Lava world plots

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1 Introduction

Throughout this project various python scripts were used to produce my plots, this document lays out what was script was used for the plots. At the end of this document you will find a figure list. All my figures have been placed in different directories, each directory corresponds to a particular list. Each list will describe the figures and the script used to make that figure.

2 Vaporock

Any plot which shows the partial pressure, density or molar elemental fraction were all created with the VapoRock notebooks. These notebooks used VapoRock and ThemoEngine to calculate the vapour and liquid species produced in a magma ocean of a lava world. The notebooks took composition and fo2 value as an input, the fo2 value was measured relative to the Iron-wustite buffer and range from $\Delta IW = -4$ to $\Delta IW = 7$. The compostion of the planet was provided by; Bulk Silicate Earth (BSE) [1], Komatiite [2], Komatiite [3] and Mercury [4].
For running these notebooks I would recommend you have each notebook in its own directory so that the output files don't get over written. These output excel files are stored in a new directory called 'Density' etc. I should point out when i created these files I didn't know the difference between the density arrays which output 34 values and the ones which output 20. So as a result I called them density for the vapor species densities and density high for the liquid species, you can obviously change these arrays and file names to something more sensible.
For instructions on installing VapoRock see:
https://gitlab.com/ENKI-portal/vaporock

3 Temperature-Pressure Plots

Helios was used to calculate the data for these plots. As Helios needs a star to model the planet K2-141b was chosen and the assumption was made that it had Earth like radius and mass. The notebook used was TP Summary plots and you can find the plots in the TP plots folder.

3.1 Spectra

The Emission spectra were produced using Helios and fast chem. Firstly the elemental abudence profiles from VapoRock were taken and imported in to Fast Chem to produce elemental mixing ratio profiles. Using Helios k-tabels were produced. Each spectrum was produced from 0.6 to 25 μm for a resolution of 3000.These wavelength range was choosen as it closely matches what JWST can observe at. The spectra were then plotted and analysed in Spectra plot notebooks, the emission features were classified using DACE[5].

4 Abstract - Figure list

4.1 List 1 BSE compostion

Figure 1 - Vapor Species density profile for $\Delta IW = 3$ was created using VapoRock-BSE.ipynb
Figure 2 - Vapor Species density profiles for all fo2 values, was created using VapoRock-BSE.ipynb
Figure 3 - Liquid Species density profiles for all fo2 values, was created using VapoRock-BSE.ipynb
Figure 4 - Elemental abudence profiles for all fo2 values, was created using VapoRock-BSE.ipynb
Figure 5 - TP plot of atompshere outgassed by the magma ocean
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Figure 10 - Vapor Species density profiles for $\Delta IW = -2$ at 1600,2200 and 2800K, was created using VapoRock-BSE.ipynb
Figure 11 - Liquid Species density profiles for all fo2 values at 1600K, was created using VapoRock-BSE.ipynb
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Figure 13 - Liquid Species density profiles for all fo2 values at 2800K, was created using VapoRock-BSE.ipynb
Figure 14 - Liquid Species density profiles for $\Delta IW = -2$ at 1600,2200 and 2800K, was created using VapoRock-BSE.ipynb
Figure 15 - Elemental abundance profiles for all fo2 values at 1600K, was created using VapoRock-BSE.ipynb
Figure 16 - Elemental abundance profiles for all fo2 values at 2200K, was created using VapoRock-BSE.ipynb
Figure 17 - Elemental abundance profiles for all fo2 values at 2800K, was created

using VapoRock-BSE.ipynb
Figure 18 - Elemental abundance profiles for $\Delta IW = -2$ at 1600,2200 and 2800K, was created using VapoRock-BSE.ipynb
Figure 21 - Partial pressure profiles for $\Delta IW = -2$ at 1600,2200 and 2800K, was created using VapoRock-BSE.ipynb
Figure 22 - Partial pressure profiles for all fo2 values and temperatures for Si species, was created using VapoRock-BSE.ipynb
Figure 23 - Partial pressure profiles for all fo2 values and temperatures for Mg species, was created using VapoRock-BSE.ipynb
Figure 24 - Partial pressure profiles for all fo2 values and temperatures for Al species, was created using VapoRock-BSE.ipynb
Figure 25 - Partial pressure profiles for all fo2 values and temperatures for O species, was created using VapoRock-BSE.ipynb
Figure 26 - Partial pressure profiles for all fo2 values and temperatures for Na species, was created using VapoRock-BSE.ipynb
Figure 27 - Partial pressure profiles for all fo2 values and temperatures for Fe species, was created using VapoRock-BSE.ipynb
Figure 28 - Partial pressure profiles for all fo2 values and temperatures for Ca species, was created using VapoRock-BSE.ipynb
Figure 29 - Elemental abundance profiles for all fo2 values at t=1950k, was created using VapoRock-BSE.ipynb

