

THERMOCALC Short Course (São Paulo): 2006

Day 2 Practical: Answers

1. Proyer eclogite

- (a) Partial THERMOCALC output for a big T range, then a small one, using the $\text{Fe}^{3+} = 0$ value for $x(\text{cpx})$:

TC	600	650	700	750	800	850	900	950	1000		
av P	30.1	29.7	29.3	28.9	28.4	27.8	27.3	26.6	25.9		
sd	2.18	2.44	3.14	4.08	5.15	6.31	7.53	8.79	10.09		
sigfit	1.2	1.2	1.5	1.8	2.1	2.4	2.7	3.0	3.3		

TC	600	610	620	630	640	650	660	670	680	690	700
av P	29.9	29.9	29.8	29.7	29.6	29.5	29.3	29.2	29.0	28.9	28.8
sd	2.23	2.23	2.26	2.31	2.39	2.48	2.61	2.75	2.91	3.09	3.30
sigfit	1.2	1.2	1.2	1.2	1.2	1.2	1.3	1.3	1.4	1.5	1.5

Note the minimum in σ_{fit} around 635°C, meaning that \overline{PT} should work (as it does):

T = 611C, sd = 56, P = 29.9 kbars, sd = 2.5, cor = -0.129, sigfit = 1.34

The reason why this T does not correspond with the g-cpx T for this $x(\text{cpx})$ is that the (relatively-large) default activity uncertainties used by THERMOCALC effectively downweight such inherently uncertain equilibria.

- (b) Partial THERMOCALC output using the Mössbauer Fe^{3+} value in cpx:

T = 620C, sd = 42, P = 30.7 kbars, sd = 1.9, cor = -0.104, sigfit = 0.37

Comparing this result with the one with the “wrong” one above, it is amazing (and good) how similar the results are (as Proyer emphasises). The main difference is that the uncertainties are much smaller (and σ_{fit} is smaller too).

Now, looking at the diagnostics, nothing stands out as bad:

	P	sd(P)	T	sd(T)	cor	fit	e*	hat
gr	30.63	1.94	629	46	-0.139	0.27	0.43	0.18
alm	30.76	1.94	620	42	-0.102	0.37	-0.08	0.01
py	30.56	1.97	601	64	0.088	0.29	0.30	0.77
di	30.72	1.93	626	45	-0.102	0.29	-0.30	0.06
hed	30.79	1.95	620	42	-0.099	0.36	0.17	0.03
mu	30.82	2.53	620	43	-0.198	0.37	0.03	0.26
cel	30.94	3.14	619	44	-0.277	0.37	-0.05	0.63
ta	30.75	1.95	621	43	-0.078	0.37	0.03	0.02
tats	30.73	1.93	620	42	-0.104	0.37	-0.05	0.00
ky	30.73	1.93	620	42	-0.104	0.37	0	0
coe	30.73	1.93	620	42	-0.104	0.37	0	0
H2O	30.73	1.93	620	42	-0.104	0.37	0	0

Omitting pyrope:

T = 575C, sd = 78, P = 30.3 kbars, sd = 1.9, cor = 0.205, sigfit = 0.08

- (c) \overline{PT} with H₂O omitted—look at the uncertainties! The reactions involving the end-members of the hydrous phases, with H₂O, are what constrain the \overline{PT}

T = 680C, sd = 111, P = 33.9 kbars, sd = 5.8, cor = 0.832, sigfit = 0.09

For $a_{\text{H}_2\text{O}} = 1$ (repeated from above)

T = 620C, sd = 42, P = 30.7 kbars, sd = 1.9, cor = -0.104, sigfit = 0.37

For $a_{\text{H}_2\text{O}} = 0.5$

T = 574C, sd = 38, P = 28.3 kbars, sd = 1.8, cor = -0.175, sigfit = 0.68

For $a_{\text{H}_2\text{O}} = 0.2$

T = 520C, sd = 36, P = 25.6 kbars, sd = 1.8, cor = -0.253, sigfit = 1.08

If one accepts $a_{\text{H}_2\text{O}} = 0.5$ as a likely lower limit (for fluid-present conditions), this is not a major dependence of PT on $a_{\text{H}_2\text{O}}$. Note that σ_{fit} increases as $a_{\text{H}_2\text{O}}$ decreases.

