dt=0.00017s

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | 0 | | 1 | | 2 | | 3 | | 4 | | 5 | | 7 | 8 | 9 | 10 |
| D0 | 1.e-09 | | 1.e-09 | | 1.e-09 | | 1.e-09 | | 1.e-09 | | 1.e-09 | | 1.e-09 | 1e-15 | 1e-15 | 1e-15 |
| poros | 1 | | 1 | | 1 | | 1 | | 1 | | 1 | | 0.1 | 0.1 | 0.1 | 0.1 |
| Modify De of interface cells | | | | | | | | | | | | | | | | |
| De | 1.e-09 | | 1.e-09 | | 1.e-09 | | 1.e-09 | | 1.e-09 | | 1.e-09 | | 1.e-09 | 1e-15 | 1e-15 | 1e-15 |
| tau | 1 | | 1 | | 1 | | 1 | | 1 | | 1 | | 1 | 0.5 | 0.5 | 0.5 |
| cphi | 1/3 | | | | | | | | | | | | | | | |
| [Ca] | 0 | | 0 | | 0 | | 0 | | 0 | | 0 | | 0.01949 | 0.01949 | 0.01949 | 0.01949 |
| CH | 0 | | 0 | | 0 | | 0 | | 0 | | 0 | | 0.54381 | 0.54381 | 0.54381 | 0.54381 |
| LB transport calculation (iteration=1) | | | | | | | | | | | | | | | | |
| [Ca] | 0 | | 0 | | 0 | | 0 | | 0 | | 0.00325 | | 0.01624 | 0.01949 | 0.01949 | 0.01949 |
| CH | 0 | | 0 | | 0 | | 0 | | 0 | | 0 | | 0 | 0.54381 | 0.54381 | 0.54381 |
| (1st CH cell: CH mass=0)After Phreeqc(iteration=1) | | | | | | | | | | | | | | | | |
| [Ca] | 0 | | 0 | | 0 | | 0 | | 0 | | 0.00325 | | 0.01624 | 0.01949 | 0.01949 | 0.01949 |
| CH | 0 | | 0 | | 0 | | 0 | | 0 | | 0 | | 0 | 0.54381 | 0.54381 | 0.54381 |
| Border cell treatment (fraction=0.004) | | | | | | | | | | | | | | | | |
| [Ca] |  | |  | |  | |  | |  | |  | | 0.01637 |  |  |  |
| CH |  | |  | |  | |  | |  | |  | | 0.54368 |  |  |  |
| Updating porous information(iteration=1) | | | | | | | | | | | | | | | | |
| poros | 1 | | 1 | | 1 | | 1 | | 1 | | 1 | | 0.10022 | 0.1 | 0.1 | 0.1 |
| De | 1.e-09 | | 1.e-09 | | 1.e-09 | | 1.e-09 | | 1.e-09 | | 1.e-09 | | 1.e-09 | 1e-15 | 1e-15 | 1e-15 |
| cphi | 0.033333333333333284 | | | | | | | | | | | | | | | |
| tau | 5.5 | | 5.5 | | 5.5 | | 5.5 | | 5.5 | | 5.5 | | 5.5 | 0.50001 | 0.50001 | 0.50001 |
| CC | 0 | | 0 | | 0 | | 0 | | 0 | | 0 | | 0 | 0 | 0 | 0 |
| [Ca] | 0 | 0 | | 0 | | 0 | | 0 | | 0.00325 | | 0.01624 | | 0.01949 | 0.01949 | 0.01949 |
| Ss\_Ca |  |  | |  | |  | |  | | -2.9e-08, | | 7.8e-02 | | 0 | 0 | 0 |
| CH | 0 | 0 | | 0 | | 0 | | 0 | | 0 | | 0.54368 | | 0.54381 | 0.54381 | 0.54381 |
| LB transport calculation (iteration=2) | | | | | | | | | | | | | | | | |
| [Ca] | 0 | 0 | | 0 | | 0 | | 9.845e-05 | | 0.0062 | | -0.0794 | | 0.141 | 0.01949 | 0.01949 |
| (1st CH cell: CH mass=0)After Phreeqc (iteration=2) | | | | | | | | | | | | | | | | |
| [Ca] | 0 | 0 | | 0 | | 0 | | 9.845e-05 | | 0.0062 | | 0 | | 0.01949 | 0.01949 | 0.01949 |
| CH | 0 | 0 | | 0 | | 0 | | 0 | | 0 | | 0 | | 0.55553 | 0.56304 | 0.56192 |
| Border cell treatment (fraction=0.004) | | | | | | | | | | | | | | | | |
| [Ca] |  |  | |  | |  | |  | |  | | 0.000777 | |  |  |  |
| CH |  |  | |  | |  | |  | |  | | 0.5436 | |  |  |  |
| Updating porous information (iteration=2) | | | | | | | | | | | | | | | | |
| poros | 1 | 1 | | 1 | | 1 | | 1 | | 1 | | 0.10034 | | 0.07992 | 0.07097 | 0.07097 |
| De | 1.e-09 | | | | | | | | | | | 1.e-09 | | 1e-15 | 1e-15 | 1e-15 |
| cphi | 0.023655594045869588 | | | | | | | | | | | | | | | |
| tau | 7.54555 | | | | | | | | | | | 7.54555 | | 0.50001 | 0.50001 | 0.50001 |
| CH |  |  | |  | |  | |  | |  | | 0.5436 | | 0.55553 | 0.56304 | 0.56192 |
| CC |  |  | |  | |  | |  | |  | |  | |  |  |  |
| [Ca] | 0 | 0 | | 0 | | 0 | | 9.84e-05, | | 0.0062 | | -0.0794 | | 0.14 | 0.19492 | 0.19492 |