4.2 List 2 - Basalt plots

Figure 1 - Vapor Species density profile for $\Delta IW = 3$ was created using VapoRock-Basalt.ipynb
Figure 2 - Vapor Species partial pressure profiles for all fo2 values, was created using VapoRock-Basalt.ipynb
Figure 3 - Liquid Species density profiles for all fo2 values, was created using VapoRock-Basalt.ipynb
Figure 4 - Elemental abudence profiles for all fo2 values, was created using VapoRock-Basalt.ipynb
Figure 5 - TP plot of atompshere outgassed by the magma ocean, was created using VapoRock-Basalt.ipynb
Figure 6 - Partial pressure for each vapor species for all fo2 values, was created using VapoRock-Basalt.ipynb
Figure 7 - Vapor Species density profiles for all fo2 values at 1600K, was created using VapoRock-Basalt.ipynb
Figure 8 - Vapor Species density profiles for all fo2 values at 2200K, was created using VapoRock-Basalt.ipynb
Figure 9 - Vapor Species density profiles for all fo2 values at 2800K, was created using VapoRock-Basalt.ipynb
Figure 10 - Vapor Species density profiles for $\Delta IW = -2$ at 1600,2200 and 2800K, was created using VapoRock-Basalt.ipynb
Figure 11 - Liquid Species density profiles for all fo2 values at 1600K, was created using VapoRock-Basalt.ipynb

Figure 12 - Liquid Species density profiles for all fo2 values at 2200K, was created using VapoRock-Basalt.ipynb
Figure 13 - Liquid Species density profiles for all fo2 values at 2800K, was created using VapoRock-Basalt.ipynb
Figure 14 - Liquid Species density profiles for $\Delta IW = -2$ at 1600,2200 and 2800K, was created using VapoRock-Basalt.ipynb
Figure 15 - Elemental abundance profiles for all fo2 values at 1600K, was created using VapoRock-Basalt.ipynb
Figure 16 - Elemental abundance profiles for all fo2 values at 2200K, was created using VapoRock-Basalt.ipynb
Figure 17 - Elemental abundance profiles for all fo2 values at 2800K, was created using VapoRock-Basalt.ipynb
Figure 18 - Elemental abundance profiles for $\Delta IW = -2$ at 1600,2200 and 2800K, was created using VapoRock-Basalt.ipynb
Figure 19 - Partial pressure profiles for all fo2 values at 1600K, was created using VapoRock-Basalt.ipynb
Figure 20 - Partial pressure profiles for all fo2 values at 2200K, was created using VapoRock-Basalt.ipynb
Figure 21 - Partial pressure profiles for all fo2 values at 2800K, was created using VapoRock-Basalt.ipynb
Figure 22 - Partial pressure profiles for $\Delta IW = -2$ at 1600,2200 and 2800K, was created using VapoRock-Basalt.ipynb
Figure 23 - Partial pressure profiles for all fo2 values and temperatures for Al species, was created using VapoRock-Basalt.ipynb
Figure 24 - Partial pressure profiles for all fo2 values and temperatures for Ca species, was created using VapoRock-Basalt.ipynb
Figure 25 - Partial pressure profiles for all fo2 values and temperatures for Fe species, was created using VapoRock-Basalt.ipynb
Figure 26 - Partial pressure profiles for all fo2 values and temperatures for Mg species, was created using VapoRock-Basalt.ipynb
Figure 27 - Partial pressure profiles for all fo2 values and temperatures for Na species, was created using VapoRock-Basalt.ipynb
Figure 28 - Partial pressure profiles for all fo2 values and temperatures for O species, was created using VapoRock-Basalt.ipynb
Figure 29 - Partial pressure profiles for all fo2 values and temperatures for Si species, was created using VapoRock-Basalt.ipynb

4.3 List 3 - Komatiite plots

Figure 1 - Vapor Species density profile for $\Delta IW = 3$ was created using VapoRock-Komatiite.ipynb
Figure 2 - Vapor Species partial pressure profiles for all fo2 values, was created using VapoRock-Komatiite.ipynb
Figure 3 - Liquid Species density profiles for all fo2 values, was created using VapoRock-Komatiite.ipynb
Figure 4 - Elemental abudence profiles for all fo2 values, was created using