- (d) See attached (actually not drawn yet!).

2. RP13

- (a) Data “as is”: Note that the σ_{fit} are large, suggesting a problem with the data:

Average pressures for RP13 (for $x(\text{CO}_2) = 0.25$)

TC	450	470	490	510	530	550	570	590	610	630	650
av P	3.8	4.7	5.5	6.3	7.1	7.9	8.7	9.5	10.3	11.1	11.9
sd	1.14	1.01	0.90	0.80	0.74	0.72	0.74	0.80	0.89	0.99	1.11
sigfit	4.9	4.2	3.6	3.2	2.9	2.7	2.7	2.9	3.1	3.4	3.7

So let's look at the diagnostics: paragonite stands out...

	P	sd	fit	e*	hat	a(obs)	a(calc)	x	y
mu	7.79	0.73	2.68	-0.9	0.02	0.740	0.674	0.59	5.60
cel	7.88	0.72	2.71	0.9	0.00	0.0117	0.0260	-0.04	-1.29
fcel	7.88	0.72	2.72	0.5	0.00	0.00260	0.0173	-0.02	-0.64
pa	8.62	0.56	1.92	6.0	0.20	0.217	0.653	1.68	7.26
phl	7.74	0.72	2.63	2.1	0.06	0.0670	0.135	-0.91	-9.32
ann	7.73	0.70	2.58	2.9	0.05	0.0150	0.0652	-0.82	-9.36
east	7.92	0.72	2.69	-1.3	0.02	0.0660	0.0429	-0.49	-2.57
py	7.89	0.72	2.72	0.5	0.00	0.00152	0.00219	0.25	1.46
gr	7.87	0.72	2.71	0.6	0.01	0.0160	0.0212	-0.40	-3.71
alm	7.84	0.72	2.69	-0.9	0.01	0.240	0.210	0.33	3.52
clin	7.90	0.71	2.67	1.6	0.00	0.0560	0.0977	0.16	-0.31
daph	7.88	0.72	2.72	0.1	0.00	0.0105	0.0111	-0.20	-1.68
ames	7.72	0.68	2.51	-3.2	0.03	0.0610	0.0206	0.68	8.52
cz	7.84	0.73	2.70	-0.6	0.01	0.650	0.630	0.42	3.93
an	7.48	0.93	2.66	1.4	0.48	0.480	0.538	-2.60	-21.90
ab	8.02	0.70	2.59	-1.6	0.01	0.700	0.645	-0.46	-1.97
cc	7.88	0.72	2.72	0	0	1.00	1.00	0	0
q	7.88	0.72	2.72	0	0	1.00	1.00	0	0

In fact, it should not have been included as it is the end-member associated with the “other” side of the muscovite-paragonite solvus. (Moreover the analysis does not look that good with $\text{Na}+\text{K} = 0.85\dots$).

- (b) Omitting the obvious outlier, paragonite

Average pressures for RP13 (for $x(\text{CO}_2) = 0.25$)

TC	450	470	490	510	530	550	570	590	610	630	650
av P	5.1	5.9	6.6	7.4	8.2	9.0	9.8	10.6	11.4	+	+
sd	0.91	0.75	0.59	0.46	0.37	0.37	0.47	0.62	0.81	1.02	1.26
sigfit	3.7	2.9	2.3	1.7	1.3	1.3	1.6	2.0	2.6	3.1	3.8

- (c) Omitting H_2O and CO_2 gives an excellent result, independent of the fluid composition:

Average pressures for RP13

TC	450	470	490	510	530	550	570	590	610	630	650
av P	7.0	7.4	7.7	8.1	8.5	8.9	9.2	9.6	10.0	10.4	10.8
sd	0.39	0.39	0.40	0.41	0.43	0.44	0.46	0.49	0.51	0.54	0.57
sigfit	1.2	1.2	1.2	1.2	1.2	1.3	1.3	1.3	1.4	1.4	1.5

Run as a \overline{PT} this gives large uncertainties:

$T = 498\text{C}$, $\text{sd} = 100$, $P = 7.9$ kbars, $\text{sd} = 1.9$, $\text{cor} = 0.972$, $\text{sigfit} = 1.32$

Clearly \overline{P} is a better option—if we have some idea of the metamorphic temperature.