3rd iteration

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| poros | | 1 | | 1 | | 1 | | 1 | | 1 | | 1 | | 0.10034 | 0.07992 | 0.07097 | 0.07097 |
| De | | 1.e-09 | | | | | | | | | | | | 1.e-09 | 1e-15 | 1e-15 | 1e-15 |
| cphi | | 0.023655594045869588 | | | | | | | | | | | | | | | |
| tau | | 7.54555 | | | | | | | | | | | | 7.54555 | 0.50001 | 0.50001 | 0.50001 |
| CC | | 0 | | 0 | | 0 | | 0 | | 0 | | 0 | | 0 | 0 | 0 | 0 |
| [Ca] | 0 | | 0 | | 0 | | 0 | | 9.84e-05, | | 0.0062 | | -0.0794 | | 0.14 | 0.19492 | 0.19492 |
| CH | 0 | | 0 | | 0 | | 0 | | 0 | | 0 | | 0.5436 | | 0.55553 | 0.56304 | 0.56192 |
| LB transport calculation (iteration=3) | | | | | | | | | | | | | | | | | |
| [Ca] | 0 | | 0 | | 0 | | 2.17e-06 | | 3.165e-04 | | 0.0077 | | -0.0197 | | 0.0144 | 0.043 | 0.0275 |
| (1st CH cell: CH mass=0)After Phreeqc | | | | | | | | | | | | | | | | | |
| [Ca] | 0 | | 0 | | 0 | | 2.17e-06 | | 3.165e-04 | | 0.0077 | | 0 | | 0.01949 | 0.01949 | 0.01949 |
| CH | 0 | | 0 | | 0 | | 0 | | 0 | | 0 | | 0 | | 0.55553 | 0.56304 | 0.56192 |
| Border cell treatment (fraction=0.004) | | | | | | | | | | | | | | | | | |
| [Ca] |  | |  | |  | |  | |  | |  | | 0.000777 | |  |  |  |
| CH |  | |  | |  | |  | |  | |  | | 0.54352 | |  |  |  |
| Updating porous information | | | | | | | | | | | | | | | | | |
| poros | 1 | | 1 | | 1 | | 1 | | 1 | | 1 | | 0.10047 | | 0.08059 | 0.06816 | 0.07003 |
| De | 1.e-09 | | 1.e-09 | | 1.e-09 | | 1.e-09 | | 1.e-09 | | 1.e-09 | | 1.e-09 | | 1e-15 | 1e-15 | 1e-15 |
| cphi | 0.022720860045403003 | | | | | | | | | | | | | | | | |
| tau | 7.8354 | | | | | | | | | | | | 7.8354 | | 0.50001 | 0.50001 | 0.50001 |
| CH | 0 | | 0 | | 0 | | 0 | | 0 | | 0 | | 0.54352 | | 0.55553 | 0.56304 | 0.56192 |
| CC |  | |  | |  | |  | |  | | 0 | | 0 | |  |  |  |
| [Ca] | 0 | | 0 | | 0 | | 2.17e-06 | | 3.165e-04 | | 0.0077 | | -0.0197 | | 0.0144 | 0.043 | 0.0275 |
| ss |  | |  | |  | |  | |  | |  | |  | |  |  |  |

