

Release Notes tc350- β

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apologies for the long delay in getting this new version to the release stage (a difficult year for all). In fact quite a lot has been done in the mean time, mainly in the realm of scripting (see the new scripting notes) and general tidying up of the code. There is not much to show for the latter work, but hopefully it will make THERMOCALC easier to maintain into the future.

- the script changes are too numerous to list on this page—see the new scripting notes—but there are several overarching ideas. The main one is that most users rely on (or would prefer to rely more on) scripting to enter information into THERMOCALC, rather than having to input the information interactively. The scripts have evolved to reflect this.
- THERMOCALC will now stop and get you to fix a script that is not understood rather than just continue, ignoring the script, and doing a calculation that may well not be what you intended. Older scriptfiles on users' computers (and on mine) commonly contain scripts that are obsolete. THERMOCALC now helps you clean up your scriptfiles.
- some scripts are now mandatory—in the prefsfile and the scriptfile. Guidance is provided by THERMOCALC about what is involved and what to do about it, if a mandatory script is missing.
- why some things are currently unavailable (or are broken)—when in tc340 they worked—relates to the history of implementing facilities in THERMOCALC. By the end of the 1980s very simple pseudosection calculations were implemented, as long as the equilibria had variance of 2 or less. For these equilibria it was as simple as calculating an equilibrium, then seeing if the equilibrium was 'seen' by the bulk composition. By the mid 90s, higher variance equilibria could be calculated because the solution of an equilibrium was combined with the requirement that the phases could make the bulk composition. The fact that these calculations are rather different meant that there ended up being a confusing duplication of code that handled the two, including making the output. Back in the 90s, rp made no attempt to remove the duplication: the code doing the two different things was kept separate. Inefficient and/or difficult to maintain. The aim now has been to remove the duplication. In this complicated process, some things got broken, and haven't been fixed yet. Be patient, I am working on it!
- **please notify us if things do not working properly or as expected** Let us know if your favourite facility is not available currently or is broken and we will prioritise trying to fix it

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- the script `drawpd`, that gives output in the drfile for manual assembly to run in the drawpd software, now has an optional code: 0 = just P and T ; 1 = P , T , G , H , S , V and ρ . Further codes will be added. Output now also in the csvfile.
- `drawpd no` now gives output in the drfile in Mathematica form, e.g. to use in the contouring code (to be made available shortly). The script `smath` is now defunct (look near the top of the logfile for info on scripts in the scriptfile which are not recognised)
- bulk composition input for pseudosection calculations has been modified, and is still evolving. The script `readbulkinf` (`rbi`) has changed, to allow better input checking. See its form by running a calculation with `printbulkinf`. Using the old `rbi` will cause THERMOCALC to exit.
- if a bulk composition range is provided, for T - X and P - x calculations, by having two `setbulk` lines, the second line can have an optional number at its end giving the number of steps across the range that will be used in calculations (default is 20).
- the script `onebulk` can be used to specify one bulk to use across a composition range, as a proportion, e.g. `onebulk 0.1`. Without the proportion specified, interactive input is requested
- the script `bulksubrange` (also called `splitbulk`) allows a subrange of a composition range to be specified. This is not yet in the form of e.g. `bulksubrange 0.1 0.2`, but this is about to be implemented (currently `bulksubrange` causes a request for interactive input)
- handling of projection info—for compatibility diagram output—now tidied up. The relevant script is `compatibility` (was `cmath`), the output being in the drfile and now in the csvfile too. If you specify `compatibility` (or `modebox`), `drawpd no` is also a consequence (one cannot mix drawpd and mathematica-form output in the drfile)
- fixed crasher in download 1, if you entered *kill* at the mode-of-operation question at the start of running THERMOCALC
- fixed bug in first download, where calculation of Gibbs energy for divariants with `tozero` did not work correctly
- density (ρ) was missing from some aspects of the output (e.g. drawpd output) in the first download, and is now instated
- more changes to scripts, partly to aid in hands-off running of THERMOCALC, the idea being to have the run information (largely) set in the scriptfile—so with no (little) interactive input. Scripting is becoming more defensive too. New script documentation soon...
- a reminder to notify us of things not working properly (thank you, already, Dave Kelsey)

- a huge amount has changed under the hood since tc347, as well as some more visible things (see below). The code is becoming more transparent and sustainable for the future. Collateral damage of this effort is that some previously-working facilities are now broken (but will be repaired as soon as I can). While this happens, new β versions will be released. If some facility has gone missing that you are keen to use, notify us.
- reference state PT : T_0 is now correct at 273.15°C and P_0 correct at 0.001 kbar (previously these were rounded). Generally there will be tiny differences in the results of calculations as a consequence.
- there is a new more thorough and transparent axfile format, allowing a complete, human-readable description of the a - x relations and end-member construction to be printed automatically in the itfile. In particular, **make**-ing of end-members is much more transparent, including specifying the state of order when an order-disorder end-member is used.
- there has been a small change from tc346-tc347 to the way that the pressure-dependence of a ΔG term is applied, in the case that an end-member is made from a single dataset end-member. It is now applied as a linear term, $c P$, consistent with what happened in tc345 and earlier, and what is stated in the metapelite and metabasite papers. This may result in small changes to results with the same thermodynamic input.
- the icfile contains a detailed summary of calculation results. It is getting this to work with all calculation types that is part of the reason why some calculation facilities are unavailable.
- population of the csvfiles is not done yet or is incomplete (ignore for the time being). Extra files that THERMOCALC creates are now erased if they are empty when you exit the program
- avT is now reinstated and it now works much more generally than before. AvP and avT select reactions for an independent set based on reaction P and T uncertainty, respectively, rather than attempting to do this on their linearity in PT
- previously, H_2O -in-excess calculations were handled behind the scenes (by adding H_2O , then normalising the mode of H_2O from the output). This must now be done explicitly (follow guidance onscreen if you meet this change).
- dogmin is upgraded. It should be faster, and there are three levels of output details for calculations at a single PT (a mode of operation that we strongly recommend now). A code can be added with the dogmin script, referred to as doglevel: 0 = minimal output; 1 = more output; 2 = all output (as previously), e.g. dogmin yes 1.