Coupled Thermal and Compositional Evolution of Photoevaporating Planet Envelopes

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Abstract

Photoevaporative mass loss sculpts the atmospheric evolution of tightly orbiting sub-Neptune-mass exoplanets. To date, models of the mass loss from warm Neptunes have assumed that the atmospheric abundances remain constant throughout the planet’s evolution. However, the cumulative effects of billions of years of escape modulated by diffusive separation and preferential loss of hydrogen can lead to planetary envelopes that are enhanced in helium and metals relative to hydrogen. We have performed the first self-consistent calculations of the coupled thermal, mass-loss, and compositional evolution of hydrogen–helium envelopes surrounding sub-Neptune-mass planets. We extended the Modules for Experiments in Stellar Astrophysics stellar evolution code to model the evolving envelope abundances of photoevaporating planets. We demonstrate that H–He fractionation can lead to planetary envelopes that are significantly enriched in helium and metals compared to their initial primordial compositions. A subset of our model planets—having $R_p \lesssim 3.00\, R_\oplus$, initial $f_{\rm env} < 0.5\%$, and irradiation flux $\sim 10^3–10^4$ times that of Earth—obtain final helium mass fractions in excess of $Y = 0.40$ after several billion years of mass loss. GJ 436b, the planet that originally inspired Hu et al. to propose the formation of helium-enhanced planetary atmospheres, requires a primordial envelope that is too massive to become helium enhanced. Planets with envelope helium fractions of $Y = 0.40$ have radii that are between 0.5% and 10% smaller (depending on their mass, irradiation flux, and envelope mass fraction) than similar planets with solar composition ($Y = 0.24$) envelopes. The results of preferential loss of hydrogen may have observable consequences for the $M_p – R_p$ relations and atmospheric spectra of sub-Neptune populations.

Unified Astronomy Thesaurus concepts: Exoplanet astronomy (486); Exoplanet evolution (491); Atmospheric effects (113); Exoplanet atmospheres (487); Planetary atmospheres (1244); Exoplanet atmospheric variability (2020); Exoplanet atmosphere composition (2021)

1. Introduction

No solar system analogs exist for the thousands of tightly orbiting sub-Neptune-mass exoplanets discovered, inspiring recent work about the nature of these planets (e.g., Howard et al. 2012; Fulton et al. 2017; Johnson et al. 2017). In recent years, observational work combined with theoretical formation and evolution models have shown the incredible diversity possible in this planetary population. Mass–radius ($M_p–R_p$) measurements and statistical analyses provide evidence that many of these planets have an envelope of light gases, increasing their observed radii (Marcy et al. 2014; Rogers 2015). A large portion of these planets are tightly orbiting (with orbits interior to 0.25 au) and have masses between 1 and 25 $M_\oplus$ (Borucki et al. 2011; Rowe et al. 2015; Mulders et al. 2016). Throughout this work, we refer to warm Neptunes and sub-Neptunes as planets with masses below 25.0 $M_\oplus$ and orbits interior to 1.0 au.

A key to understanding exoplanet demographics lies in analyzing the interplay between a planet’s H/He envelope and incident irradiation in the evolution of these tightly orbiting sub-Neptune-mass planets. Evolution and structure models have constrained the $M_p–R_p$ relations for low-density exoplanets, and have shown that the presence of a volatile envelope can greatly inflate a planet’s radius (Rogers et al. 2011). Lopez & Fortney (2014) showed that changing the H/He envelope mass fraction of a planet has a dramatic effect on planetary radius, subsuming the smaller effects due to incident flux and planet age. Evaporative mass loss depletes the gas envelopes of sub-Neptune-size planets, significantly decreasing their radii (e.g., Valencia et al. 2010; Owen & Jackson 2012; Lopez & Fortney 2013; Howe et al. 2014; Chen & Rogers 2016).

Theoretical analyses predict that photoevaporation can shape the evolution of highly irradiated sub-Neptunes, bifurcating the population based on envelope retention (Lopez & Fortney 2013; Owen & Wu 2013; Owen 2019). Under the most intense irradiation, atmospheric “boil-off” creates planets with radii similar to the radius of their heavy-element (rocky or icy) cores. Under less extreme envelope erosion, planets retain a volatile envelope, and have subsequently larger radii. Owen & Wu (2017) predict that the photoevaporative process leaves a H/He envelope (for planets with final radii $>2.6\, R_\oplus$), or strips planets of their entire envelope (with radii of $\sim 1.3\, R_\oplus$) over the course of 100 Myr.

Observational surveys have shown the existence of a bimodal radius distribution of small planets similar to that predicted by the photoevaporation valley, with occurrence rates peaked at $R_p < 1.5\, R_\oplus$ and $2.0\, R_\oplus < R_p < 3.0\, R_\oplus$ (Fulton et al. 2017). Lundkvist et al. (2016) find no exoplanets with radii between 2.2 and 3.8 $R_\oplus$ that have incident flux rates greater than 650 times that of Earth. Furthermore, a few sub-Neptune planets have been discovered with orbital periods below 2–4 days, indicating a desert of ultra-irradiated sub-Neptune-mass exoplanets (Benítez-Llambay et al. 2011; Beaugé & Nesvorný 2013; Mazeh et al. 2016).

Theories of how atmospheric erosion is shaping exoplanet populations are becoming increasingly important to interpret observational results. To date, most mini-Neptune interior structure
models have assumed solar H/He mass ratios (e.g., Valencia et al. 2007; Lopez & Fortney 2014; Howe & Burrows 2015; Chen & Rogers 2016). Additionally, models of photoevaporation (e.g., Sanz-Forcada et al. 2011; Lopez & Fortney 2013; Owen & Wu 2013, 2017; Lehmer & Catling 2017) have assumed that envelope composition stays constant over time, and that planets lose hydrogen, helium, and metals in the same proportions as they are present in their envelopes.

Preferential loss of light gases can cause planets to become enhanced in helium and metals relative to hydrogen over the course of billions of years. Hu et al. (2015) have proposed that H/He fractionation and envelope mass loss creates planets with orders-of-magnitude reductions in atmospheric hydrogen. Stellar extreme ultraviolet (EUV) radiation causes hydrodynamic outflow of atmospheric gases, with mass flux proportional to the mean molecular mass of each gas. For helium enhancement, planets must have relatively small initial envelope mass fractions ($\sim 10^{-3}$). Basing their model on previous interior structure models (Nettelmann et al. 2010), Hu et al. (2015) proposed that helium enhancement could explain the lack of CH$_4$ in GJ 436b’s emission spectrum. Although Hu et al. (2015) modeled the time-varying composition of planet envelopes, they did not couple this to a model of the interior structure of the planet and its thermal and radius evolution.

In this paper, we develop novel methods for modeling coupled thermal and compositional evolution in warm Neptunes. First, we analyze the effect of varying the envelope fraction of the interior structure and radius of exoplanet populations. We create $M_p$–$R_p$ relations with a range of initial envelope mass fractions and helium fractions. Second, we develop the first simulations of the coupled thermal, mass-loss, and envelope composition evolution of exoplanets. Third, we test the mechanism of mass loss proposed by Hu et al. (2015) with GJ 436b to determine whether it is a candidate for helium enhancement.

We present our methodology for creating planetary models with the code Modules for Experiments in Stellar Astrophysics (MESA) in Section 2. In Section 3 we describe the results of simulations of atmospheric structure and envelope mass loss. In Section 4 we discuss the effects of coupled thermal, mass-loss, and envelope composition evolution. Finally, results and conclusions are given in Section 4.5.

2. Methods

We use the code MESA (Paxton et al. 2011, 2013, 2015, 2018), an open-source Fortran library for stellar evolution, to model the evolutionary pathways of exoplanets. We specifically use MESA version 10.398. Multiple studies have already applied MESA to exoplanets with H/He-dominated envelopes (e.g., Valsecchi et al. 2015; Buhler et al. 2016; Chen & Rogers 2016; Owen & Wu 2016; Jackson et al. 2017), but all have so far assumed that the composition of the planet’s envelope (specifically, the hydrogen mass fraction, $X$, helium mass fraction $Y$, and heavy-element mass fraction, $Z$) remains constant throughout time.

