Challenges in the Forward Modeling of the Uranus Atmosphere

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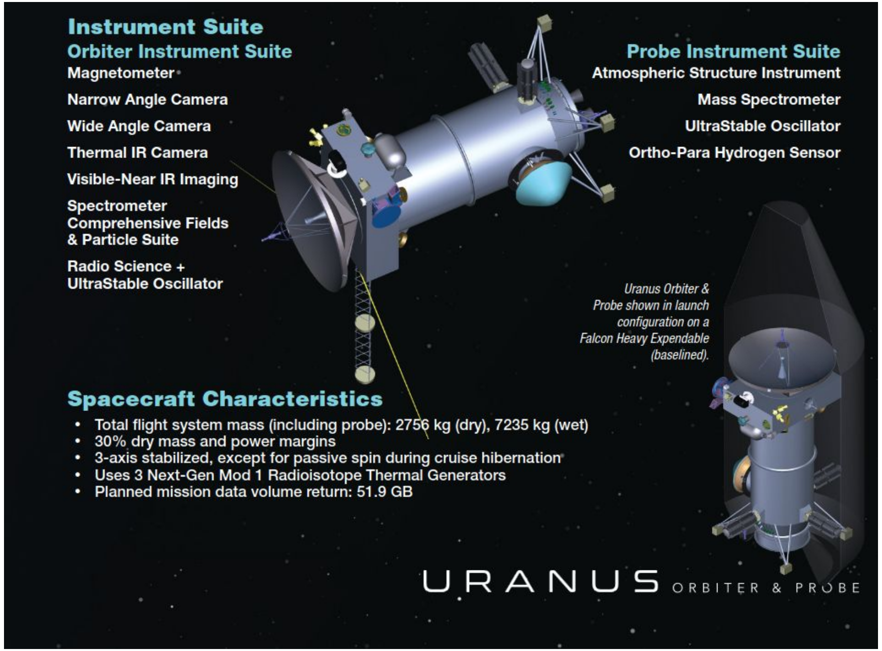
Outline

- UOP and Italian Contribution
- Overview of Uranus atmosphere
- Tools
- Modeling in the Visible-Near IR spectral range
- Modeling in the IR spectral range
- Way forward: how can *you* help

The talk does not aim to describe exciting new findings. It aims to list the main areas of further investigation required to improve the modeling - and retrieval capability from - Uranus' spectra.

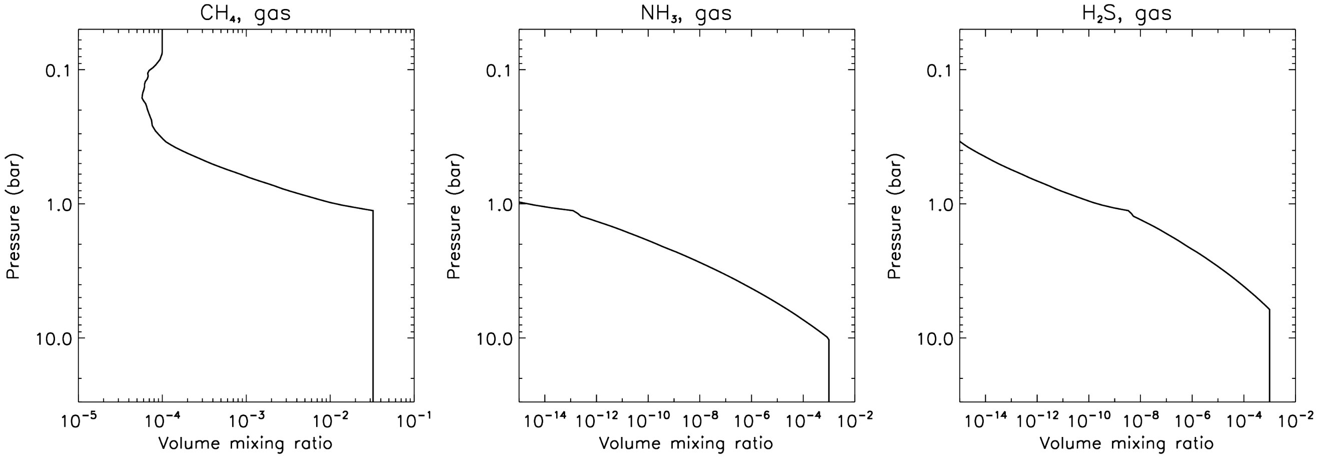
Uranus Orbiter and Probe mission

- Selected as top priority in the 2022 NASA Planetary Sciences Decadal Survey
- ASI supported a specific project to assess potential Italian contributions
- VIS-IR spectrometer included in the strawman payload
- This work initiated to quantify the scientific potential in the study of Uranus' *atmosphere*
- A 'pseudo-MAJIS' instrument was considered for the purpose (0.48-2.3 and 2.2-5.5 μm)

