TRANSMISSION SPECTRA OF TRANSITING PLANET ATMOSPHERES: MODEL VALIDATION AND SIMULATIONS OF THE HOT NEPTUNE GJ 436b FOR THE JAMES WEBB SPACE TELESCOPE

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ABSTRACT

We explore the transmission spectrum of the Neptune-class exoplanet GJ 436b, including the possibility that its atmospheric opacity is dominated by a variety of nonequilibrium chemical products. We also validate our transmission code by demonstrating close agreement with analytic models that use only Rayleigh scattering or water vapor opacity. We find broad disagreement with radius variations predicted by another published model. For GJ 436b, the relative coolness of the planet’s atmosphere, along with its implied high metallicity, may make it dissimilar in character compared to “hot Jupiters.” Some recent observational and modeling efforts suggest low relative abundances of H2O and CH4 present in GJ 436b’s atmosphere, compared to calculations from equilibrium chemistry. We include these characteristics in our models and examine the effects of absorption from methane-derived higher-order hydrocarbons. To our knowledge, the effects of these nonequilibrium chemical products on the spectra of close-in giant planets have not previously been investigated. Significant absorption from HCN and C2H2 is found throughout the infrared, while C2H4 and C2H6 are less easily seen. We perform detailed simulations of James Webb Space Telescope observations, including all likely noise sources, and find that we will be able to constrain chemical abundance regimes from this planet’s transmission spectrum. For instance, the width of the features at 1.5, 3.3, and 7 μm indicates the amount of HCN versus C2H2 present. The NIRSpec prism mode will be useful due to its large spectral range and the relatively large number of photo-electrons recorded per spectral resolution element. However, extremely bright host stars like GJ 436 may be better observed with a higher spectroscopic resolution mode in order to avoid detector saturation. We find that observations with the MIRI low-resolution spectrograph should also have high signal-to-noise in the 5–10 μm range due to the brightness of the star and the relatively low spectral resolution (R ~ 100) of this mode.

Key words: planetary systems – radiative transfer – stars: individual (GJ 436, HD 209458)

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1. INTRODUCTION

The rise of exoplanet characterization since the initial discovery of the transit of planet HD 209458b a decade ago (Charbonneau et al. 2000; Henry et al. 2000) has been truly stunning. The initial steps in atmospheric characterization of hot Jupiters came after the realization that the transmission spectra of transiting planets would be diagnostic of the temperature and chemical mixing ratios in these atmospheres (Seager & Sasselov 2000; Brown 2001; Hubbard et al. 2001). As with perhaps all subfields of astronomy and planetary science, the return on the investment in these myriad observations is amplified when the data sets are compared to models that aim to simulate the conditions in the atmospheres of these planets.

The model atmospheres, whether one-dimensional or three-dimensional, aim to predict the temperature structure, chemical mixing ratios, and wavelength-dependent opacity, as a function of height. A comparison of transmission spectra data with models can enable constraints on the mixing ratios of atomic and molecular absorbers (e.g., Charbonneau et al. 2002; Fortney et al. 2003; Tinetti et al. 2007; Swain et al. 2008; Sing et al. 2009; Madhusudhan & Seager 2009; Désert et al. 2009; Burrows et al. 2010). Of course, it then directly follows that constraints on these atmospheres are model dependent, as it is likely that the choices that one makes in constructing a model atmosphere affect the calculated spectrum. In this exciting field, the great difficulty in obtaining high signal-to-noise observations, along with the somewhat unconstrained nature of current atmosphere models, can make interpretation difficult. This was again typified by the recent works of Stevenson et al. (2010) and Beaulieu et al. (2010), who, based on separate data reductions and model fits, disagree on the probable mixing ratio of methane in the atmosphere of GJ 436b, which we discuss below.

At the forefront of exoplanet characterization, detections of lower mass objects have expanded the reservoir of constraints to parameter space beyond hot Jupiters, broadening the scope of planetary characterization. The premier hot Neptune, GJ 436b, a 22.6 M⊕ planet orbiting an M2.5 star, was detected via radial velocity reflex motion by Butler et al. (2004), and later revisited by Maness et al. (2007). The first photometric detection of transits were obtained by Gillon et al. (2007b), providing the missing link needed to determine the mass and in turn the bulk density. Gillon et al. (2007a) and Deming et al. (2007) refined system parameters with a Spitzer transit lightcurve at 8 μm, and Deming et al. (2007) and Demory et al. (2007) reported a detection of the planet’s secondary eclipse at 8 μm as well. A recent attempt at transit characterization was Pont et al. (2009), who probed the 1.4 μm water band using NICMOS on board the Hubble Space Telescope (HST). This was the first attempt at a multi-wavelength transmission spectrum obtained for GJ 436b. Ground-based efforts have yielded H- and K-band radius measurements (Alonso et al. 2008; Cáceres et al. 2009),
in addition to radius measurements from EPOXI obtained by Ballard et al. (2010) in the 0.35–1.0 μm range. Using IRAC on board Spitzer, Beaulieu et al. (2010) very recently obtained transit depth measurements at 3.6, 4.5, and 8 μm.