We extend MESA to simulate the compositional evolution of Neptune-size and sub-Neptune-size planet envelopes undergoing atmospheric escape. Our models build upon the MESA test suites irradiated_planet and make_planets, and the previous sub-Neptune planet modeling approach from Chen & Rogers (2016). We have further standardized the procedures for creating initial planet models with varied envelope compositions (Section 2.1), updated the treatment of the irradiation on the planet to include physical opacities (Section 2.2), and implemented the mass-loss prescription from Hu et al. (2015; Section 2.3). We elaborate upon each of these new developments below.

2.1. Creating Planetary Models with MESA

Our simulations are split into two distinct stages. First, we bring an initial planetary model through a series of iterative steps that gradually relax its properties until the desired initial conditions (planet mass, $M_p$, core mass, $M_{\text{core}}$, envelope composition, $X$, $Y$, $Z$, initial entropy, $S$, and irradiation flux, $F_i$) are attained. MESA natively models stars; creating starting models for Earth-mass-scale planets is nontrivial. After the initial model is brought to the desired starting conditions, the planet is evolved for several billion years. It is in this second stage that the adjustments to the planet model from one time step to the next encapsulate the physics of planetary thermal evolution and mass loss.

Although we base our procedure for creating initial planet models on the procedure outlined in Chen & Rogers (2016), we have made substantial adjustments to improve stability and to model planets across a wider parameter space. Compared to Chen & Rogers (2016), we iterate back and forth through several rounds of planet mass reduction and heavy-element core insertion, until the desired $M_p$ and $M_{\text{core}}$ are reached. We also include functionality to adjust the planetary envelope composition and create planet-starting models with nonsolar atmospheric compositions.

Our procedure for creating each initial planet model follows the steps below.

1. First we load an initial planet profile—0.001M$_\odot$ from very_low_mass_gray_models.
2. The planet is reduced in mass to 166.50 $M_\oplus$ using relax_mass.
3. Next, a rocky core is inserted with a mass of 0.67 $M_\oplus$ using relax_core. As in Chen & Rogers (2016), we use the core mass–radius relations from Rogers et al. (2011) to specify the mean density of the heavy-element core. The model core from relax_core is inert. However, we use the time-varying core luminosity routine from Chen & Rogers (2016) in the final evolution stage.
4. We then reduce the planetary mass to 30 times its final mass. Adjusting the planetary mass and core mass in stages increases model stability.
5. Next, we relax the rocky core to 10% of the final core mass using relax_core.
6. At this point, we relax $X$, $Y$, and $Z$ to the initial envelope composition desired using relax_initial_X and relax_initial_Y.
7. Next, the model evolves in isolation for 10$^6$ yr to stabilize before we continue with the ensuing parameter adjustments.
8. We then further reduce the planetary mass to its final value of between 2.0 and 25.0 $M_\oplus$.
9. We increase the core mass to the ultimate value of $M_{\text{core}}$ desired (taking care to adjust the core density, as appropriate).
10. The next two steps aim to standardize the initial thermal state of the planets by setting the initial interior entropy,
S. If the planet’s central entropy at this point is lower than the target value, we add an artificial luminosity (using \texttt{relax\_initial\_L\_center}) to the core to reinflate the planet until the target $S$ is surpassed. If the planet’s central entropy is already higher than the target value, this step is skipped.

11. The artificial core luminosity is removed (if present), and the planet is allowed to cool until the desired initial entropy is reached (specified through \texttt{center\_entropy\_lower\_limit}).

12. At this point, we iteratively solve for the appropriate value for \texttt{column\_depth\_for\_irradiation} as described in Section 2.2, and then relax the stellar irradiation incident on the planet to the desired value, $F$, using \texttt{relax\_irradiation}.

13. Finally, the planet age is reset to zero, and we evolve the model for a short time (on the order of a few million years) without mass loss.

During the final step, we adopt a value for the heat capacity of the rocky core using the same routine as in Chen & Rogers (2016), and set $c_v$ to 1.0 J K$^{-1}$ g$^{-1}$ (Guillot et al. 1995). A routine for adding the luminosity from the heavy element irradiation incident on the planet to the desired value, $F$, is the \texttt{irradiation}.

After the steps above are complete, the initial model is ready for simulating the simultaneous thermal, mass-loss, and envelope composition evolution of the planet. Upon publication, scripts and inlists for creating initial planet models following our recipe will be made available on the MESA marketplace.

### 2.2. Irradiated Atmospheric Boundary Condition

We use MESA’s built-in $F_s - \Sigma_s$ surface heating (Paxton et al. 2013) to account for the irradiation incident on the planet from its host star. This heating function deposits the specified irradiation flux, $F_s$ (corresponding to \texttt{inlist option irradiation\_flux}), in the outer layers of the planet’s envelope down to the specified column depth, $\Sigma_s$ (corresponding to \texttt{inlist option column\_depth\_for\_irradiation}). Note that we take a different approach to the atmospheric boundary conditions for irradiated planets than Chen & Rogers (2016), who used a modified version of the MESA gray_\texttt{irradiated} atmospheric boundary condition. The dayside flux ($F_s$) absorbed by the planet is determined by the stellar effective temperature, $T_{\text{eff}}$, the planet’s orbital separation, $d$, and the planet’s Bond albedo, $A$,

$$F_s = \sigma T_{\text{eff}}^4 \left( \frac{R_p}{d} \right)^2 (1 - A).$$  

(1)

The planet’s equilibrium temperature, $T_{\text{eq}}$, is related to $F_s$ via

$$T_{\text{eq}} = \left( \frac{F_s}{4\pi\kappa_s} \right)^{\frac{1}{4}}.$$  

(2)

The extent to which stellar irradiation penetrates the envelope is governed by the atmospheric opacity, $\kappa_s$, to the incoming starlight,

$$\Sigma_s = 2/\kappa_s.$$  

(3)

We use gaseous mean opacities to incident stellar radiation from Freedman et al. (2014) to determine $\Sigma_s$, as elaborated below. This goes a step beyond past studies that have specified a constant (semi-arbitrary) value of $\Sigma_s$ (e.g., Valsecchi et al. 2015). Using tabulated opacities to determine $\Sigma_s$ allows a better modeling of how stellar optical radiation is absorbed in a planet’s atmosphere.

To determine $\Sigma_s$, we use the profile output from the MESA model generated at the end of step 11 (i.e., the model prior to irradiation). The profile output provides the variation of pressure, $P_i$, temperature, $T_i$, mass interior, $m_i$, and distance from the center, $r_i$, in each radial zone within the planet envelope (indexed by $i$). The mass column density, $\Sigma_i$, above the $i$th radial zone in the planet envelope is calculated from

$$\Sigma_{s,i} = \frac{m_i - m_{i-1}}{4\pi r_i^2},$$  

(4)

where $m_i$ is the total mass at the top of the atmosphere. Making the approximation that after the irradiation is applied to the model planet, the optically thin regions of the irradiated planet’s atmosphere will be nearly isothermal at a temperature of $T_{\text{eq}}$, we interpolate within the mean opacity tables of Freedman et al. (2014) with a blackbody weighting temperature of $T_{\text{eff}}$, and $[\text{M/H}] = 0$ to obtain $\kappa_{s,i}$ in each radial zone (i.e., at a pressure $P_i$ and temperature $T_{\text{eq}}$). $\Sigma_{s,i}$ is determined by solving for the zone at which Equation (3) is satisfied. If the intersection point is unresolved, we take the column depth at the outermost layer, using Equation (4). We find $\Sigma_i$ ranging from 10.0 to 100.0 cm$^2$ g$^{-1}$ with the majority of models around 20.0 cm$^2$ g$^{-1}$. We self-consistently determine an initial value of $\Sigma_s$, and then keep $\Sigma_s$ constant throughout the planet’s evolution. Future work could update $\Sigma_s$ in time as the planet evolves.

### 2.3. H/He Mass Loss

We implement the atmospheric mass-loss prescription of Hu et al. (2015) in MESA, using the \texttt{use\_other\_adjust\_mdot\_hook}. For the close-orbiting planets that we consider, mass loss is primarily driven by EUV radiation from the host star. Previous studies of planet mass loss with MESA have solely considered hydrodynamic escape wherein the escaping gas has the same composition as the planet’s envelope (so that the envelope composition does not vary in time). In contrast, following Hu et al. (2015), we account for diffusive separation of hydrogen and helium and preferential loss of hydrogen.

