S5_Testing_Magmasat

September 8, 2020

1 This notebook tests the outputs of VESIcal to Magmasat

- Test 1 compares saturation pressures published by Bennett et al. (2019; Nature; https://www.nature.com/articles/s41586-019-1448-0?draft=collection), who used the Mac App to those calculated using VESIcal
- Test 2 compares the isobars shown in Fig. 14 of Ghiorso and Gualda (2015) to those calculated with VESIcal. We note that although the figure caption says that the composition of the Late Bishop Tuff was used, their isobars are best recreated using the composition of the Early Bishop Tuff.
- Test 3 compares X_{H_2O} calculated using the "Fluid+magma from bulk composition" option of the web app with the calculate_equilibrium_fluid_comp function of VESIcal for a set of synthetic inputs.

[1]:
```
import sys
sys.path.insert(0, '../../../../')

import VESIcal as v
import matplotlib.pyplot as plt
import numpy as np
import pandas as pd
from IPython.display import display, HTML
import pandas as pd
import matplotlib as mpl
import seaborn as sns
%matplotlib inline
from sklearn.linear_model import LinearRegression
from sklearn.metrics import r2_score
```

[2]:
```
sns.set(style="ticks", context="poster",rc={"grid.linewidth": 1,"xtick.major.
↪width": 1,"ytick.major.width": 1, 'patch.edgecolor': 'black'})
plt.style.use("seaborn-colorblind")
plt.rcParams["font.family"] = 'arial'
plt.rcParams["font.size"] =12
plt.rcParams["mathtext.default"] = "regular"
plt.rcParams["mathtext.fontset"] = "dejavusans"
plt.rcParams['patch.linewidth'] = 1
plt.rcParams['axes.linewidth'] = 1
plt.rcParams["xtick.direction"] = "in"
```

```
plt.rcParams["ytick.direction"] = "in"
plt.rcParams["ytick.direction"] = "in"
plt.rcParams["xtick.major.size"] = 6 # Sets length of ticks
plt.rcParams["ytick.major.size"] = 4 # Sets length of ticks
plt.rcParams["ytick.labelsize"] = 12 # Sets size of numbers on tick marks
plt.rcParams["xtick.labelsize"] = 12 # Sets size of numbers on tick marks
plt.rcParams["axes.titlesize"] = 14 # Overall title
plt.rcParams["axes.labelsize"] = 14 # Axes labels
plt.rcParams["legend.fontsize"]= 14
```

2 Test 1 - Comparing saturation pressures from Bennett et al., 2019 and VESIcal

[3]:
```
myfile = v.ExcelFile('S5_Testing_Magmasat.xlsx', ␣
↪sheet_name='Bennett_et_al_2019', input_type='wtpercent')
data = myfile.data
satPs_wtemps_Magmasat= myfile.calculate_saturation_pressure(temperature="Temp")
```

```
Calculating sample 1
Calculating sample 2
Calculating sample 3
Calculating sample 4
Calculating sample 5
Calculating sample 6
Calculating sample 7
Calculating sample 8
Calculating sample 9
Calculating sample 10
Calculating sample 11
Calculating sample 12
Calculating sample 13
Calculating sample 14
Calculating sample 15
Calculating sample 16
Calculating sample 17
Calculating sample 18
Calculating sample 19
Calculating sample 20
Calculating sample 21
Calculating sample 22
Calculating sample 23
Calculating sample 24
Calculating sample 25
Calculating sample 26
Calculating sample 27
Calculating sample 28
```

```
Calculating sample 29
Calculating sample 30
Calculating sample 31
Calculating sample 32
Calculating sample 33
Calculating sample 34
Calculating sample 35
Calculating sample 36
Calculating sample 37
Calculating sample 38
Calculating sample 39
Calculating sample 40
Calculating sample 41
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Calculating sample 66
Calculating sample 67
Calculating sample 68
Calculating sample 69
Calculating sample 70
Calculating sample 71
Calculating sample 72
Calculating sample 73
Calculating sample 74
Calculating sample 75
Calculating sample 76
```

```
Calculating sample 77
Calculating sample 78
Calculating sample 79
Calculating sample 80
Calculating sample 81
Calculating sample 82
Calculating sample 83
Calculating sample 84
Calculating sample 85
Calculating sample 86
Calculating sample 87
Calculating sample 88
Calculating sample 89
Calculating sample 90
Calculating sample 91
Calculating sample 92
Calculating sample 93
Calculating sample 94
Calculating sample 95
Calculating sample 96
Calculating sample 97
Calculating sample 98
Calculating sample 99
Calculating sample 100
Calculating sample 101
Calculating sample 102
Calculating sample 103
Calculating sample 104
Calculating sample 105
Done!
```