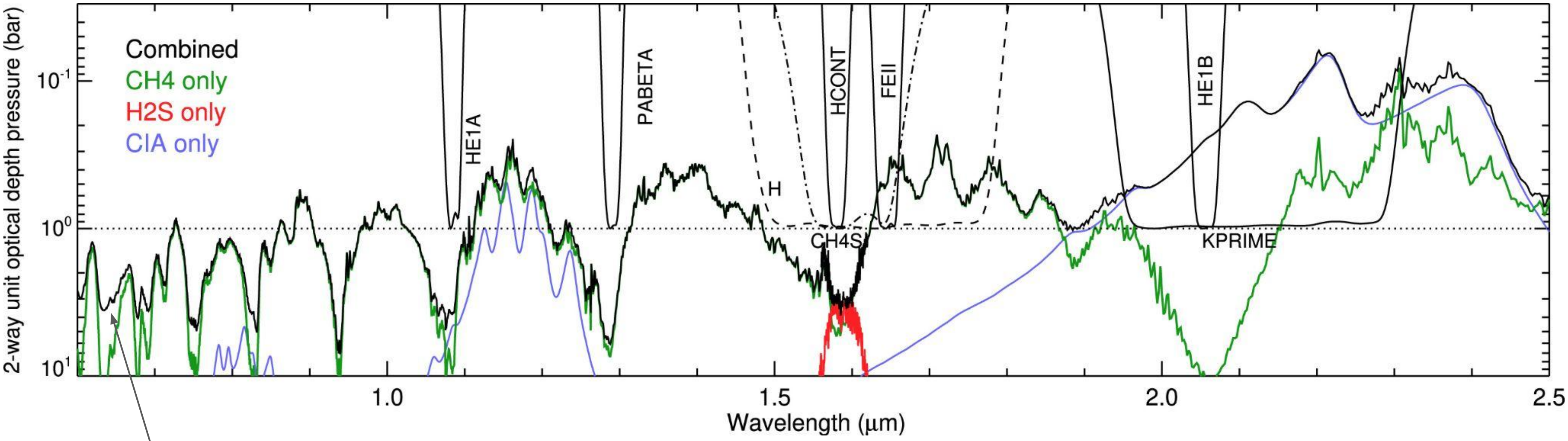


Overview of Uranus atmosphere: gases

- 'Icy Giant' class
- 'Upper' atmosphere composed mostly of H_2 and He (85% and 11%)
- Seizable amount of methane (3%), prone to condensation



Transmissivity of Uranus' atmosphere (gas components)

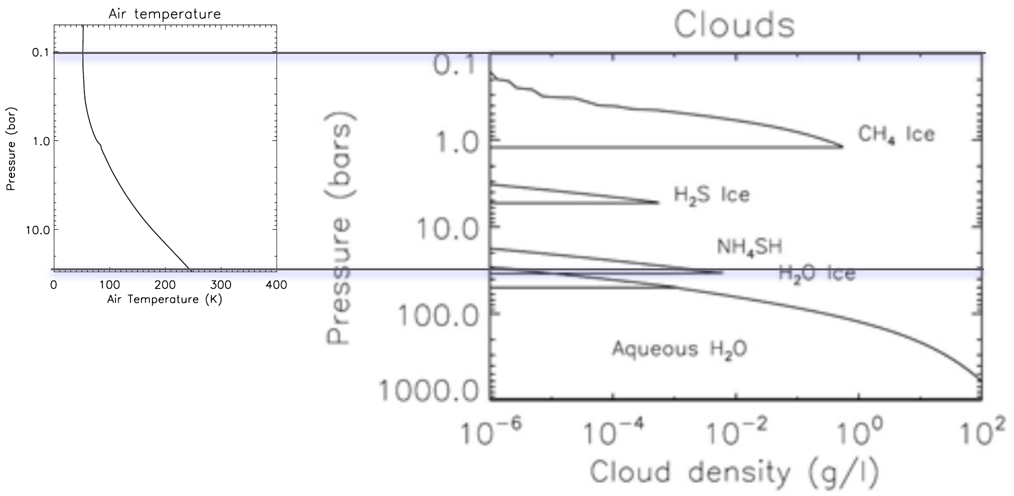


From Sromovsky et al. 2024

Significant contribution from Rayleigh scattering!

Overview of Uranus atmosphere: aerosols (1)