The planet’s energy-limited mass-loss rate, $\Phi_{\text{EL}}$ (with dimensions of mass per unit time), is given by

$$\Phi_{\text{EL}} = \frac{L_{\text{EUV}} \eta \mu^2 R_h^3}{4 K d^2 G M_p},$$  

(5)

(e.g., Lammer et al. 2003; Tian et al. 2005; Erkaev et al. 2007; Murray-Clay et al. 2009). In Equation (5), $L_{\text{EUV}}$ is the EUV luminosity of the host star, $\eta$ is the heating efficiency factor (i.e., the fraction of the EUV energy absorbed that goes into unbinding the outer layers of the planetary envelope). The factor $a$ is the ratio between the radius where EUV photons are absorbed and the planet’s homopause radius. We define the homopause radius as $R_{hp}$ and the planet-transit radius as $R_p$. We elaborate the calculation and application of $R_{hp}$ and $R_p$ in Section 2.4. Throughout this work we assume constant values for $\eta$ and $a$ of 0.10 and 1.0, respectively, following Hu et al. (2015). Finally, $K$ is a correction for the tidal effect of the planet’s Roche lobe.
The Roche potential reduction factor is calculated following Erkaev et al. (2007),
\[ K(\epsilon) = 1 - \frac{3}{2\epsilon} + \frac{1}{2\epsilon^3}, \]  
where
\[ \epsilon = \left( \frac{M_d}{3M_\star} \right)^{1/3} \frac{d}{R_\star}. \]  

To model the EUV luminosity of the host star, we adopt the empirical relation of Sanz-Forcada et al. (2011), who studied 80 stars with spectral types from M to F. They found that EUV luminosity is inversely proportional to the stellar age, 
\[ \log_{10}(L_{\text{EUV}}) = 22.12 - 1.24 \log_{10}(\tau). \]  

In Equation (8), \( \tau \) is expressed in units of Gyrs and \( L_{\text{EUV}} \) has units of J s\(^{-1}\).

The energy-limited escape rate (Equation (5)) overestimates mass loss because thermal and translational energy is carried away by escaping gas (Johnson et al. 2013). In the transonic regime, the reduction factor \( f_\epsilon \) is proportional to the ratio of the net EUV heating rate \( Q_{\text{net}} \) to the critical heating rate \( Q_\epsilon \). We adopt \( Q_{\text{net}} \) and \( Q_\epsilon \) from Hu et al. (2015),
\[ Q_{\text{net}} = \eta L_{\text{EUV}} R_\star^2, \]  
\[ Q_\epsilon = \frac{4\pi R_\star^2 \gamma U(R_\star)}{c_s \sigma T H m} \sqrt{\frac{2U(R_\star)}{\mu}}. \]

The collisional mean free path of a particle divided by the scale height \( ( \text{Knudsen number, } K_m) \), the heat capacity ratio of the atmosphere \( (\gamma) \), and the collisional cross section \( (c_s \sigma_\epsilon) \) are set to 1, 5/3, and \( 5 \times 10^{-20} \) m\(^2\), respectively (Johnson et al. 2013). Our assumption is that \( K_m = 1 \) holds as long as heat is absorbed throughout the atmospheric profile, interior to \( R_\star \). The reduction factor, \( f_\epsilon \), for transonic and subsonic escape flow is defined as

\[ f_\epsilon = \begin{cases} \frac{Q_\epsilon}{Q_{\text{net}}} \quad & \text{if } Q_{\text{net}} > Q_\epsilon, \\ 1 \quad & \text{else}. \end{cases} \]

We adjust the escape rate, \( \Phi \), to account for the reduction in mass loss relative to the energy-limited assumption,
\[ \Phi = f_\epsilon \Phi_{\text{DL}}. \]  

The mass escaping from the planet may be explicitly separated into its elemental constituents,
\[ \Phi = \Phi_{\text{H}} + \Phi_{\text{He}} = 4\pi R_\star^2 (\phi_{\text{H}} m_{\text{H}} + \phi_{\text{He}} m_{\text{He}}). \]  

where \( \phi_{\text{H}} \) and \( \phi_{\text{He}} \) represent the number fluxes (in particles per unit area per unit time), and \( m_{\text{H}} \) and \( m_{\text{He}} \) are the atomic masses of hydrogen and helium. Hydrogen is expected to be primarily in atomic (as opposed to molecular) form as it escapes. Equation (14) neglects escape of any elements heavier than helium. We return to this approximation in Section 4.

The diffusion-limited particle flux, \( \Phi_{\text{DL}} \), mediated by the momentum exchange between hydrogen and helium, from Hu et al. (2015) is
\[ \Phi_{\text{DL}} = \frac{GM_\star (m_{\text{He}} - m_{\text{H}}) b'}{R_\star^2 k T H}. \]  

where \( k \) is the Boltzmann constant, \( b' \) is the effective binary diffusion coefficient (accounting for the partial ionization of hydrogen), and \( T H \) is the temperature of the homopause. Following Hu et al. (2015), we use \( T H = 10^4 \) K as a conservative estimate of hydrogen–helium fractionation, resulting in a value of \( b' = 8.0 \times 10^{10} \) cm\(^{-1}\) s\(^{-1}\). The diffusion-limited escape rate determines the relative proportions of H and He that escape,
\[ \frac{\phi_{\text{He}}}{X_{\text{He}}} = \frac{\phi_{\text{H}}}{X_{\text{H}}} - \Phi_{\text{DL}}, \]  

where \( X_{\text{H}} \) and \( X_{\text{He}} \) represent the mixing ratios (number fractions) of H and He in the atmosphere.

Solving Equations (14) and (16), Hu et al. (2015) derived the following expressions for the hydrogen and helium mass-loss rates:

If \( \Phi \leq \Phi_{\text{DL}} X_{\text{H}} m_{\text{H}} 4\pi R_\star^2 \),
\[ \Phi_{\text{H}} = \Phi, \]  
\[ \Phi_{\text{He}} = 0. \]

If \( \Phi > \Phi_{\text{DL}} X_{\text{H}} m_{\text{H}} 4\pi R_\star^2 \),
\[ \Phi_{\text{H}} = \frac{\Phi m_{\text{H}} X_{\text{H}} + \Phi_{\text{DL}} m_{\text{He}} X_{\text{He}} X_{\text{He}} 4\pi R_\star^2}{m_{\text{H}} X_{\text{H}} + m_{\text{He}} X_{\text{He}}}, \]  
\[ \Phi_{\text{He}} = \frac{\Phi m_{\text{He}} X_{\text{He}} - \Phi_{\text{DL}} m_{\text{H}} X_{\text{H}} X_{\text{He}} 4\pi R_\star^2}{m_{\text{H}} X_{\text{H}} + m_{\text{He}} X_{\text{He}}}. \]

At each MESA time step (indexed by \( n \)), we store the envelope mass and abundance fractions. We adjust the planet mass through other_adjust_mdot in a custom run-star_extras file. However, other_adjust_mdot may be called multiple times before MESA finds an acceptable time step. In order to avoid multiple changes to the envelope abundances, we set abundance fractions in extrasFinishStep (in the same run_star_extras). This routine is only called at the end of each MESA step.

At the beginning of the \( n \)th step, H/He mass loss is calculated (according to Equations (17)–(20)), using a custom useOther_adjust_mdot. MESA then attempts to solve the model with these conditions. If MESA accepts the new model, the program proceeds to extrasFinishStep. Here, we adjust the atmospheric composition with the extrasFinishStep routine, setting atmospheric abundances through MESA’s composition variables \( xa(j, k) \) for each species and zone.

All MESA envelope models are composed of eight elemental species: \( ^1\text{H}, ^3\text{He}, ^4\text{He}, ^{12}\text{C}, ^{14}\text{N}, ^{16}\text{O}, ^{20}\text{Ne}, \) and \( ^{24}\text{Mg} \). We adjust the proportion of each species at each zone, in response to the hydrogen and helium lost by the planet at each time step \( dt \),
\[ X_n = \frac{M_{\text{env,n}} - X_{n-1} - (\Phi_{\text{H}} + \Phi_{\text{He}}) dt}{M_{\text{env},n-1} - (\Phi_{\text{He}} + \Phi_{\text{H}}) dt} \]  
\[ Y_n = \frac{M_{\text{env,n}} - Y_{n-1} - (\Phi_{\text{He}} + \Phi_{\text{H}}) dt}{M_{\text{env},n-1} - (\Phi_{\text{He}} + \Phi_{\text{H}}) dt} \]
where $Z_j$ is the mass fraction of the $j$th heavy element (i.e., heavier than $^4$He), $M_{\text{env}} = M_p - M_{\text{core}}$ is the total envelope mass, and the subscripts $n-1$ and $n$ refer to initial and final abundance fractions and envelope mass values for each step. The envelope mass is stored throughout a model step because new abundance fractions are calculated as part of extras\_finish\_step.

