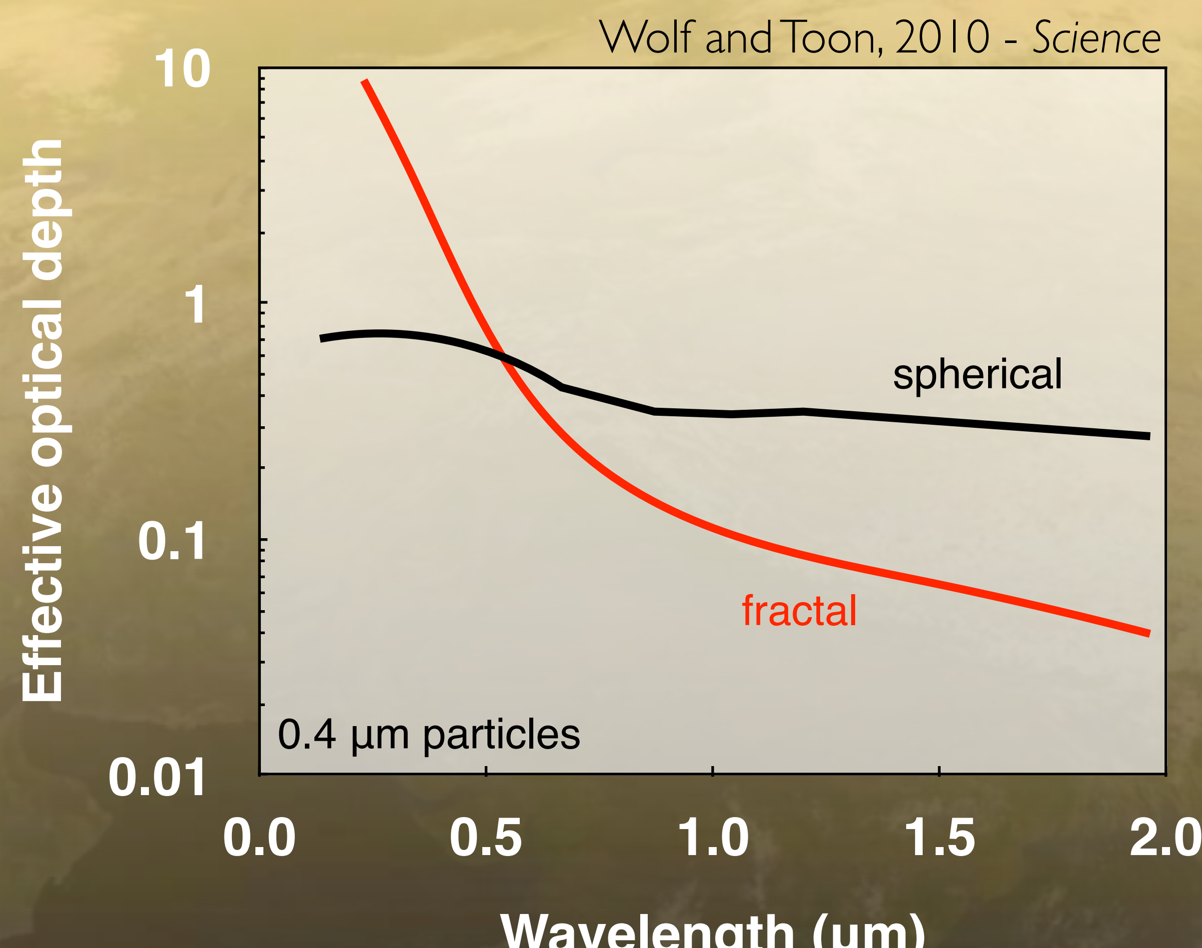

CH4
CO2
Trainer et al., 2004 - Astrobiology



Impact on atmospheric chemistry ?

Impact on planetary climate ?

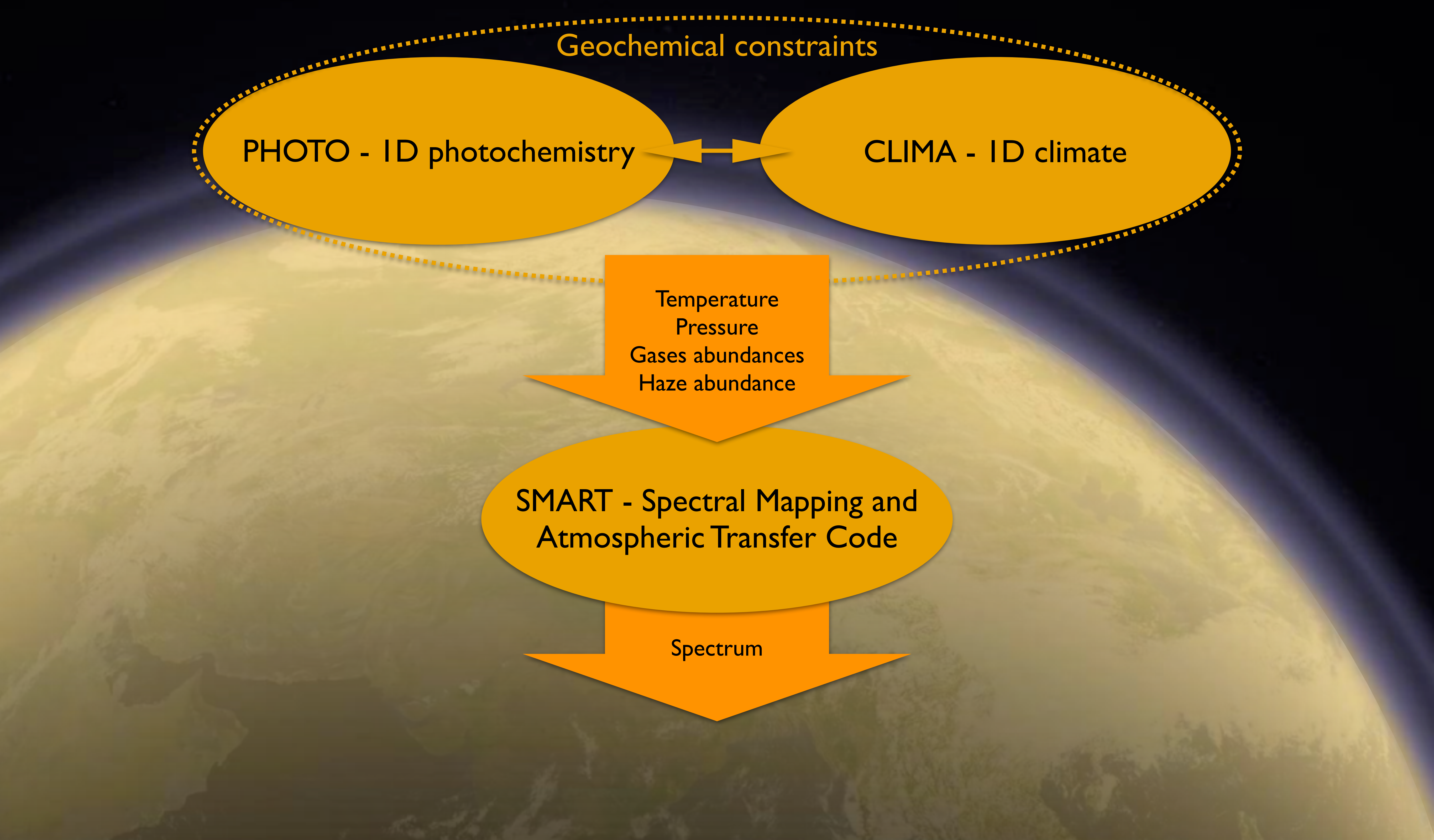
Impact on planetary spectrum ?