[4]:

```
# This calculating a Linear regression, and plots the spreadsheet outputs␣
↪against VESICal outputs
X_syn1=10*satPs_wtemps_Magmasat['Press'].values.reshape(-1, 1)
Y_syn1=satPs_wtemps_Magmasat['SaturationP_bars_VESIcal'].values.reshape(-1, 1)
lr=LinearRegression()
lr.fit(X_syn1,Y_syn1)
Y_pred_syn1=lr.predict(X_syn1)

fig, (ax1, ax2) = plt.subplots(1,2, figsize=(12,5)) # adjust dimensions of␣
↪figure here

ax1.set_xlabel('P$_{Sat}$ Bennett et al. (2019; bar)',  fontsize=14)
ax1.set_ylabel('P$_{Sat}$ VESIcal (bar)', fontsize=14)
ax1.plot(X_syn1,Y_pred_syn1, color='red', linewidth=0.5, zorder=1) # This plots␣
↪the best fit line
```

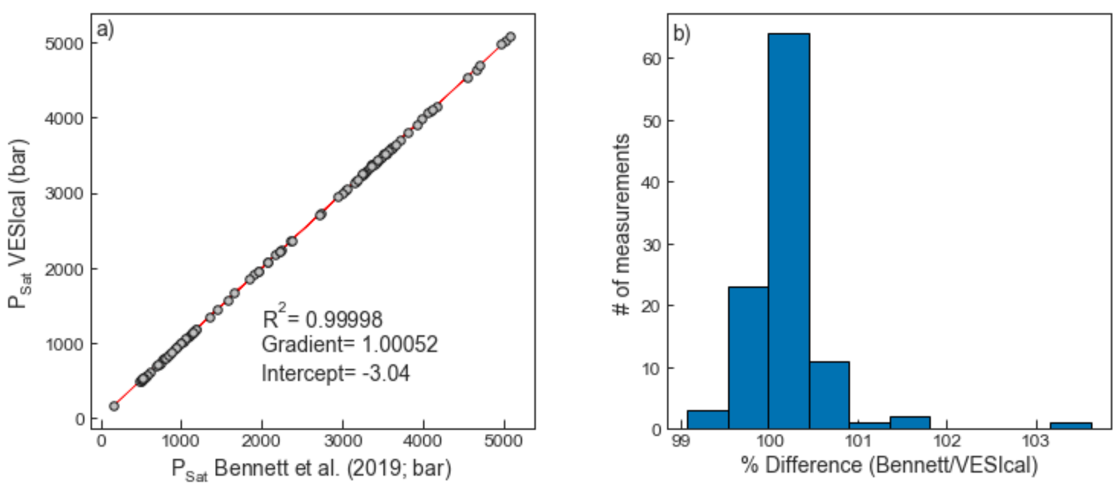
```python
ax1.scatter(X_syn1, Y_syn1,  s=30, edgecolors='k', facecolors='silver',␣
↪marker='o', zorder=5)
# This bit plots the regression parameters on the graph
I='Intercept= ' + str(np.round(lr.intercept_, 2))[1:-1]
G='Gradient= '  + str(np.round(lr.coef_, 5))[2:-2]
R='R$^2$= ' +  str(np.round(r2_score(Y_syn1, Y_pred_syn1), 5))


ax1.text(2000, 500, I, fontsize=14)
ax1.text(2000, 900, G, fontsize=14)
ax1.text(2000, 1200, R, fontsize=14)

############## Histogram showing difference as a %
ax2.set_xlabel('% Difference (Bennett/VESIcal)',  fontsize=14)
ax2.set_ylabel('# of measurements',  fontsize=14)
ax2.hist(100*10*satPs_wtemps_Magmasat['Press']/
↪satPs_wtemps_Magmasat['SaturationP_bars_VESIcal'])
plt.subplots_adjust(left=0.125, bottom=None, right=0.9, top=None, wspace=0.3,␣
↪hspace=None)

ax1.text(-50, 5100, 'a)', fontsize=14)
ax2.text(98.9, 63, 'b)', fontsize=14)

fig.savefig('Magmasat_Test1.png', transparent=True)
```



