Next Steps in Characterizing Exoplanet Atmospheres with JWST: Transit Science

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You’ve already seen some of the awesome JWST Cycle 1 transiting exoplanet science this week…

Credit: NASA, ESA, CSA, J. Olmsted (STScI)
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Exoplanet WASP-18 b

Atmospheric Spectrum & Detection of Water

Credit: NASA, JPL-Caltech (R. Hurt/IPAC)
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Credit: NASA, ESA, CSA, J. Olmsted (STScI)

Zieba et al. (2023)
JWST time-series observations are AMAZING!

Actual Data!

WASP-96b

Time in Baltimore, Maryland
June 21, 2022

Image Credit: NASA/STScI
“You can’t really know where you are going until you know where you have been”

-Maya Angelou
A solid foundation was laid for exoplanet atmospheric characterization in the era of JWST.

Increasing complexity and fidelity of exoplanet atmospheric models.

Development of 1D, 2D, and 3D atmospheric forward models.

- 1990 – Hubble Launched
- 1995 – First Exoplanet Around Sun-like Star Discovered
- 2000 – First Exoplanet Transit Detected
- 2003 – Spitzer Launched
- 2005 – First Exoplanet Directly Imaged
- 2016 – Kepler Exoplanet Demographics Released
- 2022 – JWST Launched
Hubble provided first detection of an exoplanet atmosphere.
Spitzer was among the first to measure the light (or absence thereof) from an exoplanet.
Spitzer obtained the first mid-infrared emission spectra of exoplanets.
Spitzer provided our first insights into the complex chemistry in sub-Jovian sized worlds.
Improved observational techniques brought higher fidelity multi-dimensional views of exoplanet atmospheres

The high-precision offered by Hubble’s WFC3 spatial scanning mode that came online in 2012 has given us some of the highest-definition looks at exoplanet atmospheres to date.
Atmospheric theorists rose to the challenges presented by observational data and developed models of growing complexity.

Kempton et al. (2011)

Figure 3. Same as Figure 2 but for the major carbon-bearing molecules only.

Without high levels of UV irradiation, methane remains the dominant carbon-bearing species throughout the atmosphere and is present at high abundances ranging from 0.1% for solar metallicity atmospheres to 1% when the metallicity is enhanced to $30 \times$ solar. Ammonia and $\text{N}_2$ are expected to be the most abundant nitrogen-bearing molecules with $\text{N}_2$ becoming increasingly abundant at higher metallicities. Some additional carbon-bearing species appear at moderate abundances for models with low $K_{zz}$ and high metallicity including HCN and $\text{C}_2\text{H}_6$. Molecular diffusion allows for heavy molecules to preferentially settle out of the atmosphere at pressures lower than $\sim 100 \mu$bar for models with $K_{zz}$ of $10^6 \text{ cm}^2\text{s}^{-1}$ and $\sim 10 \mu$bar for models with $K_{zz}$ of $10^7 \text{ cm}^2\text{s}^{-1}$.

For the highly irradiated models, the upper atmosphere chemistry is further complicated by UV photolysis. In these atmospheres, the chemistry is driven by photolysis of methane and ammonia. Ammonia has an appreciable photolysis cross section throughout the UV, making it unstable in the upper atmosphere (see Figure 4). Methane only has a large UV cross section shortward of 1400 Å, but it experiences significant photolysis from Ly$\alpha$ photons at 1216 Å. The heights at which $\text{CH}_4$ and $\text{NH}_3$ are removed from the atmosphere have a strong dependence on the amount of vertical mixing. At higher values of $K_{zz}$, methane and ammonia are lofted higher into the atmosphere, which results in a replenishing source that counteracts the effects of photolysis. As the models increase in metallicity, both methane and ammonia also maintain higher abundances to higher...

Figure 4. Photolysis cross sections for some of the molecules that are predicted to be present at high abundance in GJ 1214b's atmosphere. Photolysis rates are determined by $\int \sigma F_\nu e^{-\tau_\nu} d\nu$ where $F_\nu$ is the stellar flux density, $\tau_\nu$ is the optical depth, and $\sigma$ is the photolysis cross section. The photolysis cross sections plotted here are from Zahnle et al. (2009a, and references therein).

3.2. Simulations with Radiatively Active Clouds

The 3D modeling of radiatively active clouds in GJ1214b's atmosphere is challenging. Because of cloud opacity, the atmospheric radiative timescale becomes shorter in the upper atmosphere and the condensation occurs deeper in...
The development and application of exoplanet atmospheric retrieval algorithms transformed our view of exoplanet atmospheres.

