Modelling the Reactivity of Multi-Mineral Systems – Application to the Prediction of Copper Heap Leach Drain Down Chemistry

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Outline

1. Introduction
2. Kinetic database
3. Kinetic approach to numerical modelling
4. Application to Heap Leach modelling
5. Conclusions

Kinetic Database

(Declercq & Oelkers 2012, 2013)

Rationale:

- Large number of mineral dissolution data exist
- Correspondingly few aggregation efforts, beyond the single mineral or mineralogical family

Building upon earlier efforts such as Palandri and Kharaka (2004)

This work has been initiated as part of the Carbfix project, carried out at the LMTG (now GET) and is being finalized with SRK

Method:

- Literature review of existing reactivity data for a mineral
- Plot of the data
- Choosing a best fit of the data
- Inclusion of the equation in PHREEQC
- Comparison of the model with the data

Challenges:

- Variable amount of available data between minerals,
- the degree to which the data from different laboratories can be compared can be called to question.

“The dissolution equations produced represent our best estimate based on the available data and are a preliminary effort in producing a consistent database for geochemical modeling”

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Kinetic Database - Equations

After a thorough literature review, the dissolution data for the different phases considered is plotted as a function of pH and temperature, and their reactivity equation is determined or used from the literature.

Example :

$$r_+ = A_a \times \left[\exp\left(\frac{-Ea}{R \times Tk}\right)\right] \times \left(\frac{x.a_{H^+}}{a_{M^{x+}}}\right)^n + A_b \times \left[\exp\left(\frac{-Eb}{R \times Tk}\right)\right] \times \left(\frac{x.a_{OH^-}}{a_{M^{x+}}}\right)^n$$

or for carbonates

$$r_+ = \left[Aa \times \left[\exp\left(\frac{-Ea}{R \times Tk}\right)\right] \times (a_{H^+})^n\right] +$$

$$\left[Ab \times \left[\exp\left(\frac{-Eb}{R \times Tk}\right)\right] \times (a_{H_2CO_3})^n\right] +$$

$$\left[Ac \times \left[\exp\left(\frac{-Ec}{R \times Tk}\right)\right] \times (a_{H_2O})^n\right] -$$

$$\left[Ad \times \left[\exp\left(\frac{-Ed}{R \times Tk}\right)\right] \times (a_{HCO_3^-})^n\right]$$