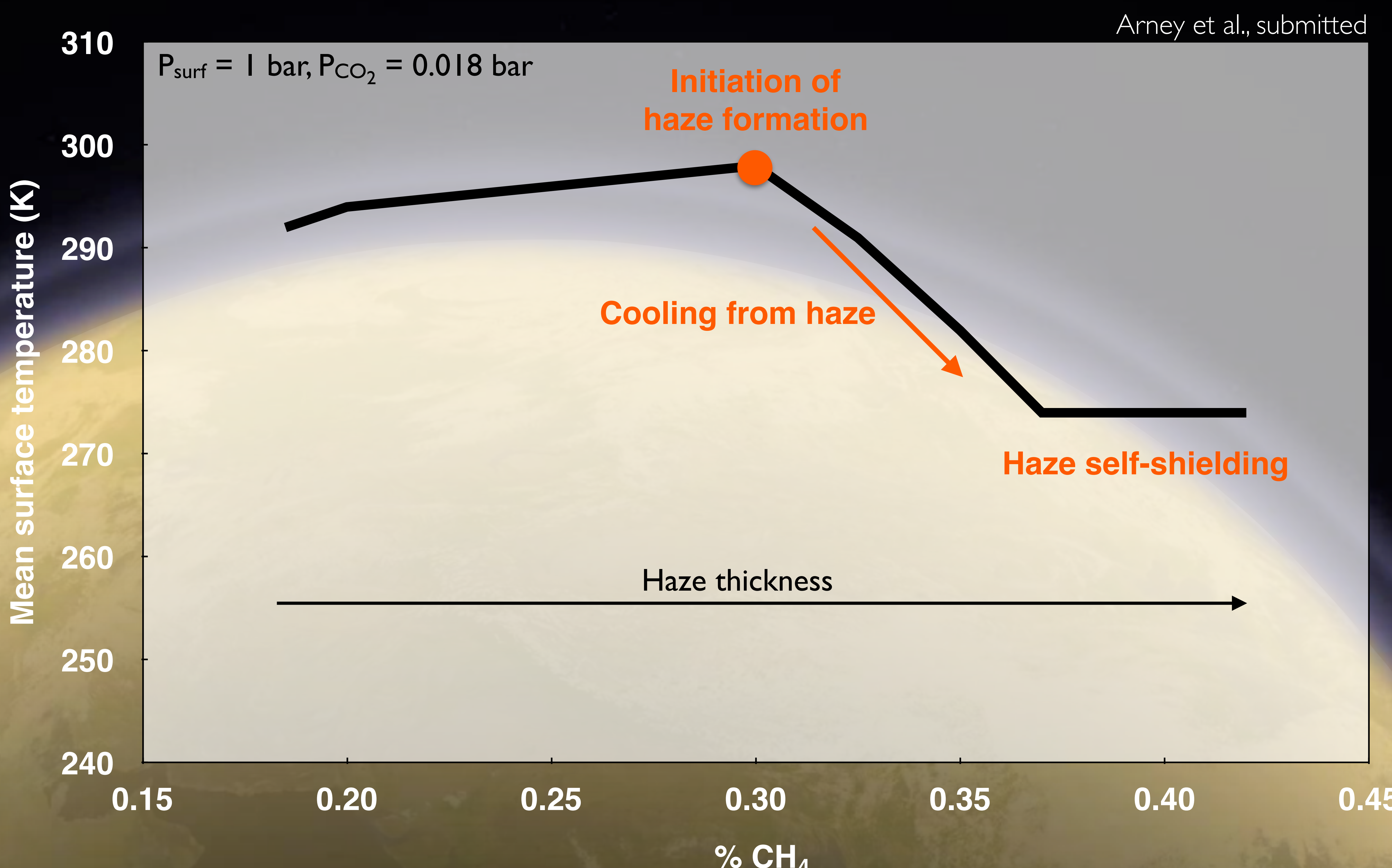
Less extinction at visible wavelengths

More extinction at UV wavelengths

vplanet

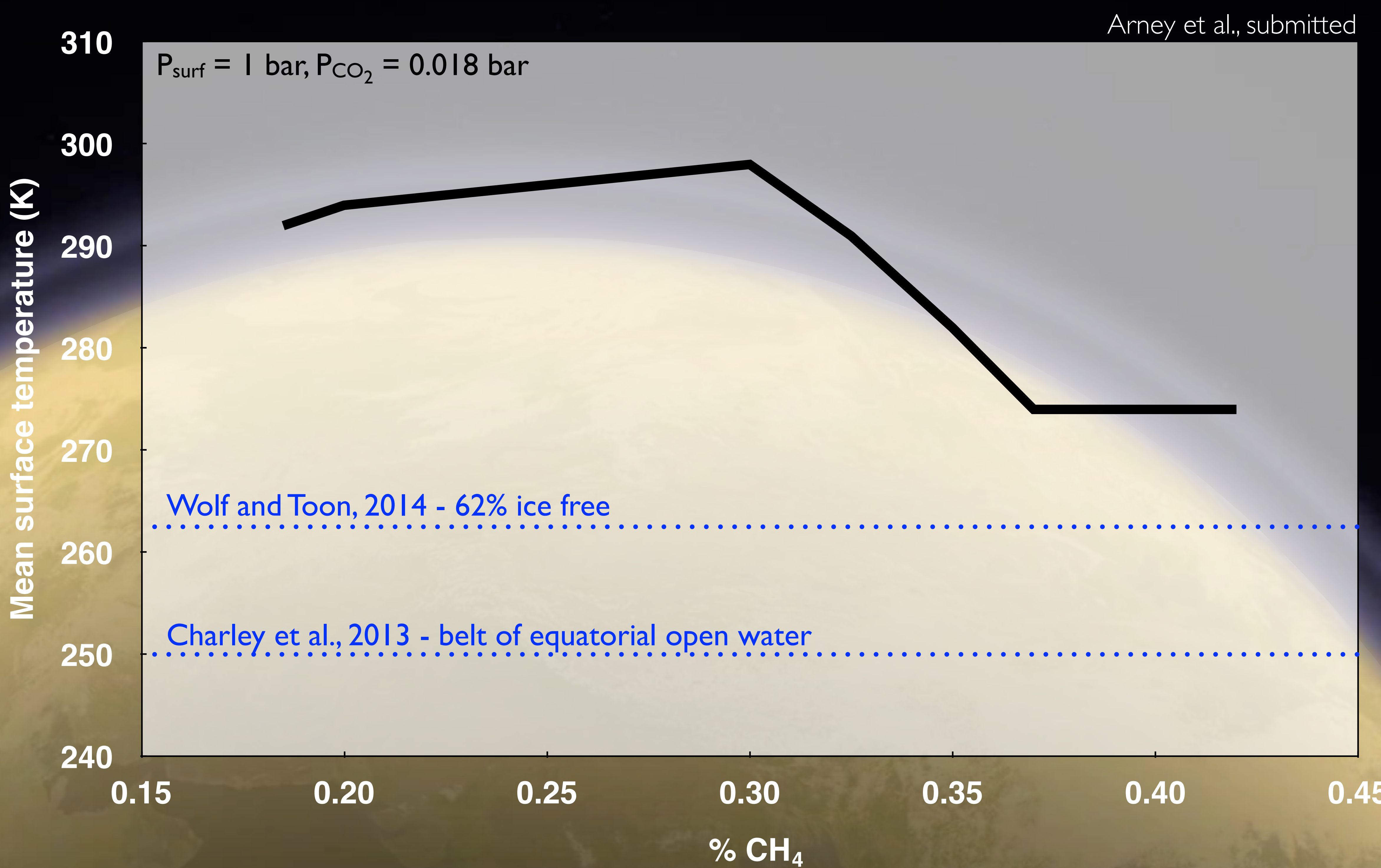

Geochemical constraints
PHOTO - 1D photochemistry
CLIMA - 1D climate
Temperature
Pressure
Gases abundances
Haze abundance
SMART - Spectral Mapping and Atmospheric Transfer Code
Spectrum

vplanet

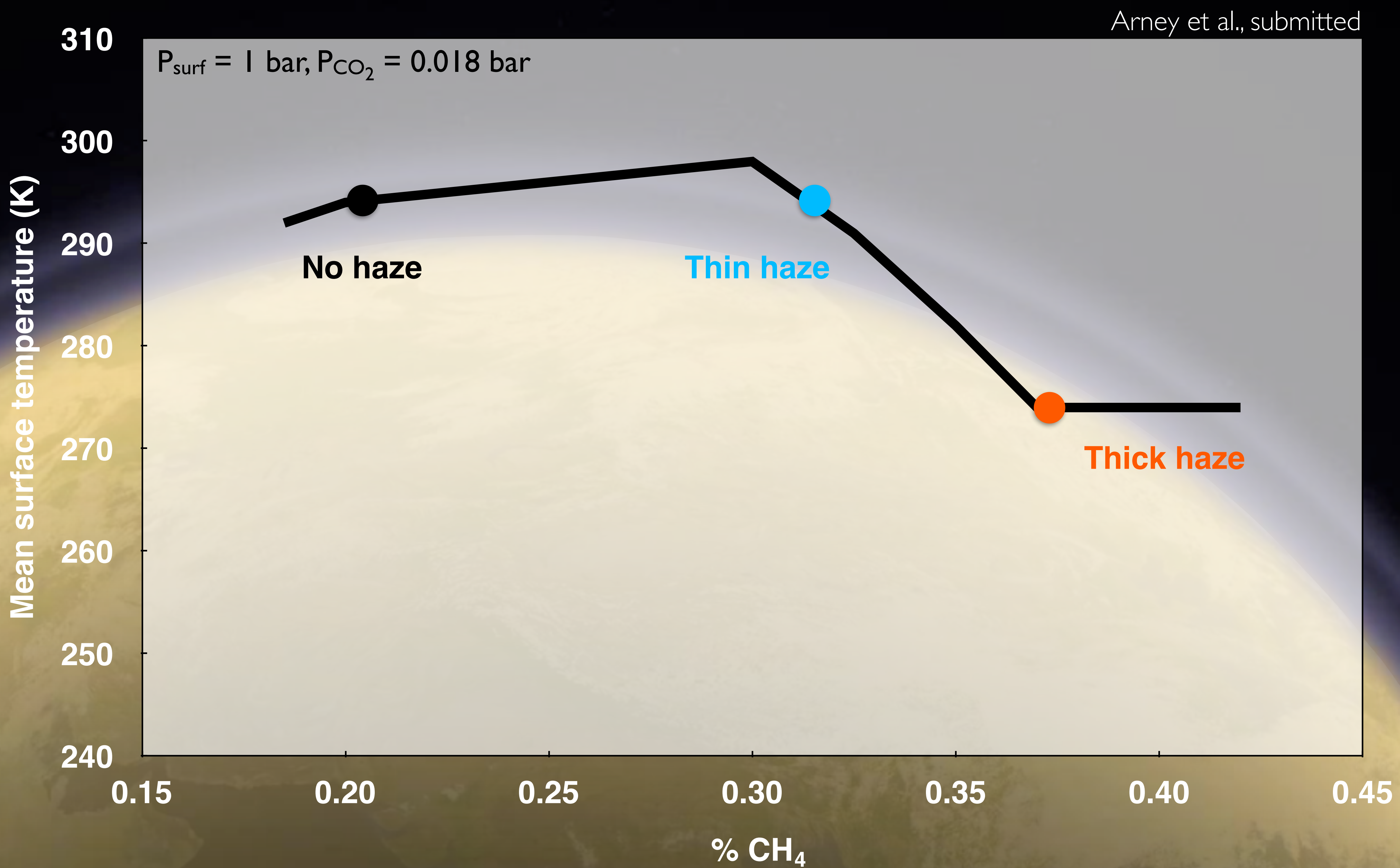


Arney et al., submitted
P_{surf} = 1 bar, P_{CO_2} = 0.018 bar
Initiation of haze formation
Cooling from haze
Haze self-shielding
Haze thickness
310
300
290
280
270
260
250
240
Mean surface temperature (K)
0.15
0.20
0.25
0.30
0.35
0.40
0.45
% CH_4