In order to study the dayside of the planet Stevenson et al. (2010) obtained secondary eclipse measurements in six Spitzer bandpasses, from 3.6 to 24 μm. They and Madhusudhan & Seager (2010) interpret their results as providing evidence of thermochemical disequilibrium in GJ 436b’s dayside atmosphere. The fits by Madhusudhan & Seager (2010) to the Stevenson et al. (2010) observations are quite interesting in the mixing ratios of CH₄, H₂O, CO, and CO₂ that they require. They postulate a metal-rich atmosphere, in line with our understanding of Uranus and Neptune. However, compared to equilibrium chemistry, CH₄ is strongly depleted, while H₂O is also depleted, and CO and CO₂ are strongly enhanced. Higher-order hydrocarbon molecules, e.g., C₂Hₓ or HCN, were not considered in their fits, even though these molecules are the first products resulting from methane destruction via photolysis (Moses et al. 2005) or reduction (Zahnle et al. 2009a), and are strong absorbers in the near- and mid-infrared. When suggesting that a low CH₄ abundance may be due to the photolysis and/or vertical mixing, these higher-order hydrocarbon molecules should be included. Alternatively, Beaulieu et al. (2010) interpret the Stevenson et al. (2010) data (some re-reduced by their team), as well as primary transit data, as potentially indicating a methane-rich atmosphere with a temperature inversion. This only further strengthens the points that differences between data reduction methods and models clearly impact conclusions.

The coming of the James Webb Space Telescope (JWST) will bring the next advancement in understanding exoplanet atmospheres and exoplanetary atmosphere modeling, as it will help to reduce the underconstrained nature of current models. For a planet like GJ 436b where there are already signs from photometry that the atmospheric chemistry is complex, the spectral capabilities of JWST will enhance our understanding, such as the identification of more complex chemical composition regimes and temperature structures. Understanding the integration times and applicable wavelength bands needed to resolve spectral features of particular atmospheres is key for planning future science initiatives with JWST.

GJ 436b is a particularly interesting planet because it is the transiting Neptune-class object that orbits the brightest parent star. This means it may long remain the best studied extrasolar Neptune-class object. Given the poor signal-to-noise of transmission spectroscopy obtained with HST (Pont et al. 2009), and the uncertainties that arise from using a small number of wide photometric bands strung together as spectra, it may well fall to JWST to enable robust atmospheric characterization.

Deriving accurate transit depths can be a complex task. Problems with Spitzer IRAC primary transit observations include the issue of variable stellar fluxes between transit visits, due to starspots. In the most common situation where a planet does not occult spots directly, the unocculted parts of the stellar surface appear less bright, due to the spots. Compared to a stellar surface that lacks spots, one would derive a deeper transit depth (see, e.g., Pont et al. 2008; Agol et al. 2010). There is also the difficulty of extracting the transit depth with great accuracy, which yields different groups to find different transit depths, with the same data sets (e.g., Beaulieu et al. 2008; Désert et al. 2009). However, given that the interpretation of transmission spectroscopy is in principle less sensitive to the atmospheric pressure–temperature profile than dayside emission spectroscopy, transmission spectroscopy may lead to the most robust determinations of atmospheric abundances.

Here we examine the transmission spectrum signatures of a variety of atmospheric chemistries, including those from thermochemical equilibrium calculations, those favored by Stevenson et al. (2010), and those that include abundant higher-order hydrocarbons not considered by these authors, guided by results from Zahnle et al. (2009a). We combine these models with a detailed simulation of the NIRSpec and MIRI low-resolution spectrograph (LRS) instruments that will be aboard JWST, for a realistic simulation of what further knowledge we may gain for this important planet. In Section 2, we make simple comparisons between our models, analytic relations, and other published work, in order to establish the robustness of derived atmospheric parameters, and to validate our code. We find large differences between our work and that of G. Tinetti and collaborators. In Section 3, we describe model transmission spectra for GJ 436b while investigating various chemistries. In Section 4, we present JWST simulations of GJ 436b transmission spectra, and discuss the possibilities for identifying important atmospheric signatures in the near future. In Section 5, we discuss implications of our transmission spectra models as well as address future endeavors for atmospheric characterization via theoretical work.

2. TRANSMISSION MODEL: DESCRIPTION AND VALIDATION

We model the transmission spectrum of planets using a descendent of the code first described in Hubbard et al. (2001). Here we ignore the effects of refraction and a glow of photons around the planet’s limb due to Rayleigh scattering, both of which Hubbard et al. (2001) found to be negligible for close-in planets. Later works using this code included Fortney et al. (2003), which investigated simple two-dimensional models of the atmosphere of HD 209458b, but included one planet-wide P–T profile, with two-dimensional changes in the atmospheric opacities. Fortney (2005) examined the possible effects of cloud opacity for the slant viewing geometry appropriate for transits. We refer the reader to Fortney et al. (2010), which described the code in some detail, and extended our treatment to three-dimensional planetary atmosphere models.

In either one dimension or three dimensions, atmospheric P–T profiles are lain atop an opaque atmosphere at a reference pressure of either 1 or 10 bar. The radius at this pressure level is adjusted to yield the best fit to observations. Along 1000 light ray paths through the atmosphere parallel to the star–planet–observer axis, the local atmospheric density and opacity are each typically sampled at 1000 points along each ray. For absorption, the wavelength-dependent cross-section is calculated based on contributions from a variety of atoms and molecules. The abundances can be based either on local chemical equilibrium at a given atmospheric P–T point (Lodders & Fegley 2002, 2006; Lodders 2009), or they can be arbitrary. The Rayleigh scattering cross-section is described in Fortney et al. (2010), and in practice for our H₂/He-dominated atmospheres, we find a cross-section of 1.645e-24 cm² molecule⁻¹.

6 Some phrases used in the original description of the code in Hubbard et al. (2001) may lead to the impression that the code replaces the true geometry of the atmosphere with a slab having the same column density. In the Hubbard et al. (2001) work this “slab” approximation was only done for the simulation of the weak glow of multiply Rayleigh-scattered photons. This approximation has never been made for one-dimensional or three-dimensional calculations of the transmission spectrum.
at 450 nm, and scale by $\lambda^{-4}$ at other wavelengths. Here we define the wavelength-dependent transit radius as the radius where the total slant optical depth reaches 0.56, following the results of Lecavelier des Etangs et al. (2008b), who use a method similar to our current one.