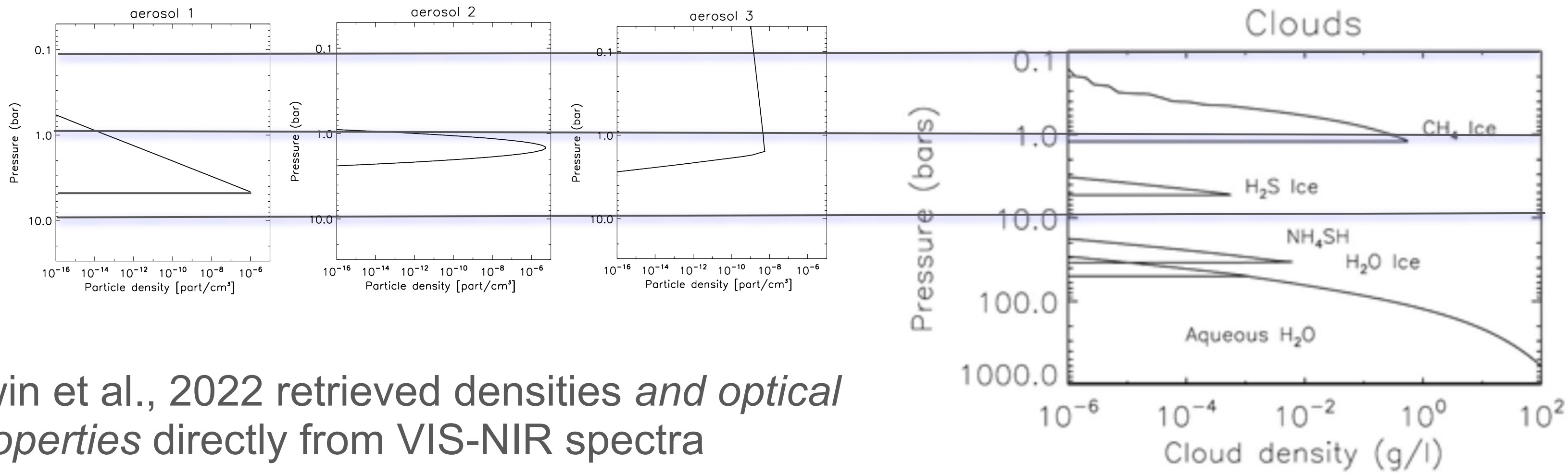
- Very (very) low temperatures induce condensation of minor components
- H_2S exceeds NH_3 (opposite holds true in Jupiter and Uranus)



Theoretical aerosol densities,
from Irwin et al. 2009

Overview of Uranus atmosphere: aerosols (2)

- As for other giant planets, pure ices can't do the job….



- Irwin et al., 2022 retrieved densities *and optical properties* directly from VIS-NIR spectra

Overview of Uranus atmosphere: aerosols (3)

Analysis of Irwin et al. 2022 led to the ‘holistic’ model for Icy Giants aerosols:

1. Deep Layer (a_1): A cloud deck at $p > 5-7$ bar, likely composed of H_2S and potentially NH_3 ice,
2. Main Cloud (a_2): A thin, reflective layer at the 1-bar level, consisting of a CH_4 ice-haze mixture,
3. Upper Haze (a_3): A layer of sub-micron particles extending into the upper atmosphere.

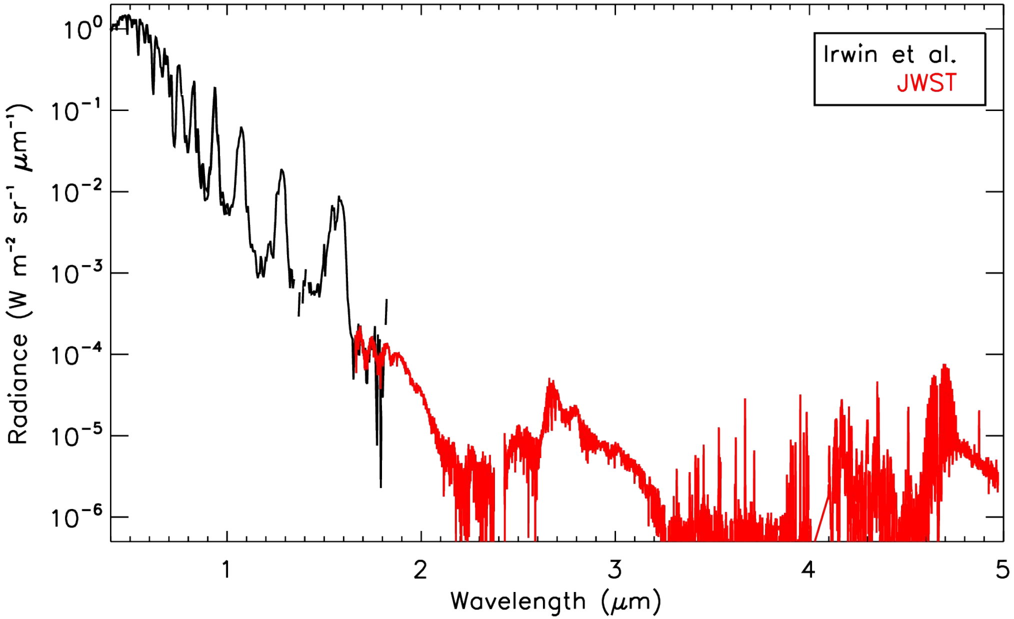
Our forward simulations

- We adopted the ARS code (Атмосфера, Радиация, Спектр - Atmosphere, Radiation, Spectrum) by N. Ignatiev (IKI-RAS, Moscow). It includes:
    - our own implementation of the correlated-k method (Irwin et al., 2008)
    - DISTORT solver for the treatment of multiple scattering (Stamnes et al., 1988)
    - treatment of Rayleigh scattering as a ‘pseudo-aerosol’, with variable formal density and explicit expansion of phase function in terms of Legendre coefficients
- Our first task was to reproduce the reference experimental spectrum #13 given in Irwin et. al, 2022, on the basis of
    - gas abundances
    - aerosol densities
    - aerosol optical properties