VapoRock-Komatiite.ipynb
Figure 5 - TP plot of atompshere outgassed by the magma ocean, was created using VapoRock-Komatiite.ipynb
Figure 6 - Partial pressure for each vapor species for all fo2 values, was created using VapoRock-Komatiite.ipynb
Figure 7 - Vapor Species density profiles for all fo2 values at 1600K, was created using VapoRock-Komatiite.ipynb
Figure 8 - Vapor Species density profiles for all fo2 values at 2200K, was created using VapoRock-Komatiite.ipynb
Figure 9 - Vapor Species density profiles for all fo2 values at 2800K, was created using VapoRock-Komatiite.ipynb
Figure 10 - Vapor Species density profiles for $\Delta IW = -2$ at 1600,2200 and 2800K, was created using VapoRock-Komatiite.ipynb
Figure 11 - Liquid Species density profiles for all fo2 values at 1600K, was created using VapoRock-Komatiite.ipynb
Figure 12 - Liquid Species density profiles for all fo2 values at 2200K, was created using VapoRock-Komatiite.ipynb
Figure 13 - Liquid Species density profiles for all fo2 values at 2800K, was created using VapoRock-Komatiite.ipynb
Figure 14 - Liquid Species density profiles for $\Delta IW = -2$ at 1600,2200 and 2800K, was created using VapoRock-Komatiite.ipynb
Figure 15 - Elemental abundance profiles for all fo2 values at 1600K, was created using VapoRock-Komatiite.ipynb
Figure 16 - Elemental abundance profiles for all fo2 values at 2200K, was created using VapoRock-Komatiite.ipynb
Figure 17 - Elemental abundance profiles for all fo2 values at 2800K, was created using VapoRock-Komatiite.ipynb
Figure 18 - Elemental abundance profiles for $\Delta IW = -2$ at 1600,2200 and 2800K, was created using VapoRock-Komatiite.ipynb
Figure 19 - Partial pressure profiles for all fo2 values at 1600K, was created using VapoRock-Komatiite.ipynb
Figure 20 - Partial pressure profiles for all fo2 values at 2200K, was created using VapoRock-Komatiite.ipynb
Figure 21 - Partial pressure profiles for all fo2 values at 2800K, was created using VapoRock-Komatiite.ipynb
Figure 22 - Partial pressure profiles for $\Delta IW = -2$ at 1600,2200 and 2800K, was created using VapoRock-Komatiite.ipynb
Figure 23 - Partial pressure profiles for all fo2 values and temperatures for Al species, was created using VapoRock-Komatiite.ipynb
Figure 24 - Partial pressure profiles for all fo2 values and temperatures for Ca species, was created using VapoRock-Komatiite.ipynb
Figure 25 - Partial pressure profiles for all fo2 values and temperatures for Fe species, was created using VapoRock-Komatiite.ipynb
Figure 26 - Partial pressure profiles for all fo2 values and temperatures for Mg species, was created using VapoRock-BSE.ipynb
Figure 27 - Partial pressure profiles for all fo2 values and temperatures for Na

species, was created using VapoRock-Komatiite.ipynb
Figure 28 - Partial pressure profiles for all fo2 values and temperatures for O species, was created using VapoRock-Komatiite.ipynb
Figure 29 - Partial pressure profiles for all fo2 values and temperatures for Si species, was created using VapoRock-Komatiite.ipynb

4.4 List 4 - Mercury plots

Figure 1 - Vapor Species density profile for $\Delta IW = 3$ was created using VapoRock-Komatiite.ipynb
Figure 2 - Vapor Species partial pressure profiles for all fo2 values, was created using VapoRock-Mercury.ipynb
Figure 3 - Liquid Species density profiles for all fo2 values, was created using VapoRock-Mercury.ipynb
Figure 4 - Elemental abudence profiles for all fo2 values, was created using VapoRock-Mercury.ipynb
Figure 5 - TP plot of atompshere outgassed by the magma ocean, was created using VapoRock-Mercury.ipynb
Figure 6 - Partial pressure for each vapor species for all fo2 values, was created using VapoRock-Mercury.ipynb
Figure 7 - Vapor Species density profiles for all fo2 values at 1600K, was created using VapoRock-Mercury.ipynb
Figure 8 - Vapor Species density profiles for all fo2 values at 2200K, was created using VapoRock-Mercury.ipynb
Figure 9 - Vapor Species density profiles for all fo2 values at 2800K, was created using VapoRock-Mercury.ipynb
Figure 10 - Vapor Species density profiles for $\Delta IW = -2$ at 1600,2200 and 2800K, was created using VapoRock-Mercury.ipynb
Figure 11 - Liquid Species density profiles for all fo2 values at 1600K, was created using VapoRock-Mercury.ipynb
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Figure 15 - Elemental abundance profiles for all fo2 values at 1600K, was created using VapoRock-Mercury.ipynb
Figure 16 - Elemental abundance profiles for all fo2 values at 2200K, was created using VapoRock-Mercury.ipynb
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Figure 19 - Partial pressure profiles for all fo2 values at 1600K, was created using VapoRock-Mercury.ipynb