vplanet

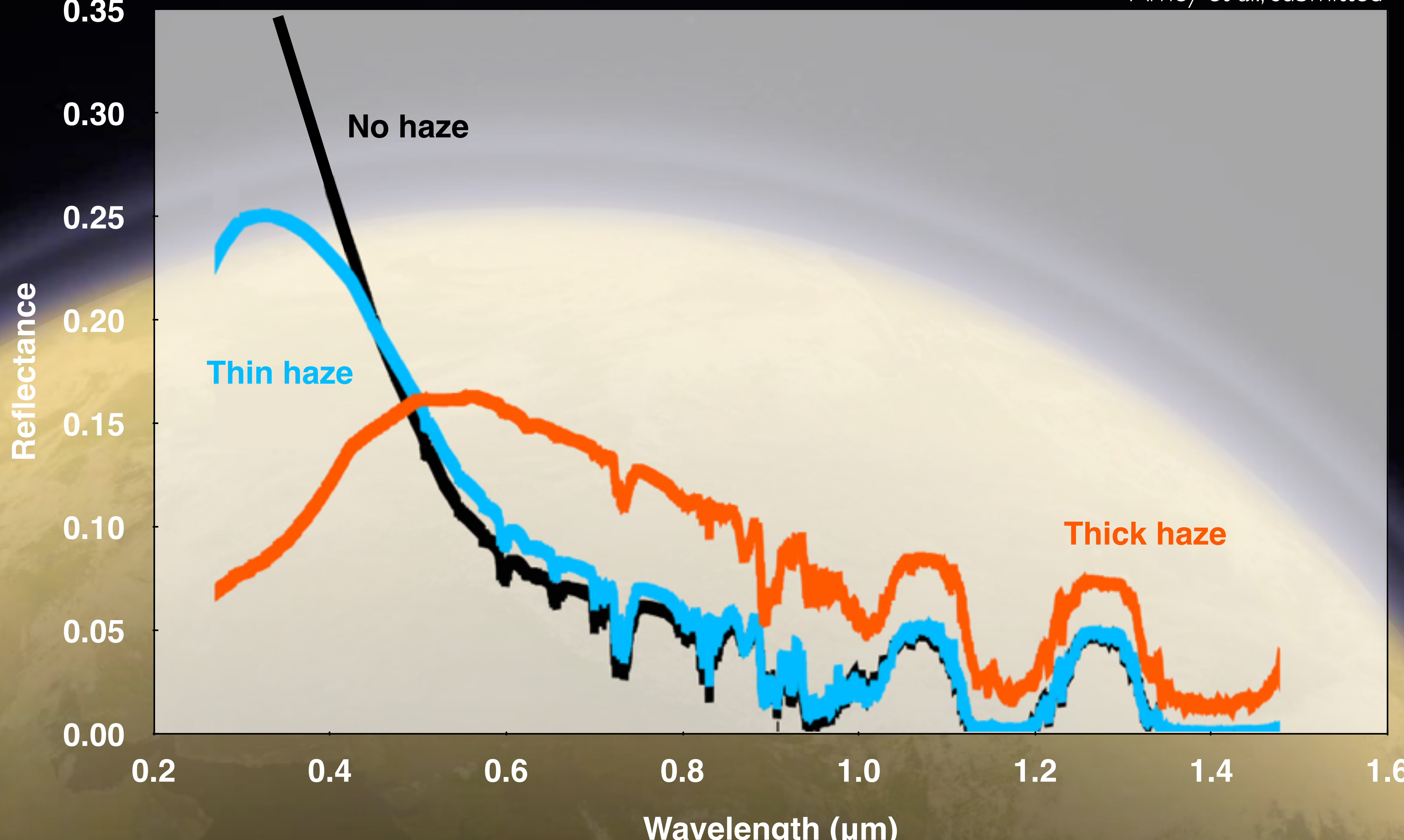


Arney et al., submitted
P_surf = 1 bar, P_CO2 = 0.018 bar
Wolf and Toon, 2014 - 62% ice free
Charley et al., 2013 - belt of equatorial open water
Mean surface temperature (K)
310
300
290
280
270
260
250
240
0.15
0.20
0.25
0.30
0.35
0.40
0.45
% CH4



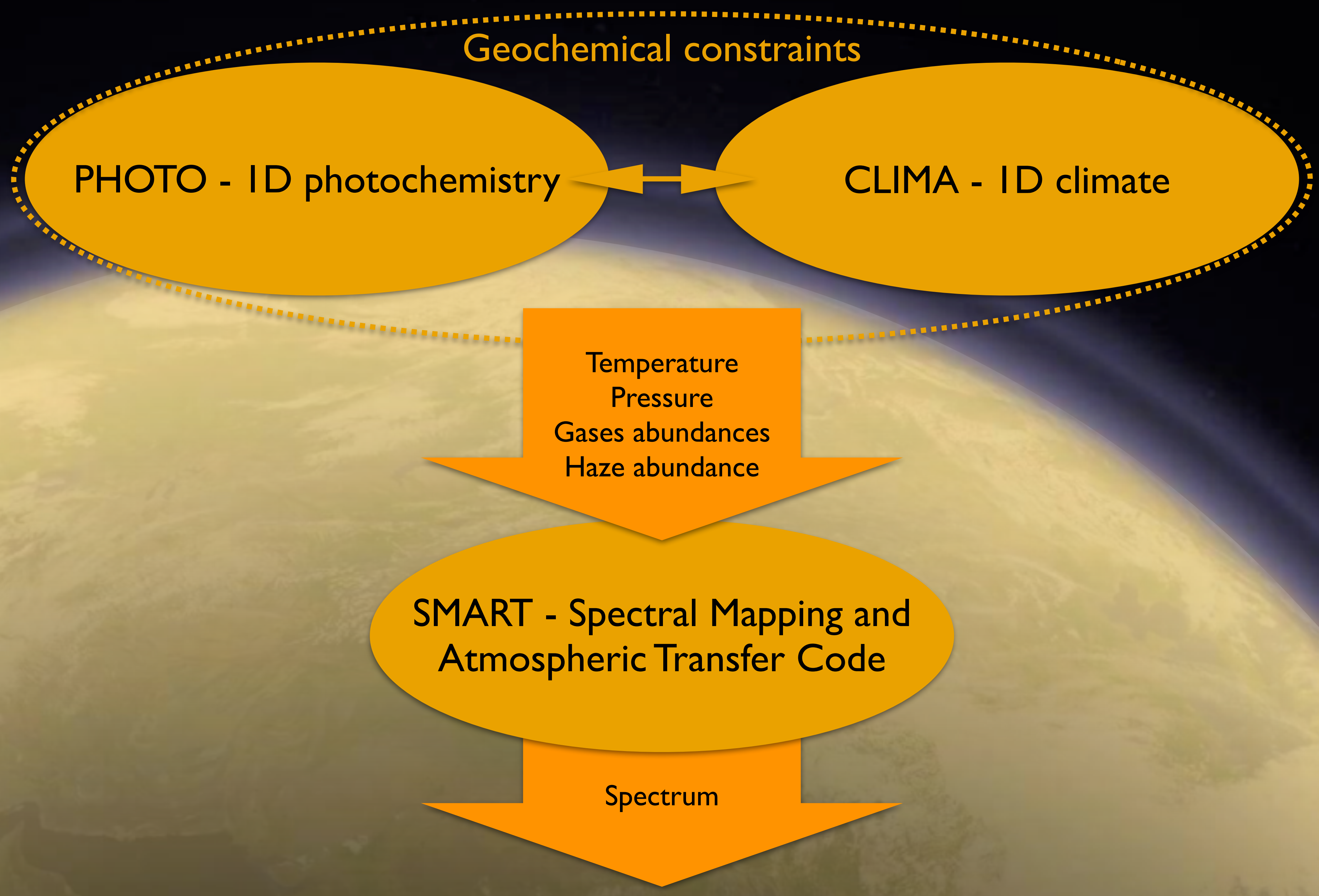
Arney et al., submitted
P_{surf} = 1 bar, P_{CO_2} = 0.018 bar
Mean surface temperature (K)
310
300
290
280
270
260
250
240
No haze
Thin haze
Thick haze
0.15
0.20
0.25
0.30
0.35
0.40
0.45
% CH_4

vplanet



Arney et al., submitted

vplanet


Geochemical constraints
PHOTO - 1D photochemistry
CLIMA - 1D climate
Temperature
Pressure
Gases abundances
Haze abundance
SMART - Spectral Mapping and Atmospheric Transfer Code
Spectrum

PHOTOCHEMICAL MODELING

- Chemical models of planetary atmospheres are complex ([0-3]D chemical-dynamical codes with thousands of highly coupled nonlinear equations)

- The chemical equations are based on **empirical parameters** :

$$\mathrm{AB} \xrightarrow{h\nu} \mathrm{A} + \mathrm{B}$$

$$\sigma_i(\lambda, T) \quad q_{i,j}(\lambda, T)$$

Photodissociations

$$\mathrm{A} + \mathrm{B} \xrightarrow{(+\mathrm{M})} \mathrm{C} + \mathrm{D}$$

$$k_i(T) = \alpha_i \left(\frac{T}{300}\right)^{\beta_i} \exp\left(-\frac{\gamma_i}{T}\right)$$

Neutral-neutral thermal reactions

- These empirical parameters are obtained from experiments, calculations and/or [more or less [but most often less]] educated-guessed estimations :

  ☞ They are always evaluated with **[[very] large] uncertainty**

  ☞ Most of the cases, **extrapolations** of these parameters are mandatory

PHOTOCHEMICAL MODELING

$$\mathrm{AB} \xrightarrow{h\nu} \mathrm{A} + \mathrm{B}$$

$$\sigma_i(\lambda, T) \quad q_{i,j}(\lambda, T)$$

Photodissociations

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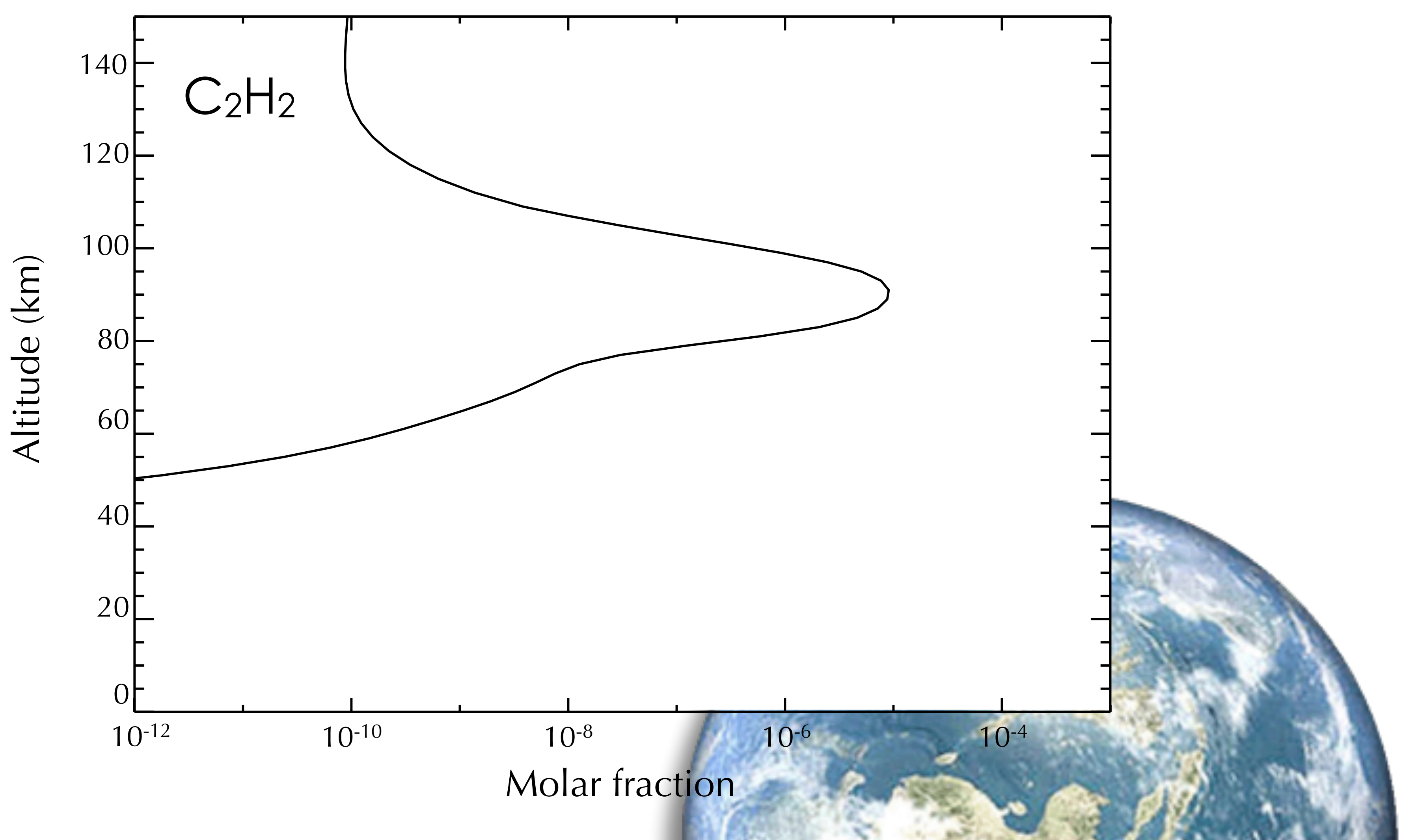
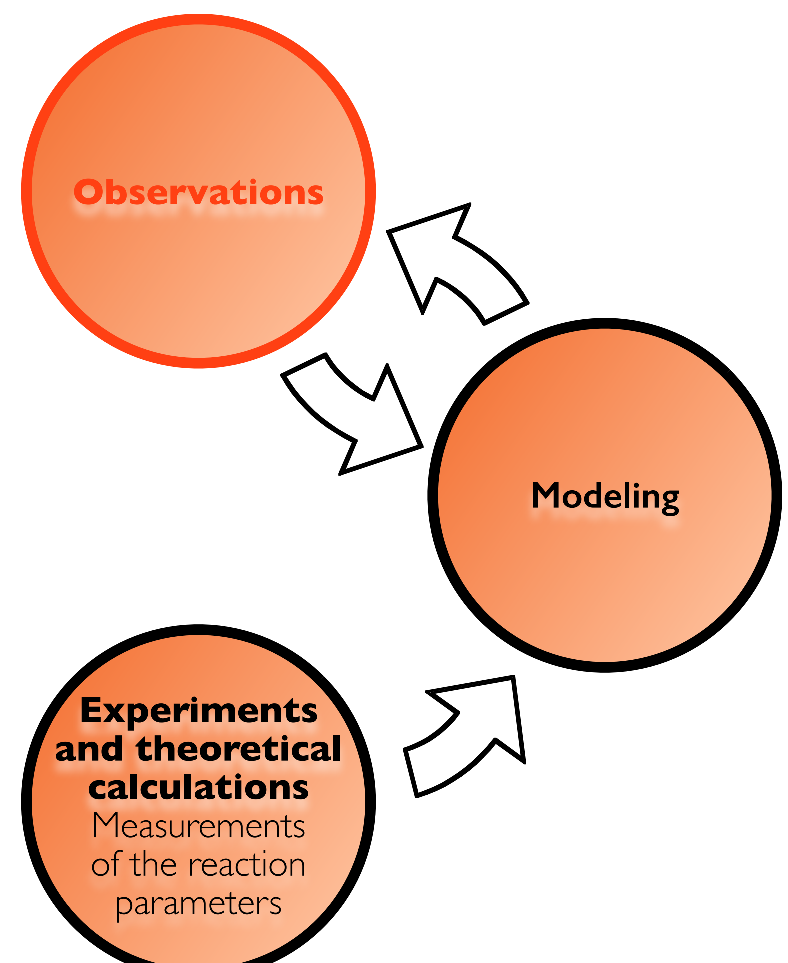
$$k_i(T) = \alpha_i \left(\frac{T}{300}\right)^{\beta_i} \exp\left(-\frac{\gamma_i}{T}\right)$$

