

*TOUGH Symposium 2015*  
*LBNL, Berkeley, California, September 28–30, 2015*



**T&T session**

Alfredo Battistelli

AMBEN Dept., Saipem SpA

## **Vanishing mass fractions in multicomponent simulations**

---

In multicomponent simulations the complete disappearance of a mass component can produce convergence problems.

**Initial conditions:** use tiny mass fractions also for those components which in principle should not be present. 1 ppm is usually enough. **Not for VOCs in TMVOC !** This is enforced by the code (minimum mole fraction 1E-30).

**Injection:** specify tiny injection rates also for all those components which should not in principle be injected (not for TMVOC !).

**Example:** with ECO2N inject some water together with the CO<sub>2</sub>. Do not inject NaCl as it will not be completely flushed away from injection elements.

**Example:** with EWASG include some NCG and NaCl in the reinjected steam condensate when modeling the production forecast for geothermal applications.



## Force at least one NR iteration

---

Forcing the code to perform at least one NR iteration is simple (small changes in CONVER subroutine).

This helps in particular when running steady-state runs: solvers may have problems close to steady-state.

You get convergence with previous set of primary variables (so no NR iteration !) and no convergence during next time step !!

**Forcing at least one NR iteration usually allows the code to go closer to a true steady-state.**

Already present in iTOUGH and TOUGH3 ?  
Add this option also in TOUGH2 V.2.0 !

## Accuracy of geometric parameters in MESH file

---

TOUGH2 V.2.0 uses 10 column fields for the geometric parameters of IFDM grids.

For cartesian grids this is usually enough (but be careful when using geographical coordinates!!).

With unstructured grids the 10 column format may not be enough. Errors in nodal distances and the cosine of angle between the connection and the vertical **can easily introduce significant spurious flows in steady-state simulations.**

**Solution:** include the option to save/read geometrical information with 20 column format (as per INCON file).

Allow the user to chose 10 or 20 column formats using a flag in the input file.

Already available in iTOUGH/TOUGH+/TOUGH3 ?

**Add this in TOUGH2 V.2.0 as well.**



## Hard single liquid $\leftrightarrow$ two-phase transitions

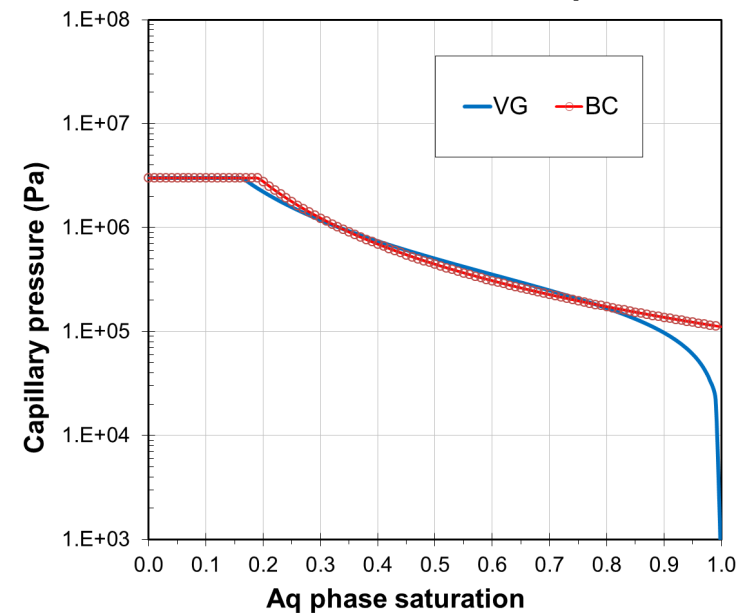
Convergence problems at phase transitions are common because of the high non linearities involved.

Often for liquid phase  $\leftarrow \rightarrow$  two-phase transitions **the steep shape of VG capillary pressure curve** close to full liquid saturation can be responsible of convergence problems.

If allowed by field/lab data, consider the use of a Brooks-Corey Pcap formulation.

When dealing with cap-rocks, or low permeability layers which may act as hydraulic barriers, VG model may be inappropriate.

**BC model includes the gas entry pressure !!**



## Density of 'non-existing' phases

---

It is recognized that the present interpolation algorithm for the density at the interface may introduce discontinuities in the derivatives when a phase transition occurs.

**Solution:** compute the density of 'non existing' phases (available in ITOUGH2/TOUGH3 !!) as suggested by J. O'Sullivan et al.

