Characterizing transiting planets with JWST spectra: Simulations and Retrievals

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Planet transit / eclipse observations

• Spectra provide best diagnosis of atmospheres:
  – Compositions: inventory of molecules requires large spectral range
  – Transmission spectra best for abundances: insensitive to T profile but only sample high atmosphere
  – Emission spectra sample more atmosphere and reveal temperature profiles with retrievals

• Photometry useful for
  – Phase curves to study response to insolation and energy transport
  – Confirming transits, e.g. small TESS objects, Kepler Earth in GV HZ
  – Eclipse mapping: temperature variations across planet disk
Some progress from transit spectroscopy

• Molecules & atoms identified in exoplanet atmospheres
  – H2O, CO (CH4, CO2), Na, other alkali, HI, CII, OI,…

• Measured temperature-pressure profiles from hot Jupiter emission spectra
  – e.g., HD 189733b (e.g., Line+ 2014), WASP-43b (Kreidberg+ / Stevenson+ 2015)

• Some Neptune-sized planets have been diagnosed
  – HAT-P-11 (Fraine+ 2014) and GJ 436b (Knutson+, etc.)

• Sub-Neptunes and super-Earths have been difficult
  – GJ 1214b: flat absorption, no sec. eclipse (many people…)
  – Promise of cooler planets like K2-3 system (Crossfield+ 2015): might be cool enough to not have clouds
Questions about exoplanet atmospheres

• **What are their compositions?**
  – Elemental abundances:
    • C/O and [Fe/H]: Both are formation diagnostics
  – Chemical processes
    • Identify equilibrium chemistry
    • Identify disequilibrium chemistry:
      – Vertical mixing, photochemistry, ion chemistry…
    • 3-D effects: spatial variations

• **Energy Budget and Transport**
  – 1-D structure: measure profiles, inversions present?
  – Dynamical transport: day/night differences

• **Clouds**
  – Cloud composition, particle sizes, vertical & spatial distribution
  – Removing cloud effects to determine bulk properties

• **Anything about low mass / small (< ~2R_e) planet atmospheres**

• **Trends with bulk parameters (mass, insolation, host stars, …)**
  – Requires a population of diverse planets
New JWST Transiting Planet Assessment

Model some known planet types, assess information in simulated JWST spectra

• Select archetypal planets from known system parameters
  – Hot Jupiter, warm Neptune, warm sub-Neptune, cool super-Earth

• Create model transmission and emission spectra (M. Line)

• Simulate JWST spectra using performance models (TG)
  – Simulate slitless modes with large bandpasses & good bright limits: NIRISS SOSS, NIRCam grisms, MIRI LRS slitless 1 – 11 µm
  – My code is based on validated instrument models, detector parameters, JWST background models, random & systematic noise

• Perform atmospheric retrievals (M. Line) to assess uncertainties in abundances, T-P profiles
  – Focus on uncertainties, not absolute parameters
  – *Identify what wavelengths give most useful information for what planets*
Forward models & retrievals

• Use 1-D forward models:

• Transmission model has 11 free parameters:
  – $T(SH)$, $R(P=10b)$, hard clouds ($P_c$, $\sigma_0$, $\beta$), $H_2O$, $CH_4$, $CO$, $CO_2$, $NH_3$, $N_2$ absorbers, constant with altitude

• Emission model has 1D T-P profile & 10 free params
  – $H_2O$, $CH_4$, $CO$, $CO_2$, $NH_3$, 5 gray atm parameters for T-P (Line+ 2013a)

• CHIMERA Bayesian retrieval suite (Line+ 2013a,b)
  – Updated with emcee MCMC
  – Uniform & Jeffreys priors
Simulated Planet Signals ($S_\lambda$) & Noise ($N_\lambda$)

\[
T_{r,\lambda} = \frac{S_\lambda(F_*) + Bkg - (S_\lambda(F(\star + p)_{Tr}) + Bkg)}{S_\lambda(F_*) + Bkg - \langle Bkg \rangle}
\]

and

\[
E_{m,\lambda} = \frac{S_\lambda(F(\star + p)_{Em}) + Bkg - (S_\lambda(F_*) + Bkg)}{S_\lambda(F_*) + Bkg - \langle Bkg \rangle}
\]

\[
N_\lambda = \sqrt{S_\lambda + Bkg + N_{d,tot}^2}
\]

\[
N_{d,tot} = N_d \frac{\sqrt{n_{pix}n_{ints}R_{native}}}{R}
\]