3 Test 2 - Recreating isobars in Fig. 14 of Ghioso and Gualda, 2015

[5]:
```
myfile_Isobars= v.ExcelFile('S5_Testing_Magmasat.xlsx',  ␣
↪input_type='wtpercent', sheet_name='Isobars')
data_Isobars = myfile_Isobars.data
```

[6]:
```
"""To get composition from a specific sample in the input data:"""
# Note, - In Ghiorso and Gualda, 2015, it says that the isobars in Fig. 14 are␣
↪calculated using the Late Bishop Tuff composition.
#However, we get a far better match if we use the Early Bishop Tuff␣
↪composition, so presume this was a typo in the original paper.
SampleName_EarlyBT = 'EarlyBishop'

bulk_comp_EarlyBT = myfile_Isobars.get_sample_oxide_comp(SampleName_EarlyBT,␣
↪norm='standard')
"""Define all variables to be passed to the function for calculating isobars␣
↪and isopleths"""
"""Define the temperature in degrees C"""
temperature = 750

"""Define a list of pressures in bars:"""
pressures = [1000, 2000, 3000]

isobars_EarlyBT, isopleths_EarlyBT = v.
↪calculate_isobars_and_isopleths(sample=bulk_comp_EarlyBT, points=51,␣
↪smooth_isobars=False,
                                            temperature=temperature,
                                            pressure_list=pressures,
                                            isopleth_list=[0, 0.01, 0.05, 0.1,␣
↪0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1],
                                            print_status=True).result
smoothed_isobars = v.smooth_isobars_and_isopleths(isobars_EarlyBT)
```

```
Calculating isobar at 1000 bars
Calculating isopleth at XH2Ofluid = 0
Calculating isopleth at XH2Ofluid = 0.01
Calculating isopleth at XH2Ofluid = 0.05
Calculating isopleth at XH2Ofluid = 0.1
Calculating isopleth at XH2Ofluid = 0.2
Calculating isobar control point at XH2Ofluid = 0.25
Calculating isopleth at XH2Ofluid = 0.3
Calculating isopleth at XH2Ofluid = 0.4
Calculating isopleth at XH2Ofluid = 0.5
Calculating isopleth at XH2Ofluid = 0.6
Calculating isopleth at XH2Ofluid = 0.7
Calculating isobar control point at XH2Ofluid = 0.75
```