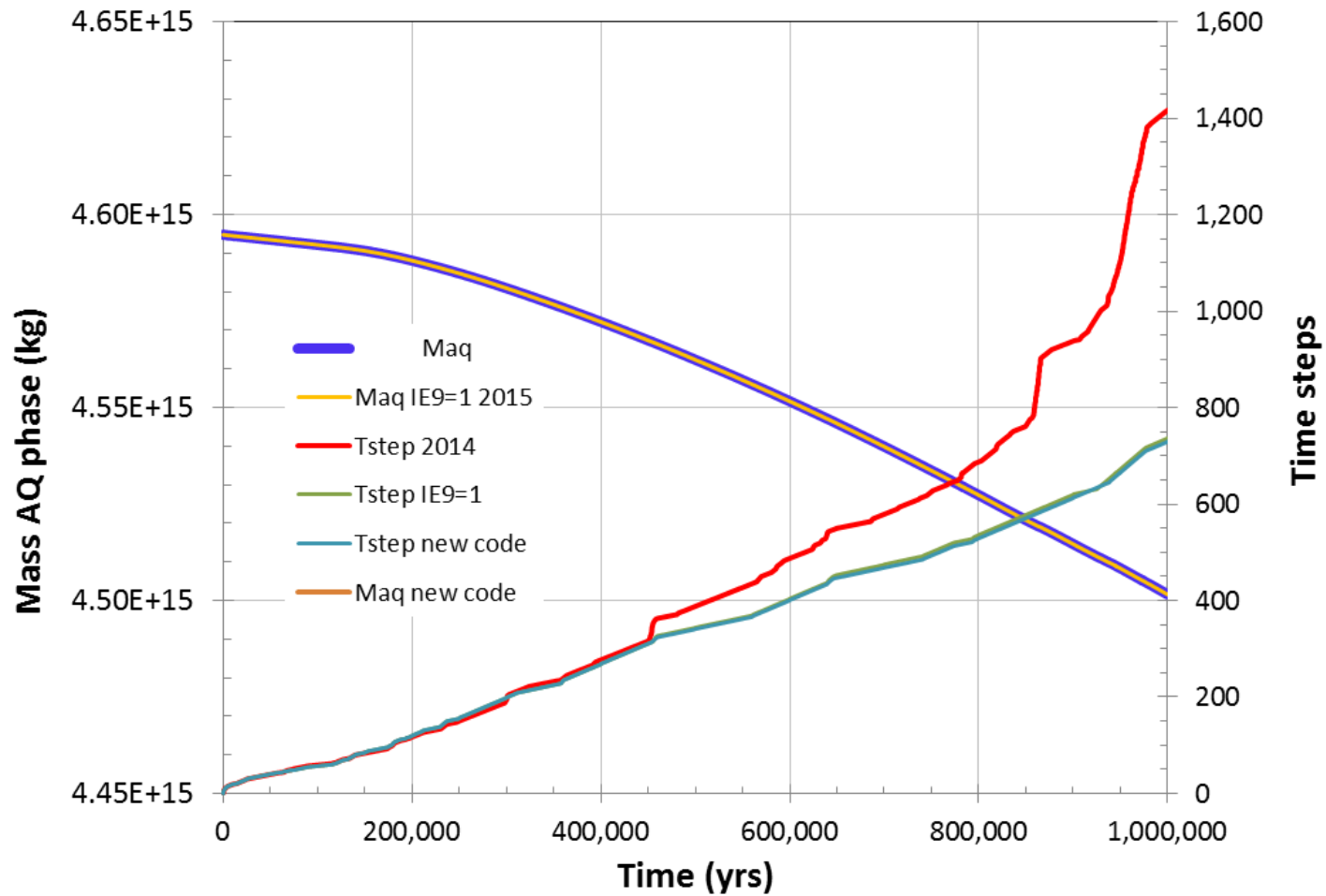
**Easy for EOS with few components and 'simple' thermodynamics.**

We found many convergence problems when running with TMGAS the migration of NCGs in a large deep sedimentary formation, when the NCG plume is migrating under density driven flow.