Neutral-neutral thermal reactions





Eric Hébrard (NASA-GSFC / ORAU)

« NEXT-GENERATION » PHOTOCHEMICAL MODELING

$$\mathrm{AB} \xrightarrow{h\nu} \mathrm{A} + \mathrm{B}$$

$$\sigma_i(\lambda, T) \quad q_{i,j}(\lambda, T)$$

$$F_{\sigma_i(\lambda,T)} \quad F_{q_{i,j}(\lambda,T)}$$

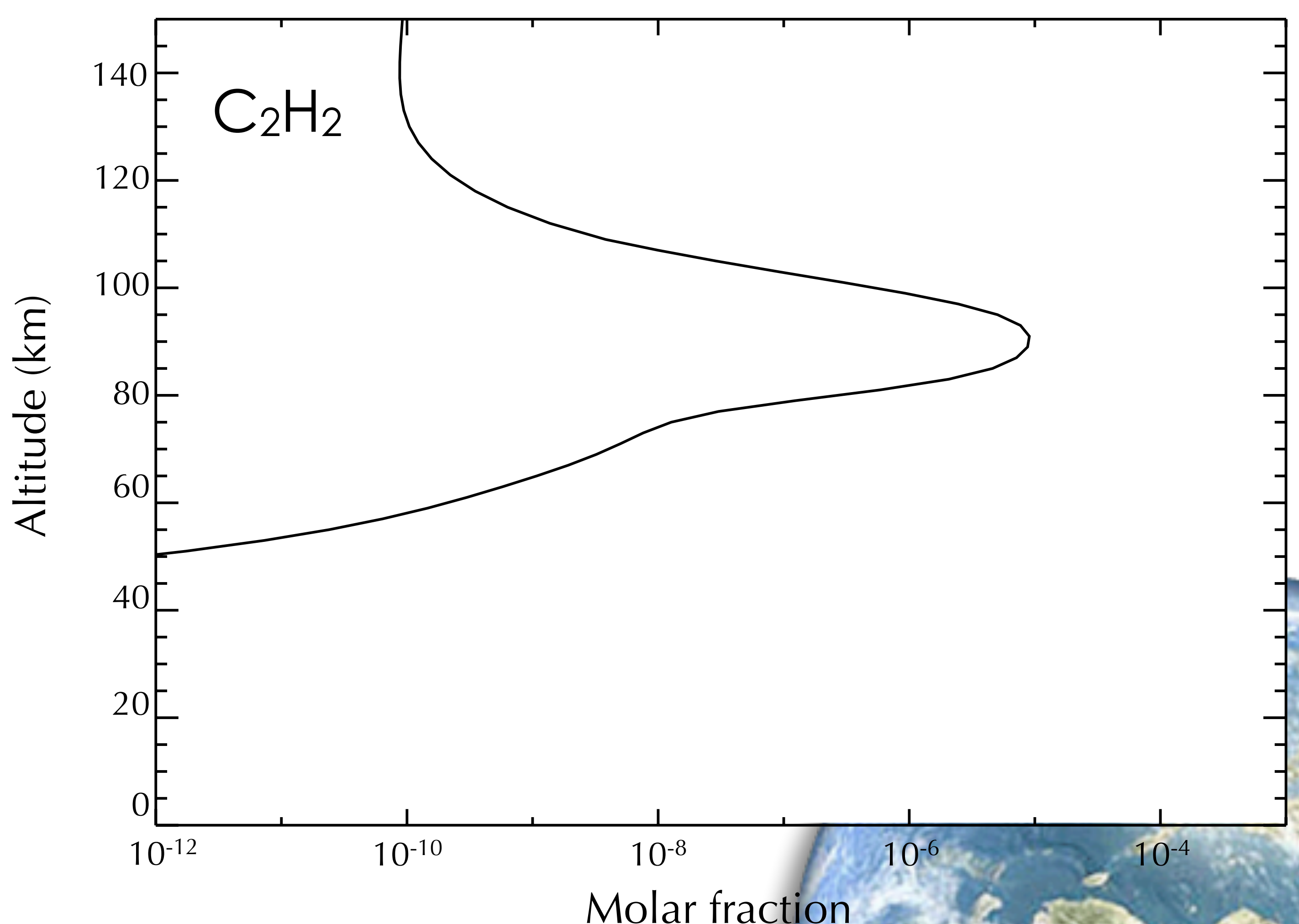
Photodissociations

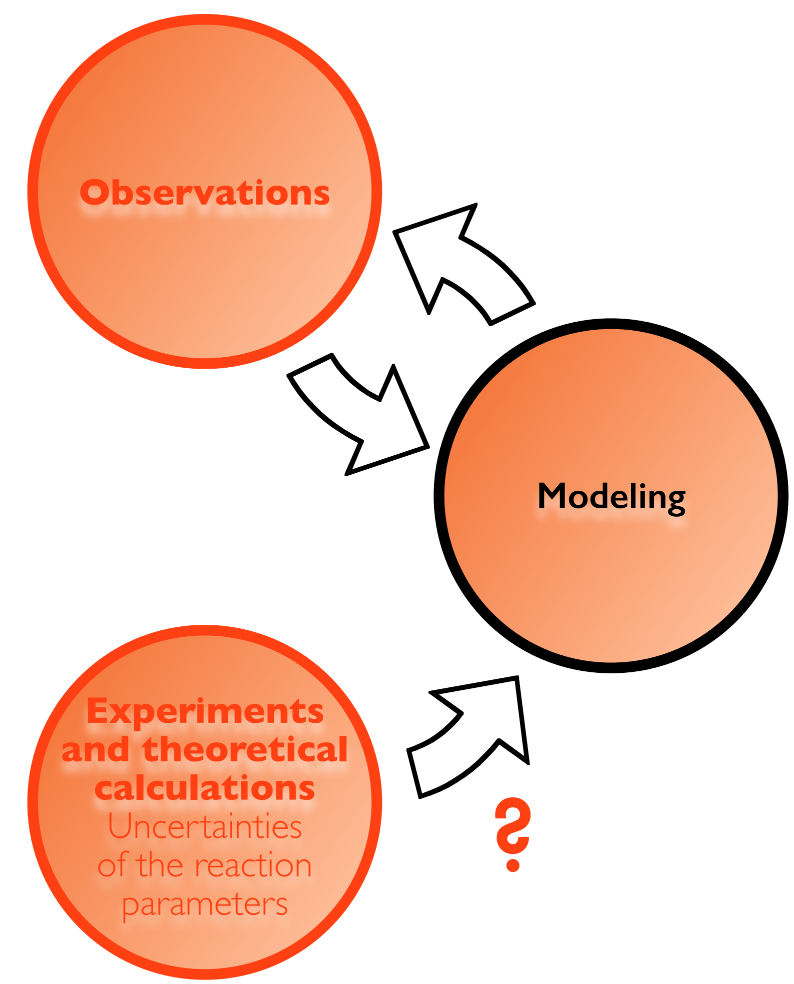
$$\mathrm{A} + \mathrm{B} \xrightarrow{(+\mathrm{M})} \mathrm{C} + \mathrm{D}$$

$$k_i(T) = \alpha_i\left(\frac{T}{300}\right)^{\beta_i} \exp\left(-\frac{\gamma_i}{T}\right)$$

