Transport Modeling of Oilfield Brines

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Outline

- Need for Modeling
- Background Information and Context
- Data and Original Study
- Phreeqc Modeling
- Results
- Research Possibilities
- Questions/Discussion

Background Information/Context

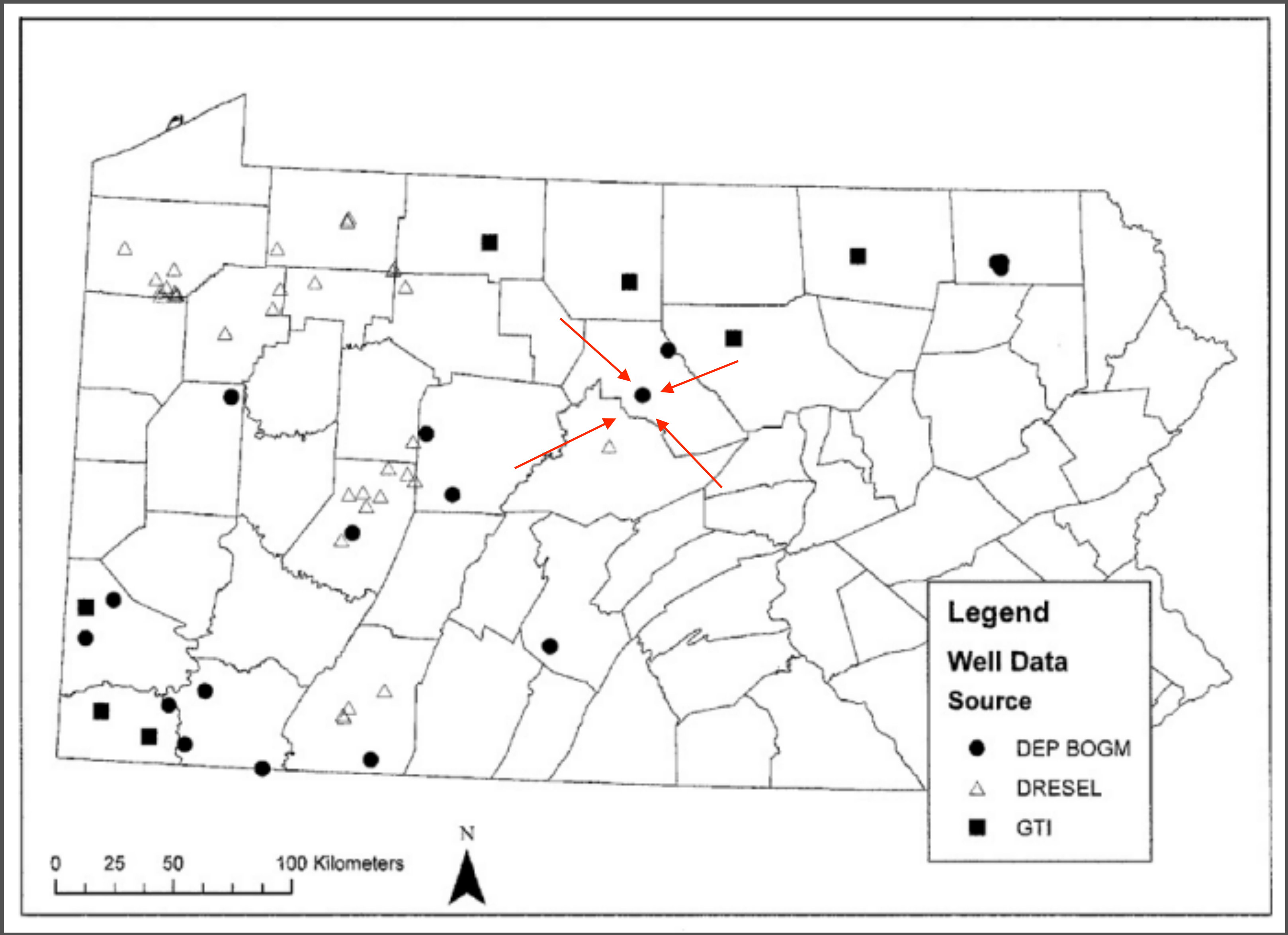
- Oil wells generate oil, natural gas, and production water
- Production water is a byproduct; not useful
- Typically have very high TDS and can contain harmful levels of heavy metals
  - TDS<30,000
- Wells can have significant output of these brines
- There is a large potential for spills
  - Pipeline leaks, injection well, illegal dumping
- 24 reported production water spills of >100 barrels in last 12 months in ND
  - Largest was 24,000 barrels
  - None were contained

Interest in Modeling

- Worked on several cleanups this past summer
- Interested in modeling the interaction of brines with groundwater
- Modeling transport through a water column
- Interested in an enhanced understanding as to potential impact