<table>
<thead>
<tr>
<th>$\lambda$ ((\mu)m)</th>
<th>Noise floor</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0 – 2.5</td>
<td>20 ppm</td>
</tr>
<tr>
<td>2.5 – 5.0</td>
<td>30 ppm</td>
</tr>
<tr>
<td>5.0 - 12</td>
<td>50 ppm</td>
</tr>
</tbody>
</table>

15 Oct 2015

JWST Exoplanet Spectra
Selected Model Systems

<table>
<thead>
<tr>
<th>Planet Type</th>
<th>System Parameters</th>
<th>Composition</th>
<th>Clouds</th>
<th>Geometry</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hot Jupiter</td>
<td>HD 209458b</td>
<td>1x Solar</td>
<td>Clear 1 mbar</td>
<td>Trans, Emis</td>
</tr>
<tr>
<td>Warm Neptune</td>
<td>GJ 436b</td>
<td>1x Solar</td>
<td>Clear 1 mbar</td>
<td>Trans, Emis</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1000x Solar</td>
<td>Clear</td>
<td>Trans, Emis</td>
</tr>
<tr>
<td>Warm Sub-Neptune</td>
<td>GJ 1214b</td>
<td>1x Solar</td>
<td>Clear 1 mbar</td>
<td>Trans, Emis</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1000x Solar</td>
<td>Clear</td>
<td>Trans, Emis</td>
</tr>
<tr>
<td>Cool Super-Earth</td>
<td>K2-3b</td>
<td>1x Solar</td>
<td>Clear 1 mbar</td>
<td>Trans, Emis</td>
</tr>
<tr>
<td></td>
<td></td>
<td>100% H₂O</td>
<td>Clear</td>
<td>Trans, Emis</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Planet Type</th>
<th>System Parameters</th>
<th>$T_*(K)$</th>
<th>$R_*(R_⊙)$</th>
<th>$K$ (mag)</th>
<th>$T_{eq}(K)$</th>
<th>$M_p$ ($M_{Jup}$)</th>
<th>$R_p$ ($R_{Jup}$)</th>
<th>$H^a$ (km)</th>
<th>$T_{14}$ (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hot Jupiter</td>
<td>HD 209458b</td>
<td>6065</td>
<td>1.155</td>
<td>6.3</td>
<td>1500</td>
<td>0.69</td>
<td>1.359</td>
<td>580</td>
<td>11,000</td>
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<tr>
<td>Warm Neptune</td>
<td>GJ 436b</td>
<td>3350</td>
<td>0.464</td>
<td>6.1</td>
<td>700</td>
<td>0.073</td>
<td>0.377</td>
<td>200</td>
<td>2740</td>
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<tr>
<td>Warm Sub-Neptune</td>
<td>GJ 1214b</td>
<td>3030</td>
<td>0.211</td>
<td>8.8</td>
<td>600</td>
<td>0.020</td>
<td>0.239</td>
<td>240</td>
<td>3160</td>
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<tr>
<td>Cool Super-Earth</td>
<td>K2-3b</td>
<td>3900</td>
<td>0.561</td>
<td>8.6</td>
<td>500</td>
<td>0.017</td>
<td>0.191</td>
<td>160</td>
<td>9190</td>
</tr>
</tbody>
</table>
Model Transmission Spectra

Hot Jupiter $R \leq 100$
- Clear Solar
- Cloudy Solar

Warm Neptune $R \leq 100$
- Clear Solar
- Cloudy Solar
- 1000x Solar

Warm Sub-Neptune $R \leq 100$
- Clear Solar
- Cloudy Solar
- 1000x Solar

Cool Super-Earth $R = 35$
- Clear Solar
- Cloudy Solar
- 100% H2O
Simulated JWST Trans Spectra (1 transit)

- **Hot Jupiter (R ≲ 100)**
  - Cloudy Solar
  - Clear Solar

- **Warm Neptune (R ≲ 100)**
  - Cloudy Solar
  - Clear Solar
  - 1000x Solar

- **Warm Sub-Neptune (R ≲ 100)**
  - Cloudy Solar
  - Clear Solar
  - 1000x Solar