(A color version of this figure is available in the online journal.)

2.1. Opacities

Opacities generally used in the field of exoplanet atmospheres are discussed in detail in Sharp & Burrows (2007) and Freedman et al. (2008). Freedman et al. (2008) outline the opacities that we use in modeling the atmospheres of hot Jupiters, other Jupiter-class planets, Neptune-class planets, and brown dwarfs (e.g., Fortney et al. 2008a, 2008b; Saumon et al. 2006; Cushing et al. 2008). We will not repeat the discussions in that paper, but we will touch on the issues of water opacity and higher-order hydrocarbons in turn.

It is well established theoretically (Burrows et al. 1997; Marley et al. 1999; Seager & Sasselov 2000; Sudarsky et al. 2000; Barman et al. 2001) that water vapor opacity is the dominant infrared opacity source in warm giant planet atmospheres. There is also inescapable observational evidence that this is true for brown dwarfs (e.g., Kirkpatrick 2005), and this clearly appears to be true for hot Jupiters as well (e.g., Swain et al. 2008; Grillmair et al. 2008). Comprehensive ab initio calculations of line lists of hundreds of millions of lines for H$_2$O have been tabulated by, for instance, Partridge & Schwenke (1997) and by Barber et al. (2006). Both tabulations are widely used. One of us (R. S. Freedman) has done extensive comparisons of these two particular line lists at the temperatures of interest for planets and brown dwarfs, those below 2500 K, and these differences are described in Freedman et al. (2008) at being “slight.” In the detailed fits of M. S. Marley and collaborators to L- and T-type brown dwarfs, there is no hint that the Partridge & Schwenke (1997) database is insufficient to match the high signal-to-noise medium-resolution NIR and mid-IR spectra that have been achieved for scores of objects (e.g., Cushing et al. 2008; Stephens et al. 2009). In Figure 1 we show calculated absorption cross-sections at 1500 K and 1 mbar. Clearly the Partridge & Schwenke (1997) and Barber et al. (2006) line lists are nearly identical in this pressure/temperature regime. If transmission spectra calculated by two different atmosphere codes differ (see Section 2.3), the choice between these two water line lists cannot be an important contributing factor.

2.2. Transmission Model Validation

We can validate the predictions of the transmission spectrum code by turning to previous work. In particular, Lecavelier des Etangs et al. (2008a) have shown that the relation between absorption cross-section, mixing ratio, atmospheric temperature structure, and transit radius can be treated analytically. There is a particularly straightforward relation for the wavelength-dependent transit radius for an atmosphere that obeys a few simple constraints. These constraints are an isothermal temperature structure, a constant gravitational acceleration with height, and an opacity cross-section $\sigma$ that varies as

$$\sigma = \sigma_o(\lambda/\lambda_o)^4,$$

(1)

where $\sigma$ and $\sigma_o$ are the wavelength-dependent cross-section and a reference cross-section, respectively, and $\lambda$ and $\lambda_o$ are the wavelength and a reference wavelength, respectively. Given these constraints, the planet’s radius can be written as

$$\frac{dR_p}{d\ln \lambda} = aT/\mu g = aH,$$

(2)

where $R_p$ is the transit radius, $\lambda$ is the wavelength, $k$ is Boltzmann’s constant, $T$ is the temperature, $\mu$ is the mean molecular mass, $g$ is the surface gravity, and $H$ is the scale height. For a pure Rayleigh scattering atmosphere, $\alpha = -4$. In Figure 2 we present an isothermal model at $T = 1500$ K, $g = 25$ m s$^{-2}$, and $\mu = 2.32$, with all opacity turned off, save Rayleigh scattering. We find a model slope that is within 1%
of the analytic relation from Equation (2), which we regard as excellent agreement.

2.3. Comparison with Other Work for Simple Models

In Section 2.1, we described our implementation of the water vapor line list of Partridge & Schwenke (1997). As a further test of the transmission code we can isolate specific wavelength ranges where water opacity closely obeys the $\alpha$-relation from Equation (1). In particular, in Figure 3(a) we show the absorption cross-section versus wavelength at 1500 K and 10 mbar. We have overplotted fits for $\alpha$ in three spectral regions. The bluest and reddest wavelength ranges have a large negative slope, while the middle wavelength range has a positive slope. If our transmission spectrum model is working correctly, we should be able to match the transit radius slope of $dR_p/d\ln \lambda$ from Equation (2), for an atmosphere with a constant gravity and scale height, with water vapor being the only opacity source.

We choose 1500 K and the surface gravity of HD 209458b, $980 \text{ cm s}^{-2}$. This model is plotted in Figure 3(b). One can readily see that over the three defined wavelength ranges our model matches the analytic relation.

Our choice of an isothermal HD 209458b-like model was based on models presented by G. Tinetti and collaborators in a recent paper by Beaulieu et al. (2009). These authors used Spitzer IRAC observations to measure the transit depth in four bandpasses from 3 to 10 $\mu$m. Their nice model fit, compared to the data (shown in their Figure 10), allowed the authors to assert that water vapor was the main absorber in that atmosphere. This may well be true. However, as shown in Fortney et al. (2010), our own HD 209458b models were not able to reproduce the large variation in absorption depths. As discussed in Fortney et al. (2010), we are generally unable to match the much larger variation in transit radius of the models of Tinetti and collaborators (e.g., Tinetti et al. 2007, 2010). Although our two groups use different water opacity databases (Tinetti et al. use the BT2 list), it does not appear that can be a contributing factor.