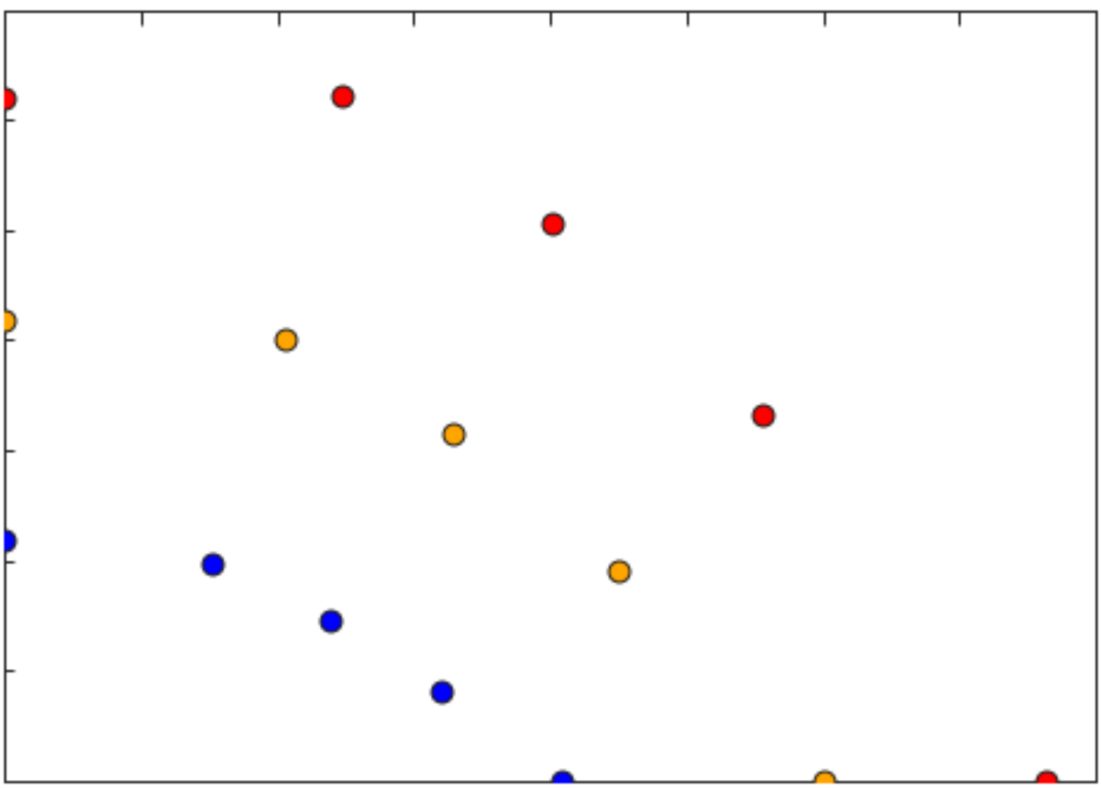
```
Calculating isopleth at XH2Ofluid = 0.8
Calculating isopleth at XH2Ofluid = 0.9
Calculating isopleth at XH2Ofluid = 1
Calculating isobar at 2000 bars
Calculating isopleth at XH2Ofluid = 0
Calculating isopleth at XH2Ofluid = 0.01
Calculating isopleth at XH2Ofluid = 0.05
Calculating isopleth at XH2Ofluid = 0.1
Calculating isopleth at XH2Ofluid = 0.2
Calculating isobar control point at XH2Ofluid = 0.25
Calculating isopleth at XH2Ofluid = 0.3
Calculating isopleth at XH2Ofluid = 0.4
Calculating isopleth at XH2Ofluid = 0.5
Calculating isopleth at XH2Ofluid = 0.6
Calculating isopleth at XH2Ofluid = 0.7
Calculating isobar control point at XH2Ofluid = 0.75
Calculating isopleth at XH2Ofluid = 0.8
Calculating isopleth at XH2Ofluid = 0.9
Calculating isopleth at XH2Ofluid = 1
Calculating isobar at 3000 bars
Calculating isopleth at XH2Ofluid = 0
Calculating isopleth at XH2Ofluid = 0.01
Calculating isopleth at XH2Ofluid = 0.05
Calculating isopleth at XH2Ofluid = 0.1
Calculating isopleth at XH2Ofluid = 0.2
Calculating isobar control point at XH2Ofluid = 0.25
Calculating isopleth at XH2Ofluid = 0.3
Calculating isopleth at XH2Ofluid = 0.4
Calculating isopleth at XH2Ofluid = 0.5
Calculating isopleth at XH2Ofluid = 0.6
Calculating isopleth at XH2Ofluid = 0.7
Calculating isobar control point at XH2Ofluid = 0.75
Calculating isopleth at XH2Ofluid = 0.8
Calculating isopleth at XH2Ofluid = 0.9
Calculating isopleth at XH2Ofluid = 1
Done!
```