2.4. Planetary Radius

We define the planetary radius to be at 1.0 mbar. This is approximately the depth at which the atmosphere becomes optically thin, and it is useful as a benchmark transit radius (Miller et al. 2009). To calculate this, we extrapolate radially from the outermost zone in MESA, assuming a constant scale height. Generally, this increases the planetary radius by approximately 10%–20%. However, low-mass planets that are highly irradiated can have even larger differences between their transit radii and MESA’s outermost zone. The only exception in using 1.0 mbar as a radius definition is when we calculate mass-loss rates, as explained below.

Above the homopause, the H–He binary diffusion coefficient is greater than the eddy diffusion coefficient ($K_{z2}$) (Hu et al. 2012, 2015). For Equations (5)–(23) we defined the planetary radius as the homopause—the level in the atmospheres below which the constituent molecules are well mixed.

The binary mixing (molecular diffusion) coefficient between hydrogen and helium is (Fuller et al. 1966; Bird et al. 2007)

$$D_{\text{H,He}} = \frac{10^{-3}T_h^{1.75}}{P_h\left(\sum_{\text{He}} V_{\text{He}}\right)^{1/3} + \left(\sum_{\text{H}} V_{\text{H}}\right)^{1/3}}^{1/2},$$

where $P_h$ is the pressure at the homopause radius, and $V_{\text{H}}$ and $V_{\text{He}}$ are the atomic diffusion volumes (Fuller et al. 1966; O’Connell 1981; Tang et al. 2014).

Like the transit radius, the homopause is not resolved by the topmost zone of our MESA planet models. To calculate the planetary radius at the homopause, we thus extrapolate the atmospheric pressure profiles to lower pressures, assuming an isothermal temperature profile (appropriate to the outer radiative zones of these strongly irradiated planets). We find the scale height of the atmosphere using Equation (25). Equating $D_{\text{H,He}}$ and $K_{z2}$ determines the pressure level of the homopause, $P_h$, from which the radius at the homopause is estimated using Equation (26),

$$H = \frac{kT_{\text{eq}}}{\mu g},$$

$$P_h = \frac{1}{2} Pe^{2\pi},$$

where $g$ is the surface gravity, $\mu$ is the mean molecular mass of the atmosphere, $P_1$ is the pressure at the outermost profile zone, and $Z$ is the radius above the outermost zone. We use the value of the scale height at MESA’s outermost zone and extrapolate using constant values for $g$ and $\mu$.

We find that the homopause typically adds between 5% and 25% to the planetary radius, decreasing as the planet cools and contracts. In the more extreme cases, the homopause could be approximately 50% larger than the planetary transit radius. The large variability comes from the most extreme of our models, subject to the most intense irradiation with the lowest surface gravity. For planets with masses above 15.0 $M_\oplus$, the homopause is typically 20% larger than the transit radius. Below the homopause, the atmosphere is well mixed, and the species’ mass fractions are constant with depth.

The surface boundary conditions for our MESA models are set through atm\_option and atm\_T\_tau\_relation (Paxton et al. 2015). We take the default control option of a simple gray Eddington boundary condition. These specify a set of temperature and pressure conditions for the outermost zone in MESA. However, different surface boundary conditions may be useful in subsequent work.

2.5. Default Parameters

Unless otherwise specified, we consider planets orbiting Sun-twin host stars (with $M_\ast = M_\odot$, $R_\ast = R_\odot$, and $T_{\text{eff,\ast}} = 6000$ K). In our GJ 436b case study, however, we adjust the host star properties to those of GJ 436 (see Section 3.4).

In all the simulations presented herein, we specified an initial entropy of

$$S = 7.0 + \frac{M_p}{25.0 M_\oplus} \frac{k_B}{\text{baryon}} (27)$$

and allow the planet to evolve for $6 \times 10^9$ yr before applying atmospheric mass loss. Unless otherwise specified, we initialize our planets with solar composition envelopes ($X = 0.74$, $Y = 0.24$, $Z = 0.02$). In determining $\kappa_\ast$ and $\Sigma_\ast$, we take the opacity table from Freedman et al. (2014) for [M/H] = 0. We adopt a Bond albedo of $A = 0.2$ to relate $F_\ast$ and orbital separation $d$, and set $K_{z2}$ to $10^9$ cm$^2$ s$^{-1}$ throughout.

3. Results

3.1. Helium Fraction Dependent Mass–Radius Relations

We present the first planet mass–radius ($M_p$–$R_p$) relationships that quantify the effect of the envelope helium mass fraction, $Y$, on planetary radii (Figure 1). To create the $M_p$–$R_p$ relations, we evolved models for 10 Gyr over a range of orbital separations (from $d = 0.1$ to 0.5 au), envelope mass fractions ($f_{\text{env}} = M_{\text{env}}/M_p = 0.005$–0.20), and helium fractions ($Y = 0.18$–0.40).

Variations in atmospheric helium mass fraction have a significant effect on planet radius. For planets exterior to 0.20 au, the effect of $Y$ on the planetary radii is second only to the effect of $f_{\text{env}}$ (within the parameter range explored). For two similar models (at $M_p = 10.0 M_\oplus$, $f_{\text{env}} = 0.05$, and $d = 0.20$ au), we find that a planet with $Y = 0.40$ had a 9.11% smaller radius than a planet with $Y = 0.24$ (3.69 $R_\oplus$, compared to 4.06 $R_\oplus$) after 10 Gyr. The stronger the irradiation and the larger $f_{\text{env}}$, the greater the effect of $Y$ on the planetary radius because the envelope contributes a larger overall fraction to the total planet radius.

$Y$ influences the planetary radii in Figure 1 at a level that may be detected by transit surveys. In the era of Gaia, planet-transit radii may be commonly determined to ~3% (Stassun et al. 2017). Figure 1 shows that across a wide range of $d$, $f_{\text{env}}$, and $M_p$, planets with an atmospheric helium fraction of $Y = 0.40$ are between 0.5% and 10% smaller than similar planets with a solar composition ($Y = 0.24$). Differences in helium content should not be discounted when considering radius
measurements, and they present an additional dimension of planetary compositional diversity that to date has largely been neglected.

We note that atmospheric escape will not increase the ratio of hydrogen relative to helium in primordial planetary envelopes. However, other atmospheric sources such as outgassing and cometary delivery of volatiles will preferentially contribute hydrogen and not helium (e.g., Elkins-Tanton & Seager 2008; Rogers & Seager 2010; Rogers et al. 2011). Although this is not the primary emphasis of this paper, we include models with $Y = 0.18$ in Figure 1 to highlight how, in theory, a decrease in the helium mass fraction below solar proportions would affect the $M_p - R_p$ relations. In Section 3.3 we investigate the range of planetary configurations (mass, envelope composition, and envelope mass fraction) that can be achieved by escape from initially solar composition primordial envelopes.

3.2. Effect of Helium on the Envelope $P-T$ Structure

Physically, the helium mass fraction has multiple effects on the interior structure of a planet’s envelope that in turn affect the planet’s transit radius. Figure 2 presents atmospheric pressure-temperature ($P-T$) profiles for planets having various values of $Y$.

The higher the concentration of helium in a planet’s envelope, the higher the mean molecular weight (for a given envelope metallicity, $Z$). As a result, helium-enhanced planets have smaller atmospheric scale heights (Equation (25)) and smaller radii (as observed in Figure 1).

Changing the relative mass fractions of hydrogen and helium also affects the adiabatic temperature gradient in the convection zones of planetary envelopes because hydrogen has a higher heat capacity than helium. Based on the Saumon et al. (1995) equations of state, the specific heat capacity (per unit mass), $c_P$, of hydrogen is 2.7–5.6 times higher than that of helium at pressures of $10^5$–$10^{10}$ Pa and temperatures of $10^{2.5}$–$10^{3.3}$ K. Molecular dissociation of hydrogen begins at $\sim$2500 K, further increasing the specific heat capacity of hydrogen to as much as 50 times that of helium. However, the majority of our atmospheric profiles do not encounter temperatures this high. The adiabatic temperature gradient depends on the heat capacity as in Equation (28),

$$\left(\frac{dT}{dP}\right)_S = \frac{\alpha_v T}{\rho c_P},$$

where $\rho$ is the density, and $\alpha_v = 1/v(\partial v/\partial T)_p$ is the coefficient of thermal expansion. The lower heat capacities of hydrogen-depleted and helium-enhanced envelopes in turn lead to steeper temperature gradients in their convecting regions (i.e., with larger changes in temperature with pressure) than in envelopes with solar hydrogen-to-helium ratios. For example, in two $M_p = 10.0\ M_\oplus$, $d = 0.50$ au, and $f_{env} = 0.01$ planet models, the $Y = 0.24$ and $Y = 0.40$ models have a convective
were all evolved for 500 Myr. Each model was run at 10.0 AU, and 0.30, 0.20, and 0.20 au. These correspond to the pink, blue, green, and purple lines, respectively. Planet envelopes with larger atmosphere and optically thick radiative zones of true planets.