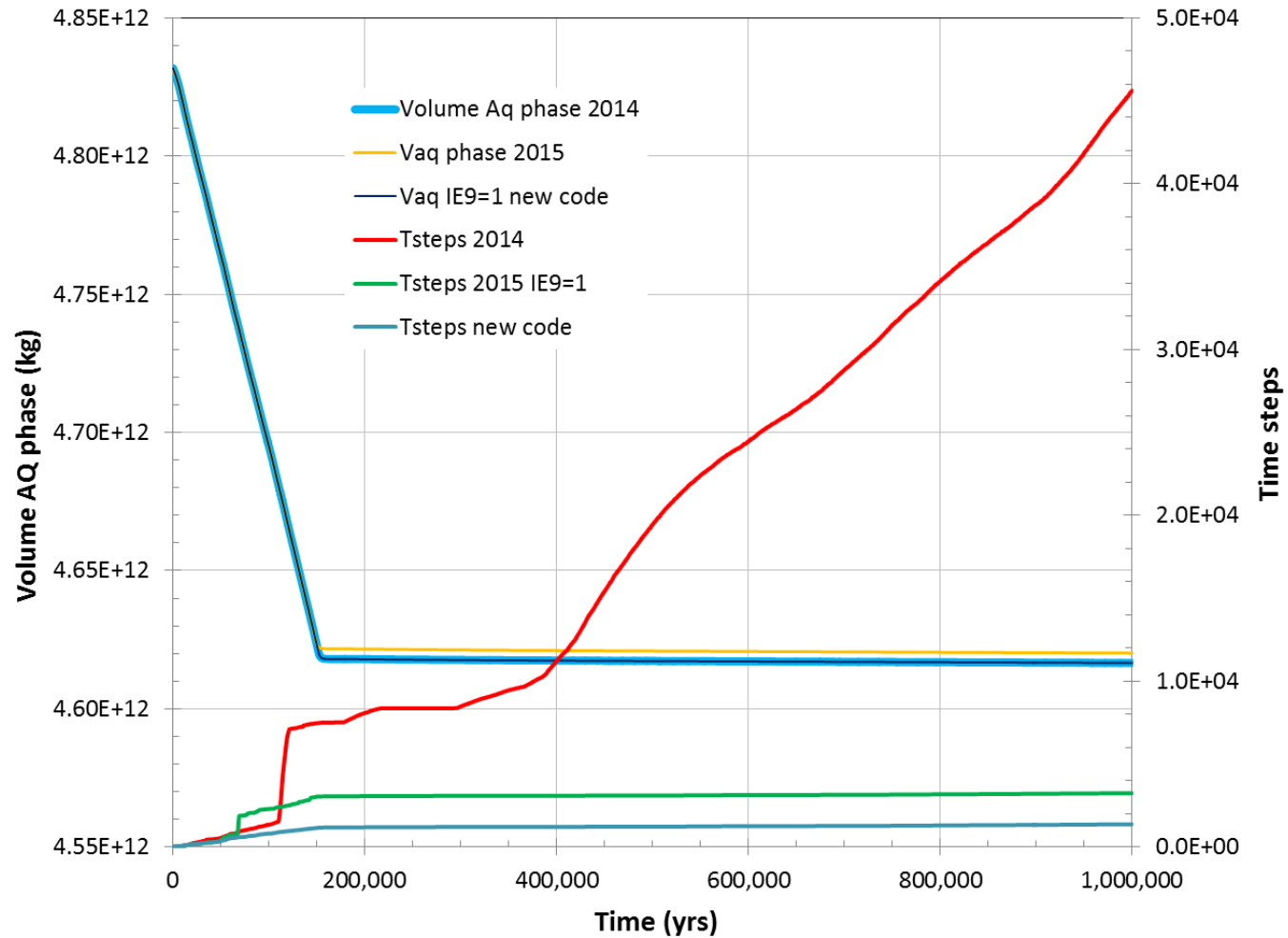
A preliminary attempt to fix the problem gave a remarkable improvement of converge speed in 90% of the simulations.



# H2S injection run



# CH4 injection run





## And more....

---

**SAVE file** : for very long runs allows writing of SAVE file any time you have a printout. If for any reason the run stops before the expected end, you have the possibility to restart from the last printout time.

**RELP, PCAP, PERMRED, VPL**: include an option to print for any rock domain the RELP, PCAP and VPL values as function of SW and PERMRED as function of SS (depending on the EOS used). Useful to check/remember which functions you used for any run.

**INPUT file** : add the input file at the end of the output file. After years you will always be able to recover the correct input file (inappropriate for the multimillion grids used by George ...)

**BALLA output**: allows the saving of BALLA info at any time step on a dedicated file. Quite useful for checking steady state conditions



---

*Thanks for your kind attention !*