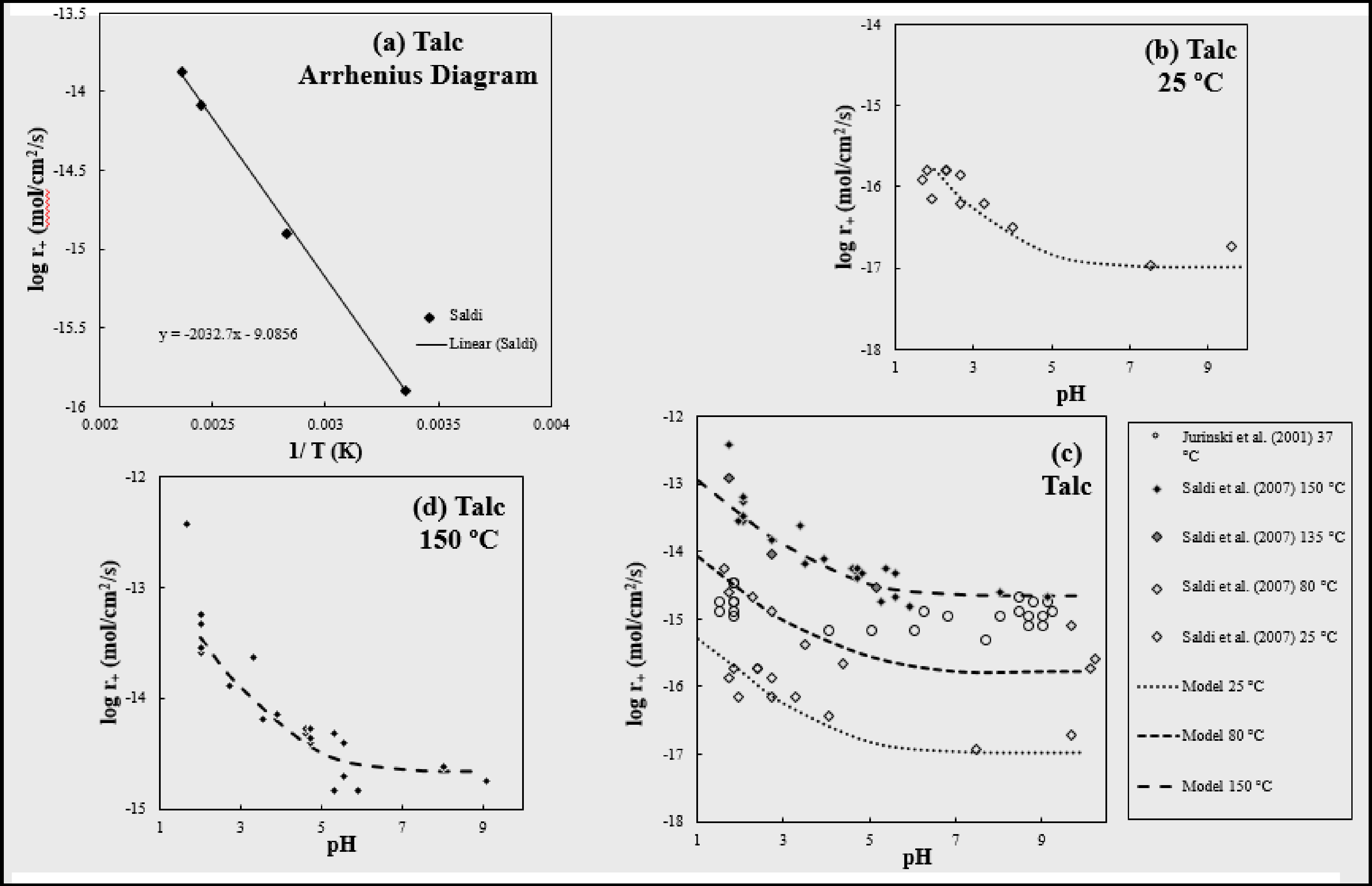
and

$$\text{rate} = r_+ \times \left(\frac{1 - SR\,(\text{"Mineral"})}{\Sigma}\right)$$

Equations of this form have been integrated in a database based on the LLNL database, which is used by PHREEQC

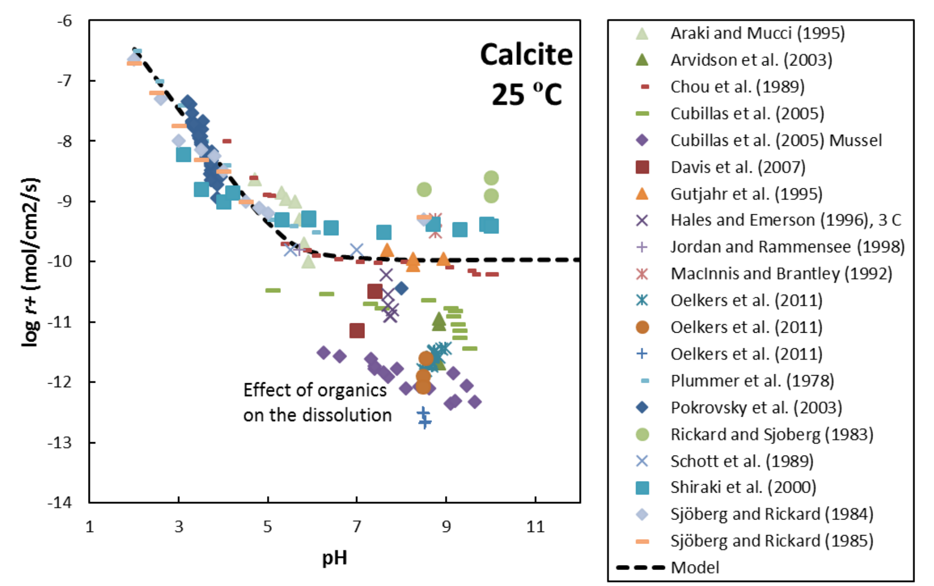
The database contains 107 minerals across the various mineralogical groups