    retrieved by the authors for this specific observation

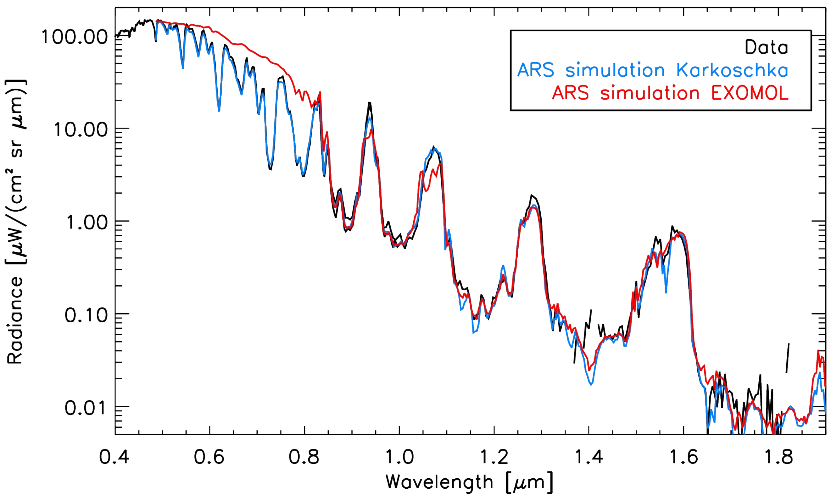
Reference spectrum for VIS-NIR range

- Irwin et al., 2022 spectra are collections from different sources
  - HST/STIS (2002): Visible and near-infrared observations covering 0.3–1.0 µm.
  - IRTF/SpeX (2000): Near-infrared reference spectra covering 0.8–2.5 µm.
  - Gemini/NIFS (2009): High-resolution H-band observations covering 1.47–1.8 µm.
- They shall be considered as full disk spectra. For our purposes we adopted $i=\varepsilon=\varphi=0°$
- Signal variations span over four orders of magnitude!
- Spectrum #13 is assumed to be representative of equatorial regions



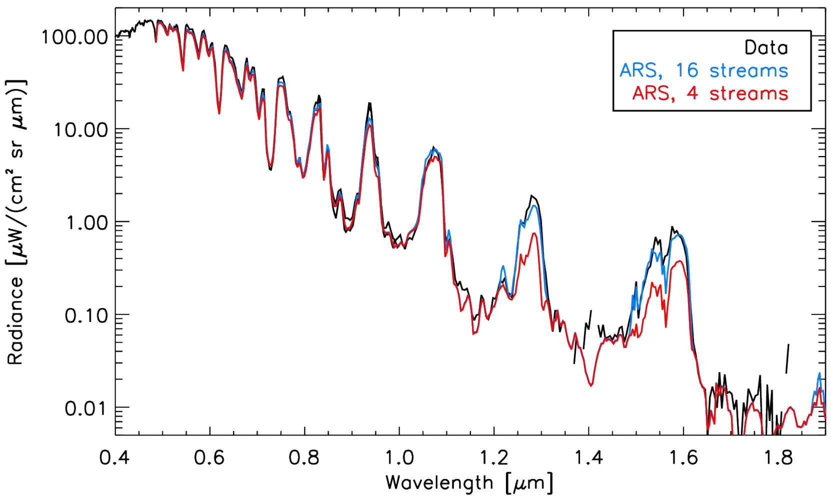
Modeling in the VIS-NIR: gases

- Methane line lists are largely incomplete in the VIS-NIR range, mostly for the difficulties in isolating - in experiments - individual lines for higher polyads. We had to resort to the empirical dataset of Karkoschka & Tomasko, 2010
- NH_3 and H_2S were modeled directly from the latest ExoMol cross-sections, given as input to the *exo-k* Python package to compute correlated-k tables. Foreign broadening for H_2, He and CH_4 not available in this spectral range
- Collision-induced absorption
  - H_2-H_2: Borysow et al., 2002 remains the latest reference for λ<1μm
  - H_2-He: updated estimates from Abel et al. 2011 not available below 200K, extrapolated
  - H_2-CH_4: entirely missing for λ<7μm