Figure 20 - Partial pressure profiles for all fo2 values at 2200K, was created using VapoRock-Mercury.ipynb
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Figure 23 - Partial pressure profiles for all fo2 values and temperatures for Al species, was created using VapoRock-Mercury.ipynb
Figure 24 - Partial pressure profiles for all fo2 values and temperatures for Ca species, was created using VapoRock-Mercury.ipynb
Figure 25 - Partial pressure profiles for all fo2 values and temperatures for Fe species, was created using VapoRock-Mercury.ipynb
Figure 26 - Partial pressure profiles for all fo2 values and temperatures for Mg species, was created using VapoRock-BSE.ipynb
Figure 27 - Partial pressure profiles for all fo2 values and temperatures for Na species, was created using VapoRock-Mercury.ipynb
Figure 28 - Partial pressure profiles for all fo2 values and temperatures for O species, was created using VapoRock-Mercury.ipynb
Figure 29 - Partial pressure profiles for all fo2 values and temperatures for Si species, was created using VapoRock-Mercury.ipynb

4.5 List 5 - TP plots, spectra and chemistry

Figure 1 - Chemistry abundance profile for Basalt fo2=0, created using fastchem
Figure 2 - Chemistry abundance profile for Basalt fo2=1, created using fastchem
Figure 3 - Chemistry abundance profile for Basalt fo2=-1, created using fastchem
Figure 4 - Chemistry abundance profile for Basalt fo2=2, created using fastchem
Figure 5 - Chemistry abundance profile for Basalt fo2=-2, created using fastchem
Figure 6 - Chemistry abundance profile for BSE fo2=0, created using fastchem
Figure 7 - Chemistry abundance profile for BSE fo2=1, created using fastchem
Figure 8 - Chemistry abundance profile for BSE fo2=-1, created using fastchem
Figure 9 - Chemistry abundance profile for BSE fo2=2, created using fastchem
Figure 10 - Chemistry abundance profile for BSE fo2=-2, created using fastchem
Figure 11 - Chemistry abundance profile for Komatiite fo2=0, created using fastchem
Figure 12 - Chemistry abundance profile for Komatiite fo2=1, created using fastchem
Figure 13 - Chemistry abundance profile for Komatiite fo2=-1, created using fastchem
Figure 14 - Chemistry abundance profile for Komatiite fo2=2, created using fastchem
Figure 15 - Chemistry abundance profile for Komatiite fo2=-2, created using fastchem
Figure 16 - Chemistry abundance profile for Mercury fo2=0, created using fastchem
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fastchem
Figure 18 - Chemistry abundance profile for Mercury fo2=-1, created using fastchem
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Figure 20 - Chemistry abundance profile for Mercury fo2=-2, created using fastchem
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Figure 25 - Chemistry abundance profile for Basalt vs Komatiite, I cant find what the fo2 values. Was created using Chemistry abudance plots.ipynb
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Figure 33 - Area under the emission hump at 0.75 μm for each composition for $fo2 = -2$. Was created using Spectra hump at 0.75 microns.ipynb
Figure 34 - TP summary plots for all compositions and fo2 values from -2 to 2. Was created using TP Summary plots.ipynb

References

[1] L. Schaefer and B. Fegley, "Chemistry of silicate atmospheres of evaporating super-earths," *The Astrophysical Journal*, vol. 703, p. L113, sep 2009.

[2] A. S. Wolf, N. Jäggi, P. A. Sossi, and D. J. Bower, "VapoRock: Thermodynamics of vaporized silicate melts for modeling volcanic outgassing and magma ocean atmospheres," *The Astrophysical Journal*, vol. 947, p. 64, apr 2023.

[3] L. Schaefer and B. Fegley, "A thermodynamic model of high temperature lava vaporization on io," *Icarus*, vol. 169, no. 1, pp. 216–241, 2004. Special Issue: Io after Galileo.

[4] J. W. Morgan and E. Anders, "Chemical composition of earth, venus, and mercury," *Proceedings of the National Academy of Sciences*, vol. 77, no. 12, pp. 6973–6977, 1980.

[5] DACE, "Opacity visualization," 2023. Last Accessed 6th September 2023.