Data and Original Study

- Data for Brine came form Marcellus Shale in Pennsylvania
  - Study was on fracking by-products
- Very little research done on the Bakken
- Not very much modeling done on interaction of brines with the ground
- Modeled my groundwater after possible earth constituents in Western North Dakota


Legend
Well Data
Source
DEP BOGM
DRESEL
GTI
0
25
50
100 Kilometers
N

Assumptions for Modeling

- No interaction with organic material ie. topsoil, vegetation
- Composition of earth
  - K-feldspar, Quartz, Kaolinite
- Homogeneous composition throughout region of transport
- Chemistry of groundwater is the sole result of pure water interacting with K-feldspar, Quartz, Kaolinite
- Groundwater is in contact with atmosphere
- Assumption of inputs for transport modeling
  - Time interval, dipsersivities, distance, number of cells, number of shifts

tial
nditions for
oundwater

e Equilibrium Phases function
s used to simulate groundwater
eraction

: pure water in equilibrium with
eldspar, Quartz, and Kaolinite,
2 and 02

```
SOLUTION 1-400 Initial solution in earth
    temp       25
    pH         7 charge
    units      mg/l

EQUILIBRIUM_PHASES 1-400 bedrock geology
    K-feldspar 0 10
    Kaolinite 0 10
    Quartz     0 10
    CO2(g)     0 10
    O2(g)      0 10
```

```
---------------------------Description of solution-------------------------

                                       pH  =   7.088      Charge balance
                                       pe  =  13.711      Adjusted to redox e
      Specific Conductance (µS/cm, 25°C)  = 24350
                          Density (g/cm³)  =   1.01386
                               Volume (L)  =   1.00594
                        Activity of water  =   0.991
                           Ionic strength  =   2.544e-01
                       Mass of water (kg)  =   9.932e-01
                 Total alkalinity (eq/kg)  =   2.541e-01
                       Total CO2 (mol/kg)  =   2.861e-01
                         Temperature (°C)  =  25.00
                  Electrical balance (eq)  =  -3.792e-13
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                               Iterations  =  13
                                  Total H  = 1.105078e+02
                                  Total O  = 5.595094e+01
```

Transport Modeling

Explanation of Inputs

- Cells:
  - Number of individual spaces fluid will be transferred to
- Length
  - 4 meters per cell
- Shifts
  - Number of times solution 0 passes through the cells
- Time-Step
  - Time for solution to react in each cell
  - Overal time of transport is shifts*time-step
- Dispersivities
  - Variation between cells

```
TRANSPORT
    -cells                 400
    -length                4
    -shifts                60
    -time_step             43200 # seconds
    -dispersivities        400*1
    -correct_disp          true
    -thermal_diffusion     1   0
    -print_cells           40
    -print_frequency       20
    -punch_cells           40
    -warnings              false
```

Transport Modeling Continued

- Transport modeling assumes a column with a variable number of cells
  - Cell size and amount of time in each cell is variable
- The model is run by shifting solution one into the first cell and reacting it
- The same is done for all the other cells in the column
- This is carried on continuously for a set number of shifts which is variable
- The inputs were chosen to achieve the most meaningful results possible
  - Through reading and trial and error

Brine Analysis

```
LE Brine Calculation
UTION 0 Brine
 temp        25
 pH          6.3
 pe          12.5 O2(g) 0
 redox       pe
 units       mg/l
 density     1
 Alkalinity 235
 Ba          6270
 Br          613
 Ca          12500
 Cl          83500
 K           224
 Mg          0
 Mn          5
 Na          34300
 Sr          3570
 -water      1 # kg
```

```
----------------------------Description of solution---------------------

                                          pH  =   6.300
                                          pe  =  14.516      Equilibrium wit
       Specific Conductance (µS/cm, 25°C)  = 186253
                          Density (g/cm³)  =   1.10767
                               Volume (L)  =   1.05135
                        Activity of water  =   0.916
                           Ionic strength  =   3.171e+00
                       Mass of water (kg)  =   1.000e+00
                    Total carbon (mol/kg)  =   6.044e-03
                       Total CO2 (mol/kg)  =   6.044e-03
                         Temperature (°C)  =  25.00
                  Electrical balance (eq)  =  -8.521e-02
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -1.57
                               Iterations  =   7
                                  Total H  = 1.110179e+02
                                  Total O  = 5.552499e+01
```

