

- When some mass components are not present in (parts of) the flow domain, or disappear in the course of a simulation, mass balances there reduce to "0=0".
- For example, TOUGH2/ECO2N and TOUGH2/ECO2M have components water, salt, CO2. Any of these may be absent or may disappear during the simulation in (parts of) the flow domain.
- This leads to poorly conditioned Jacobian matrices that have many zeros on the main diagonal, with adverse effects on convergence rates, time stepping, and execution times.

### Example fragment from file LINEQ

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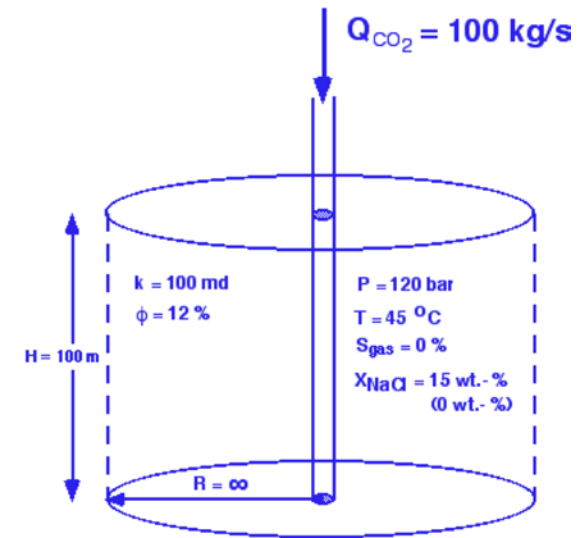
AT KCYC= 24 AND ITER= 3, IZEROD= 30, ZPROCS = Z2 AND OPROCS = O3
  AT [ 24, 3] DELT=0.327680E+05 IERR=0& ERR=7.830485E-09 IT= 27 ITC= 1033
AT KCYC= 24 AND ITER= 4, IZEROD= 20, ZPROCS = Z2 AND OPROCS = O3
  AT [ 24, 4] DELT=0.327680E+05 IERR=0& ERR=5.956149E-09 IT= 32 ITC= 1065
AT KCYC= 25 AND ITER= 1, IZEROD= 30, ZPROCS = Z2 AND OPROCS = O3
  AT [ 25, 1] DELT=0.327680E+05 IERR=0& ERR=5.814066E-09 IT= 30 ITC= 1095
  AT [ 25, 2] DELT=0.327680E+05 IERR=0& ERR=9.751440E-09 IT= 29 ITC= 1124
  AT [ 25, 3] DELT=0.327680E+05 IERR=0& ERR=7.587229E-09 IT= 24 ITC= 1148
  AT [ 26, 1] DELT=0.655360E+05 IERR=0& ERR=2.316058E-09 IT= 39 ITC= 1187
AT KCYC= 26 AND ITER= 2, IZEROD= 40, ZPROCS = Z2 AND OPROCS = O3
  AT [ 26, 2] DELT=0.655360E+05 IERR=0& ERR=6.444737E-09 IT= 41 ITC= 1228
  AT [ 26, 3] DELT=0.655360E+05 IERR=0& ERR=8.181143E-09 IT= 34 ITC= 1262
  AT [ 26, 4] DELT=0.655360E+05 IERR=0& ERR=8.874454E-09 IT= 34 ITC= 1296
AT KCYC= 26 AND ITER= 5, IZEROD= 31, ZPROCS = Z2 AND OPROCS = O3

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## Example (Jos Maas, TNO):

TOUGH2/ECO2M simulation of CO<sub>2</sub> injection into a 10-layer 2-D R-Z system (2-D version of the rcc3 sample problem).

- Initial conditions: aqueous-gas, with  $P = 20.e5$  Pa,  $X_{sm} = 0.15$ ,  $S_{aq} = 0.1$ ,  $T = 100$  deg-C.
- Inject CO<sub>2</sub> at  $T = 20$  deg-C, at a rate of 10 kg/s per layer.
- When injecting pure CO<sub>2</sub>, aqueous phase will be removed by dissolution into the flowing CO<sub>2</sub> stream, and water component will disappear in a region that expands outward from the injection well.
- Alternatively, co-inject water at a small rate, 1.e-6 kg/s per layer. Water solubility in CO<sub>2</sub> is of order 1.e-3, so co-injecting water at a relative rate of 1.e-7 will have negligible impact on water dissolution in the CO<sub>2</sub>.
- Co-injection of water will avoid the "0=0" issues, and will allow better advance of the simulation.



time steps	simulation times (s)	
	pure CO <sub>2</sub> injection	with co-injection of water
100	0.948096E+07	0.334735E+08
200	0.330489E+08	0.954056E+08
300	0.615995E+08	0.170221E+09
400	0.919015E+08	0.257621E+09
500	0.144961E+09	0.338490E+09