$$F_{k_i(T)}$$

Neutral-neutral thermal reactions





« NEXT-GENERATION » PHOTOCHEMICAL MODELING

$$\mathrm{AB} \xrightarrow{h\nu} \mathrm{A} + \mathrm{B}$$

$$\sigma_i(\lambda, T) \quad q_{i,j}(\lambda, T)$$

$$F_{\sigma_i(\lambda,T)} \quad F_{q_{i,j}(\lambda,T)}$$

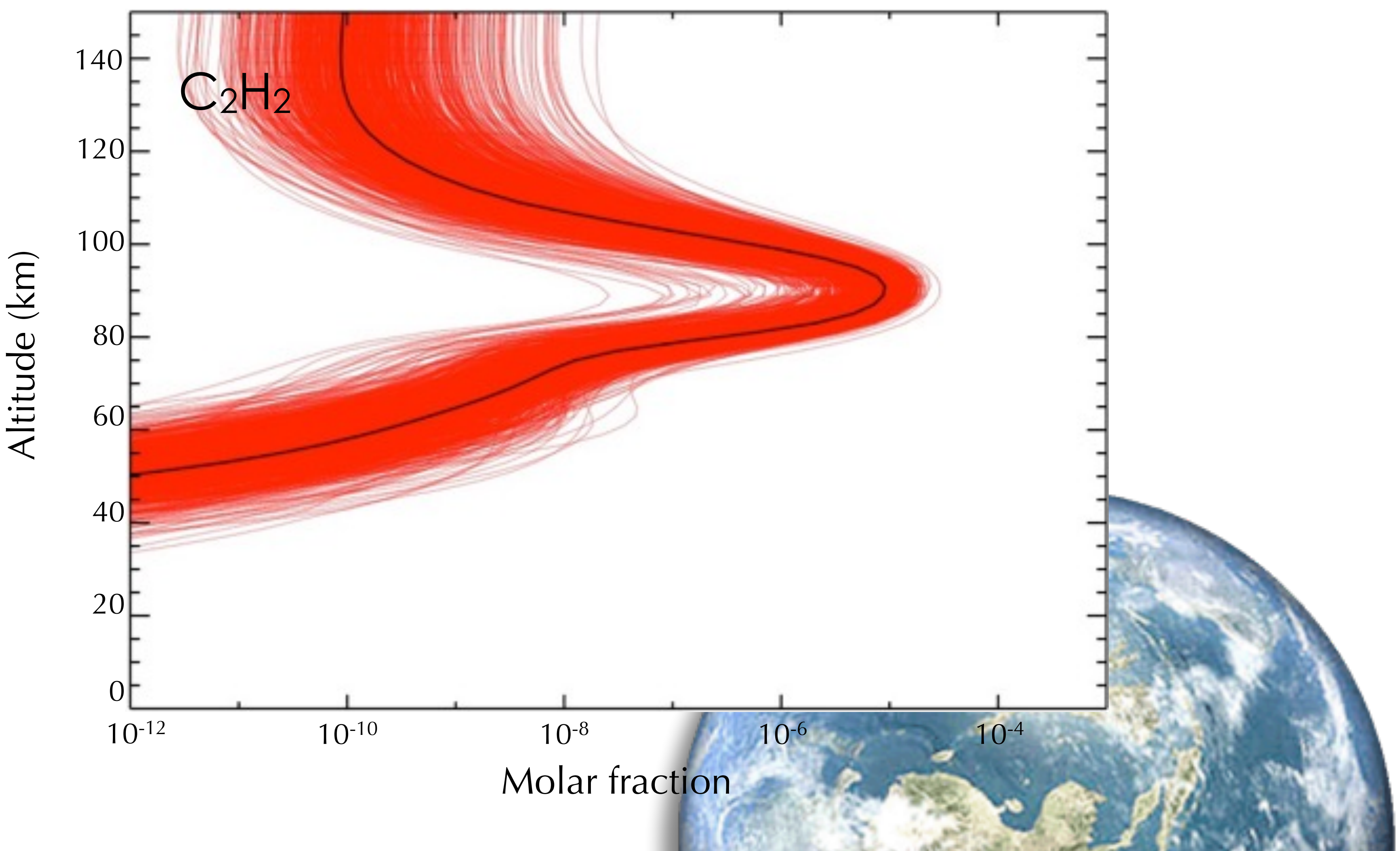
Photodissociations

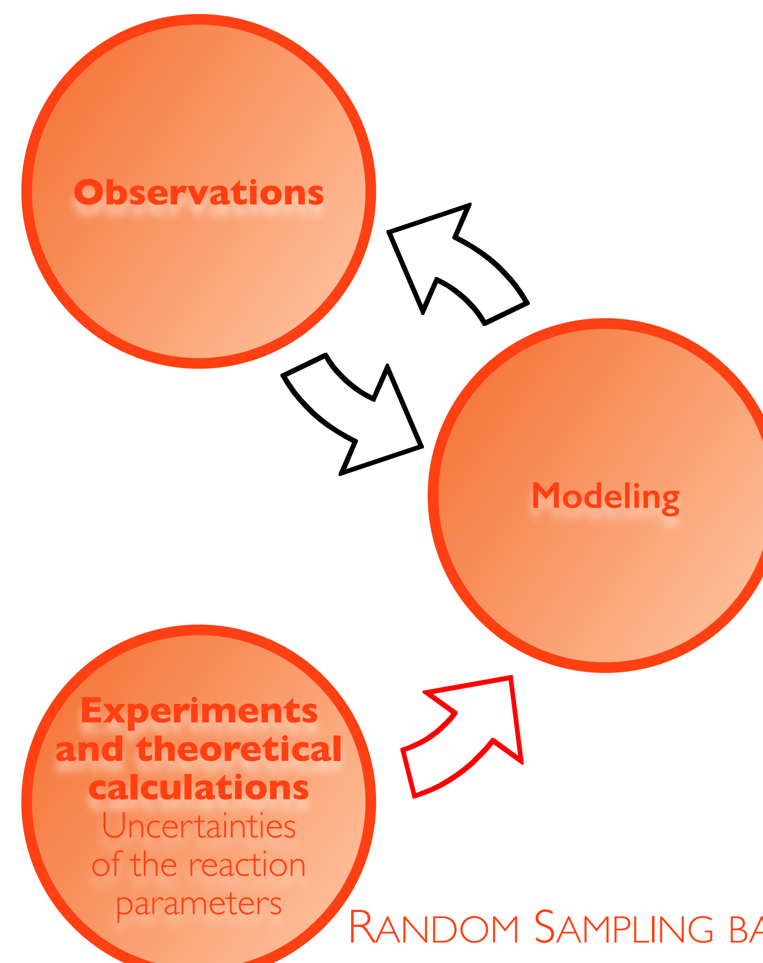
$$\mathrm{A} + \mathrm{B} \xrightarrow{(+\mathrm{M})} \mathrm{C} + \mathrm{D}$$

$$k_i(T) = \alpha_i \left(\frac{T}{300}\right)^{\beta_i} \exp\left(-\frac{\gamma_i}{T}\right)$$