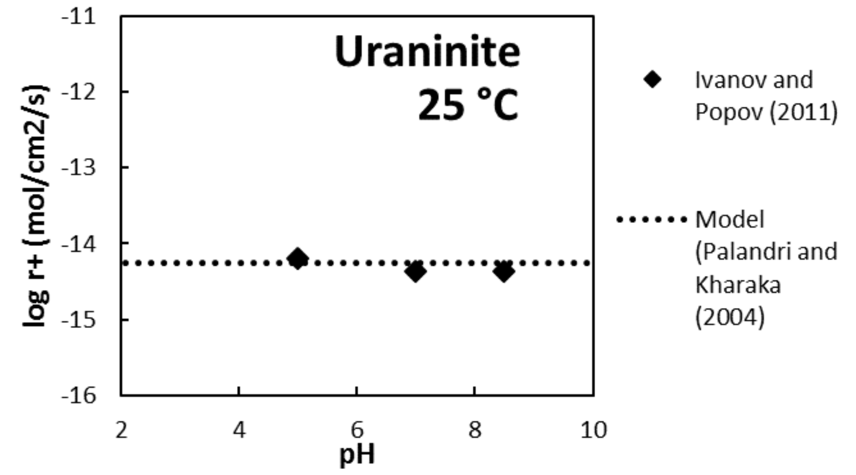
Kinetic Database – Parameters

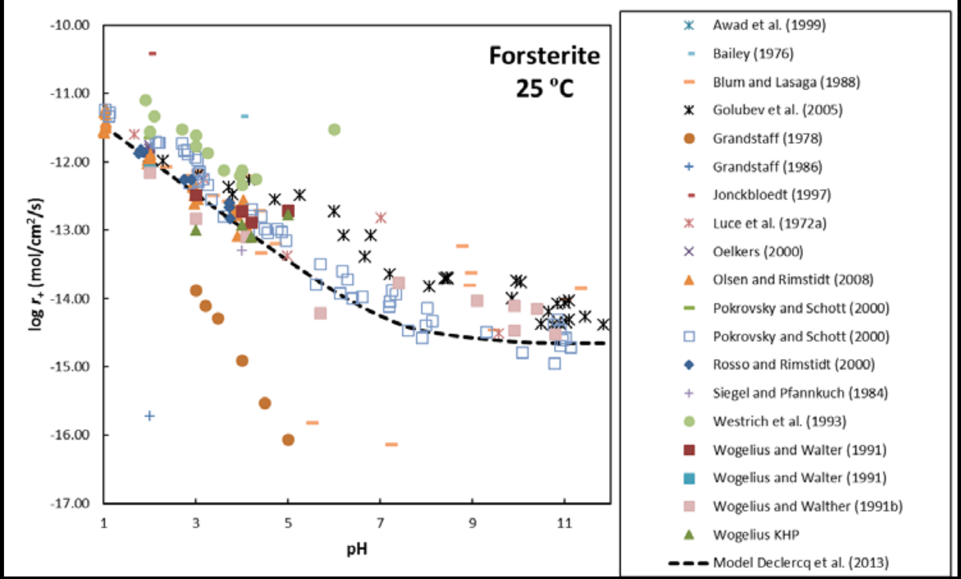


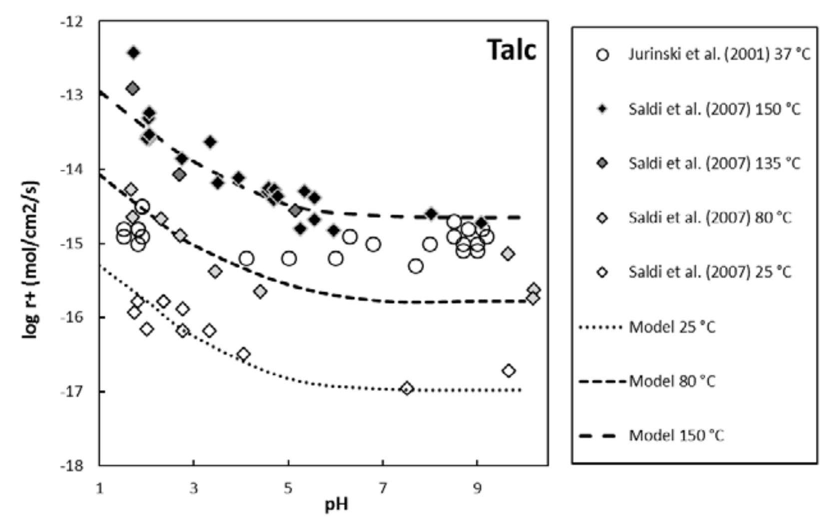
(a) Talc ($Mg_3Si_4O_{10}(OH)_2$) dissolution as a function of the inverse of temperature allowing the recalculation of equation 1 parameters. (b and d) Talc dissolution rates as a function of pH at 25 and 150 °C showing the good adequation of the model in dashed line and the data in diamonds. (c) is the entirety of the data available for talc. (Declercq & Oelkers, 2013)

Kinetic Database – A few Examples