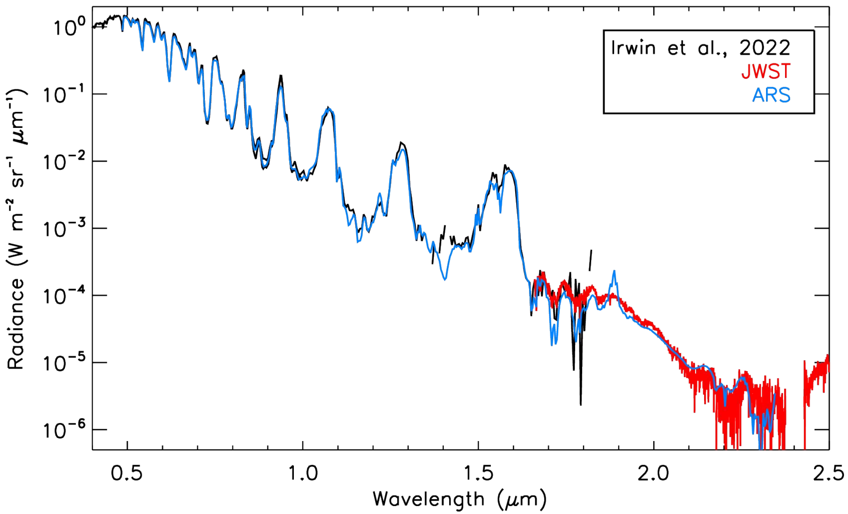
Modeling in the VIS-NIR: scattering

- Retrievals from Irwin et al., 2022 provided directly the phase (as double H-G asymmetry parameters) and densities for the three aerosol populations
- Direct tests demonstrated that 16 streams are adequate for DISORT to reach 'asymptotic' solutions
- Irwin et al., 2022 states that aerosol properties retrieved from data does not match refractive indices of pure ices ⇒ *no way to make reasonable assumptions on the spectral behaviour at other wavelengths*



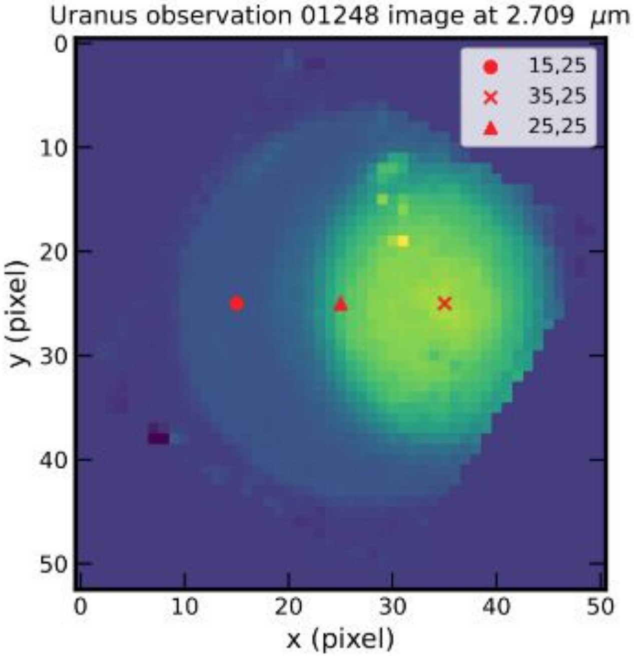
Moving to longer λ….

- The model developed for VIS-NIR provided reasonable agreement with JWST data between 1.6 and 2.3 µm
- The model has an excess of methane opacity at 1.7 amd 1.78 µm. underestimation on aerosol-2 reflectivity also possible.



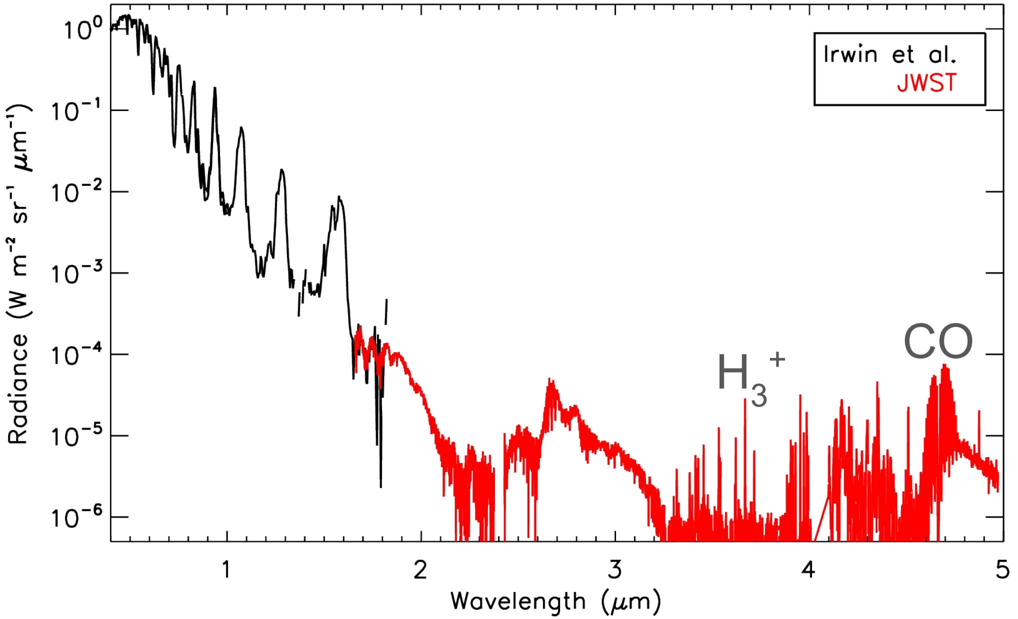
Reference spectrum for IR range

- By far, the most complete dataset is from JWST data of Proposal ID 01248, acquired in Jan. 2023. Spectral cubes with corresponding geometric information.
- We considered spectrum x=15, y=25 to match the ‘mostly-equatorial’ conditions considered in the VIS-NIR discussion
- Notably, data analysis of the troposphere from the proponent team still unpublished



