Used Fuel Disposition Campaign

PFLOTRAN Process Modeling: Density Dependence on Salinity

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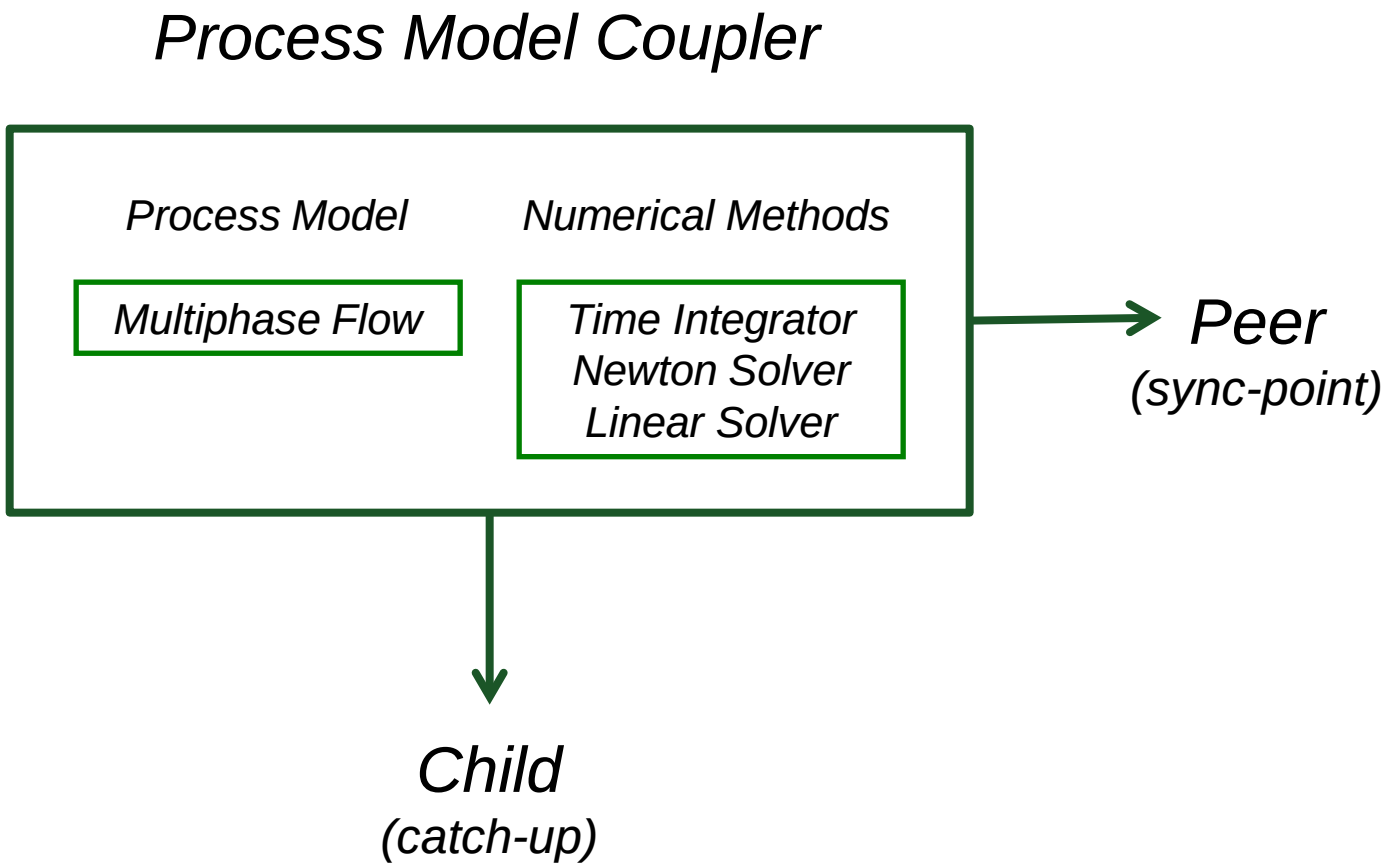
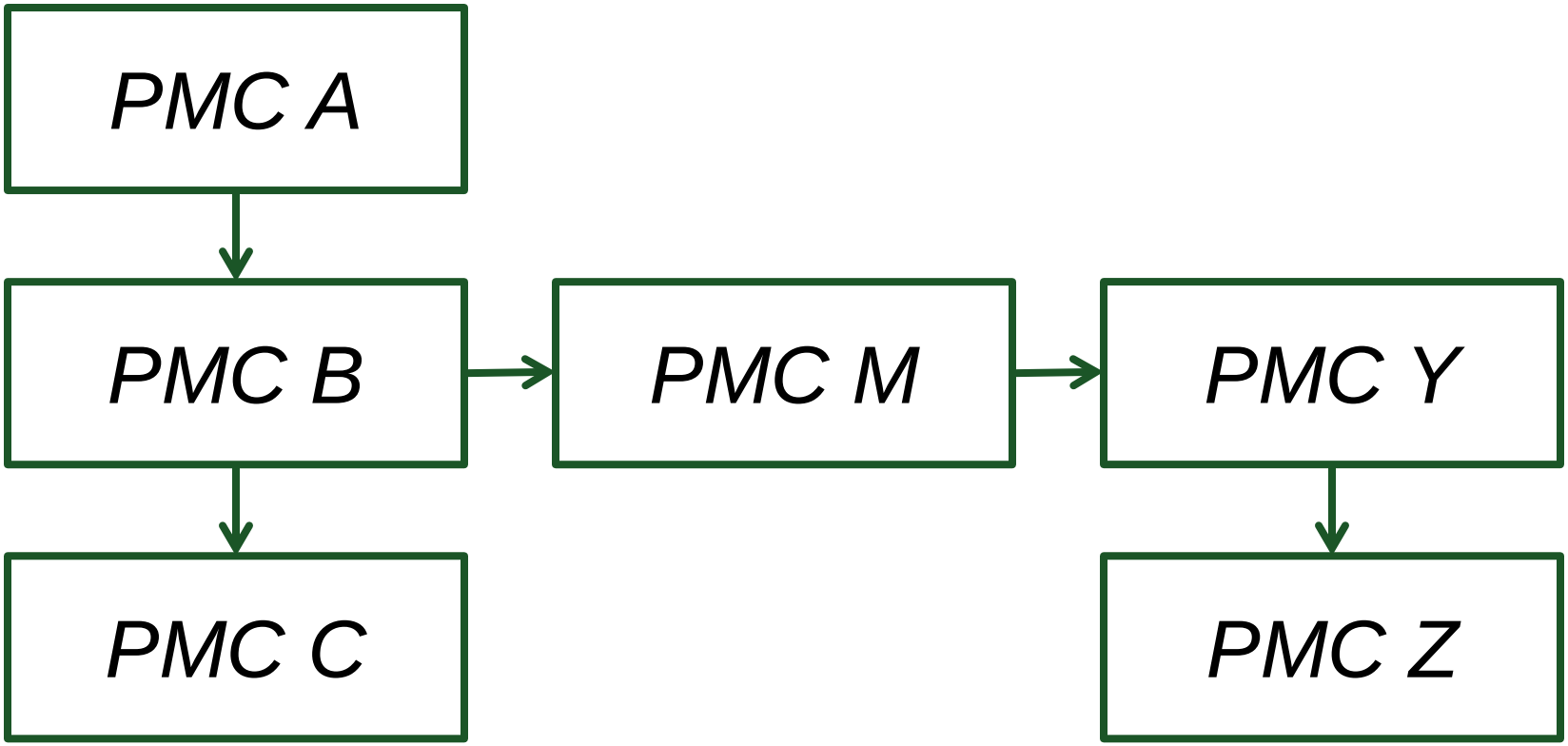
Motivation

- Brine density is heavily dependent upon solute concentrations in saline aquifers.
- How to implement a salinity-dependent brine density for all flow process models within PFLOTRAN without doubling the number of flow process models?