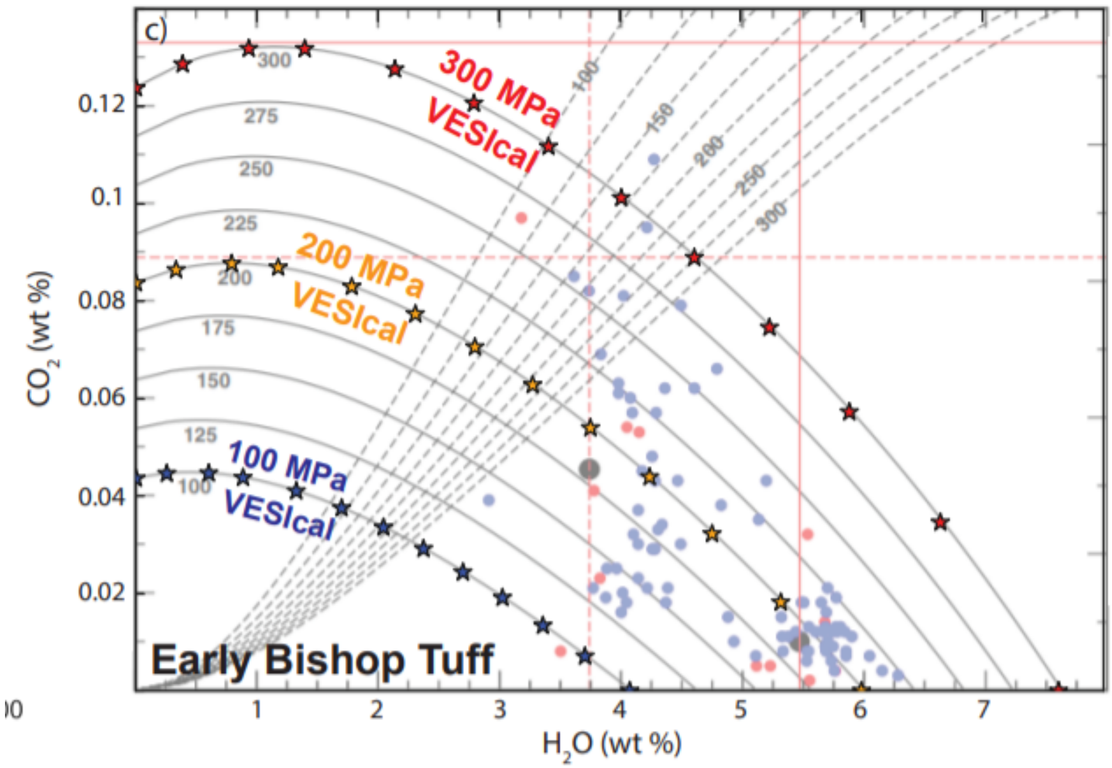
```
../../../../VESIcal.py:1720: RuntimeWarning: temperature (750.0 oC) is outside
the calibration range of the MagmaSat model (800.0-1400.0 oC).
  w.warn(self.calib_check,RuntimeWarning)
```

[7]:
```
# Overlaid in adobe illustator - pasted below
index1000bars_Early=isobars_EarlyBT["Pressure"]==1000
index2000bars_Early=isobars_EarlyBT["Pressure"]==2000
index3000bars_Early=isobars_EarlyBT["Pressure"]==3000
H2O=isobars_EarlyBT["H2O_liq"]
CO2=isobars_EarlyBT["CO2_liq"]
fig, ax1 = plt.subplots(figsize = (6*1.38,4.*1.50))
```

```
plt.scatter(H2O[index1000bars_Early], CO2[index1000bars_Early], s=80,␣
 ↪edgecolors='k', facecolors='blue', marker='o', zorder=5, label='100 Mpa')
plt.scatter(H2O[index2000bars_Early], CO2[index2000bars_Early], s=80,␣
 ↪edgecolors='k', facecolors='orange', marker='o', zorder=5, label='200 Mpa')
plt.scatter(H2O[index3000bars_Early], CO2[index3000bars_Early],  s=80,␣
 ↪edgecolors='k', facecolors='red', marker='o', zorder=5, label='300 Mpa')

plt.xlim([0, 8])
plt.ylim([0, 0.14])
ax1.yaxis.tick_left()
ax1.xaxis.tick_top()
plt.xticks([0, 1, 2, 3, 4, 5, 6, 7])
plt.yticks([0, 0.02, 0.04, 0.06, 0.08, 0.1, 0.12, 0.14])
plt.setp(ax1.get_xticklabels(), visible=False)
plt.setp(ax1.get_yticklabels(), visible=False)
fig.savefig('Magmasat_isobars_EarlyBishopTuff.svg', transparent=True)
```