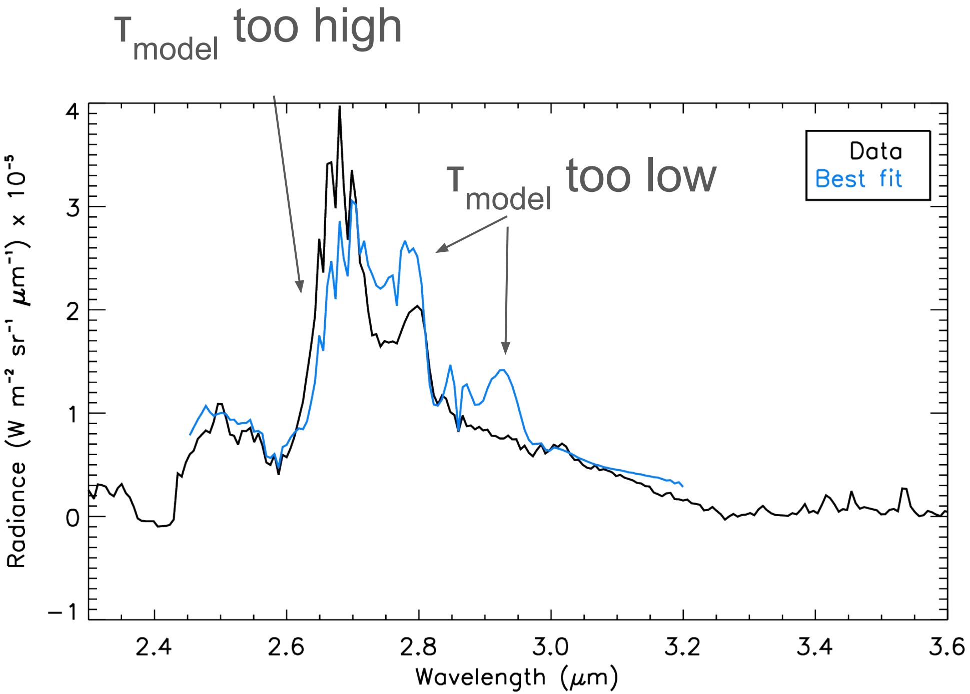
Modeling in the IR: gases (1)

- Region for 3.2 < λ < 4.1 μm dominated by H_3^+ emission, not discussed here, but properly described by *h3ppy* model (Melin et al., 2025)
- CO stratospheric emission 4.65-4.8 μm also not considered here
- No obvious CH_4 non-LTE emission observed in data



Modeling in the IR: aerosols (1), *the* issue

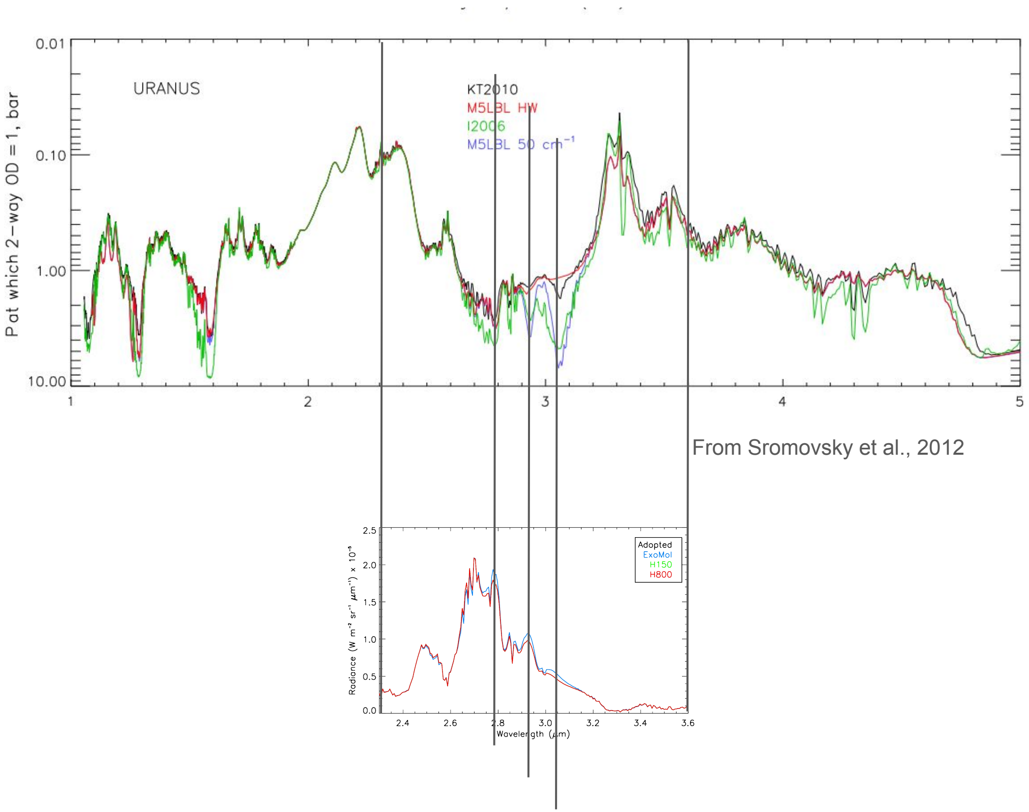
- Rayleigh scattering must be included in computations
- Mere extrapolation of Irwin et al., optical properties of aerosols (σ, ω_0, g) from VIS-NIR to longer λ does not produce reasonable signal levels
- σ, ω_0, g was adjusted with a Levenberg-Marquardt scheme, *assuming constant values over 1 μm intervals*. Density profiles from Irwin et al. analysis on VIS-NIR. Result not satisfactory
- Let's check gas role before….