Parameterisation has also evolved in modelling of primary transit spectra. The different geometries of primary and secondary transit observations mean that each is sensitive to different aspects of the atmospheric state, and so different parameters are included depending on the type of observation.

The transit depth in primary transit is given by

\[ d = R_p - \tau_R_s \]

where \( R_p \) is the radius of the planet and \( \tau \) the radius of the star. A transit spectrum is the variation in transit depth as a function of wavelength, which results from the change in atmospheric opacity due to the presence of absorbing gases and aerosols (Figure 2).

Barstow & Heng (2020)

Kreidberg et al. (2014)
Eventually a comparative sample of exoplanet atmospheres evolved...

Observations from *Hubble* and *Spitzer* have provided detections of H$_2$O, Na, K, TiO, H, He, aerosols, and hints of many other atmospheric components.
With *Spitzer* and *Hubble* we embarked on our first probes of the atmospheres of habitable zone worlds.

K2-18b

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**Figure 3.** Transmission spectrum of K2-18b computed from our global spectroscopic and broadband transit light-curve analysis (black points), and a random sampling of the model transmission spectra in the retrieval MCMC chain (blue). The shaded regions indicate 1σ and 2σ credible intervals in the retrieved spectrum (medium and light blue, respectively), relative to the median fit (dark blue line) and the overall best-fitting model (red). The main feature of the transmission spectrum is the prominent increase in transit depth within the 1.4 µm vibrational band of water vapor covered by the HST/WFC3 data. The K2 data point is plotted at visible wavelengths and the Spitzer/IRAC measurements are indicated at 3.6 and 4.5 µm. The secondary vertical axis on the right indicates the atmospheric pressure for the best-fitting model.

explore the most extreme scenarios where the spot and faculae covering fractions can be as high as 100%, but even those stellar inhomogeneity models fail to explain the amplitude of the observed transit depth variation. They deliver an absolute maximum of 20 ppm at 1.4 µm, which still only corresponds to less than a quarter of the transit depth variation in the observations. We conclude that stellar inhomogeneities and activity cannot explain the measured transmission spectrum.

**ATMOSPHERIC MODELING**

We compute quantitative constraints on the atmosphere of K2-18b using the SCARLET atmospheric retrieval framework (*Benneke & Seager* 2012, 2013, *Knutson et al.* 2014a, *Kreidberg et al.* 2014, *Benneke* 2015, *Benneke et al.* 2019). To be as independent of model assumption as possible, we employ the "free retrieval" mode, which parameterizes the mole fractions of the molecular gases, the pressure of the cloud deck, and the atmospheric temperature as free fitting parameters. SCARLET then determines their posterior constraints by combining the atmospheric forward model with a Bayesian MCMC analysis.

To evaluate the likelihood for a particular set of parameters, the atmospheric forward model first computes a model atmosphere in hydrostatic equilibrium, then determines the opacities of molecules at each layer, and finally computes the transmission spectrum. Beyond H₂/He, our model allows for H₂O, CH₄, CO, CO₂, NH₃, HCN, and N₂ with a log-uniform prior for mixing ratios between 10⁻¹ and 1. We find that only H₂O is required by the data and that including the other molecules has virtually no impact on the best fit to the data. Following *Benneke & Seager* (2012, 2013), we also include a cloud deck at a freely parameterized cloud top pressure with a log-uniform prior between 0.1 mbar and 10 bar. The cloud deck is assumed to be opaque to grazing light beams below the cloud top pressure as would occur for large droplets. We also explored a more complex three-parameter Mie-scattering cloud description as introduced in *Benneke et al.* (2019); however, we find no significant improvement in the fit to the observed transmission spectrum compared to gray clouds. Our atmospheric temperature is parameterized using a single free parameter for the mid-atmosphere probed by the observations because low-resolution transmission spectra are largely insensitive to the exact vertical temperature structure (*Benneke & Seager* 2012). We also considered a five-parameter analytic model (*Parmentier & Guillot* 2018).
A reminder of the instrument systematics and other noise sources tackled in the era of *Hubble* and *Spitzer*

Bean et al. (2018), adapted from Knutson et al. (2012)

**Precision “records”: Spitzer ~ 20 ppm, Hubble ~30 ppm**
In the era of *Hubble* & *Spitzer*
>100 transiting exoplanets with atmospheric characterization observations

In the era of *JWST*
Potential for >500 transiting exoplanets with atmospheric characterization observations
JWST Transiting Exoplanets Cycle 1 & 2 Targets

~120 Individual Targets
300+ Observations
~2800 hours
20% of JWST GO Time

207 Transits
90 Eclipses
20 phase-curves

Figure Credit: Hannah Wakeford/Sarah Moran
“Your future is whatever you make it, so make it a good one.”