- **Cool Super-Earth (R = 35)**
  - Cloudy Solar
  - Clear Solar
  - 100% H2O
Model Emission Spectra

- Hot Jupiter R≤100
  - Clear Solar
  - T Inversion

- Warm Neptune R=35
  - Clear Solar
  - 1000x Solar

- Warm Sub-Neptune R=35
  - Clear Solar
  - 1000x Solar

- Cool Super Earth R=35
  - Clear Solar
  - 100% H2O
Simulated JWST Emission Spectra (1 eclipse)

- Hot Jupiter R≤100, 1 eclipse
  - Clear Solar
  - T Inversion

- Warm Neptune R=35, 1 eclipse
  - Clear Solar
  - 1000x Solar

- Warm Sub-Neptune R=35, 1 eclipse
  - Clear Solar
  - 1000x Solar

- Cool Super Earth R=35, 1 eclipse
  - Clear Solar or 100% H2O
Retrieval Birds & Bees

Figure 3. Unique constraints on the atmospheric properties based on observables in the transmission spectrum. The transmission spectrum of an atmosphere with \( n \) relevant absorbers contains \( n+4 \) independent pieces of information that constrain the \( n \) mixing ratios of these absorbers, up to two mixing ratios of the two spectrally inactive components \( \text{H}_2 + \text{He} \) and \( \text{N}_2 \), the planetary radius at a reference pressure level, \( R_{P;10} \), and the surface/cloud-top pressure. The left panel illustrates conceptually the individual observables in the transmission spectrum that carry the \( n+4 \) pieces of information for an example with \( n = 3 \) absorbers. For well-mixed atmospheres, the three observables “slope of the Rayleigh signature,” “shapes of individual features,” and “relative transit depths in features of same molecule” are redundant and provide only one independent piece of information. Note that to uniquely constrain any of the \( n+4 \) atmospheric properties on the far right, all \( n+4 \) pieces of information need to be available, unless additional assumptions are made.

Benneke & Seager (2012)
Retrieval: Hot Jupiter Gasses

HOT JUPITER

Emission Clear Solar

Transm. Cloud Solar

Transm. Clear Solar

Priors

15 Oct 2015

JWST Exoplanet Spectra
Retrieval: Warm Neptune Gasses

WARM NEPTUNE

<table>
<thead>
<tr>
<th>Emission Clear Solar</th>
<th>H₂O</th>
<th>CH₄</th>
<th>CO</th>
<th>CO₂</th>
<th>NH₃</th>
<th>C/O</th>
<th>[Fe/H]</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Emission Clear</strong></td>
<td><img src="image1" alt="Graph" /></td>
<td><img src="image2" alt="Graph" /></td>
<td><img src="image3" alt="Graph" /></td>
<td><img src="image4" alt="Graph" /></td>
<td><img src="image5" alt="Graph" /></td>
<td><img src="image6" alt="Graph" /></td>
<td><img src="image7" alt="Graph" /></td>
</tr>
<tr>
<td><strong>Emission High MMW</strong></td>
<td><img src="image8" alt="Graph" /></td>
<td><img src="image9" alt="Graph" /></td>
<td><img src="image10" alt="Graph" /></td>
<td><img src="image11" alt="Graph" /></td>
<td><img src="image12" alt="Graph" /></td>
<td><img src="image13" alt="Graph" /></td>
<td><img src="image14" alt="Graph" /></td>
</tr>
<tr>
<td><strong>Transm. Clear</strong></td>
<td><img src="image15" alt="Graph" /></td>
<td><img src="image16" alt="Graph" /></td>
<td><img src="image17" alt="Graph" /></td>
<td><img src="image18" alt="Graph" /></td>
<td><img src="image19" alt="Graph" /></td>
<td><img src="image20" alt="Graph" /></td>
<td><img src="image21" alt="Graph" /></td>
</tr>
<tr>
<td><strong>Transm. High MMW</strong></td>
<td><img src="image22" alt="Graph" /></td>
<td><img src="image23" alt="Graph" /></td>
<td><img src="image24" alt="Graph" /></td>
<td><img src="image25" alt="Graph" /></td>
<td><img src="image26" alt="Graph" /></td>
<td><img src="image27" alt="Graph" /></td>
<td><img src="image28" alt="Graph" /></td>
</tr>
<tr>
<td><strong>Transm. Cloud Solar</strong></td>
<td><img src="image29" alt="Graph" /></td>
<td><img src="image30" alt="Graph" /></td>
<td><img src="image31" alt="Graph" /></td>
<td><img src="image32" alt="Graph" /></td>
<td><img src="image33" alt="Graph" /></td>
<td><img src="image34" alt="Graph" /></td>
<td><img src="image35" alt="Graph" /></td>
</tr>
<tr>
<td><strong>Transm. Clear Solar</strong></td>
<td><img src="image36" alt="Graph" /></td>
<td><img src="image37" alt="Graph" /></td>
<td><img src="image38" alt="Graph" /></td>
<td><img src="image39" alt="Graph" /></td>
<td><img src="image40" alt="Graph" /></td>
<td><img src="image41" alt="Graph" /></td>
<td><img src="image42" alt="Graph" /></td>
</tr>
</tbody>
</table>