To help sort out this issue, we became interested in simple tests. Figure 9 of Beaulieu et al. (2009) additionally shows transmission spectra for isothermal model atmospheres of HD 209458b at 1500, 2000, and 2500 K, with opacity due only to water vapor (with a mixing ratio of $4.5 \times 10^{-4}$, the same value we use here). We compare our 1500 K model to that of Beaulieu et al. (2009), as well as the analytic relations, in Figure 4. (The model from Beaulieu et al. 2009 was obtained using a data extraction software package.) The differences are large. Here we are able to match the analytic relations, while the model from Beaulieu et al. (2009) cannot.

It is not immediately clear what causes these dramatic differences between the two models. The large differences remain at 2000 K and 2500 K as well. As shown in Figure 1, differences in water opacity databases cannot be a culprit. Differences in abundances can generally not be a reason either, as a higher (lower) water abundance would move the transit radius up (down) at all wavelengths. Also, that issue was eliminated for the simple test presented here. We are left in the position of identifying what we believe is a problem with the Tinetti et al. models, but we are not in a position to speculate as to its cause.

We only dwell on this issue at length because it is the match of models to observations that allows for the identification of
absorption features, and the determination of the mixing ratios of specific components. We are left to doubt the validity of the Tinetti transmission models, and the derivations of atmospheric abundances from some of the papers in which those models were used. We further wish to stress that at this time we have only compared to transmission spectrum models, and not to dayside emission spectrum models. Certainly the comparison between models is an area in need of future work. An interesting avenue would be to model the transmission spectrum of solar system planets, such as Earth (Pallé et al. 2009) or Saturn (Nicholson et al. 2006), which we will pursue in the near future. Our description of our methods complete, we can now turn our application to GJ 436b.

3. APPLICATION TO GJ 436B

GJ 436b is a relatively small planet with a bulk density similar to Neptune (Gillon et al. 2007b; Torres et al. 2008). It may be mostly composed of fluid water, but a layer of H–He-dominated atmosphere is clearly needed to account for the observed radius (Gillon et al. 2007b; Adams et al. 2008; Nettelmann et al. 2010). GJ 436b is one of the least-irradiated transiting planets, which makes its atmosphere cooler than many other well-studied planets. Based on thermochemical equilibrium models, the low temperatures suggest that the dominant carbon-bearing molecule in the gaseous envelope is methane (Spiegel et al. 2010; Madhusudhan & Seager 2010; Lewis et al. 2010). The recent Stevenson et al. (2010) secondary eclipse measurements from warm Spitzer, however, have been interpreted by these authors as suggesting otherwise. An atmosphere whose carbon chemistry is methane-dominant would tend to yield a small flux ratio in the 3.6 μm band, with more flux in the 4.5 μm band. However, Stevenson et al. (2010) report a strong detection at 3.6 μm, and non-detection at 4.5 μm. This could be indicative of extensive methane depletion, which would allow one to probe deeply, to hotter gas, in the 3.6 μm band, while a large mixing ratio for CO and CO2, which both absorb strongly in the 4.5 μm band, could suppress flux in this bandpass (Stevenson et al. 2010; Madhusudhan & Seager 2010). Large CO and CO2 abundances have been shown to be indicators of high metallicity (Lodders & Fegley 2002; Visscher et al. 2006; Zahnle et al. 2009b).

In the favored scenarios, the CO/CH4 and CO2/CH4 mixing ratios are enhanced due to vertical mixing from hotter, CH4-poor gas below, along with the photochemical destruction of CH4 by incident UV photons. If relatively abundant CH4 is indeed destroyed, this will give rise to a whole host of higher-order hydrocarbons, which is well understood for our solar system’s giant planets (e.g., Moses et al. 2005). Detailed chemical models, including photochemistry and vertical mixing, were applied to cool transiting planets by Zahnle et al. (2009a), which predicted the formation of abundant C2H2, C2H4, C2H6, and HCN. More recently, the theory of a methane-poor atmosphere for GJ 436b was challenged by Beaulieu et al. (2010), who, with a combination of modestly different eclipse depths at 3.6 and 4.5 μm, compute emission and transmission spectra models that allow abundant methane.

3.1. Abundances and Opacities at the Terminator

Since a goal of the work is to explore the prospects for broad-wavelength-coverage spectra with JWST, we choose to explore a diverse set of model atmospheres. Our choices are guided by predictions from equilibrium chemistry, nonequilibrium chemistry, and fits to published spectra of the planet. Cross-sections for the main molecules expected from thermochemical equilibrium are shown in Figure 5. There are certainly a rich number of molecular bands, particularly at wavelengths blueward of 5 μm, where NIRCam and NIRSpec will be sensitive.

In Figure 6, we present GJ 436b model transmission spectra, using these cross-sections. One model is for a 30× solar metallicity atmosphere in thermochemical equilibrium (black), as well as two models (red and blue) with abundances taken directly from the “red model” and “blue model” in Table 2 of Stevenson et al. (2010). These mixing ratios are somewhat depleted in water, strongly depleted in methane, and CO and CO2 rich compared to our equilibrium calculations. In all cases, we include the atomic sodium and potassium abundances derived from the equilibrium model. For the three chemistry cases, we use two different P–T profiles. In the upper panel, a hotter “dayside average” profile (named “2 pi”), which simulates inefficient day night energy redistribution. The bottom panel uses a cooler planet-wide average profile (named “4 pi”; Fortney et al. e.g., 2005). The two P–T profiles are plotted in Figure 7. These models (which we will refer to as models “a”–“f”), as well as models discussed in the following sections, are described in Table 1. At the current time we do not investigate time-variable temperature structure or abundances. The only published model of the atmospheric dynamics of GJ 436b shows little variability (Lewis et al. 2010), and there is no observational evidence as yet. For the two P–T profile cases, we adjust the 10 bar radius of all models so that the radii align in the optical. The main chemical difference between the hotter and cooler profiles is that the hotter model yields a larger mixing ratio of Na and K, yielding stronger features in the optical. A structural difference is that the larger scale height in the warmer model leads to modestly larger changes in radius as a function of wavelength.