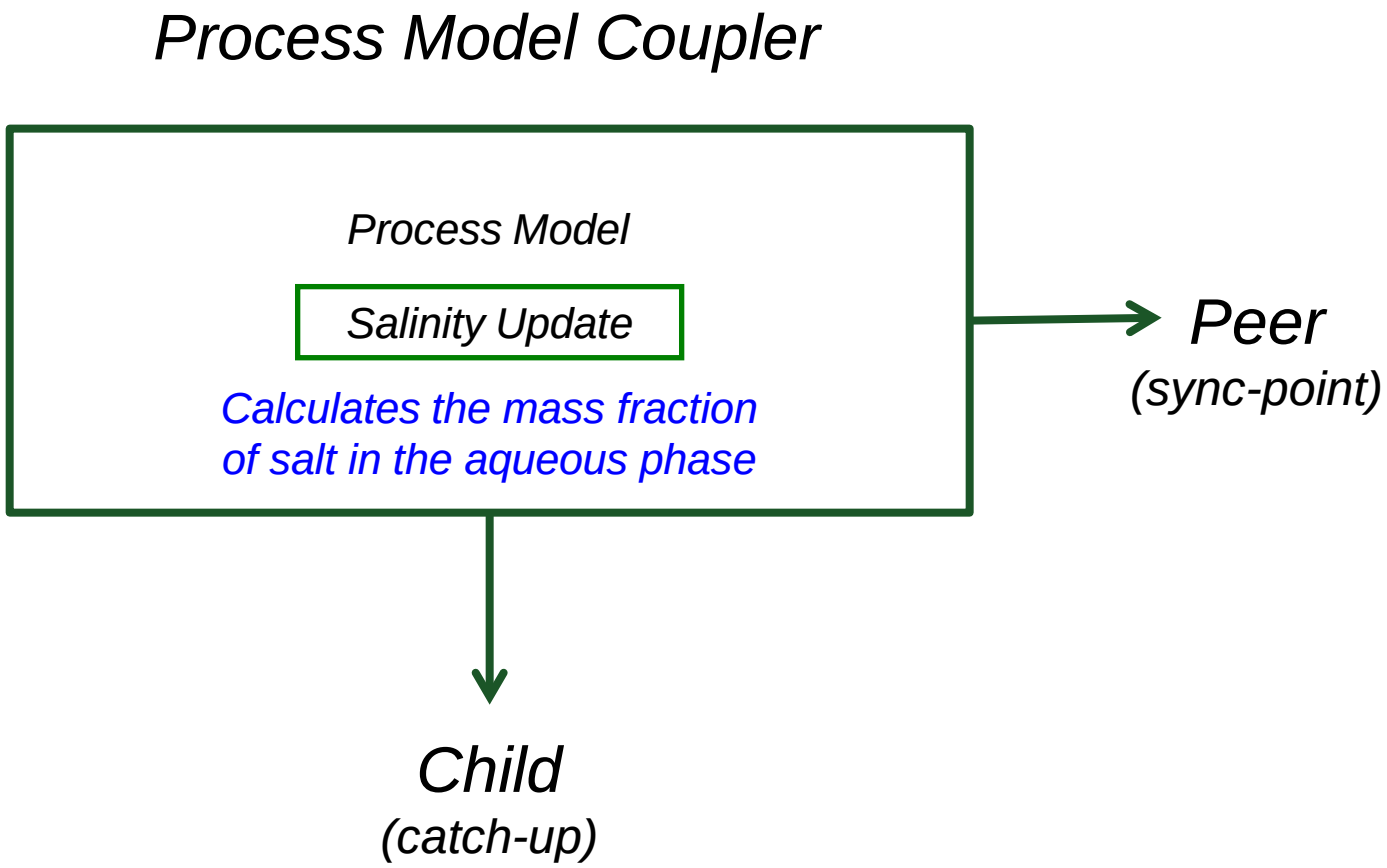
PFLOTRAN Process Model Coupler (PMC)