Our "best" fit…

Modeling in the IR: gases (2)

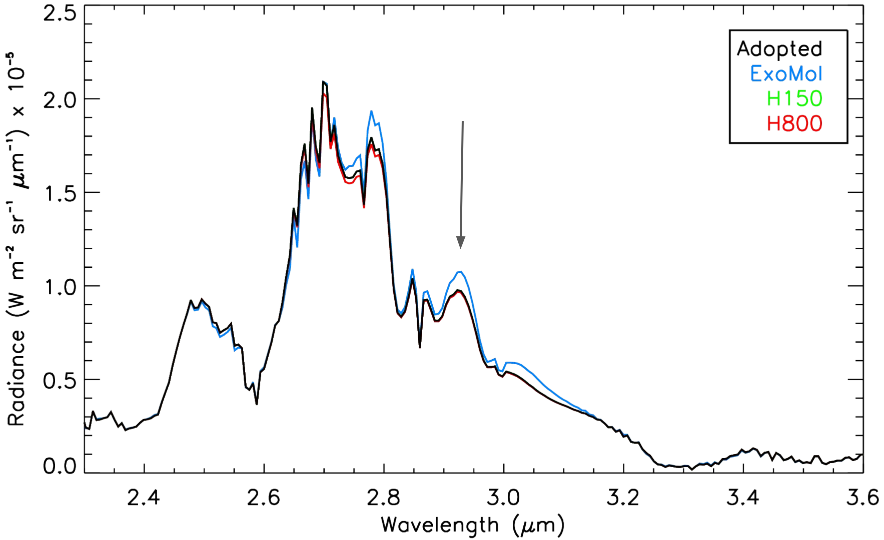
- Methane modeling expected as particularly critical between 2.6 and 3.1 μm
    - Methane lines from STDS theoretical dataset (Wenger and Champion, 1998).
    - Line-mixing according Tran when available for lines in v_3 band. Voigt truncated at 25 cm^{-1} otherwise
    - Foreign broadening by H_2 according Brown et al.



From Sromovsky et al., 2012

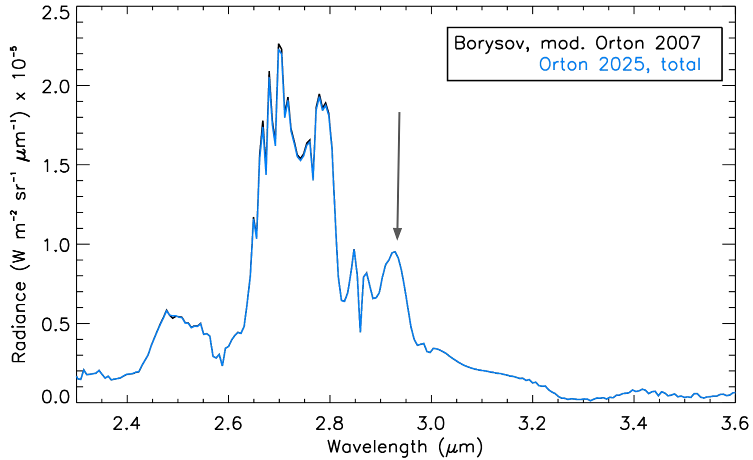
Modeling in the IR: gases (3)

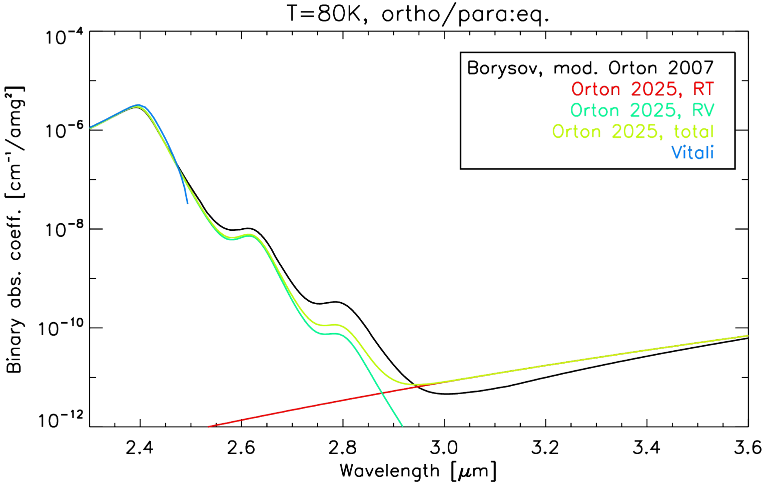
- Improvement in Methane modeling would benefit from:
  - new comparison among recent databases (ExoMol opacity appears lower, despite more lines)
  - line-mixing in other bands
  - theoretical line positions for other isotopes
- regions of opacity deficiency in our model are the ones prone to largest changes among different models. This deserves a deeper analysis.