Compared to our equilibrium model, the two models from Stevenson et al. (2010; models “c”–“f” in Table 1) show considerably smaller radii in the near- and mid-infrared, which is predominantly due to the smaller mixing ratio of water. Therefore, a clear probe of the water mixing ratio is the near-IR radius, compared to the optical radius, where water vapor

![Figure 5. Cross-sections for the main equilibrium chemistry molecules at 10 mbar and 1500 K. NH3, CH4, H2O, CO, and CO2 are represented by the black, red, blue, green, and purple curves, respectively.](image-url)
3.2. Nonequilibrium Chemical Products: Absorption Features

Stevenson et al. (2010) and Madhusudhan & Seager (2010) suggested that there could be evidence for a very low CH₄ mixing ratio in the atmosphere of GJ 436b due to a combination of vertical mixing and photolysis of CH₄. However, they did not investigate how the methane-derived nonequilibrium chemical products may affect the spectra of the planet’s atmosphere. Recently, Zahnle et al. (2009a) have investigated nonequilibrium carbon for isothermal “warm Jupiter” atmospheres (800 < T < 1200 K) at a range of metallicities. These temperatures are similar to those suggested for GJ 436b. Zahnle et al. (2009a) find that methane is sustained at higher regions in the atmosphere, water is more stable, and OH and H₂ quickly combine to form H₂O and H. This effectively increases the C-to-O ratio leading to increased abundances of molecules such as HCN, C₂H₂, C₂H₄, and C₂H₆. Given the uncertainties in modeling this chemistry, and the wide range of atmosphere models that are consistent with the GJ 436b data to date, our next aim is to explore transmission spectra with a range of nonequilibrium chemical products, guided by the results of Zahnle et al. (2009a).

The cross-sections for these first generation products of methane, which are strong absorbers in the infrared, can be found in Figure 8. Data for C₂H₂, C₂H₄, and C₂H₆, which are likely incomplete, are from the HITRAN database, while that for HCN is from the calculations of Harris et al. (2008). The cross-sections are similar in magnitude to those of the equilibrium chemistry products (Figure 5). HCN and C₂H₂ have prominent features at 1.5, 3.3, 7, and 13 μm; C₂H₄ has a significant impact to absorption at 9.5 μm, but C₂H₆ has very little effect, with most of its opacity residing between 10 and 13 μm. In Figure 9 we explore transmission spectra including the opacities with these nonequilibrium products. We begin with model “e” from Table 1, also shown as the red model from the top panel of Figure 6. This model uses a dayside average P–T profile with the same best-fit mixing ratios as the “red model” from Table 2 of Stevenson et al. (2010).

In addition to the original parameters of model “e,” we include absorption from HCN, C₂H₂, C₂H₄, and C₂H₆, with mixing ratios of $1 \times 10^{-3}$, $1 \times 10^{-4}$, $1 \times 10^{-5}$, and $1 \times 10^{-8}$ respectively, shown as the cyan model in Figure 9 (model “g” from Table 1). We derive these chemical abundances based on Zahnle et al. (2009a), where they depict mixing ratios as a function of height and $K_{zz}$ (eddy diffusion coefficient) for an atmosphere at 1000 K. The mixing ratios chosen are similar to what is expected for an atmosphere that is vigorously mixing ($K_{zz} = 10^{11}$).

It is worthwhile to explore some variations on this model. One variation removes the blanketing effects of hydrogen cyanide (HCN), shown in purple (model “h” from Table 1). This model illustrates the difference in the width of the features at 3.3, 7, and 13 μm, where HCN and C₂H₂ have overlapping opacity. When the features are thick, they are dominated by HCN opacity. When we remove HCN, we see thinner features, indicating that C₂H₂ dominates over HCN. This characteristic may allow further constraints on the mixing ratios of cool transiting planet atmospheres. In green is a model with these nonequilibrium products:

H₂O and H. This effectively increases the C-to-O ratio leading to increased abundances of molecules such as HCN, C₂H₂, C₂H₄, and C₂H₆. Given the uncertainties in modeling this chemistry, and the wide range of atmosphere models that are consistent with the GJ 436b data to date, our next aim is to explore transmission spectra with a range of nonequilibrium chemical products, guided by the results of Zahnle et al. (2009a).
products absent at pressures below 10 mbar (model “i” from Table 1). The green model illustrates the condition of modest vertical mixing, with \( K_z \) on the order of \( 10^6 \text{ cm}^2 \text{s}^{-1} \), similar to that favored by Madhusudhan & Seager (2010). In this case, nonequilibrium products are not stable higher in the atmosphere than the \( \sim 10 \text{ mbar} \) pressure level (Zahnle et al. 2009a). The main absorption features in the infrared will be weakened, as the green model confirms. The strength of these features could be constraints on vertical mixing and \( K_z \).

Absorption from these nonequilibrium products may mask features that would otherwise show an underabundance of water in the transmission spectrum, as Figure 9 shows. The red model, which generally shows smaller radii in the near- and mid-IR than in the optical, instead shows significantly larger radii when the nonequilibrium products are introduced. Spectroscopy, rather than photometry, will be key toward disentangling the effects of various molecules on the transmission spectrum.