Results

```
-------------Description of solution---------------------------

                         pH  =   7.088      Charge balance
                         pe  =  13.711      Adjusted to redox equilibrium
c Conductance (µS/cm, 25°C)  = 24350
             Density (g/cm³)  =   1.01386
                  Volume (L)  =   1.00594
           Activity of water  =   0.991
              Ionic strength  =   2.544e-01
          Mass of water (kg)  =   9.932e-01
    Total alkalinity (eq/kg)  =   2.541e-01
         Total CO2 (mol/kg)   =   2.861e-01
           Temperature (°C)   =  25.00
     Electrical balance (eq)  =  -3.792e-13
, 100*(Cat-|An|)/(Cat+|An|)   =  -0.00
                  Iterations  =  13
                     Total H  = 1.105078e+02
                     Total O  = 5.595094e+01
```

l groundwater

```
----------------------------Description of solution------------------------

                                       pH  =   6.987      Charge balance
                                       pe  =  13.823      Adjusted to redox
        Specific Conductance (µS/cm, 25°C)  = 119300
                           Density (g/cm³)  =   1.08491
                                Volume (L)  =   1.03284
                         Activity of water  =   0.942
                            Ionic strength  =   1.918e+00
                        Mass of water (kg)  =   9.900e-01
                  Total alkalinity (eq/kg)  =   3.786e-01
                        Total CO2 (mol/kg)  =   3.969e-01
                          Temperature (°C)  =  25.00
                   Electrical balance (eq)  =  -4.793e-02
Percent error, 100*(Cat-|An|)/(Cat+|An|)    =  -1.37
                                Iterations  =   3
                                   Total H  = 1.102721e+02
                                   Total O  = 5.611104e+01
```

Groundwater after 20 Shifts

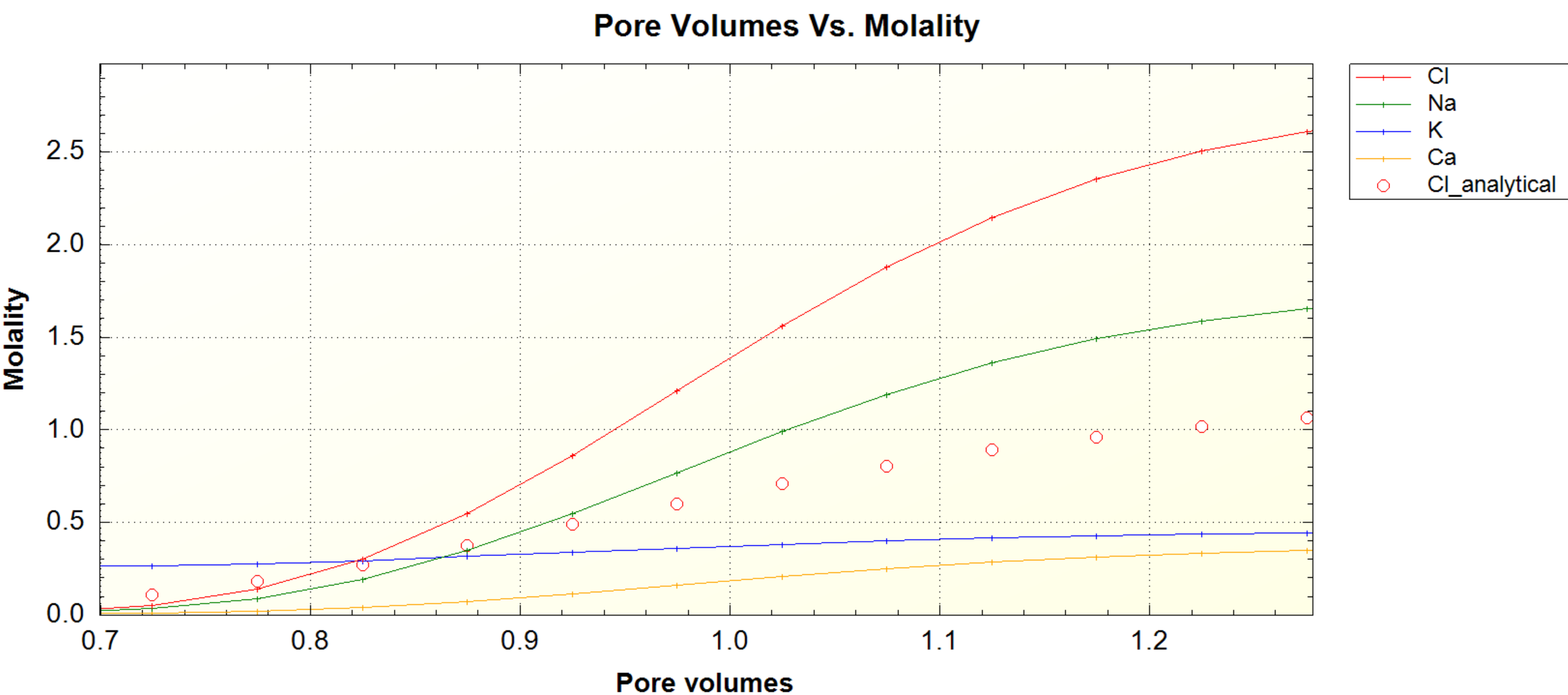
- Only major changes are those related to dilution of the solution

