Irradiated ocean planets bridge super-Earth and sub-Neptune populations

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With radii ranging between those of the Earth (1 $R_\oplus$) and Neptune ($\sim$3.9 $R_\oplus$), small planets constitute more than half of the inventory of the 4000-plus exoplanets discovered so far1. This population follows a bimodal distribution peaking at $\sim$1.3 $R_\oplus$ (super-Earths) and 2.4 $R_\oplus$ (sub-Neptunes), with few planets in between2,3. Smaller planets are sufficiently dense to be rocky, but those with radii larger than $\sim$1.6 $R_\oplus$ are thought to display large amounts of volatiles, including in many cases hydrogen/helium gaseous envelopes up to $\sim$30% of the planetary mass4,5. With orbital periods less than 100 days, these low-mass planets are highly irradiated and their origin, evolution, and possible links are still debated6−10. Here we show that close-in ocean planets11 affected
by greenhouse effect display hydrospheres in supercritical state, which generate inflated atmospheres without invoking the presence of large H/He gaseous envelopes. We derive a new set of mass-radius relationships for ocean planets with different compositions and different equilibrium temperatures, well adapted to low-density sub-Neptune planets. Our model suggests that super-Earths and sub-Neptunes\textsuperscript{2,3} could belong to the same family of planets. The differences between their interiors could simply result from the variation of the water content in those planets. Close-in sub-Neptunes would have grown from water-rich building blocks compared to super-Earths, and not concurrently from gas coming from the protoplanetary disk. This implies that small planets should present similar formation conditions, which resemble those known for the terrestrial and dwarf planets in the solar system.

Theoretical mass/radius relationships are at odds to explain the composition of the largest members of the small planet population. When available, mass and radius measurements show that super-Earths are sufficiently dense to be rocky while sub-Neptunes fall near curves of planets composed of pure water, suggesting instead a solid core surrounded by a hydrogen/helium gaseous envelope up to $\sim$30\% of the planetary mass\textsuperscript{2−10}. However, even though the vast majority of the known small planets are close-in, current mass/radius relationships exclude the physical properties of highly irradiated ocean planets\textsuperscript{11}, whose formation mechanisms do not deviate from those of super-Earths, contrary to sub-Neptunes. This category of planets should be ubiquitous in the universe given the large number of water-rich worlds (Europa, Titan, Enceladus, Pluto, etc) existing in our own solar system.

Here we present new mass/radius relationships of irradiated ocean planets that can easily
explain the large observed radii of the sub-Neptunes population. These relationships are derived from the combination of two one-dimensional models, i.e. a fully differentiated planet interior model\textsuperscript{12} and a steam atmosphere model\textsuperscript{13,14} connected at a 1000-bar pressure. The interior model takes as inputs the planetary mass and chemical composition (Mg/Si, Fe/Si mole ratios and water mass fraction), and computes the resulting radius and internal structure of the planet\textsuperscript{12}. The internal structure relies on the pressure $P(r)$, the temperature $T(r)$, the gravity acceleration $g(r)$, and the density $\rho(r)$ as a function of radius. These quantities are integrated following an iterative scheme until convergence is reached. Along the radius $r$ of the planet, the pressure $P(r)$ is calculated via different equations of state (EOS), which are chosen depending on the material composing the considered layer. The different layers include the core, the lower and upper mantles, the high pressure ice, and a liquid hydrosphere\textsuperscript{12}. To account for the effects of irradiation, as expected for the close-in population, a water phase in supercritical state has been added to the hydrosphere. For given density and temperature, the supercritical layer pressure is calculated via an EOS (see Methods) obtained from data generated by molecular level computer simulations that consider simple point-charge potential models to which average polarization corrections have been added\textsuperscript{15}. The resulting EOS (hereafter DZ06) agrees within a $\pm 0.6\%$ deviation with the well-known IAPWS95 formulation\textsuperscript{16}, which provides an accurate EOS based on experimental data within the $\sim 0$–1.0 GPa pressure range. At higher pressure, the DZ06 EOS has been shown to compute the pressure within a $\pm 1.3\%$ deviation up to 10.0 GPa, and should remain within a $\pm 5.0\%$ deviation up to 35 GPa, from comparisons with simulated data\textsuperscript{15,17}.