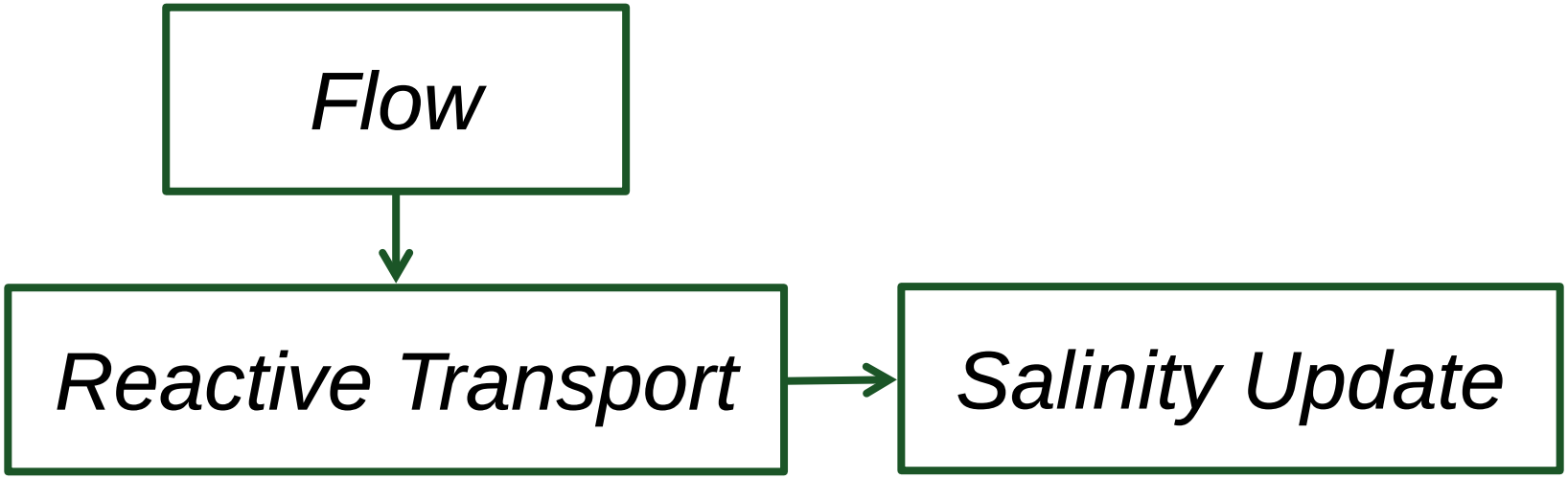
Hypothetical PFLOTRAN PMC Hierarchy



Salinity Update Process Model



PFLOTRAN Salinity Update



PFLOTRAN::EOS::EOS_Water:: EOSXXXBatzleAndWang()

Batzle, M and Z. Wang, (1992) Seismic properties of pore fluids, Geophysics, V57, N11, P 1396-1408.

Water Density [g/cm^3]

$$\rho_W = 1 + 1 \times 10^{-6}(-80T - 3.3T^2 + 0.00175T^3 + 489P - 2TP + 0.016T^2P - 1.3 \times 10^{-5}T^3P - 0.333P^2 - 0.002TP^2) \quad (27a)$$

Brine Density [g/cm^3]

$$\rho_B = \rho_W + S\{0.668 + 0.44S + 1 \times 10^{-6}[300P - 2400PS + T(80 + 3T - 3300S - 13P + 47PS)]\}, \quad (27b)$$

Brine Viscosity [mPa-s]