- (d) Looking for the overall minimum in σ_{fit} : x_{CO_2} is the first number

0.1: $T = 522\text{C}$, $\text{sd} = 19$, $P = 8.2$ kbars, $\text{sd} = 1.0$, $\text{cor} = 0.761$, $\text{sigfit} = 2.17$
0.2: $T = 535\text{C}$, $\text{sd} = 14$, $P = 8.5$ kbars, $\text{sd} = 0.7$, $\text{cor} = 0.760$, $\text{sigfit} = 1.52$
0.25: $T = 538\text{C}$, $\text{sd} = 13$, $P = 8.6$ kbars, $\text{sd} = 0.6$, $\text{cor} = 0.760$, $\text{sigfit} = 1.38$
0.3: $T = 539\text{C}$, $\text{sd} = 12$, $P = 8.6$ kbars, $\text{sd} = 0.6$, $\text{cor} = 0.760$, $\text{sigfit} = 1.29$
0.35: $T = 540\text{C}$, $\text{sd} = 12$, $P = 8.7$ kbars, $\text{sd} = 0.6$, $\text{cor} = 0.760$, $\text{sigfit} = 1.22$
0.4: $T = 541\text{C}$, $\text{sd} = 11$, $P = 8.7$ kbars, $\text{sd} = 0.5$, $\text{cor} = 0.760$, $\text{sigfit} = 1.16$
0.45: $T = 541\text{C}$, $\text{sd} = 11$, $P = 8.7$ kbars, $\text{sd} = 0.5$, $\text{cor} = 0.760$, $\text{sigfit} = 1.16$
0.5: $T = 540\text{C}$, $\text{sd} = 11$, $P = 8.7$ kbars, $\text{sd} = 0.5$, $\text{cor} = 0.761$, $\text{sigfit} = 1.17$
0.55: $T = 539\text{C}$, $\text{sd} = 12$, $P = 8.7$ kbars, $\text{sd} = 0.6$, $\text{cor} = 0.761$, $\text{sigfit} = 1.22$
0.6: $T = 537\text{C}$, $\text{sd} = 12$, $P = 8.7$ kbars, $\text{sd} = 0.6$, $\text{cor} = 0.762$, $\text{sigfit} = 1.32$
0.65: $T = 534\text{C}$, $\text{sd} = 14$, $P = 8.7$ kbars, $\text{sd} = 0.7$, $\text{cor} = 0.763$, $\text{sigfit} = 1.46$
0.7: $T = 529\text{C}$, $\text{sd} = 15$, $P = 8.6$ kbars, $\text{sd} = 0.8$, $\text{cor} = 0.764$, $\text{sigfit} = 1.66$

- (e) The “answer” is $T = 540 \pm 25^\circ\text{C}$, $P = 8.7 \pm 1.3$ kbar in a fluid composition range, $x_{\text{CO}_2} = 0.25\text{--}0.62$, with the PT hardly varying across this x_{CO_2} range.

The σ_{fit} is about 1 at the minimum. In fact it was our experience with \overline{PT} on rocks such as this one—with our prejudice that they do represent an equilibrium mineral assemblage—that helped us decide how big the default uncertainties should be (recognising that, for example, if all the activity uncertainties are halved, then the σ_{fit} is doubled, then in this case failing the χ^2 test).

- (f) The garnet-biotite Fe-Mg thermometer gives $420 \pm 160^\circ\text{C}$, so it will have hardly contributed to constraining the T of RP13.