The adiabatic temperature profile within the supercritical layer depends on the Grüneisen parameter, which shows strong dependence with both density and temperature. In the supercritical layer, this parameter is derived from a bilinear interpolation of a grid of data available in the python library for IAPWS standard calculation of water and steam properties\textsuperscript{18}. This grid
gives a range of Grüneisen parameters for temperatures up to $10^4$ K and supercritical water densities up to 2500 kg/m$^3$, corresponding to pressures up to $\sim$150 GPa, a value exceeding the one at the center of a 20 $M_{\oplus}$ planet fully made of water. It shows good agreement with available experimental data up to 1GPa/1273K$^{16}$. When deriving this grid, the IAPWS team focused on the extrapolation behavior of the formulation, and ensured it behaves physically at high pressure/temperature domains, which are relevant to (exo)planetary interiors. The Grüneisen parameter’s profile is expected to have a correct physical behavior, albeit with increasing uncertainties when going deeper in the planet. However, we find this to be of secondary importance regarding planetary radius as the Grüneisen parameter is basically a proxy of thermal expansivity along pressure variations, which rapidly becomes of second order when pressure increases.

The atmosphere model$^{13,14}$ takes over at water column pressures lower than $\sim$1000 bar, where the H$_2$O envelope behaves more and more like a hot and dense steam atmosphere as the pressure drops. The used model is based on a $T(P)$ profile prescription$^{19}$ starting from the 1000-bar level (unsaturated since $T(1000 \text{ bar}) > T_{\text{critical}}$) upwards, assuming a dry adiabat, and switching optionally to a moist adiabat (where $T(P) = T_{\text{saturation}}(P)$) if/when saturation reaches unity. Once the temperature reaches the skin temperature $T_{\text{skin}}$, which is related to the equilibrium temperature $T_{\text{eq}}$ via $T_{\text{skin}} = T_{\text{eq}}/2^{1/4}$, an isothermal radiative mesosphere $T = T_{\text{skin}}$ is assumed up to the 0.1 Pa topmost level. Moreover, steam is not treated as an ideal gas, and the EOS is taken instead from the NBS/NRC steam tables$^{20}$. This enables a smooth transition of the $T(P)$ profile with the interior model. Altitudes are computed assuming hydrostatic equilibrium. Shortwave and thermal fluxes are then computed using 4-stream approximation. Gaseous (line and continuum) absorptions are computed using the $k$-correlated method. Rayleigh opacity is also included. $T(1000 \text{ bar})$ is iteratively chosen so that the thermal flux at the top of the atmosphere is equal to $\sigma T_{\text{eq}}^4$. We finally chose the radius/altitude of the 20 mbar level as the observable, transiting radius$^{21}$. 

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Figure 1 displays the pressure and temperature profiles (hereafter \((P, T)\) profiles) of hydrospheres of 1–15 \(M_{\oplus}\) supercritical ocean planets with equilibrium temperatures of 300, 650, and 1200 K, superimposed onto the water phase diagram. The \((P, T)\) profiles expand from the base of the hydrosphere to the top of the \(H_2O\)-dominated atmosphere set to 0.1 Pa. Most of the hydrospheres remain in the supercritical regime and those of smallest planets are located well below ice VII, with a fluid-ice VII transition law valid up to 60 GPa in the water phase diagram. Beyond this pressure range, the phase change from supercritical to high pressure ices (VII or X) is neglected because the temperature/pressure region remains widely unknown in this region.

Figure 2 represents the mass/radius relationships of supercritical ocean planets calculated in the 0.6–20 \(M_{\oplus}\) range for equilibrium temperatures of 300, 650, and 1200 K, corresponding to distances of 0.72, 0.15, and 0.04 AU from a solar-type star, respectively, assuming an Earth-like albedo. The presence of a thick \(H_2O\)-dominated atmosphere generates a strong runaway greenhouse effect causing the presence of a supercritical hydrosphere, even if the equilibrium temperature of the planet is lower than the critical temperature of water \(T_{\text{critical}} \sim 650\) K. Because the core-mantle boundary is not firmly defined at very high pressure and temperature, we assume here the core and mantle form a unique magma phase of mantelic composition. Figure 2 shows that sub-Neptunes can be well matched by mass/radius curves corresponding to ocean planets with significant supercritical hydrospheres.

Our model suggests that super-Earths and sub-Neptunes could belong to the same family of planets, rather than being distributed in two distinct families, i.e. rocky and Neptune-like planets. Sub-Neptunes would be richer in water and, because of the proximity to their host star, the strong insolation associated to runaway greenhouse effect in their atmospheres generates inflated supercritical hydrospheres, compared to similar bodies with a very low water content located at higher distances to the star. We also note that planets possessing exactly the masses
and radii of Uranus and Neptune could be matched by ocean planets if these latter contain more than 70% of supercritical water, depending on their orbital distance and the type of their host star. Our model does not require the accretion of sub-Neptunes from gas coming from the protoplanetary disk. It implies that both super-Earths and sub-Neptunes would have formed from the accretion of building blocks in a manner similar to those known for the terrestrial and dwarf planets in the solar system. Sub-Neptunes would have grown from water-rich building blocks beyond the snowline in protoplanetary disks and would have then migrated inwards. On the opposite, super-Earths would have grown in water-depleted regions of protoplanetary disks.