Modeling in the IR: gases (4)

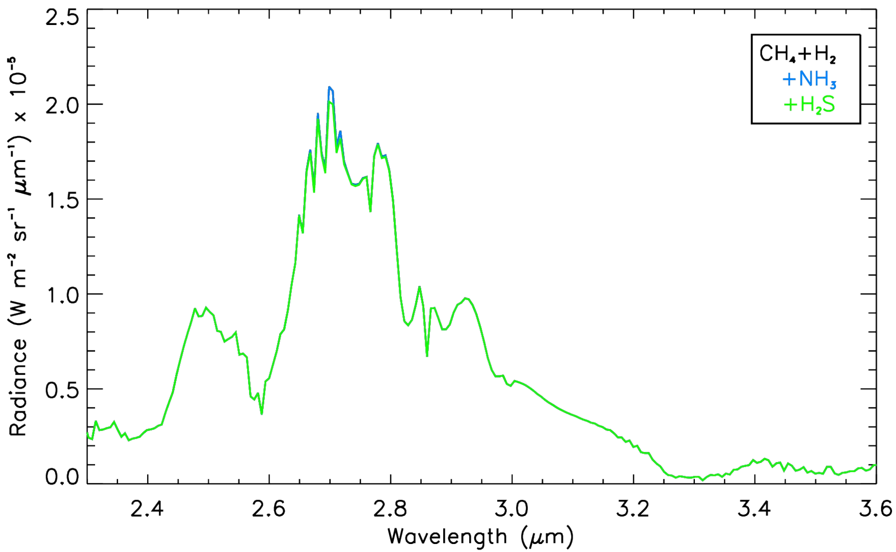
- Collision-induced absorption
  - H_2-H_2: Borysow et al., 2002 still preferred for coverage at low temperatures
  - H_2-He: Borysow et al., 1998 Preferred for still preferred for coverage at low temperatures
  - H_2-CH_4: <u>entirely missing for λ<7µm</u>





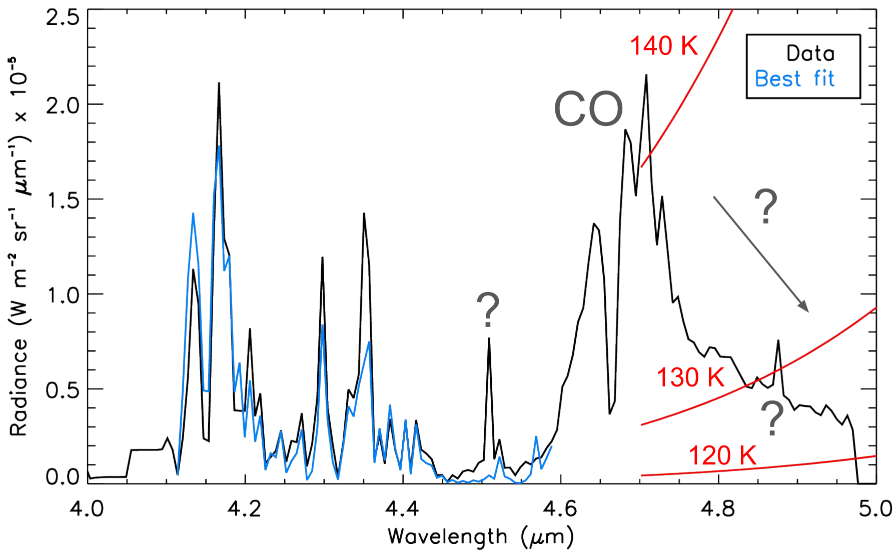
Other investigations

- Neither NH_3 nor H_2S help to solve the macroscopic discrepancies between our model and observed data
- aerosol retrieval properties on smaller ranges also failed, being incapable to reproduce the slopes observed in spectra



Thermal range

- Signal drop beyond 4.7 μm requires a strong opacity source, rapidly increasing with λ, currently missing in our model. Not compatible with H_2-H_2 CIA alone. Most likely, a strong variation in ω_0 for the deepest aerosol-1
- Stratospheric species not yet included in our analysis



Current status

- Missing sources of opacity
- Correspondence of problematic fit areas with more transparent methane regions suggest a role of this gas
  - Integrated effect of very weak lines?
  - dymers?
- H_2-CH_4 CIA still missing
  - Very urgent to address, but even a κ comparable to H_2- H_2 in the same spectral regions would not help
- Retrieval of empirical aerosol from JWST data in progress from proponent team. Our analysis suggests rapid variations with wavelengths.

How can *you* help

- High sensitivity opacity measurements on pure CH_4 and Uranian CH_4-H_2-He mixtures at 2.93 and 2.78 μm. Ideally, cavity ring-down on very long paths.
- Theoretical models for H_2-CH_4 CIA
- Experiment for synthesis of haze analogues in Icy Giants conditions: high CH_4 and H_2, virtually no NH_3, low amounts of H_2S, low air temperature, low UV flux