We describe below how the decrease in helium. We quantify the effect of this approximation in our opacity with -lapse rate of 0.24 K km\(^{-1}\) and 0.27 K km\(^{-1}\), respectively, at a pressure of 10\(^9\) Pa.

In addition to changing the temperature profile in zones where convection occurs, the \( Y \) dependence of the adiabatic lapse rate also influences the location of the radiative–convective boundary. With a steeper adiabatic temperature gradient, helium-enhanced envelopes are more stable against convection and have narrower convecting zones (Figure 2).

In general, increasing the proportion of helium relative to hydrogen in a planet’s envelope lowers the opacity. In the planet models presented herein, we have neglected the effect of nonsolar \( Y \) on opacity; the opacities from Freedman et al. (2014) and the lowT_Freedman11 table implemented in MESA (Freedman et al. 2008) are only available for solar ratios of hydrogen and helium. We quantify the effect of this approximation in our models in Section 4.3. We describe below how the decrease in opacity with \( Y \) is expected to influence both the optically thin atmosphere and optically thick radiative zones of true planets.

In the optically thin atmosphere, the helium mass fraction of an envelope affects the depth at which the stellar irradiation penetrates the planetary atmosphere. The higher the helium content in a planetary envelope, the lower the wavelength-averaged (irradiation mean) opacity to incoming starlight, \( \kappa_{\nu} \). As a result, the irradiation from the host star penetrates farther into helium-enhanced planetary atmospheres.

Within optically thick radiative zones, helium-enhanced planets with lower Rosseland mean opacities can more easily transport energy by radiative diffusion and will have shallower radiative temperature gradients. Based on the low-T_fa05_gs98 opacity tables (Ferguson et al. 2005), increasing the \( Y \) from 0.18 to 0.36 decreased the Rosseland mean opacity by 5–15%, depending on temperature and density. In addition to changing the temperature profile in optically thick radiative zones, the \( Y \) dependence of opacity would lead helium-enhanced envelopes to be more stable against convection and to have narrower convecting zones.

### 3.3. The Effect of Mass Loss on Atmospheric Structure and Composition

In the previous two sections, we explored how varying the \( X \) and \( Y \) of a mini-Neptune could affect the planetary radius and atmospheric structure. Now we turn to considering a mechanism by which planets may become enhanced in helium relative to hydrogen.

To investigate diffusion-modulated atmospheric escape as a pathway for creating helium-enhanced planets, we simulated a grid of planets with varying masses, orbital separations, and envelope mass fractions for three different mass-loss regimes. Figure 3 shows the resulting \( M_{\text{p}}-R_{\text{p}} \) relations after 5.0 Gyr of evolution. Models ranged from 2.0 \( M_{\oplus} \) to 25.0 \( M_{\oplus} \), 0.001 to 0.20 \( f_{\text{env}} \), initial abundances of \( Y = 0.24 \), \( Z = 0.02 \), \( X = 0.74 \), and were evolved around a 6000 K host star.

In Figure 3 we show three simulated regimes of mass loss. First, we simulated the mass-loss regime from Hu et al. (2015). Fractionation between hydrogen and helium leads to preferential hydrogen loss. Next, we computed evolution tracks for planets with mass loss but no fractionation. The rate of mass loss was calculated in the same manner as in Hu et al. (2015). These planets had constant envelope compositions throughout their evolution. Last, we modeled a third set of planets without mass loss.

We find that preferential hydrogen loss can shape the \( M_{\text{p}}-R_{\text{p}} \) relations of sub-Neptune-mass planet populations. Planets simulated with fractionation often had atmospheric helium mass fractions significantly higher than their initial abundance of \( Y = 0.24 \). We found \( Y \) fractions as high as 0.35 within our simulated grid, and would expect to find even more helium enhancement if we had simulated a denser grid of highly irradiated planets with small initial envelopes.

Low-mass \( (M_{\text{p}} \lesssim 10 M_{\oplus}) \) highly irradiated planets with envelope fractions below 1.0% showed the largest differences in radii between planets evolved with fractionation mass loss and planets evolved with nonfractionation (constant envelope composition) mass loss. These effects can be seen in Figure 3. In this low-mass, low-\( f_{\text{env}} \) regime, planets run with mass loss are significantly smaller than planets run without mass loss. Planets that evolve with preferential hydrogen loss are smaller still than planets run with constant composition mass loss. Over the remaining parameter space we explored, the envelope mass fraction dominates the \( M_{\text{p}}-R_{\text{p}} \) relations, being the most important input factor affecting planet radii at 5.0 Gyr.
dramatically reduced the radii of modeled planets. Additionally, all models were evolved for 5.0 Gyr around a host star with a temperature of 6000 K. Although the envelope mass fraction is the input factor with the strongest influence on the $M_\text{f}-R_\text{p}$ relations, the mass-loss mode assumed leads to significant differences in radius—particularly for small and highly irradiated planets. The most irradiated planets had envelopes that became unbound at the lowest masses modeled. Below 15.0 $M_\oplus$, envelope erosion and helium enhancement dramatically reduced the radii of modeled planets.

### 3.4. GJ 436b

Hu et al. (2015) first proposed the possibility of helium-enhanced mini-Neptunes to explain the lack of CH$_4$ observed in the emission spectrum of GJ 436b. This transiting Neptune-size planet (4.22$^{+0.09}_{-0.10} M_\oplus, 23.17 \pm 0.79 M_\oplus$; Torres 2007) has an orbital semimajor axis of 0.02872 ± 0.00027 au. Its host star is type M2.5V ($M_*=0.452^{+0.014}_{-0.012} M_\odot$, $R_*=0.464^{+0.009}_{-0.011} R_\odot$; Torres 2007), and has an effective temperature of $T_\text{eff}=3350\pm300$ K (Deming et al. 2007). There is significant uncertainty on GJ 436b’s age. Bourrier et al. (2018) places the age of the system between 4 and 8 Gyr. For the purposes of our model, we assume GJ 436b has an age of 5.0 Gyr unless otherwise specified. This is well within the age range where helium enhancement is possible. Hu et al. (2015) theorized that if hydrodynamic mass loss was to significantly alter the atmospheric composition of GJ 436b, the planet must begin evolution with the presence of an initial H/He envelope fraction lower than or equal to $10^{-3}$ of the planetary mass.

We find that GJ 436b cannot be significantly enhanced in helium or depleted in hydrogen compared to its host star via the mechanism proposed by Hu et al. (2015). The radius and orbital separation of GJ 436b places it outside the realm of possible helium enhancement that we modeled. GJ 436b is too large and requires too massive a primordial envelope to become sufficiently helium-enhanced via atmospheric mass loss. We ran a large suite of models with characteristics similar to GJ 436b and its host star (Figure 5), and found that GJ 436b was significantly outside the domain of helium enhancement. This conclusion is robust against small changes in the mass, radius, orbital separation, and age of GJ 436b. In our modeled grid, no planet with a radius exceeding 3.00 $R_\oplus$ reached a helium fraction above $Y=0.40$ within 10 Gyr. Furthermore, 23.0–24.0 $M_\oplus$ models from 0.01 to 1.00 au and with final radii such that 4.0 $R_\oplus < R_\text{p} < 5.0 R_\oplus$ all had final envelope fractions between 0.05 and 0.20—an order of magnitude larger than was typical for helium enhancement. Envelope fractions this large preclude hydrodynamic mass loss from significantly changing a planet’s atmospheric composition. GJ 436b’s radius of 4.22 $R_\oplus$ necessitates the presence of a significant gaseous envelope and places it outside the domain of envelope mass-fraction parameter space for which helium enhancement is possible.