This first quantitative exploration of the role of supercritical water in planetary envelopes, which underlines the importance of composition in case of strong irradiation, will be extended by the development of a model describing the planets’ interior and atmosphere in a more consistent way. This work also highlights the need for improved EOS in the high pressure and high temperature regime of the water phase diagram.
Methods

Equation of state of supercritical water

The EOS of supercritical water used in this study is written as\textsuperscript{15}:

\[
Z = \frac{PV}{RT} = 1 + \frac{BV_c}{V} + \frac{CV_c^2}{V^2} + \frac{DV_c^4}{V^4} + \frac{EV_c^5}{V^5} + \frac{FV_c^2}{V^2} \times \left( \beta + \frac{\gamma V_c^2}{V^2} \right) \exp \left( -\frac{\gamma V_c^2}{V^2} \right), \quad (1)
\]

where \( R = 83.14467 \text{ cm}^3 \text{ bar/(K mol)} \) is the universal gas constant. Parameters \( B, C, D, E, \) and \( F \) in Eq. 1 are calculated via the following equations:

\[
B = a_1 + \frac{a_2}{T_r^2} + \frac{a_3}{T_r^3} \quad (2)
\]

\[
C = a_4 + \frac{a_5}{T_r^2} + \frac{a_6}{T_r^3} \quad (3)
\]

\[
D = a_7 + \frac{a_8}{T_r^2} + \frac{a_9}{T_r^3} \quad (4)
\]

\[
E = a_{10} + \frac{a_{11}}{T_r^2} + \frac{a_{12}}{T_r^3} \quad (5)
\]

\[
F = \frac{\alpha}{T_r^3} \quad (6)
\]

\[
T_r = \frac{T}{T_c} \quad (7)
\]

\[
F = \frac{RT_c}{P_c} \quad (8)
\]
Table 1: EoS Parameters

| Parameter | Value                  |
|-----------|------------------------|
| $a_1$     | $4.68071541 \times 10^{-02}$ |
| $a_2$     | $-2.81275941 \times 10^{-01}$ |
| $a_3$     | $-2.43926365 \times 10^{-01}$ |
| $a_4$     | $1.10016958 \times 10^{-02}$ |
| $a_5$     | $-3.86603525 \times 10^{-02}$ |
| $a_6$     | $9.30095461 \times 10^{-02}$ |
| $a_7$     | $-1.15747171 \times 10^{-05}$ |
| $a_8$     | $4.19873848 \times 10^{-04}$ |
| $a_9$     | $-5.82739501 \times 10^{-04}$ |
| $a_{10}$  | $1.00936000 \times 10^{-06}$ |
| $a_{11}$  | $-1.01713593 \times 10^{-05}$ |
| $a_{12}$  | $1.63934213 \times 10^{-05}$ |
| $\alpha$ | $-4.49505919 \times 10^{-02}$ |
| $\beta$  | $-3.15028174 \times 10^{-01}$ |
| $\gamma$ | $1.25000000 \times 10^{-02}$ |

where $T_c$ and $P_c$ are the critical temperature and critical pressure respectively. Here, $T_c = 647.25$ K, and $P_c = 221.19$ cm$^3$/mol. Parameters $a_1$–$a_{12}$, $\alpha$, $\beta$, and $\gamma$ are summarized in Table 1. We refer the reader to the study of Duan & Zhang (2006) for details.
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Figure 1: Pressure and temperature profiles of hydrospheres of 1 and 15 $M_\oplus$ supercritical ocean planets with equilibrium temperatures of 300, 650, and 1200 K superimposed onto the water phase diagram. Colored solid and dashed curves correspond to 1 and 15 $M_\oplus$ planets, respectively. The fluid–ice VII transition law is fitted from data between 3 and 60 GPa$^{22}$. The grey dashed line delimits an hypothetical transition between the supercritical phase and high pressure ice (see text). The other phase-change laws are collected from a compilation of thermodynamic data$^{16}$, and from the website of the International Association for the Properties of Water and Steam (IAPWS)$^{24}$. 
Figure 2: Mass-radius diagrams determined for exoplanets with masses in the 0.6–20 $M_\oplus$ range, and equilibrium temperatures of 300 K, 650 K, and 1200 K. Mass-radius curves are calculated for several planetary compositions: 100% core and 100% mantle (red curves), liquid water (LW) hydrosphere (brown curves) and supercritical water (SW) hydrosphere (blue curves) topping mantle-like composition interiors. Planetary data are taken from the NASA exoplanet archive and updated to 20th July 2019. Hydrostatically unstable atmospheres (defined when the altitude at 0.1 Pa tends towards infinity) around the hotter and smaller planets are excluded from the mass-radius relationships.