$$F_{k_i(T)}$$

Neutral-neutral thermal reactions





RANDOM SAMPLING BASED UNCERTAINTY PROPAGATION

« NEXT-GENERATION » PHOTOCHEMICAL MODELING

$$AB \xrightarrow{h\nu} A + B$$

$$\sigma_i(\lambda, T) \quad q_{i,j}(\lambda, T)$$

$$F_{\sigma_i(\lambda,T)} \quad F_{q_{i,j}(\lambda,T)}$$

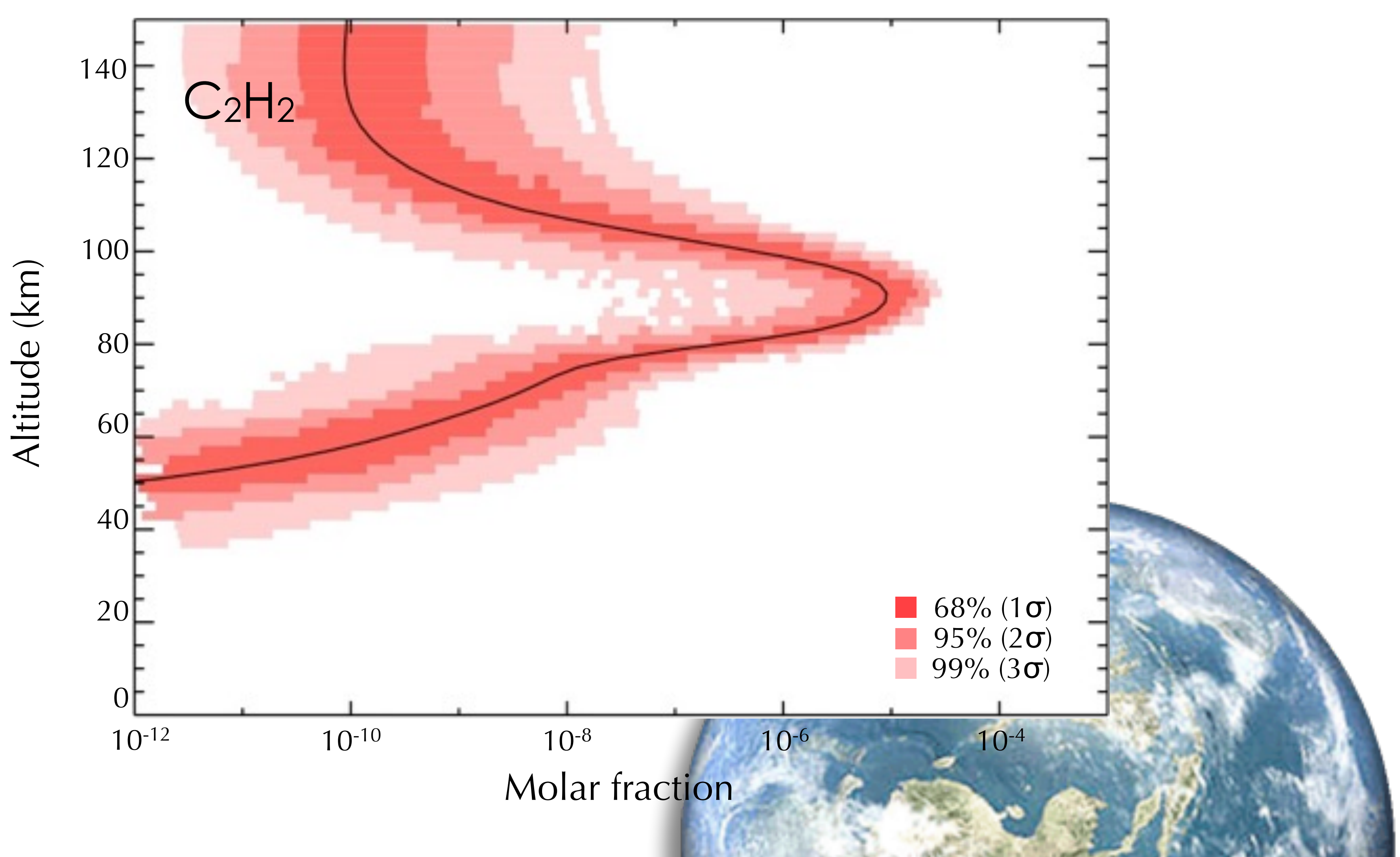
Photodissociations

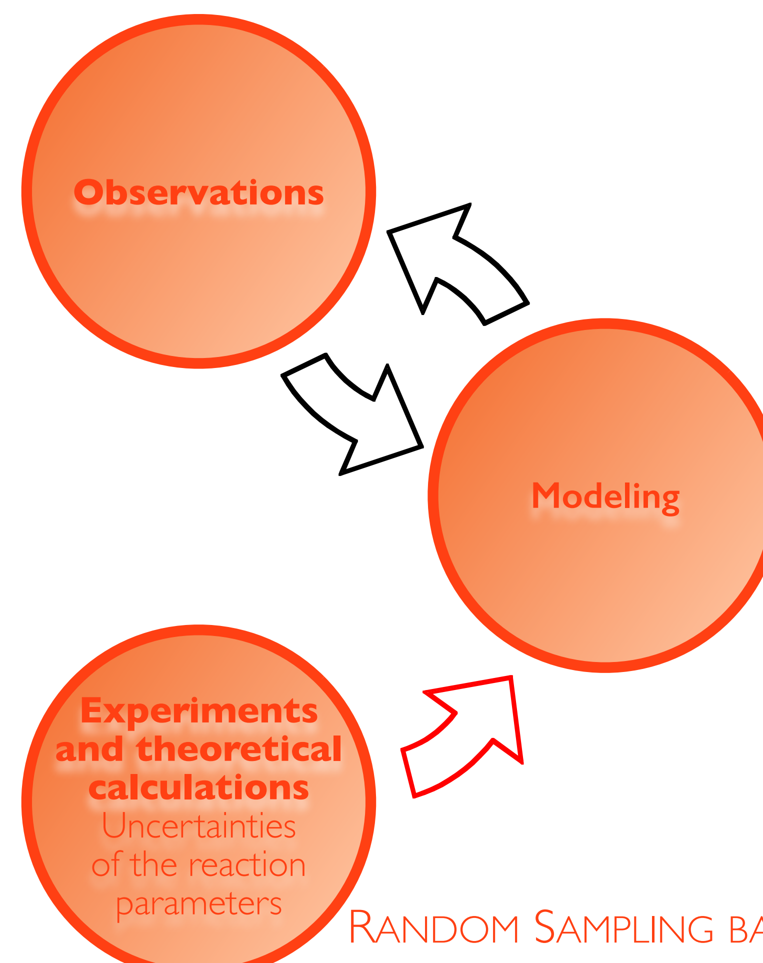
$$A + B \xrightarrow{(+M)} C + D$$

$$k_i(T) = \alpha_i\left(\frac{T}{300}\right)^{\beta_i} \exp\left(-\frac{\gamma_i}{T}\right)$$

$$F_{k_i(T)}$$

Neutral-neutral thermal reactions





RANDOM SAMPLING BASED UNCERTAINTY PROPAGATION

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$$\mathrm{AB} \xrightarrow{h\nu} \mathrm{A} + \mathrm{B}$$

$$\sigma_i(\lambda, T) \quad q_{i,j}(\lambda, T)$$

$$F_{\sigma_i(\lambda,T)} \quad F_{q_{i,j}(\lambda,T)}$$

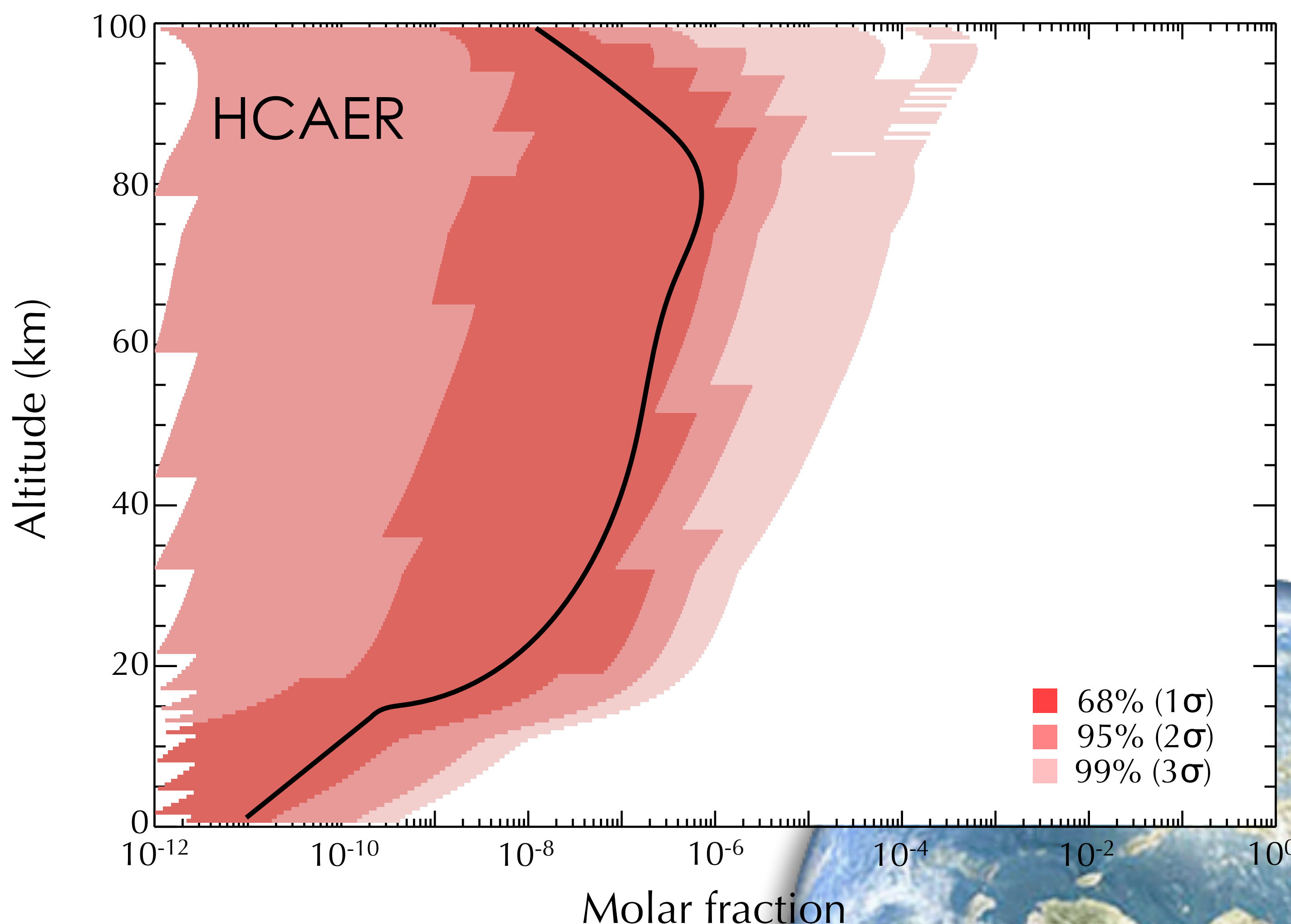
Photodissociations

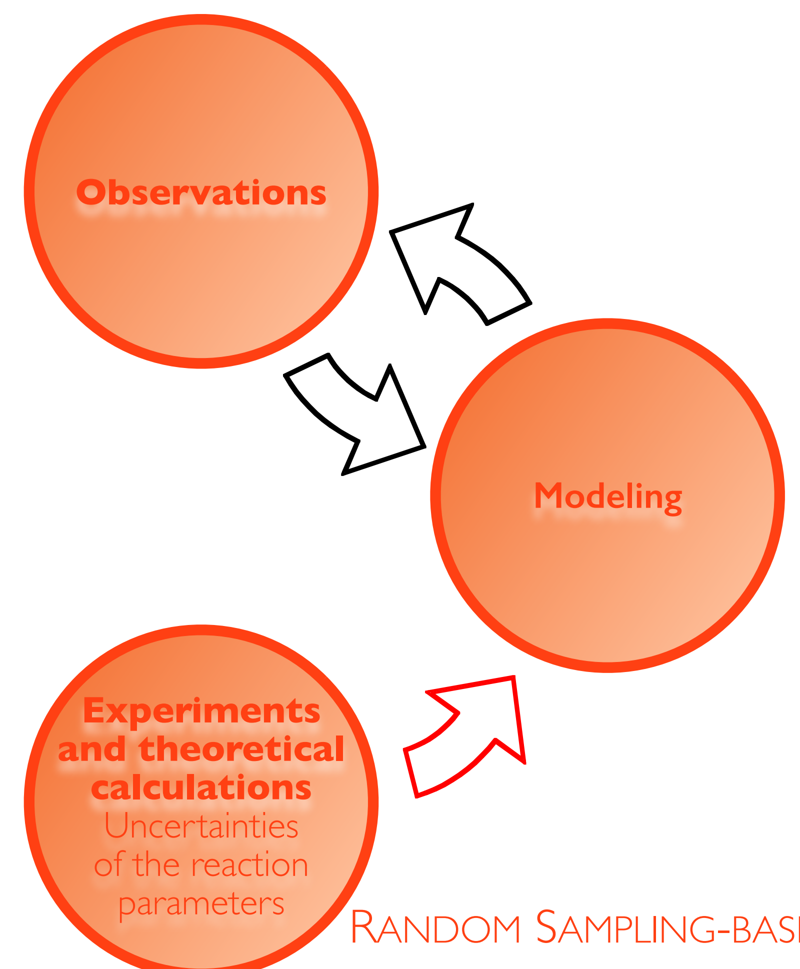
$$\mathrm{A} + \mathrm{B} \xrightarrow{(+\mathrm{M})} \mathrm{C} + \mathrm{D}$$

$$k_i(T) = \alpha_i\left(\frac{T}{300}\right)^{\beta_i} \exp\left(-\frac{\gamma_i}{T}\right)$$