We found good agreement between our simulated mass-loss rate for GJ 436b and previous work. For a 23.5 $M_\oplus$ model run at 0.026 au and with a final radius of 4.21 $R_\oplus$, we found a mass-loss rate of $1.98 \times 10^9$ g s$^{-1}$ at 5.0 Gyr. In comparison, Hu et al. (2015) modeled the escape rate of GJ 436b at $10^8–10^{10}$ g s$^{-1}$. Lyα transit transmission spectra show a current mass-loss rate of $10^8–10^9$ g s$^{-1}$ for GJ 436b (Ehrenreich et al. 2015). Furthermore, Ehrenreich et al. (2015) show that the escape rate of GJ 436b would have been significantly greater during the earlier evolution of its host star. Overall, our models agree with Hu et al. (2015), as well as with observational estimates of GJ 436b’s loss rate.

### 3.5. Helium Enhancement in GJ 436b Mass Planets

Although we find that GJ 436b cannot be significantly helium enhanced, it is possible that exoplanets with smaller initial envelope fractions could be. We ran an extensive grid of simulations for planets with similar masses to GJ 436b. For Figure 5, we evolved planets from 0.01 to 1.00 au, and 0.001 to 0.20 $f_{\text{env}}$, and masses from 23.0 to 24.0 $M_\oplus$ around a 3350 K, star. In future work we will explore helium enhancement for a larger range of sub-Neptune-mass models.

A key takeaway of our simulations of planet evolution is that helium enhancement is possible. Preferential escape of light gases causes planetary atmospheres to increase in helium and metals relative to hydrogen over billions of years. Through mass loss, planets can progress from solar helium abundances to having atmospheric helium mass fractions greater than $Y=0.40$. We describe this in detail below.

The outcomes of our evolution simulations can be divided into three categories based on helium enhancement and envelope erosion. Figure 4 shows the evolution of three planets—i.e., one from each category. First, for planets with large initial envelopes (>1.0%), or at distances farther away than 0.50 au, there was no significant helium enhancement. These planets did not experience significant mass loss, and obeyed the same $M_\text{f}-R_\text{p}$ relations as shown in Figure 1. Their final radius is largely determined by their initial envelope mass fraction and mass. Second, we found planets that had
progressed in atmospheric helium abundance from $Y = 0.24$ to $Y$ in excess of 0.40 over a timescale of several billion years. These planets were along the lower radius boundary of the planets that retained their H/He envelopes for a given mass, and were highly irradiated. Last, the most highly irradiated planets became remnant cores through envelope erosion, and had envelopes that became unbound before 10 Gyr had passed.

Models exterior to 1.00 au or with initial envelope fractions greater than 1.0% did not become helium enhanced over 10 Gyr. The rate of helium mass loss relative to hydrogen was not high enough to significantly change the composition of these planets. The physical structure of these models was similar to previous sub-Neptune interior structure models (e.g., Valencia et al. 2007; Lopez & Fortney 2014; Howe & Burrows 2015; Chen & Rogers 2016).

After 5.0 Gyr of mass loss, we found that helium-enhanced models had final radii between 2.34 $R_\oplus$ and 2.90 $R_\oplus$. These models were among the most highly irradiated, and had some of the smallest initial envelope fractions. Helium-enhanced models lost between 35% and 90% of their initial envelope mass. Furthermore, they had irradiation fluxes from 7.0 to 1130.0 $F_{\odot}$, initial envelope fractions below 0.0047, final envelope mass fractions below 0.0025, Z fractions from 0.033 to 0.225, and transit radii from 5% to 29% above that of their rocky cores.

The progression of helium enhancement for 23.5 $M_\oplus$, models can be seen in Figure 5. Planets initially lose helium and hydrogen in relatively equal proportions, and we do not find planets with $Y \gtrsim 0.40$ before approximately 2.5 Gyr. As planets continue to evolve, helium enhancement becomes a prominent feature along the lower radius boundary. However, after 5.0 Gyr, changes in atmospheric composition and planet radius largely abate. This is due to a decrease in mass-loss rates and a decrease in envelope contraction, respectively.

Last, the most highly irradiated planets had envelopes that became completely unbound in our simulations. We define these remnant cores as models that failed to evolve for the full 10 Gyr, and lost more than 75% of their initial envelope before failing. We manually assigned these planets radii equal to their rocky cores, and placed them in the appropriate location within the flux—radius relations of Figure 5. They occupy a parameter space within the F–R chart along the lowest radius boundary, and are more strongly irradiated than models that evolved the full 10 Gyr.

Figure 4. Plot of changing atmospheric abundances throughout the 10 Gyr evolution of three planetary models. All three models were run with hydrodynamic mass loss and began with $M_p = 23.5 M_\oplus$ and initial envelope fractions of 0.003. From left to right, the planets were run with orbital separations of 0.01, 0.03, and 1.00 au. From left to right, we can see the different extremes of mass loss. First we show a planet that was so irradiated that it failed the full 10 Gyr evolution. Before failing, this planet had become basically a remnant core, with no envelope remaining. Second we show a model that became helium enhanced. A significant fraction of the total atmospheric hydrogen has been lost. Last, no significant composition change occurred throughout the planet evolution at 0.50 au. The choice of $M_p = 23.5 M_\oplus$ for each of the three models shows specifically how the magnitude of irradiation flux affects the mass-loss evolution of models that are similar in mass, radius, and orbital separation radius to GJ 436b.

Figure 5. The flux–radius distribution of models evolved around a GJ 436-like star, with the presence of hydrodynamic H/He loss. The above models had an initial mass of 23.5 $M_\oplus$, orbital separations from 0.01 to 1.00 au, and $f_{\text{env}}$ between 0.001 and 0.200. Above are the distributions at 2.5, 5.0, and 7.5 Gyr. The black cross corresponds to the flux and radius of GJ 436b, solidly in a parameter space where helium enhancement did not occur. However, we see significant helium enhancement along the lower radius boundary after 5.0 Gyr of mass loss. The red diamonds correspond to remnant core models that failed to evolve for the time frame plotted, and whose envelopes became unbound by the incident flux. We assigned these models radii corresponding to the core radius at 23.5 $M_\oplus$. These models constrain the progression of helium enhancement for a planet with the mass of GJ 436b, and the parameter space for which final $Y$ fractions might exceed 0.40.
We found remnant cores for planets that were irradiated at rates of at least 30.0 $F_{\odot}$. The higher the planet mass, the higher the surface gravity, and the higher the flux necessary to evaporate the envelope. These remnant cores show a clear demarcation between planets that had managed to retain some of their envelope, and planets that had lost their entire envelope due to hydrodynamic mass loss. This complete or nearly complete envelope loss is similar to that found in previous studies (e.g., Lopez & Fortney 2013; Owen & Wu 2013, 2016; Jin et al. 2014; Chen & Rogers 2016; Lehmer & Catling 2017; Ginzburg et al. 2018). We discuss the remnant cores in detail in Section 4.3.

4. Discussion

4.1. Helium Enhancement in Tightly Orbiting Sub-Neptunes

Under irradiation approximately $10^3–10^4$ times that of Earth, helium enhancement was possible for planets with masses similar to GJ 436b. We found helium-enhanced planets primarily along the lower radius boundary of all planets that had retained a gaseous H/He envelope (Figure 5). These planets usually had final radii $10–30$ times larger than the radius of their rocky core. Helium enhancement necessitates that planets begin their evolution with relatively small envelope fractions. Compounding this, helium-enhanced planets ($Y > 0.40$) further lost a minimum of 35% of their envelope mass through envelope erosion. Planets with high envelope masses do not lose enough mass to significantly change their atmospheric abundances. All models that eventually became helium enhanced began their evolution with $f_{\text{env}} < 0.005$. As a result, helium enhancement occurs within a narrow range of simulated planet radii (Figure 5).

Helium enhancement appeared as a prominent feature after approximately 2.5 Gyr of hydrodynamic mass loss. Planets with small envelope fractions ($f_{\text{env}} < 0.0025$) become helium enhanced in the shortest time frame. After several billion years, however, larger-envelope planets undergoing steady mass loss with diffusive separation of hydrogen and helium can become helium enhanced. Figure 5 shows a set of 23.5 $M_\odot$ models at various evolution snapshots to show the progression of helium enhancement. Helium enhancement occurs first along the lower radius boundary, and subsequently spreads to planets with larger envelopes and larger radii.