**Priors**

NIRISS+NIRCam+MIRI (1-11μm)-NIRISS+NIRCam (1-5μm)-NIRISS (1-2.5μm)
Retrieval: Warm Sub-Neptune Gasses

WARM SUBNEPTUNE

![Graph showing various emission and transmission spectra for different gases such as H$_2$O, CH$_4$, CO, CO$_2$, NH$_3$, C/O, and Fe/H. The graphs are labeled with priors such as P$_{cloud}$ and log(P$_{dust}$).]
Retrieval: Cool Super-Earth Gasses

COOL SUPER EARTH

H₂O  CH₄  CO  CO₂  NH₃  C/O  [Fe/H]  P_{cloud}

NIRISS+NIRCam+MIRI (1-11 μm)-NIRISS+NIRCam (1-5 μm)-NIRISS (1-2.5 μm)

Transm. Clear Solar

Transm. Clear

Transm. All H₂O

Priors
Emission retrievals: T-P Profiles

Dashed: True value
Solid line: Retrieved mean value
Shaded: 1 sigma

Detect inversion at 4 sigma with NIRISS only (red)
JWST Exoplanet Spectra

Warm Neptune Solar

Warm Neptune High MMW

Warm SubNeptune Solar

Warm SubNeptune High MMW

NIRISS+NIRCam+MIRI (1-11μm)-NIRISS+NIRCam (1-5μm)-NIRISS (1-2.5μm)
Constraining C/O from $\text{H}_2\text{O} + T_{\text{eq}}$

Transmission spectra
Mass - Metallicity

Transmission spectra
Dis-equilibrium Chemistry (v mixing)
Summary / Conclusions (1)

- NIRISS (1 – 2.5 μm) transmission spectra alone often constrain mixing ratios of dominant molecules in clear solar atmosphere planets
  - C/O and [Fe/H] sometimes also constrained with only NIRISS
  - \( \lambda \geq 5 \) μm spectra needed in a number of cases

- Cloudy solar atmospheres are often constrained (~1 dex or better mixing ratios) with \( \lambda = 1 - 11 \) μm spectra
  - Transmission is better than emission for warm sub-Neptune
  - Hot Jupiter and warm Neptune do better with emission
    - Need sufficient \( F_p \) and high \( F_p/F*_\star \) for useful emission spectra

- High MMW atmospheres can be identified by high [Fe/H]

- C/O is constrained to 0.2 dex for hot Jupiters with \( \lambda = 1 – 5+ \) μm spectra. Also: C/O for hot planets with H2O + Teq

- \( \sigma[Fe/H] < 0.5 \) dex for warm, clear planets (\( \lambda = 1-5+ \) μm tr)
Summary / Conclusions (2)

• Non-equilibrium vertical mixing cannot be detected via mixing ratios
  – May be better to look for unexpected spectral features

• Observing 5 planets from Uranus to Jupiter mass should measure [Fe/H] vs. Log (M) slope to $1\sigma = 0.13$
  – $\lambda = 1$-5+ $\mu$m transmission spectra
  – More than adequate (~5%) for detecting Solar System slope

• These results are for observations of single transits or eclipses. We will not know the actual JWST data quality – and how noise will decrease with co-adding – until after launch

• Many more retrieval issues to be explored (binning, Bayesian estimators, priors, 3D, parameterization), but will largely be driven by future data
The End