$$F_{k_i(T)}$$

Neutral-neutral thermal reactions





RANDOM SAMPLING-BASED UNCERTAINTY PROPAGATION

« NEXT-GENERATION » PHOTOCHEMICAL MODELING

$$\mathrm{AB} \xrightarrow{h\nu} \mathrm{A} + \mathrm{B}$$

$$\sigma_i(\lambda, T) \quad q_{i,j}(\lambda, T)$$

$$F_{\sigma_i(\lambda,T)} \quad F_{q_{i,j}(\lambda,T)}$$

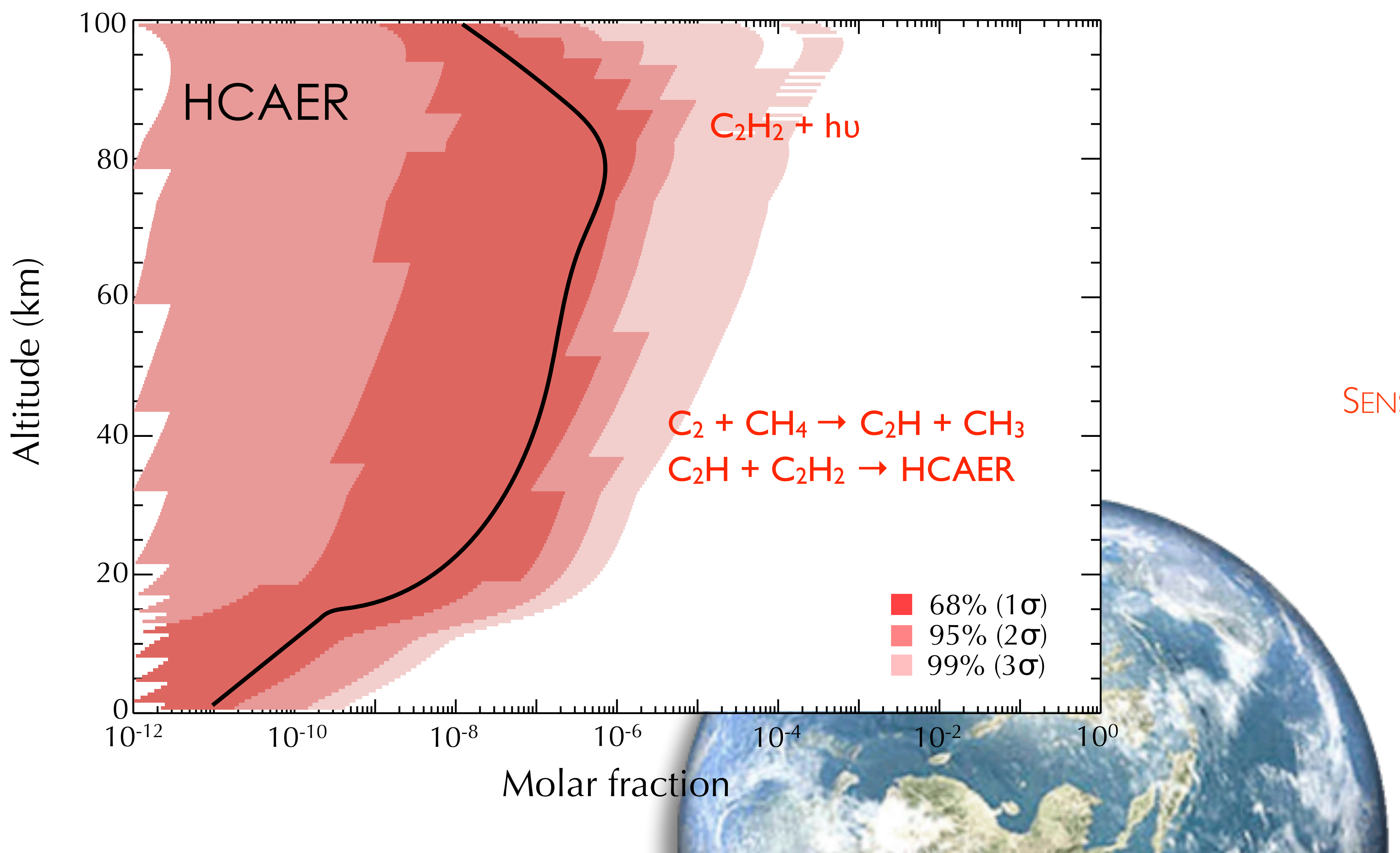
Photodissociations

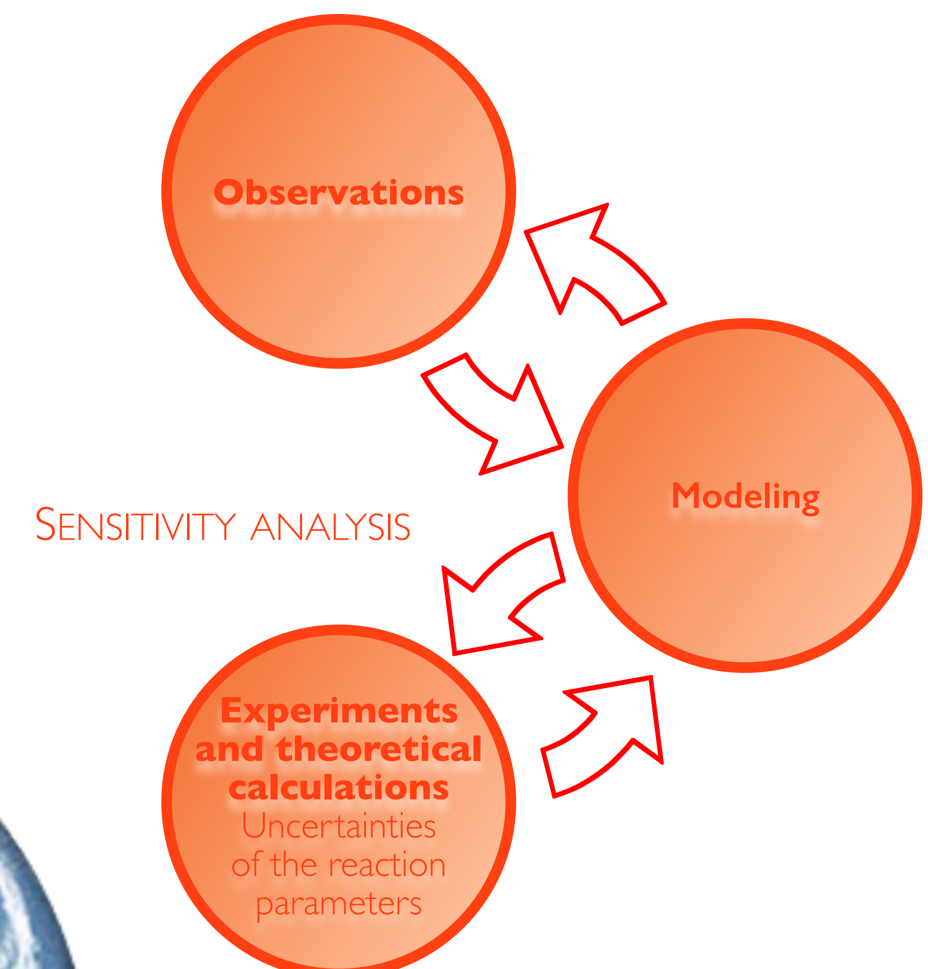
$$\mathrm{A} + \mathrm{B} \xrightarrow{(+\mathrm{M})} \mathrm{C} + \mathrm{D}$$

$$k_i(T) = \alpha_i\left(\frac{T}{300}\right)^{\beta_i} \exp\left(-\frac{\gamma_i}{T}\right)$$