### 3.3. Comparison with Data

In Figure 10, we explore model fits to recent Spitzer IRAC data for 3.6, 4.5, and 8 \( \mu \text{m} \) (Beaulieu et al. 2010), as well as data from EPOXI in the 0.35–1.0 \( \mu \text{m} \) range (Ballard et al. 2010), \( \text{HST NICMOS} \) in the 1.1–1.9 \( \mu \text{m} \) range (Pont et al. 2009), ground-based \( H \) band (Alonso et al. 2008), and ground-based \( K \) band (Cáceres et al. 2009). We plot our models in high resolution, and as band averages, where appropriate. Looking at the optical and near infrared, the best match is to the model that uses abundances from equilibrium chemistry, shown in gray (model “a” from Table 1).

In the mid-infrared, for the Spitzer IRAC data we see the same trend that we found in Fortney et al. (2010): in comparison to Beaulieu et al. (2008) data for HD 189733b and to Beaulieu et al. (2009) data for HD 209458b, our models cannot match the larger amplitude of the features—the implied dramatic change in absorption depth as a function of wavelength. The models of G. Tinetti and collaborators, used in the Beaulieu et al. (2010) paper, do fit the observation reasonably well. However, as discussed in Section 2.3, we find that the Tinetti et al. models overestimate the amplitude of absorption features.

It is clear that our models do not agree with the large peak to trough variation of spectra required by Beaulieu et al. (2010) to fit their data. If the methods employed by Beaulieu et al. (2008, 2009, 2010) are correct, and the error bars are underestimated, the results for all of these planets imply that dramatic revisions to models of these atmospheres are needed. Given the uncertainties in the reduction of IRAC transit data, it may be up to JWST to confirm speculations about the molecules present at the terminator of GJ 436b.

### Table 1

| Model | Profile | H₂O | CH₄ | CO | CO₂ | HCN | C₂H₂ | C₂H₄ | C₂H₆ |
|-------|---------|-----|-----|----|-----|-----|------|------|------|
| a     | 2pi     |     |     |    |     | 30× Solar |     |      |      |
| b     | 4pi     |     |     |    |     | 30× Solar |     |      |      |
| c     | 2pi     | \( 1 \times 10^{-4} \) | \( 1 \times 10^{-7} \) | \( 1 \times 10^{-4} \) | \( 1 \times 10^{-6} \) | \( \cdots \) | \( \cdots \) | \( \cdots \) | \( \cdots \) |
| d     | 4pi     | \( 1 \times 10^{-4} \) | \( 1 \times 10^{-7} \) | \( 1 \times 10^{-4} \) | \( 1 \times 10^{-6} \) | \( \cdots \) | \( \cdots \) | \( \cdots \) | \( \cdots \) |
| e     | 2pi     | \( 3 \times 10^{-6} \) | \( 1 \times 10^{-7} \) | \( 7 \times 10^{-4} \) | \( 1 \times 10^{-7} \) | \( \cdots \) | \( \cdots \) | \( \cdots \) | \( \cdots \) |
| f     | 4pi     | \( 3 \times 10^{-6} \) | \( 1 \times 10^{-7} \) | \( 7 \times 10^{-4} \) | \( 1 \times 10^{-7} \) | \( \cdots \) | \( \cdots \) | \( \cdots \) | \( \cdots \) |
| g     | 2pi     | \( 3 \times 10^{-6} \) | \( 1 \times 10^{-7} \) | \( 7 \times 10^{-4} \) | \( 1 \times 10^{-7} \) | \( 1 \times 10^{-4} \) | \( 1 \times 10^{-5} \) | \( 1 \times 10^{-3} \) | \( 1 \times 10^{-8} \) |
| h     | 2pi     | \( 3 \times 10^{-6} \) | \( 1 \times 10^{-7} \) | \( 7 \times 10^{-4} \) | \( 1 \times 10^{-7} \) | \( \cdots \) | \( 1 \times 10^{-5} \) | \( 1 \times 10^{-3} \) | \( 1 \times 10^{-8} \) |
| i     | 2pi     | \( 3 \times 10^{-6} \) | \( 1 \times 10^{-7} \) | \( 7 \times 10^{-4} \) | \( 1 \times 10^{-7} \) | \( \cdots \) & \( \cdots \) | \( \cdots \) | \( \cdots \) | \( \cdots \) | Same as g, but absent at \( P < 10 \text{ mbar} \)
4. PROSPECTS FOR JWST FOR GJ 436

We now evaluate the observability of the differences in the GJ 436b models by comparing them through the eyes of JWST. We have developed a code that simulates JWST spectra by computing the number of photons detected using a model of the host star, a transmission model of the planet, and estimates of the total efficiency (detected electrons per incident photon) at each wavelength for the various JWST dispersive spectroscopic modes. Noise is also modeled and added to the simulated spectra.

The star GJ 436 is relatively bright over the 0.7–5 μm spectral range, and the transmission models predict that GJ 436b will have absorption features from many species over this wavelength range. Therefore, we illustrate the model similarities and differences with simulations of JWST observations using the NIRSpec $R \equiv \lambda/\delta\lambda \sim 100$ spectroscopic mode over this spectral range. The double-pass CaF$_2$ prism used in this mode provides spectroscopic resolution varying from $R \approx 30$ at $\lambda \sim 1.2$ μm to $R > 200$ at $\lambda > 4.3$ μm. We approximate this with a fourth-order polynomial fit over the 0.7–5 μm range, and we assume that the prism has total transmission efficiency of 0.81 after two passes. We estimate that the optical efficiency of NIRSpec’s 14 reflective surfaces (te Plate et al. 2005) is approximately 0.58 over $\lambda = 1–5$ μm, consistent with the values calculated by the NIRSpec team (P. Jakobsen, private communication 2003) and assumed by Deming et al. (2009) after removing the grating blaze function. We adopt a quantum efficiency of 0.75 across the entire $\lambda = 1–5$ μm spectral range, consistent with the NIRSpec detector requirements (Rauscher et al. 2007). The telescope is estimated to have total reflectivity of 0.9 across this wavelength range. Total efficiency was modeled to decrease linearly by a factor of two as wavelength decreases from 1.0 to 0.7 μm, driven mostly by reduction in reflectivity in the 14 reflective NIRSpec surfaces.