-Doc Brown

JWST Cycle 3 GO deadline = Wednesday October 25th, 2023
JWST High-Precision Bright-Object Time-Series Modes

**NIRCam**
- 0.6-5 microns
- Spectroscopy: 2.5-5.0 microns
- Photometry: 0.7-4.8 microns

**NIRSpec BOTS**
- 1-5 microns
- Spectroscopy: 
  - J > 5, R~2700
  - J > 6, R~1000
  - J > 9.5, R~100

**MIRI**
- 5-28 microns
- Slitless Spectroscopy: K > 5, R~100
- IFU Spectroscopy: 4.9-27.9 microns
- Photometry: 5.6-25.5 microns

**https://jwst-docs.stsci.edu/methods-and-roadmaps/jwst-time-series-observations**
JWST High-Precision Bright-Object Time-Series Modes: New for Cycle 3!

1.0-2.0 μm spectra can be taken at the same time as the standard, longer wavelength, F322W2 (2.5-4.0 μm) or F444W (4.0-5.0 μm) spectra on the long wavelength detectors.

NIRCam DHS produces 10 R~300 spatially separated spectra.

Targets as bright as K~1 can be observed with this mode!
JWST Transiting Exoplanet Proposal Roadmap

1) Science Question
2) Targets and Models
3) Modes and Precision
4) Make sure you have the team necessary to tackle proposal and future observations
5) Iterate, polish, submit and wait..

Batalha et al. (2017),
https://natashabatalha.github.io/PandExo/

https://jwst.etc.stsci.edu/

Astronomer's Proposal Tool (APT)
apt.stsci.edu
“There are no insurmountable challenges to Transiting Exoplanet Observations with JWST.”

-Nikole Lewis
Surmountable challenges for JWST transiting exoplanet atmospheric characterization observations

Espinoza et al. 2022

Bell et al. 2023
Surmountable challenges for JWST transiting exoplanet atmospheric characterization observations

Mirror Tilt Events

1/f and background noise

Rigby et al. (2023)

Radica et al. (2023)
Surmountable Challenges for JWST exoplanet atmospheric characterization observations

Noise Sources

NASA SAG21 Report

Robust chemistry/opacity databases
Supporting laboratory investigations

See Fortney and 80+ co-authors whitepapers

Gharib-Nezhad et al. (2021)
Hörst et al. (2018)
MacDonald & Lewis (2022)

3D atmospheric structure and processes
Surmountable challenges for JWST transiting exoplanet atmospheric characterization observations

Rigby et al. (2023)
“If you want to go fast, go alone. If you want to go far, go together.”

-African Proverb
Community-driven workshops, data challenges, collaborations and open-source software can accelerate the rate at which new insights into exoplanet atmospheres are gained in the coming decade.

Spitzer Data Reduction Challenge (Ingalls et al. 2016)

Ariel Atmospheric Retrieval Challenge (Barstow et al. 2022)

JWST Transiting Exoplanet ERS Collaboration (ers-transit.github.io)
In the coming decade JWST will not be the only space-based facility spectroscopically probing transiting exoplanet atmospheres.

- **CUTE** – Cubesat launched in 2021
- **Pandora** – Smallsat launch in mid-2020s
- **Ariel** – M4 Mission launch in 2029
In the era of JWST, *Hubble* will still provide critical access to UV, Optical, and NIR wavelengths necessary for understanding exoplanet atmospheric chemistry and evolution.

Strategic Exoplanet Initiatives with HST and JWST Working Group

https://sites.google.com/view/exoplanet-strategy-wg

Townhall on July 31st, 2023 is reserved for early career researchers!

Credit: Mercedes Lopez-Morales
Opportunities for synergies between ground and space-based observatories for transiting exoplanet atmospheric characterization

Low-resolution optical/NIR transmission spectroscopy and stellar monitoring

High-resolution optical/NIR spectroscopy

Kirk et al. (2021)

Van Sluijs al. (2023)
Early-career researchers have an important opportunity shape JWST transiting exoplanet science in the coming decade...

My First Exoplanet Meeting (~ 50 people)

2008

Molecules in the Atmospheres of Extrasolar Planets - a Workshop in Paris

2023

Sagan Summer Workshop Characterizing Exoplanet Atmospheres: The Next 20 Years

To today.... (1000+ people)