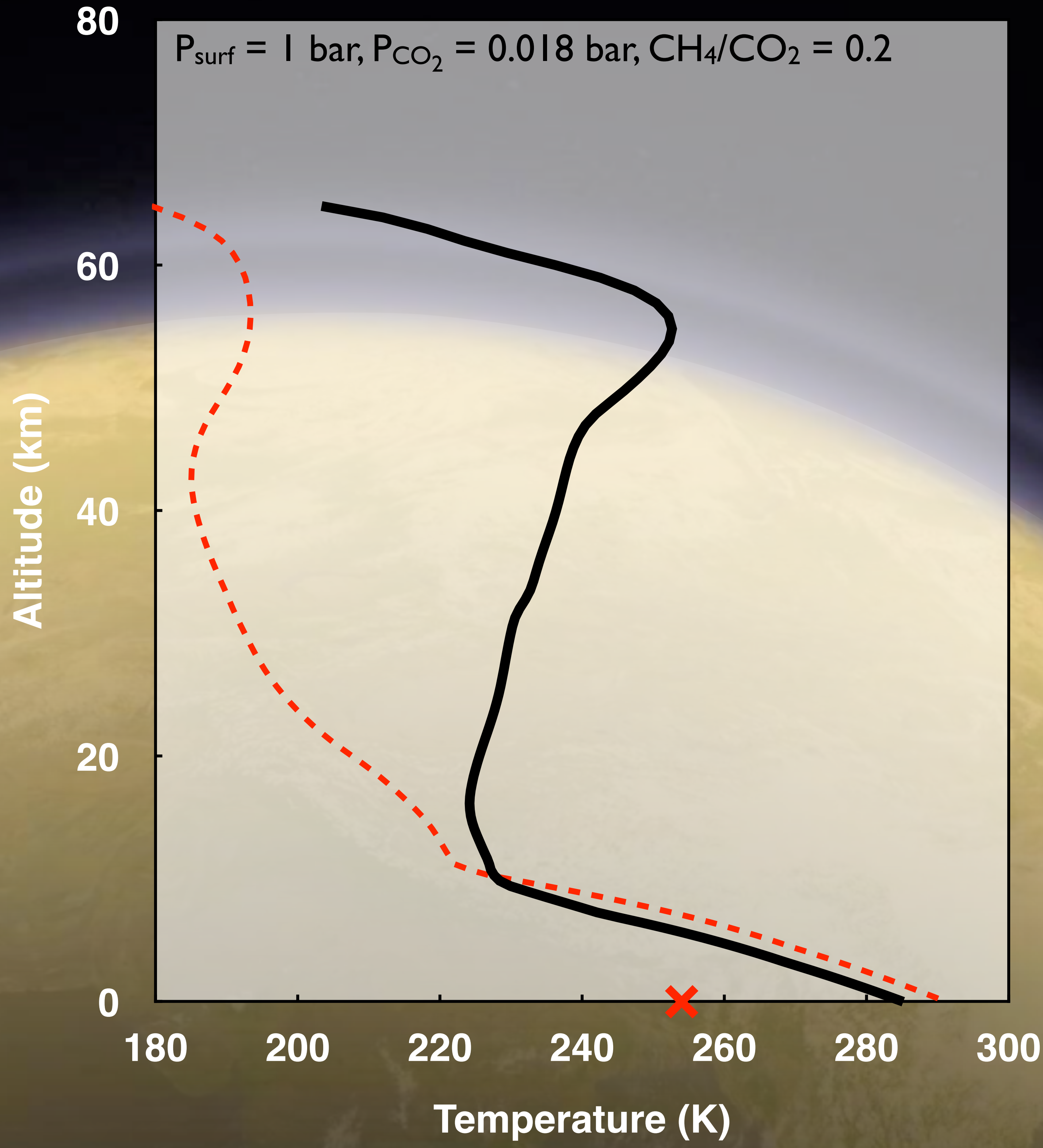
$$F_{k_i(T)}$$

Neutral-neutral thermal reactions

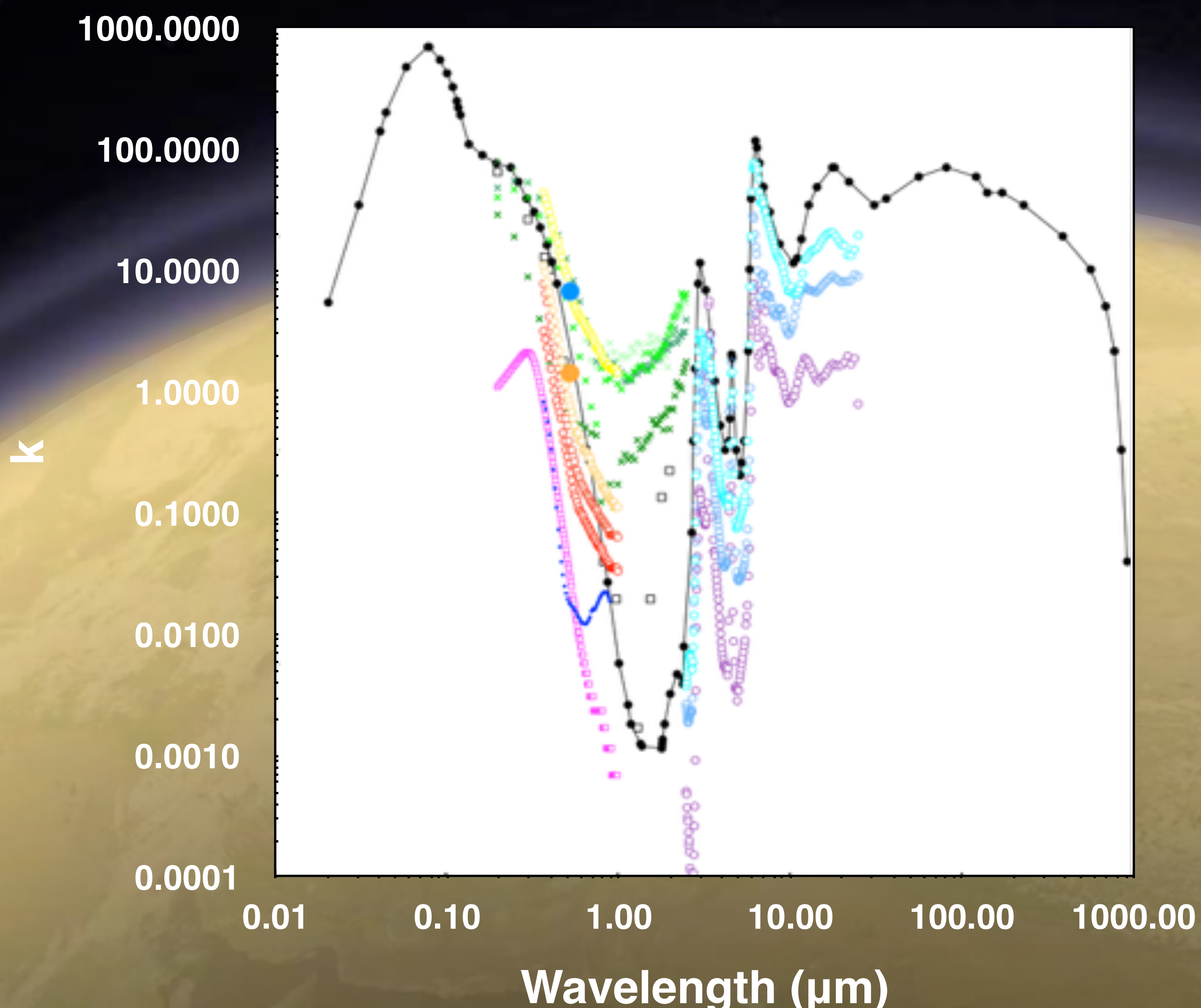


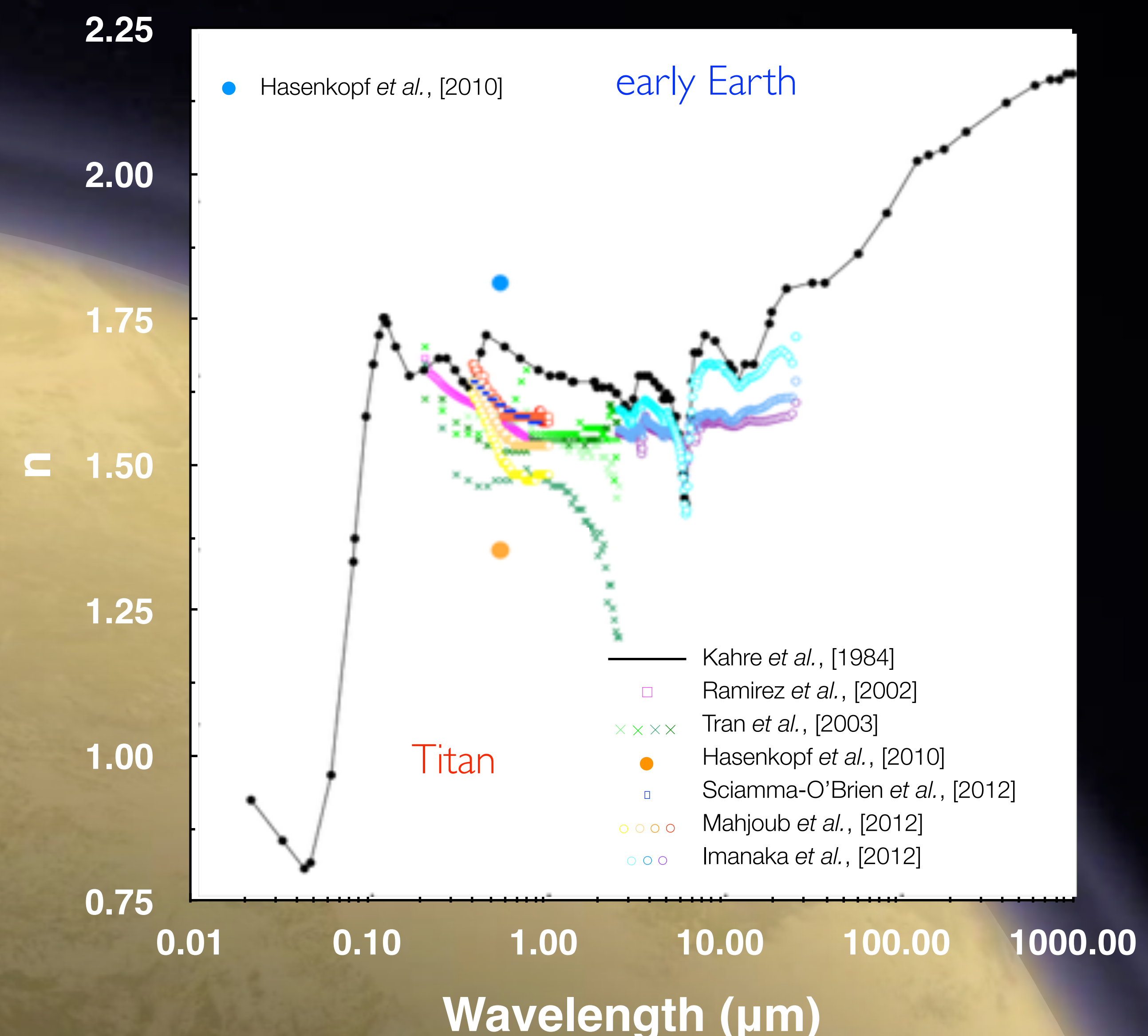


« NEXT-GENERATION » CLIMATE MODELING

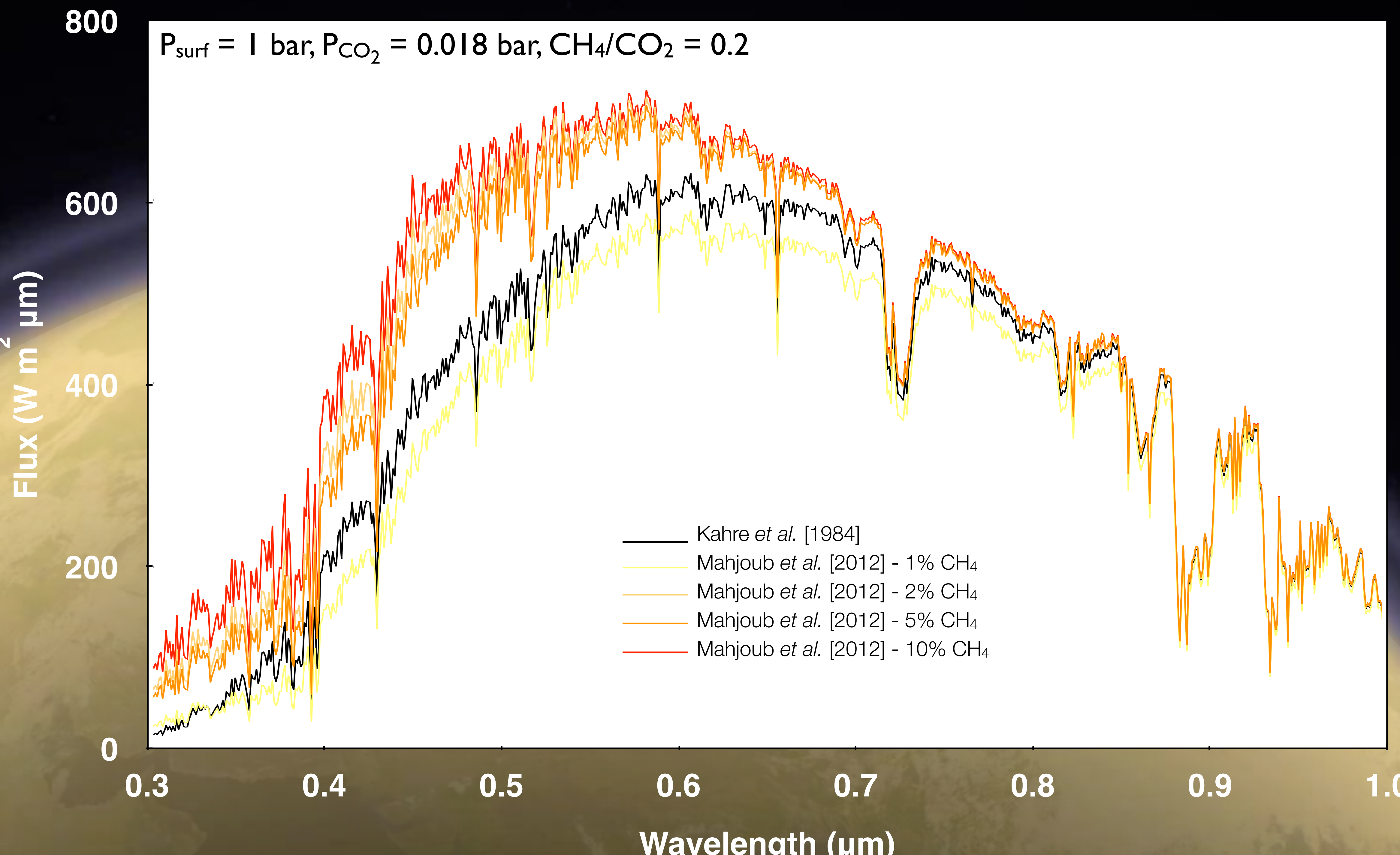


« NEXT-GENERATION » CLIMATE MODELING





« NEXT-GENERATION » CLIMATE MODELING



NASA ROSES-EXO

Chemical Formation Pathways and Optical Properties for Early Earth's Organic Haze : A Combined Theoretical and Experimental Approach

Institutional PI: Melissa G. Trainer; NASA Goddard Space Flight Center, Greenbelt, MD
Science PI: Eric Hébrard (NASA-GSFC)
Co-Is: Shawn D. Domagal-Goldman, Thomas Gautier and Jennifer C. Stern (NASA-GSFC)
Collaborator: Giada Arney (University of Washington, Seattle, WA)

+ vplanet

PHOTO - 1D photochemistry
CLIMA - 1D climate
SMART - Spectral Mapping and Atmospheric Transfer Code


TAKE AWAYS...
HYDROCARBONS HAZES DO NO PRECLUDE HABITABLE SURFACE TEMPERATURES
HYDROCARBONS HAZES HAVE STRONG, DETECTABLE SPECTRAL FEATURES AT SHORT WAVELENGTHS
A BETTER KNOWLEDGE OF THEIR CHEMICAL FORMATION PATHWAYS AND OPTICAL PROPERTIES ARE NEEDED