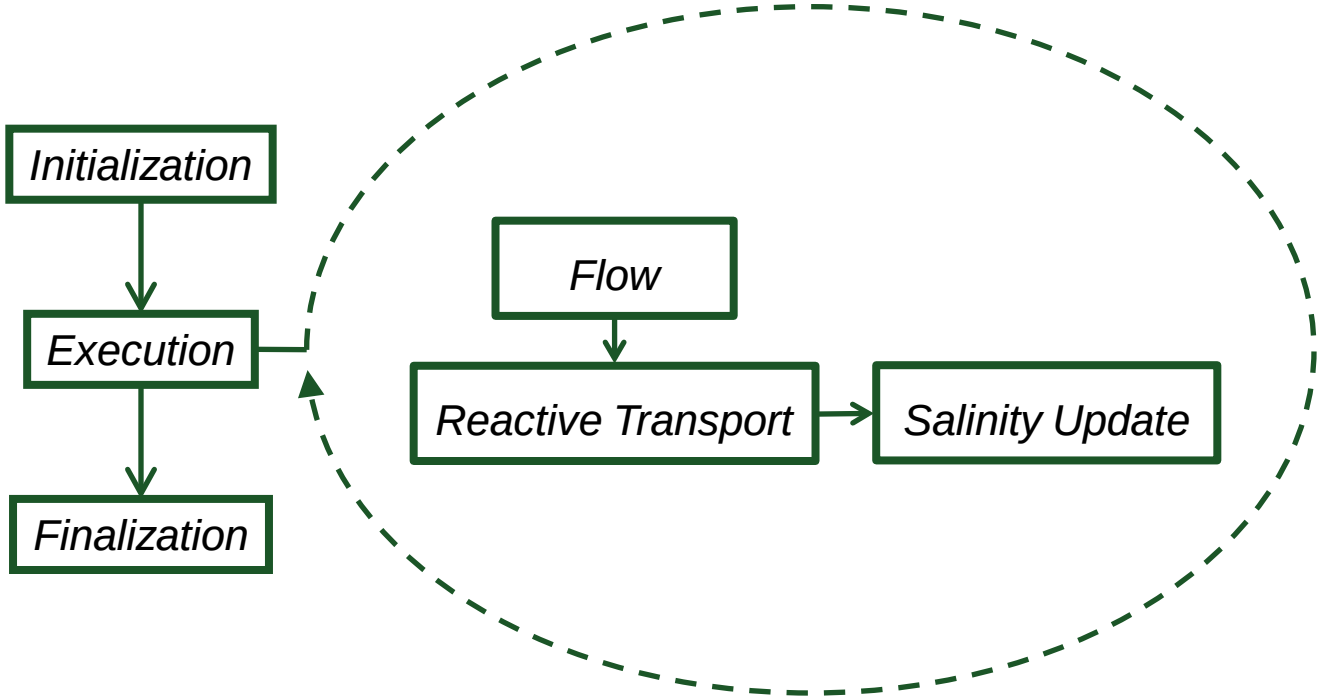
$$\eta = 0.1 + 0.333S + (1.65 + 91.9S^3) \exp\{-[0.42(S^{0.8} - 0.17)^2 + 0.045]T^{0.8}\}. \quad (32)$$

P = pressure [Pa], T = temperature [C], S = mass fraction [-]