The Hu et al. (2015) model that we implemented treated the loss of hydrogen and helium, but not metals. Therefore, complete envelope erosion was not possible. Additionally, our model assumed constant values for $\eta$ and the EUV absorption radius ratio ($\omega$) in Equation (5). Future work could expand on our mass-loss routine, and include metal loss and better treatment of the most extreme edge cases.

Although GJ 436b is not significantly helium enhanced, atmospheric mass loss may significantly alter the envelope compositions of similar-mass planets with smaller initial envelopes. At 5.0 Gyr, GJ 436b mass planets (23.5 $M_\odot$) with $Y > 0.40$ had final radii between 2.38 $R_\odot$ and 2.84 $R_\odot$, and $F_\odot > 10 F_\odot$ (Figure 5). The final helium mass fraction gradually declines (approaching the primordial solar value assumed) as the planetary radius increases and irradiation flux decreases. In the population of GJ 436b mass planets we modeled, only models with radii below 3.00 $R_\odot$ had helium abundances above $Y = 0.40$. Furthermore, given sufficient irradiation, we expect to find helium enhancement in the broader sub-Neptune population as well.

4.2. Metallicity Enhancement

In addition to engendering supersolar proportions of helium, preferential loss of light gases may lead to metallicity enhancements in sub-Neptune atmospheres. In our simulations, the planets that became enhanced in helium also became enhanced in metals. The planets along the lower (small-radius) boundary of Figure 5 experienced significant atmospheric metallicity enhancement (relative to their initial solar-metallicity starting envelope composition, $Z = 0.02$), achieving final metal mass fractions between $Z = 0.04$ and 0.23.

Theoretical work by Fortney et al. (2013) has pointed to links between planet atmospheric metallicity and formation process (e.g., the size distribution of planetesimals, and the mass of H/He gas accreted). Our results highlight that evolution (specifically, atmospheric escape) in addition to the formation process could impact planet atmospheric metallicities—contributing (over several billion years) to Neptune-mass and sub-Neptune-mass planets having more metal-rich atmospheres than their massive Jovian cousins. Although this is beyond the scope of this paper, expanding the model to include the loss of heavy elements could be a future endeavor.

4.3. Model Caveats

4.3.1. EOS Limitations

Some of our planet models failed to evolve for the full 10 Gyr evolution because they exceeded the $\rho - T$ boundary limits in the equation-of-state (EOS) module of MESA. In particular, models with masses $\geq 15.0 M_\odot$, $f_{\text{env}} = 0.01–0.10$, and outer envelope temperatures between 750 and 1500 K failed after approximately 8 Gyr. The low-density and low-temperature SCVH tables within MESA’s EOS module (Saumon et al. 1995) roughly cover calculations for which $\log(\rho) - 2 + \log(T) + 12 < 5.0$. As our models cooled and contracted, they pushed the limits of what MESA was able to simulate. Future versions of MESA aim to expand the range of temperatures and densities in the EOS tables, allowing densities from $10^{-8}$ to $10^{6}$ g cm$^{-3}$, pressures from $10^{-9}$ to $10^{13}$ GPa, and temperatures from $10^5$ to $10^7$ K (Chabrier et al. 2019; J. Schwab 2019, private communication).

4.3.2. Remnant Cores

Planets with orbits interior to 0.05 au and with initial envelope fractions lower than 0.003 are likely to become remnant cores. MESA experienced time-step convergence issues with these models, and failed to evolve them past approximately $3.0 \times 10^9$ yr. Often, they had final radii in excess of 10 $R_\odot$, suggesting that the atmosphere had become gravitationally unbound before model failure. Additionally, most of the mass lost for these simulations was in the energy-limited escape regime. This meant that the remnant cores lost both hydrogen and helium, and at rates approximately equal to their abundances. This means that before becoming unbound, they did not become appreciably enhanced in helium relative to hydrogen.

Owen & Wu (2016) described this phenomenon, and suggested that rapid atmospheric boil-off could deplete the gaseous envelopes of $M_p \leq 10.0 M_\oplus$ planets over a period of
10^5 yr. They point to boil-off as a possible cause of the dearth of Kepler planets with orbits interior to 0.50 au and radii above 2.50 \( R_{\oplus} \).

Numerically, remnant cores are (not unexpectedly) challenging to model in MESA. These simulations are extremely sensitive to small changes in envelope fraction and orbital separation, and were only found for the most unstable conditions that we modeled. We differentiate these models from the super helium-enhanced models that have evolved for the full 10 Gyr (Figure 5), and manually assign the remnant cores the radii of their rocky core.

4.3.3. Opacities

We chose the \texttt{lowT\_Freedman11} opacity tables to model atmospheric opacity because they had the most accurate data for the atmospheric temperature ranges that our models spanned. However, the \texttt{lowT\_Freedman11} opacity tables do not include the effects of varying helium concentrations on atmospheric opacity (Freedman et al. 2014). Other opacity tables within MESA, such as \texttt{lowT\_fa05\_gs98}, include the effects of varying \( Y \), but have more restrictive temperature ranges (Ferguson et al. 2005). The tables from Freedman et al. (2014) extend from 75 to 4000 K, while the tables from Ferguson et al. (2005) cover 500–30,000 K. Our models have outer envelope temperatures from approximately 250 to 3000 K, necessitating the choice of the \texttt{lowT\_Freedman11} tables.

To benchmark how the choice of opacity table influences our results, we reran the suite of planets in Figure 2 with \texttt{lowT\_fa05\_gs98}. Using \texttt{lowT\_fa05\_gs98}, we find that planets had slightly (less than 2.0%) larger final radii than planets run with \texttt{lowT\_Freedman11}.

Notably, the level of helium enhancement was almost identical between the opacity table choices. Thus, the choice of opacity table does not change our overall qualitative results: that GJ 436b is not helium enhanced, but that similar planets with smaller envelopes may be.

4.3.4. Homopause Temperature

Our choice of \( T_H = 10^4 \) K results in a conservative estimate of the hydrogen–helium fractionation effect. Murray-Clay et al. (2009) show that above the photoionization base, \( \text{Ly}\alpha \) cooling regulates the temperature to at most \( \sim 10^4 \) K. Further increasing incident UV power is balanced out by larger radiative losses. Choosing \( T_H = 10^3 \) as opposed to a lower estimate such as the planet equilibrium temperature—decreases fractionation in two ways. First, the coupling between neutral hydrogen and helium increases with temperature. Second, a larger fraction of hydrogen is ionized at higher temperatures. From \( 10^3 \) to \( 10^4 \) K, \( \text{H} – \text{He} \) is more strongly coupled than neutral \( \text{H} – \text{He} \). Therefore, increasing the ionized fraction increases the average coupling weight for all atmospheric \( \text{H} – \text{He} \) (Mason & Marrero 1970; Schunk & Nagy 1980; Hu et al. 2015). Both effects result in more helium being carried with escaping hydrogen. Even with the conservative estimate, however, we found extensive helium enhancement.

4.3.5. The Eddy Diffusion Coefficient

The self-consistent calculations of coupled, thermal, mass-loss, and compositional evolution of primordial envelopes presented so far have adopted a nominal eddy diffusion coefficient of \( K_{zz} = 10^9 \) cm^2 s^-1. The strength of eddy diffusion in planetary envelopes is very uncertain, however (e.g., Hu et al. 2015). In this section, we evaluate the sensitivity of our results to the value of \( K_{zz} \).

Our simulations of helium enhancement in sub-Neptune-size planets are robust against changes in \( K_{zz} \) over multiple orders of magnitude. We simulated planets experiencing fractionated mass loss and for values of \( K_{zz} \), spanning from 1/100th of our nominal value of \( 10^9 \) cm^2 s^-1 to 100 times greater (Figure 6). For the model with \( M_p = 25 \ M_{\oplus} \), \( a = 0.05 \text{ au} \), and \( f_{\text{env}} = 0.004 \), adopting an eddy diffusion coefficient of \( 10^7 \) cm^2 s^-1 instead of \( 10^9 \) cm^2 s^-1 decreased envelop helium mass fraction, \( Y \), by approximately 3% after 10 Gyr. Similarly, an eddy diffusion coefficient of \( 10^{11} \) cm^2 s^-1 increased the final \( Y \) at an age of 10 Gyr by approximately 3%, as compared to an analogous planet simulated with our nominal value of \( K_{zz} = 10^9 \) cm^2 s^-1. Varying \( K_{zz} \) had an even smaller influence on the simulated planets with larger initial \( f_{\text{env}} \). Overall, we find that the choice of eddy diffusion coefficient does not significantly change how the planetary envelope composition evolves in our simulations.