4th iteration

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| poros | | 1 | | 1 | | 1 | | 1 | | 1 | | 1 | | 0.10047 | 0.08059 | 0.06816 | 0.07003 |
| De | | 1e-9 | | | | | | | | | | | | 1e-9 | 1e-15 | 1e-15 | 1e-15 |
| cphi | | 0.022720860045403003 | | | | | | | | | | | | | | | |
| tau | | 7.8354 | | | | | | | | | | | | 7.8354 | 0.50001 |  |  |
| CC | | 0 | | 0 | | 0 | | 0 | | 0 | | 0 | | 0 | 0 | 0 | 0 |
| [Ca] | 0 | | 0 | | 0 | | 2.17e-06 | | 3.165e-04 | | 0.0077 | | -0.0197 | | 0.0144 | 0.043 | 0.0275 |
| CH | 0 | | 0 | | 0 | | 0 | | 0 | | 0 | | 0.54352 | | 0.55553 | 0.56304 | 0.56192 |
| After LB | | | | | | | | | | | | | | | | | |
| [Ca] | 0 | | 0 | | 4.6e-8 | | 1e-5 | | 6.6e-4 | | 8.5e-3 | | -0.0786 | | 0.114 | 0.0115 | 0.017 |
| After Phreeqc | | | | | | | | | | | | | | | | | |
| [Ca] | 0 | | 0 | | 4.6e-8 | | 1e-5 | | 6.6e-4 | | 8.5e-3 | | 0 | | 0.0195 | 0.0195 | 0.0195 |
| CH | 0 | | 0 | | 0 | | 0 | | 0 | | 0 | | 0 | | 0.56314 | 0.5625 | 0.56174 |
| Border cell treatment | | | | | | | | | | | | | | | | | |
| [Ca] |  | |  | |  | |  | |  | |  | | 0.000776 | |  |  |  |
| CH |  | |  | |  | |  | |  | |  | | 0.54344 | |  |  |  |
|  | | | | | | | | | | | | | | | | | |
| poros |  | |  | |  | |  | |  | |  | |  | |  |  |  |
| De |  | |  | |  | |  | |  | |  | |  | |  |  |  |
| cphi |  | | | | | | | | | | | | | | | | |
| tau |  | |  | |  | |  | |  | |  | |  | |  |  |  |
| CH |  | |  | |  | |  | |  | |  | | 0.54344 | | 0.56314 | 0.5625 | 0.56174 |
| CC |  | |  | |  | |  | |  | |  | |  | |  |  |  |
| [Ca] | 0 | | 0 | | 5e-8 | | 1e-5 | | 0.00066 | | 0.00848 | | -0.0786 | | 0.0114 | 0.0115 | 0.017 |

