# Troubleshooting for phase diagram calculations in THERMOCALC

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New users of THERMOCALC sometimes find that they can't seem to calculate anything at all. Or, THERMOCALC calculates part of the way along a line and then stops. Here is a short troubleshooter guide that might help you in these situations. This guide is not a substitute for understanding how stable phase diagrams are built up – for that you need to read Roger Powell's documents, *phase-diagram-introduction.pdf* and *phase-diagram-calculations-in-TC.pdf*, or the THERMOCALC tutorials, all available from the $P$–$T$ projection and pseudosection sections of the website.

## Contents

## 1   Looking for a successful calculation

Suppose you are just starting to calculate a phase diagram, hopefully with a related, published diagram to look at for guidance. You have pasted a `xyzguess` script block into your script file from the *starting_guesses.txt* file in the appropriate thermodynamic input file distribution. You start by trying to calculate along a curve – ideally, a univariant reaction, but more likely (in a big chemical system like NCKFMASHTO) a phase-out boundary. However, you can't make THERMOCALC calculate anything at all. What can you do?

- Check that the compositions implied by your starting guesses are reasonable.

- Try switching between calculating temperatures at specified pressure (`calctatp yes`, for curves that are steep in $P$–$T$ space) and calculating pressures at specified temperature (`calctatp no`, for curves that are shallow in $P$–$T$ space).

- Try widening the $T$ window (for `calctatp yes`) or $P$ window (for `calctatp no`). Also, remember that the starting guess for $P$ or $T$ is important – THERMOCALC uses the middle of the specified window.

- If THERMOCALC generates '8' errors, use the `c8` script to find useful compositional starting guesses as discussed in section 3. The results of any successful calculations are printed in the `log` file in `xyzguess` form, and can be copied into the scriptfile for use in subsequent calculations.

- Instead of calculating the curve, try doing calculations over a $P$–$T$ grid in the next-door field to find useful compositional starting guesses (again, use the `c8` script if you get any '8' errors).

## 2   Why does my calculation along a line stop?

Sometimes, THERMOCALC is happily calculating a series of points along a curve, when suddenly it stops calculating and produces error codes. Usually, if this happens, you simply need to replace the `xyzguess` script block with the most recent one that was generated during calculations, found near the bottom of the `log` file. If this doesn't work:

- Does one of the phases run out, i.e. fall to a modal proportion of zero, along the curve?

- If the boundary or reaction is strongly curved, consider changing from `calctatp yes` to `calctatp no` or vice versa (see section 1).

- Look carefully at the most recent compositional and order variables calculated. Are some of them heading towards the edges of their allowed ranges? (see *composition_spaces_and_phases.pdf*). If you're calculating a $P$–$T$ projection, your system may have reached its terminus in a subsystem – check this against the site fraction information in the `-ic` file. If you're calculating a pseudosection, and your phases are heading into unexpected regions of composition space, does it indicate that you should have added a new phase to the assemblage?

- Do any of your phases contain a solvus? Calculations can run into a solvus and stop. See Johann Diener's pseudosection tutorial (tutorial 6 in the White & Diener tutorial collection) for more information and help with this.

## 3   THERMOCALC **error codes**

THERMOCALC prints an error code when a calculation fails. These give hints about what has gone wrong with a calculation:

| Error code | Meaning |
| --- | --- |
| 1–5 | Non-linear equation solver is not making any progress, or compositions are heading for a bad place. Change starting guesses or look in a different part of $P$–$T$ space for this assemblage. |
| 6-7 | The solution is outside the allowed $P$–$T$ range, or in a non-physical part of composition space. Try a different part of $P$–$T$ space or a different assemblage. |
| 8 | The calculation is successful, but the modal proportions of one or more phases is negative, i.e. the assemblage is non-physical – see note on c8 script below. |

Error code 8 can be really useful, because it indicates a calculation that is thermodynamically successful, even though the result is non-physical with respect to mass balance. If you're struggling to find successful calculations, but you see this error code, setting the script c8 yes causes THERMOCALC to print the results of calculations with negative modes. Although you don't want to include these calculations in the final phase diagram, the equilibrium phase compositions obtained can provide useful starting guesses for subsequent calculations.