Although the evolution of the envelope compositions are not strongly affected by \( K_{zz} \) in our simulations, \( K_{zz} \) does have a substantive effect on the location of the homopause. The higher the value of \( K_{zz} \), the higher our calculated value for the homopause radius, according to Equation (26). Changing from \( K_{zz} = 10^7 \) cm^2 s^-1 to \( K_{zz} = 10^{11} \) cm^2 s^-1 for a \( M_p = 25 \ M_{\oplus} \) model with an orbital separation of 0.05 au and \( f_{\text{env}} = 0.01 \) resulted in a ~30% increase in \( R_h \). Smaller envelope fractions or larger orbital separation further decrease the effect of \( K_{zz} \) on \( R_h \). Larger homopause radii lead to higher planet mass-loss rates. Thus, although helium-enhanced planetary envelopes are a robust outcome of our simulations, the cumulative mass lost by the simulated planets (and hence the mapping from observed planet properties today back to the initial planet compositions) is sensitive to the choice of \( K_{zz} \). We note that in contrast to variations in the mass-loss efficiency, \( \eta \), which scale the mass-loss rate of all models equally, variations in \( K_{zz} \) have a stronger impact on the mass-loss rates of low-mass planets with low surface gravities.
4.4. Observational Consequences of He Enhancement

Our models have shown that although GJ 436b is not enhanced in helium relative to hydrogen, other smaller planets may be. Nonsolar ratios of hydrogen and helium could have multiple observable consequences for exoplanet mass, radius, and atmospheric spectral characterization.

Inferences of planet compositions from transit, transit-timing variation, and radial velocity observations rely on comparing the observational constraints on the planet mass and radius to mass–radius relations computed from planet interior structure and evolution models. As discussed in Section 3.1, increasing the helium mass fraction \( Y \) of a primordial envelope from solar to \( Y = 0.40 \) can decrease modeled planet radii by more than a few percent—a level exceeding the observational precision of planetary radii in the era of Gaia (Stassun et al. 2017). This additional dimension of planet compositional diversity has so far been largely neglected in the interpretation of planet mass–radius measurements. Assuming solar ratios of hydrogen to helium in the primordial envelopes of close-orbiting sub-Neptune-size planets would lead to a systematic underestimation of the envelope mass fractions of planets that have been sculpted by atmospheric escape.

A depletion of hydrogen and relative enhancement of helium in sub-Neptune-size planet envelopes could have observable consequences for their atmospheric spectra. Increasing the mean molecular weight and decreasing the proportion of hydrogen relative to helium in a planet’s atmosphere will decrease the atmospheric scale height and lead to less pronounced absorption features (Miller-Ricci et al. 2009). The proportion of hydrogen relative to helium can also affect the atmospheric chemistry and equilibrium molecular abundances (e.g., decreasing the proportions of \( \text{CH}_4 \) relative to \( \text{CO} \)). Hu et al. (2015) originally proposed a helium-enhanced scenario to explain the lack of methane observed in GJ-436b’s emission spectrum. Finally, the recent detection of the theoretically predicted (Seager & Sasselov 2000; Oklopić & Hirata 2018) forbidden 10,830 Angstrom He line (e.g., Allart et al. 2018; Mansfield et al. 2018; Spake et al. 2018) opens the possibility of directly detecting the escape of helium from sub-Neptune planets.

4.5. Summary

We implemented the new MESA routine from Section 2 to iterate the stages of planet evolution, including modeling planets with varying initial atmospheric helium mass fractions. We ran models across a wide parameter space of mass, envelope fraction, orbital separation, and composition to observe the effects of coupled thermal and compositional evolution. We evolved models starting from 2.0 to 25.0 \( M_{\oplus} \), 0.18–0.40 helium fraction, \( f_{\text{env}} = 0.001–0.200 \), and orbital separations from 0.01 to 1.00 au. We showed the results of helium enhancement on atmospheric structure, as well as the effect of helium enhancement on \( M_{\text{p}} - R_{\text{p}} \) relations of sub-Neptune-mass planets.

 Preferential loss of hydrogen can lead to planetary envelopes that are significantly enriched in helium and metals. Evolving planets with initial solar abundances under the mass-loss regime from Hu et al. (2015), we found planets with helium mass fractions in excess of 0.40 and metal mass fractions in excess of 0.10. In addition to helium enhancement, we found planets that had become remnant cores through envelope erosion. We characterized how initial envelope mass, planet mass, and irradiation flux influence the evolution of planet atmospheres.

Helium enhancement is constrained to highly irradiated planets with small initial envelopes. We showed that GJ 436b mass planets older than \( \sim 2.5 \) Gyr with \( R_{\text{p}} \lesssim 3.00 R_{\oplus} \), \( f_{\text{env}} < 0.5\% \) and irradiation flux \( \sim 10^{11}–10^{13} \) times that of Earth are likely candidates to have atmospheres with significant helium enhancement. In light of the abundance of short-period sub-Neptune-mass exoplanets that have been recently discovered, this result further expands on the expected diversity of an already incredibly varied population.

Last, we found GJ 436b to not be a suitable candidate to have undergone helium enhancement. The radius of GJ 436b places it outside the regime for which hydrodynamic mass loss produced noticeable changes in atmospheric helium abundance. However, we find that many GJ 436b mass planets with a smaller initial envelope could become helium enriched, as shown by Figure 5. Future work will expand these results and compare our models with the observed planet populations. Helium-enhancement models, along with our interior structure simulations, can be valuable predictive techniques to be used in conjunction with new observational surveys.

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References

Allart, R., Bourrier, V., Lovis, C., et al. 2018, Sci, 362, 1384
Beaugé, C., & Nesvorný, D. 2013, ApJ, 763, 12
Benítez-Llambay, P., Massei, F., & Beaugé, C. 2011, A&A, 528, A2
Bird, R., Stewart, W., & Lightfoot, E. 2007, Transport Phenomena (New York: Wiley)
Borucki, W. J., Koch, D. G., Basri, G., et al. 2011, ApJ, 728, 117
Bouffard, L., Koch, D. G., Basri, G., et al. 2011, ApJ, 728, 117
Bourrier, V., Lovis, C., Beust, H., et al. 2018, Natur, 553, 477
Buehler, P. B., Knutson, H. A., Batygin, K., et al. 2016, ApJ, 821, 26
Chabrier, G., Mazevet, S., & Soubrain, F. 2019, ApJ, 787, 51
Chen, H., & Rogers, L. A. 2016, ApJ, 831, 180
Deming, D., Harrington, J., Laughlin, G., et al. 2007, ApJL, 667, L119
Ehrenreich, D., Bourrier, V., Wheatley, P. J., et al. 2015, Natur, 522, 459
Elkins-Tanton, L. T., & Seager, S. 2008, ApJ, 688, 628
Erkaev, N. V., Kulikov, Y. N., Lammer, H., et al. 2007, A&A, 472, 329
Ferguson, J. W., Alexander, D. R., Allard, F., et al. 2005, ApJ, 623, 585
Fortney, J. J., Mordasini, C., Nettelmann, N., et al. 2013, ApJ, 775, 80
Freedman, R. S., Lustig-Yaeger, J., Fortney, J. J., et al. 2014, ApJS, 214, 25
Freedman, R. S., Marley, M. S., & Lodders, K. 2008, ApJS, 174, 504
Fuller, E. N., Schettler, P. D., & Giddings, J. C. 1966, Industrial & Engineering Chemistry, 58, 18
Fulton, B. J., Petigura, E. A., Howard, A. W., et al. 2017, AJ, 154, 109
Ginzburg, S., Schlichting, H. E., & Sari, R. 2018, MNRAS, 476, 759
Guillot, T., Chabrier, G., Gautier, D., & Morel, P. 1995, ApJ, 450, 463
Howard, A. W., Marcy, G. W., Bryson, S. T., et al. 2012, ApJS, 201, 15
Howe, A. R., & Burrows, A. 2015, ApJ, 808, 150
Howe, A. R., Burrows, A., & Verne, W. 2014, ApJ, 787, 173
Hu, R., Seager, S., & Bains, W. 2012, ApJ, 761, 166
Hu, R., Seager, S., & Yung, Y. L. 2015, ApJ, 807, 8
Jackson, B., Arras, P., Pennev, K., Peacock, S., & Marchant, P. 2017, ApJ, 835, 145