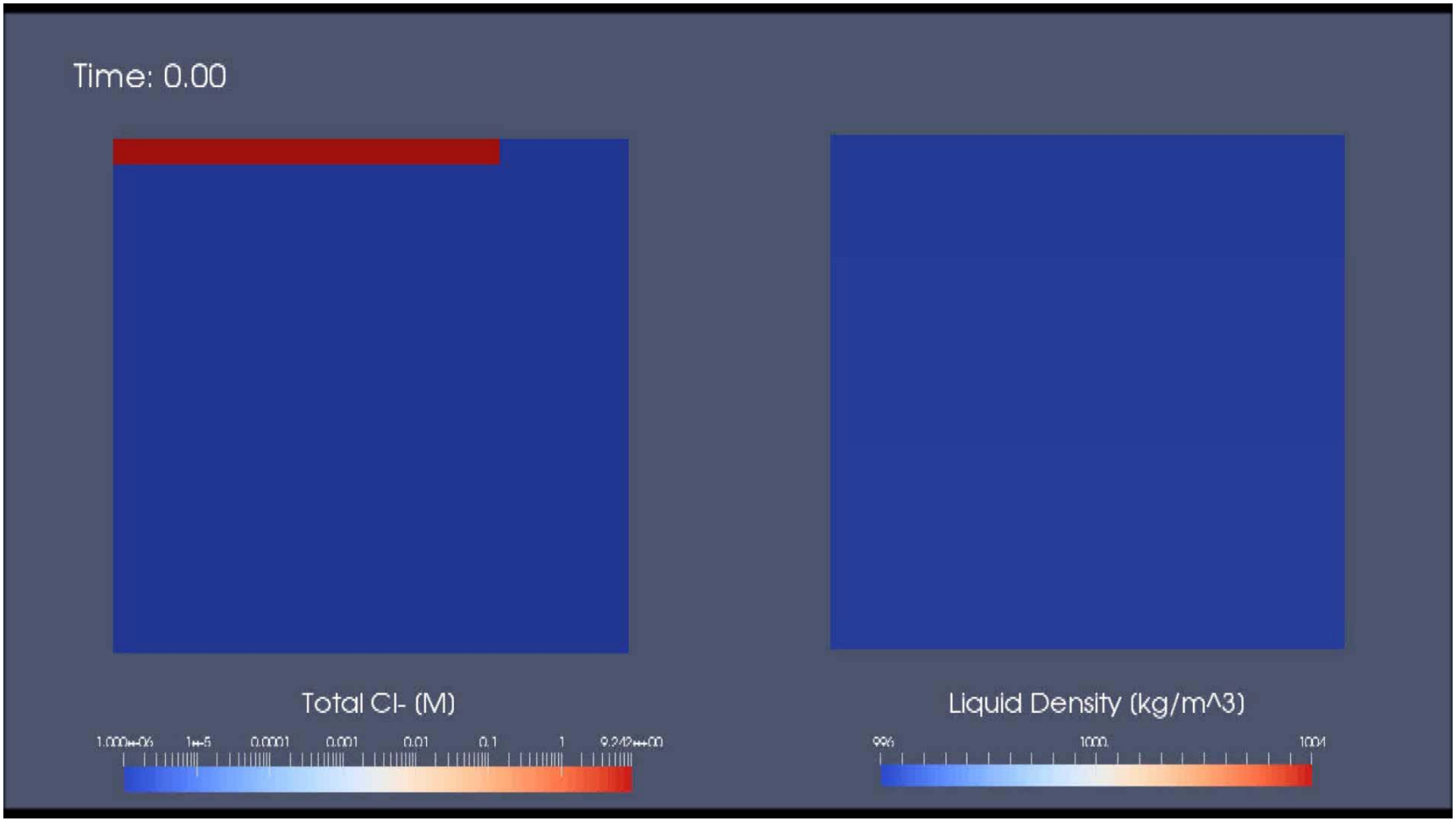
Modifications to the PFLOTRAN Input Deck

```
SIMULATION
  SIMULATION_TYPE SUBSURFACE
  PROCESS_MODELS
    SUBSURFACE_FLOW flow
      MODE RICHARDS
    /
    SUBSURFACE_TRANSPORT transport
      GLOBAL_IMPLICIT
    /
    AUXILIARY SALINITY
      SPECIES Na+ 22.9898
      SPECIES Cl- 35.4527
    /
  /
/

...

EOS WATER
  DENSITY BATZLE_AND_WANG
  VISCOSITY BATZLE_AND_WANG
/
```

PFLOTRAN Workflow



Density Driven Flow from Salt Layer



Kuhlman, 2016