100 iteration

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| poros | 1 | | 1 | | 1 | | 1 | | 1 | | 0.99938 | | 0.10644 | 0.0655 | 0.0696 | 0.07 |
| De | 1e-9 | | 1e-9 | | 1e-9 | | 1e-9 | | 1e-9 | | 1.6e-11 | | 2.7e-10 | 1e-15 | 1e-15 | 1e-15 |
| tau | 8.1289 | | | | | | | | | | 0.62049, | | 2.57438, | 0.50001 |  |  |
| cphi | 0.021846846528027264 | | | | | | | | | | | | | | | |
| [Ca] | 0.0027 | | | | | | | | | 0.00336 | | 0.00825 | | 0.0195 | 0.0195 | 0.0195 |
| SS\_Ca | 0 | -1.3e-4 | | -4.2e-5 | | -7e-6 | | -5e-8 | | -0.065 | | 0.27 | | -0.001 | 0.014 | 0.01 |
| CH | 0 | 0 | | 0 | | 0 | | 0 | | 0 | | 0.53988 | | 0.5646 | 0.562 | 0.5619 |
| CC | 0 | 0 | | 0 | | 0 | | 0 | | 3.378e-4 | | 3.445e-05 | | 0 | 0 | 0 |
| [C] | 0.0046 | 0.0038 | | 0.0031 | | 0.0027 | | 0.0024 | | 7e-4 | | 6.7e-4 | | 1e-4 | 8e-9 | 3e-13 |
| After LB | | | | | | | | | | | | | | | | |
| [Ca] | 0.0027 | 0.0027 | | 0.0027 | | 0.0027 | | 0.0027 | | 0.0034 | | 0.0084 | | 0.0196 | 0.0195 | 0.0195 |
| [C] | 4.60646e-03, | 3.86856e-03 | | 3.18182e-03, | | 2.71878e-03, | | 2.4053  e-3 | | 6.95551e-04 | | 6.70820e-04, | | 1.11909e-04 | 8.24744e-09, | 3.29705e-13 |
| After Phreeqc | | | | | | | | | | | | | | | | |
| [Ca] | 0.0027 | 0.0027 | | 0.0027 | | 0.0027 | | 0.0027 | | 0.0034 | | 0.0084 | | 0.0195 | 0.0195 | 0.0195 |
| CH | 0 | 0 | | 0 | | 0 | | 0 | | 0 | | 0 | | 0.565 | 0.562 | 0.562 |
| [C] | 4.90631e-03, | 3.86853e-03, | | 3.18181e-03, | | 2.71878e-03, | | 2.4053  e-3 | | 6.84731e-04, | | 6.71546e-04, | | 1.11909e-04, | 8.24744e-09, | 3.29705e-13 |
| CC | 0 | 0 | | 0 | | 0 | | 0 | | 3.48566e-04, | | 3.43693e-05 | | 0 | 0 | 0 |
| Border cell treatment | | | | | | | | | | | | | | | | |
| [Ca] |  |  | |  | |  | |  | |  | | 0.00882 | |  |  |  |
| CH |  |  | |  | |  | |  | |  | | 0.539835 | |  |  |  |
|  | | | | | | | | | | | | | | | | |
| poros |  |  | |  | |  | |  | |  | |  | |  |  |  |
| De |  |  | |  | |  | |  | |  | |  | |  |  |  |
| cphi |  | | | | | | | | | | | | | | | |
| tau |  |  | |  | |  | |  | |  | |  | |  |  |  |
| CH |  |  | |  | |  | |  | |  | |  | |  |  |  |
| CC |  |  | |  | |  | |  | |  | |  | |  |  |  |
| [Ca] | 0 | 0 | |  | |  | |  | |  | |  | |  |  |  |

**@ Overlap of nodetype:**

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| cells | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| border |  |  |  |  |  |  | yes |  |  |  |
| CH |  |  |  |  |  | no | No | Yes | Yes | Yes |
| CC |  |  |  |  |  | yes | yes | No | No | no |

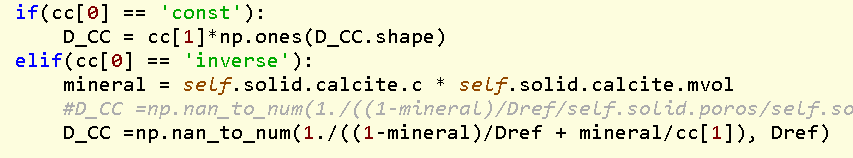
is\_border = self.solid.border

is\_port = (self.solid.portlandite.c >0) & (~is\_border) port is not border

is\_calc = np.logical\_and(self.solid.calcite.c >0,~is\_port) calc is not port, but it can be border

De = D\_CH\*is\_port + D\_CC\*is\_calc + D\_CC\*is\_border + Dref\*is\_liquid wheb border has CC precipitation, D\_CC at border will be counted twice

**@De of the border: both CH and CC exist at the border**



**@ D0 and De**

De = D\_CH\*is\_port + D\_CC\*is\_calc + D\_CC\*is\_border + Dref\*is\_liquid

self.fluid.set\_attr('D0',De,component\_dict=False)

in LB:

@property

def \_De(self):-----------🡪tau

#D = self.\_D0 \* self.app\_tort \* self.poros

D = self.\_D0 \* np.ones(self.poros.shape)

return D

**@Mixing factor model at border CH cell:**

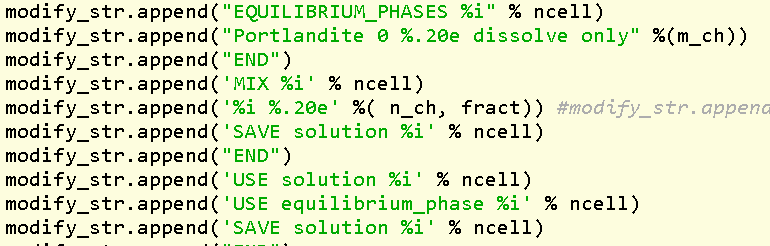
border cell has CH=0.53992, [Ca]= 0.00825,, pros=0.10636

Mixing: fraction=0.004/0.10636=0.0376

1st mixing:

1dx2 Virtual cell solution is mixed with 0.0376 dx2 of the border cell solution?

Φdx2 Virtual cell solution is mixed with 0.4% dx2 of the border cell solution?



virtual cell: poros= 0.003999994625707339->0.003999994609787787,

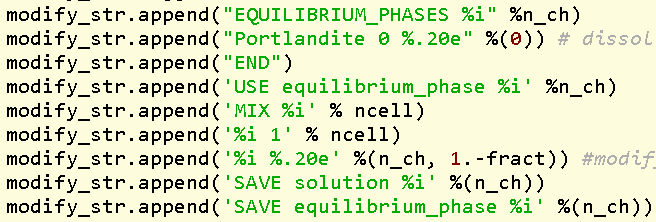
Ca=0.00825🡪 0.019499309883052665,

CH= 0🡪0.5398798057755456

2nd mixing:

1dx2 Virtual cell mixture solution is mixed with (1- 0.0376) dx2 of the border cell solution?

Φdx2 Virtual cell mixture solution is mixed with (Φ-0.4%) dx2 of the border cell solution?



border cell: poros= 0.10636, [Ca]= 0.008676364522645058, [CH]= 0.0,

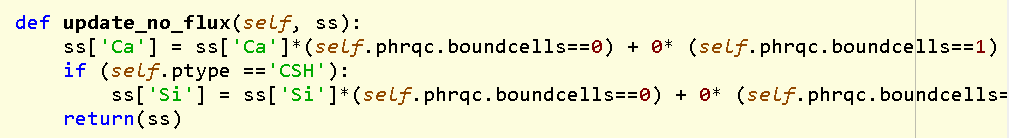
overall: 0.0004 CH is dissolved and [Ca] increases from 0.00825-0.008676

*('1st mixing', [[u'soln', u'pH', u'Alk(eq/kgw)', u'mu', u'H2O', u'poros', u'C', u'Ca', u'H', u'O', u'portlandite', u'SI\_portlandite', u'calcite', u'SI\_calcite'], [123456, 12.139492423507395, 0.016506863625579394, 0.02259405720461326, 55.50929780738274, 0.003999994625707339, 0.0006706915767152457, 0.008253431812791543, 111.037746308278, 55.52581165033512, 0.0, -0.91956782915695, 0.0, 8.881784197001252e-16], [123456, 12.479900834863473, 0.038998619766101625, 0.04988396785148464, 55.50929780738274, 0.003999994609787787, 0.000670691579384543, 0.019499309883052665, 111.06023850627122, 55.548303627396756, 0.5398798057755456, 0.0, 0.0, 0.04239578192169269]])*

*('2nd mixing', [[u'soln', u'pH', u'Alk(eq/kgw)', u'mu', u'H2O', u'poros', u'C', u'Ca', u'H', u'O', u'portlandite', u'SI\_portlandite', u'calcite', u'SI\_calcite'], [123456, 12.159498218747522, 0.017352729045286244, 0.02367639633666324, 55.50929780738274, 0.10636077711009206, 0.0006706915768323437, 0.008676364522645058, 111.0385921930856, 55.526657525448556, 0.0, -0.8646836837704726, 0.0, 0.0028342623141206502]])*

**@why add no flux boundary solution ?**

ss = self.update\_no\_flux(ss)



**@argument of the acceleration procedure for such a dynamic system**

**@define active nodes in Phreeqc**