Like Deming et al. (2009), we assume there will be no losses from the 1/6 wide entrance slit and that the only significant noise sources are photon noise and systematic noise due to small guiding errors during exposures. Photon noise is simulated by adding Poisson noise appropriate for the number of detected photo-electrons in each resolution bin. We adopt the systematic noise value of $5 \times 10^{-5}$ estimated by Deming et al. (2009). We do assume that this noise is Gaussian in its distribution although Deming et al. (2009) found that it was somewhat non-Gaussian. Even with high precision JWST instruments, we will suffer systematic noise at these modest but significant levels. In the “1 − (in-transit/star)” computation, any additional natural or instrumental noise occurring at frequencies greater than the inverse of the transit observation period will impact the extracted spectrum. This simulation program was coded in C, and it uses the public domain RANLIB package for simulating photon noise and Gaussian systematic noise.

A high-fidelity stellar model of the GJ 436 host star was not readily available, so we used a model of GJ 411 which has M2 V spectral type, similar to the M2.5 V type of GJ 436. Using our simulation code, we re-binned the Kurucz (2009) $R = 1000$ model of GJ 411 to the instrumental resolution of the JWST NIRSpec prism at each wavelength interval over $\lambda = 0.7–5$ μm. Next, our code computed the number of stellar photons from this binned flux, reducing it by the ratio of the squared model planet radius divided by the squared stellar radius (assumed to be $3.2 \times 10^{10}$ cm) at each wavelength. We used a distance of 10.2 pc to GJ 436 and an integration time of 1800 s for these calculations. This integration time is ∼33% shorter than the 2740 s duration of the transit (Pont et al. 2009). We used the resultant simulated in-transit spectrum and the simulated stellar spectrum of equal integration time to compute the absorption depth at each wavelength, $1 − (\text{in-transit/star})$. This is plotted for GJ 436b models in Figure 11.

Models “a,” “c,” and “e” (shown in black, blue, and red respectively) are plotted in the top panel of Figure 11. These are JWST simulations of the models in the top panel of Figure 6. Models “e,” “g,” “h,” and “i” are plotted in the bottom panel in red, purple, cyan and green respectively, and are JWST simulations of the models in Figure 9. The absorption features are labeled here for clarity. In particular, in the top panel the differences between the water rich model (black) and water poor models (red and blue) are readily apparent, as is the strong CO$_2$ feature at 4.3 μm and CO feature at 4.5 μm. In the bottom panel, the absorption features due to nonequilibrium HCN and C$_2$H$_2$ are clearly apparent, as is CH$_4$ absorption from 3–4 μm. The prospects for detailed characterization of this planet and others with JWST are good.

Given the high brightness of GJ 436b ($K = 6.1$ or $K_{AB} = 7.9$ mag), it is likely that its observation will require use of a detector subarray that is smaller in the dispersion direction than the ∼350 pixel length of the complete 0.6–5 μm $R \sim 100$ spectrum (Turnlinson 2008). Therefore, we find that acquiring the entire spectrum shown at the signal-to-noise in Figure 11 may require two or three transits. These observations may be best acquired in the higher resolution $R = 1000$ mode for stars as bright as GJ 436.

At $\lambda = 5–10$ μm MIRI LRS ($R \sim 100$) observations were also simulated for these models in a similar fashion using details of LRS models and actual measured performance. These simulations are shown in Figure 12 and are another independent way of looking at the effects of nonequilibrium chemistry in the atmosphere of GJ 436b. In the top panel (models “a,” “c,” and “e” are shown as black, blue, and red, respectively), water is the main opacity source in this wavelength range. The bottom panel (showing models “e,” “g,” “h,” and “i” as red, purple, cyan, and green, respectively) shows the clear distinction of HCN and C$_2$H$_2$ between the different models shown at 7 μm. Absorption
Figure 12. Simulated JWST MIRI LRS observations of the absorption depth of the transiting planet GJ 436b relative to its host star at each wavelength. Models “a,” “c,” and “e” are shown in black, blue, and red, respectively. Models “g,” “h,” and “i” are shown in red, purple, cyan, and green, respectively. In the top panel, water is the main absorber in this wavelength range. In the bottom panel, HCN and C$_2$H$_2$ features are labeled at 7 μm, and C$_2$H$_2$ absorption is labeled at 9.5 μm for clarity.

(A color version of this figure is available in the online journal.)

from C$_2$H$_4$ is shown at 9.5 μm as well. Observations using MIRI will be the only way to probe the 9.5 μm feature created by the presence of C$_2$H$_4$. The simulations were also made for a total integration time of 30 minutes in transit and 30 minutes on the star. The flux of GJ 436 is less than 1 Jy over this wavelength range, faint enough for its entire $\lambda = 5–10$ μm spectrum to be acquired simultaneously, which is an advantage MIRI will have over NIRSpec observations that require multiple transits to obtain the full spectrum.

