Review of Riel et al., GMD-2024-197

This is plainly a useful and important contribution. The essential motivation and results are clear. Nonetheless, before publication some minor revisions are needed to make the presentation as clear and unambigious as it can be.

Lines 40-48: People are starting to explore a new cheap work-around, namely neural net emulators of thermodynamic models. See, for example, https://agu.confex.com/agu/agu24/meetingapp.cgi/Paper/1708197 … just an abstract at this point, but maybe worth mentioning.

Line 70: Fix grammar: "…inequality constraint in gradient-based methods results in…"

Line 77: "…avoids the need to express …"

Line 79: Just "conjugate", not "conjugated"

Line 88: "combinations", plural

Equation 2: $a_{i(\lambda)}^{id}$ as defined here is NOT an "ideal activity coefficient". It is an "ideal activity". I think everybody agrees that the activity coefficient defines the deviation from ideality and is given by $\gamma_{i(\lambda)}^{id}$ such that $g_{i(\lambda)}^{ex} = RT\log(\gamma_{i(\lambda)}^{id})$. A "coefficient" is a multiplicative quantity that modifies some variable term in an equation. So, for example in the polynomial $f(x) = a + bx + cx^2$, the coefficients are a, b, and c. The term "bx" is not a coefficient. Also, better specify, because the usage is not universal, that here "log" means natural logarithm.

Line 113: "functions"

Line 138: c is defined incorrectly. Obviously, it is equal to X_{Ca}^{M2}, not X_{Fe}^{M1} !

Equation 17: The meaning of the Jacobian matrix is vague unless you explicitly spell out the order of the terms in the vectors, i.e. $\boldsymbol{X}_{e_s}^{s} = \{X_{Mg}^{M1}, X_{Fe}^{M1}, X_{Mg}^{M2}, X_{Fe}^{M2}, X_{Ca}^{M2}\}$ and $\boldsymbol{x}_{cv} = \{x, c, Q\}$.

Equations 17-18: make up your mind about notation. Is the numerator in the Jacobian matrix and in the null-space expression $X_{e_{s,i}}^{s}$, x, or X_e? Recommend you use a bold character since it is really a vector.

Equation 21: Again, make up your mind: x or x_{cv}?

Equation 22: What is b? Here it appears to be {1, 1}, but this is never stated. Equation 18 is not the set of equality constraints, it is just the definition of the matrix A (which, again, ought to have a distinctive symbol to indicate it is a matrix).

Line 183: It is not obvious (to those that don't do QR decompositions for a living) that Q is a matrix whose columns are $q^1 \ldots q^m$, or that these are ordered into Q_1 and Q_2 where Q_1 has n columns corresponding to the image and Q_2 has $m–n$ columns corresponding to the null space. Please say that.

Do you really need to introduce the matrix F? Isn't it just Q_2? Or for that matter, N_z as the nullspace matrix of A when A is already the nullspace matrix of the Jacobian?

Bottom line: I really think equations 17-27 could be presented in a manner that is less confusing and introduces fewer throw-away symbols.

Lines 196-198: The sentence beginning "Considering …" is not a sentence.

Line 262: I am confused about whether this is a valid test of the acceleration available from this algorithm, if the global minimum hyperplane first has to be calculated by MAGEmin (i.e., using the old, slow algorithm!).

Figure 2 caption: "Least", not "Levast"; "Conjugate Gradient", not "conjugated gradiend"; "method presented in", not "present in"; "number of minimizations", not "minimization".

Line 299: What is Γ?

Line 310: The conclusion section starts here, give it a section header.