4 Test 3

- compares X_{H_2O} calculated using the "Fluid+magma from bulk composition" option of the web app with the calculate_equilibrium_fluid_comp function of VESIcal

[8]:
```
myfile_FM= v.ExcelFile('S5_Testing_Magmasat.xlsx', ␣
↪sheet_name='Calculate_Eq_Fluid', input_type='wtpercent') # Loads outputs␣
↪from web app.
data_FM = myfile_FM.data
eqfluid_wtemps = myfile_FM.calculate_equilibrium_fluid_comp(temperature='Temp',␣
↪pressure='Press')
```

[11]:
```
# This calculating a Linear regression, and plots the spreadsheet outputs␣
↪against VESICal outputs
X_syn1=eqfluid_wtemps['H2Ofluidfrac_web'].values.reshape(-1, 1)
Y_syn1=eqfluid_wtemps['XH2O_fl_VESIcal'].values.reshape(-1, 1)
lr=LinearRegression()
lr.fit(X_syn1,Y_syn1)
Y_pred_syn1=lr.predict(X_syn1)

fig, (ax1, ax2) = plt.subplots(1,2, figsize=(12,5)) # adjust dimensions of␣
↪figure here

ax1.set_xlabel('X$_{H_{2}O}$ Web App',  fontsize=14)
```

```
ax1.set_ylabel('X$_{H_{2}O}$ VESIcal', fontsize=14)
ax1.plot(X_syn1,Y_pred_syn1, color='red', linewidth=0.5, zorder=1) # This plots␣
↪the best fit line
ax1.scatter(X_syn1, Y_syn1,  s=30, edgecolors='k', facecolors='silver',␣
↪marker='o', zorder=5)
# This bit plots the regression parameters on the graph
I='Intercept= ' + str(np.round(lr.intercept_, 2))[1:-1]
G='Gradient= '  + str(np.round(lr.coef_, 3))[2:-2]
R='R$^2$= ' +  str(np.round(r2_score(Y_syn1, Y_pred_syn1), 3))


ax1.text(0.9, 0.77, I, fontsize=14)
ax1.text(0.9, 0.79, G, fontsize=14)
ax1.text(0.9, 0.81, R, fontsize=14)
ax1.tick_params(axis="x", labelsize=12)
ax1.tick_params(axis="y", labelsize=12)
############## Histogram showing difference as a %
ax2.set_xlabel('Absolute Difference',  fontsize=14)
ax2.set_ylabel('# of measurements',  fontsize=14)
X_syn1=eqfluid_wtemps['H2Ofluidfrac_web'].values.reshape(-1, 1)
Y_syn1=eqfluid_wtemps['XH2O_fl_VESIcal'].values.reshape(-1, 1)
ax2.set_xlim([-0.005, 0.005])
ax2.set_xticks([-0.005, 0, 0.005])
ax2.hist(eqfluid_wtemps['H2Ofluidfrac_web']-eqfluid_wtemps['XH2O_fl_VESIcal'])
plt.subplots_adjust(left=0.125, bottom=None, right=0.9, top=None, wspace=0.3,␣
↪hspace=None)
ax1.text(0.75, 0.99, 'a)', fontsize=14)
ax2.text(-0.0047, 3, 'b)', fontsize=14)
fig.savefig('Magmasat_Test2.png', transparent=True)
#fig.suptitle('Test 2 - Comparing dissolved H$_2$O contents', fontsize=15)
```