Results

-----------------------------Saturation indices-----------------------------

Phase	SI**	log IAP	log K(298 K, 1 atm)	
Al(OH)3(a)	-3.12	7.68	10.80	Al(OH)3
Albite	-2.02	-20.02	-18.00	NaAlSi3O8
Anorthite	-5.67	-25.38	-19.71	CaAl2Si2O8
Aragonite	2.65	-5.68	-8.34	CaCO3
Ca-Montmorillonite	-2.36	-47.39	-45.03	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	2.80	-5.68	-8.48	CaCO3
CH4(g)	-140.66	-143.50	-2.84	CH4
Chalcedony	-0.43	-3.98	-3.55	SiO2
CO2(g)	-0.00	-1.46	-1.46	CO2 Pressure 1.0 atm, phi 0.994
Gibbsite	-0.43	7.68	8.11	Al(OH)3
H2(g)	-41.67	-44.77	-3.10	H2
H2O(g)	-1.53	-0.03	1.50	H2O
Halite	-1.72	-0.15	1.57	NaCl
Hausmannite	5.04	66.07	61.03	Mn3O4
K-feldspar	-0.00	-20.57	-20.57	KAlSi3O8
K-mica	4.81	17.51	12.70	KAl3Si3O10(OH)2
Kaolinite	0.00	7.44	7.43	Al2Si2O5(OH)4
Manganite	3.60	28.94	25.34	MnOOH
O2(g)	-0.00	-2.89	-2.89	O2 Pressure 1.0 atm, phi 0.999
Pyrochroite	-7.07	8.13	15.20	Mn(OH)2
Pyrolusite	8.35	49.73	41.38	MnO2:H2O
Quartz	0.00	-3.98	-3.98	SiO2
Rhodochrosite	1.14	-9.99	-11.13	MnCO3
SiO2(a)	-1.27	-3.98	-2.71	SiO2
Strontianite	2.63	-6.64	-9.27	SrCO3
Sylvite	-1.61	-0.71	0.90	KCl
Witherite	2.03	-6.53	-8.56	BaCO3

- After 20 Shifts
- Highlighted are the super-saturated minerals
- Primarily minerals with carbonate ions or manganese ions
- Chance for several ions to precipitate out
  - Ca, Mn, Ca, CO3



- Pore volumes definition:
  - *PV* = (number of shifts + 0.5) / (number of cells)
- Essentially this is a graph of concentration at the bottom of the column as fluid is shifted through it
- Can see the comparatively rapid increase in concentration of Cl and Na compared with K and Ca

Results

- Element concentrations in original production water sample and groundwater after 20 shifts (approximately 1 pore volume)
- There is a decrease of approximately 40 percent
  - Still significant concentrations though
- Would require significant dilution to return water to normal levels

Elements	Molality	Moles
Alkalinity	5.468e-03	5.468e-03
Ba	5.316e-02	5.316e-02
Br	8.933e-03	8.933e-03
Ca	3.632e-01	3.632e-01
Cl	2.743e+00	2.743e+00
K	6.671e-03	6.671e-03
Mn	1.060e-04	1.060e-04
Na	1.737e+00	1.737e+00
Sr	4.744e-02	4.744e-02

Elements	Molality	Moles
Al	1.737e-08	1.719e-08
Ba	3.021e-02	2.990e-02
Br	5.076e-03	5.025e-03
C	3.969e-01	3.929e-01
Ca	2.063e-01	2.043e-01
Cl	1.558e+00	1.543e+00
K	3.792e-01	3.755e-01
Mn	6.022e-05	5.962e-05
Na	9.871e-01	9.773e-01
Si	5.987e-05	5.927e-05
Sr	2.696e-02	2.669e-02

Possible Future Research

- With a greater understanding of phreeqc
  - Modeling of production water contaminating streams
  - Larger scale modeling of contamination from injection well
  - Better modeling of distance of impact per volume
    - 3D modeling
- Analysis of production water for potentially harmful heavy metals
- More data on production water from other oil fields
  - Other fields might contain drastically different chemical constituents

References

- Haluszczak, Lara O., Arthur W. Rose, and Lee R. Kump. "Geochemical Evaluation of Flowback Brine from Marcellus Gas Wells in Pennsylvania, USA." *Applied Geochemistry* 28 (2013): 55-61. Web.
- "North Dakota Department of Health." http://www.ndhealth.gov/

Questions?