The noise included in the spectral simulations and shown in Figures 11 and 12 are likely lower limits to the actual noise recorded in JWST spectra. Common-mode low-frequency noises due to the observatory will likely be eliminated by the differential measurement of the star and planet. All data for the simulated spectra shown are obtained on timescales of 2–3 eclipses, so any global variation in the star on longer timescales (i.e., subsequent transits or eclipses) will also be removed. Variation of the planet between transits will be recorded, and this could, in principle, limit the usefulness of co-adding multiple spectra. Variations in the JWST instrumentation, the host star, or the planet on timescales shorter than 2–3 transit or eclipse events will appear in the data as systematic or random noise. Nevertheless, we expect that JWST should be able to obtain high signal-to-noise exoplanet spectra given that Spitzer was able to obtain signal-to-noise approaching 10$^4$ (e.g., Machacek et al. 2010, and references therein) with its older detectors, about a factor of two less than we predict for the systematic noise of JWST.

5. DISCUSSION AND CONCLUSIONS

We have explored possible transmission spectra of GJ 436b, including nonequilibrium chemical products (due to mixing and photochemistry) a self-consistent code is needed. This would ensure that the molecular mixing ratios, and their impact on opacities, are consistent with the atmospheric P–T profile. This alone is difficult, but should be addressed in the future. In principle, all of this should be done in a three-dimensional model. Perhaps someday exquisite observations will warrant such a treatment. Clearly JWST will be an effective tool for reducing the underconstrained nature of current models, yet the brightness of GJ 436 may be a limitation. The NIRSpec prism mode will be able to observe a larger spectral range at high signal-to-noise with fewer transits for planets orbiting stars that are relatively dimmer than GJ 436. This issue, however, does not pertain to obtaining spectra in the 5–10 μm range using the MIRI LRS. This study is the first in a series of papers that will investigate models of transmission and emission spectra of transiting planets, convolved with our realistic model of JWST observations. For a complementary approach over a large phase space of JWST exoplanet observations, see Belu et al. (2010).

The model-dependent nature of our understanding of the composition and structure of exoplanet atmospheres ensures that it will always be useful to refine atmosphere models. Thus developing, scrutinizing, and refining these models brings us closer order hydrocarbons for close-in giant planet atmosphere models. Specifically, we have included absorption from HCN, C$_2$H$_2$, C$_2$H$_4$, and C$_2$H$_6$. The special condition that favors production of these molecules the most is the relatively low temperatures found in this planet.

HST and Spitzer may be limited in the capabilities needed to observe this planet’s transmission spectrum. The Pont et al. (2009) near-IR spectrum from Hubble suffered from instrumental systematics that could not be overcome. Reduction of Spitzer IRAC transit data suffers from the problem that different groups reducing the same data sets achieve different results, with errors bars that do not overlap (Beaulieu et al. 2008; Désert et al. 2009). Transit depths observed at different epochs allow for stellar variability to complicate the interpretation. These observations are extremely challenging, such that many results for GJ 436b, and many of the transiting planets, must be regarded as provisional.

We have shown that JWST should be able to make important breakthroughs in answering questions about the chemical mixing ratios in the planet’s atmosphere. Specifically, the presence of higher-order hydrocarbons in the transmission spectrum of this planet would reinforce the recent claim of non-detection of methane in the emission spectrum. We also may be able to constrain the composition and structure at the planetary limb. If hydrocarbon chemistry is present, it will be possible to constrain the abundances of these species. For example, HCN and C$_2$H$_2$ have strong absorption overlapping at 1.5, 3.3, 7, and 13 μm. The thickness of the feature in each wavelength region will tell us which molecule is more abundant in the atmosphere. When there is minimal HCN, the signature of C$_2$H$_2$ in these wavelength regions will be characteristically thinner. This phenomenon is depicted for JWST’s NIRSpec in the lower panel of Figure 11 for the 1.5 and 3.3 μm features as well as for the MIRI LRS in the lower panel of Figure 12 at 7 μm. The strength of the features in the infrared produced by these hydrocarbons may also be instrumental in constraining information regarding atmospheric mixing. Weak features may indicate a small eddy diffusion coefficient ($K_{zz}$), providing weak vertical mixing in the planet’s atmosphere, with these molecules forming at higher pressure levels.

In order to produce accurate model spectra of an exoplanet, including nonequilibrium chemical products (due to mixing and photochemistry) a self-consistent code is needed. This would ensure that the molecular mixing ratios, and their impact on opacities, are consistent with the atmospheric P–T profile. This alone is difficult, but should be addressed in the future. In principle, all of this should be done in a three-dimensional model. Perhaps someday exquisite observations will warrant such a treatment. Clearly JWST will be an effective tool for reducing the underconstrained nature of current models, yet the brightness of GJ 436 may be a limitation. The NIRSpec prism mode will be able to observe a larger spectral range at high signal-to-noise with fewer transits for planets orbiting stars that are relatively dimmer than GJ 436. This issue, however, does not pertain to obtaining spectra in the 5–10 μm range using the MIRI LRS. This study is the first in a series of papers that will investigate models of transmission and emission spectra of transiting planets, convolved with our realistic model of JWST observations. For a complementary approach over a large phase space of JWST exoplanet observations, see Belu et al. (2010).
to the true nature of these planets. In Section 2, we validated our model against analytic relations, but found that a similar Tinetti et al. model could not match these same relations. Recent work on including nonequilibrium and photophysical products (Li et al. 2004; Zahnle et al. 2009a, 2009b) will yield better predictions of chemical mixing ratios. Transmission spectrum models that incorporate the full three-dimensional nature of the planetary atmosphere, which is particularly important at the terminator region (Fortney et al. 2010; Burrows et al. 2010), will yield a more accurate understanding of the temperature structure and chemical abundances. The conditions of GJ 436b coupled with JWST will provide the chance to explore the possibility of a compositionally complicated atmosphere in great detail, expanding our knowledge of planets as unique to their particular circumstance.

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