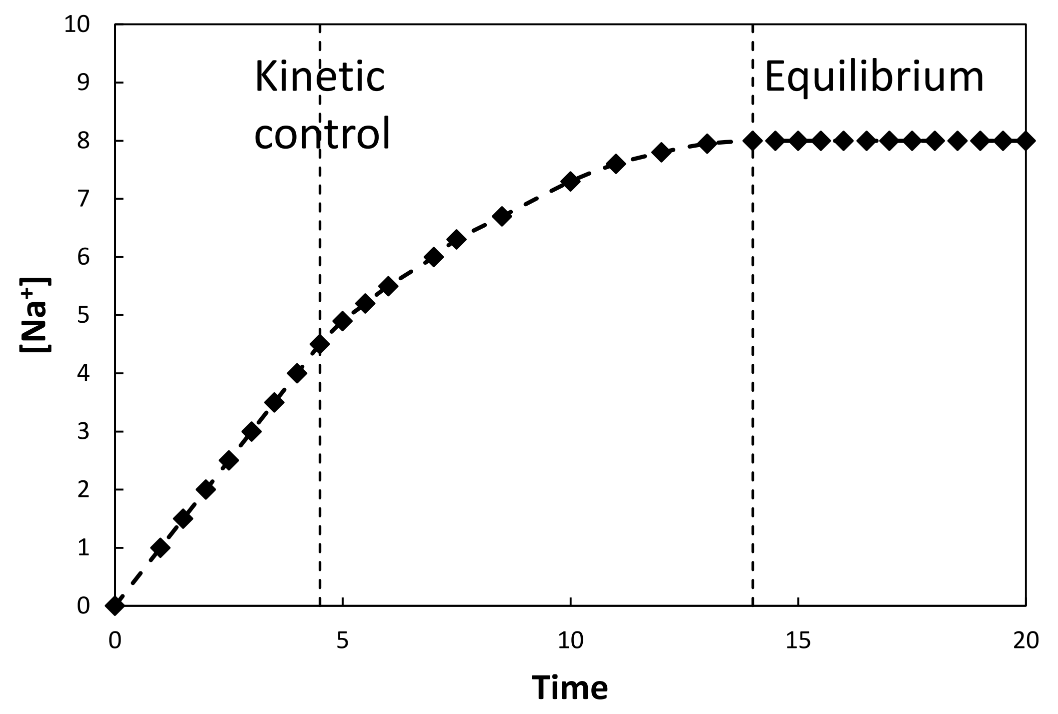






Modelling at Equilibrium

- Thermodynamic equilibrium
- Caveat: apart from fast reacting phases, no mineral is at equilibrium on the timescale considered in our calculations
- When possible compensation measures have to be employed, such as fixing SI values
- But they are educated guesses
- Or slow reacting phases have to be left out of the calculation (e.g. silicates)
- Use the results of leach tests to define a "reaction rate" such as HCT



Halite dissolution in deionised water

Modelling with Kinetics

Kinetic approach, A more natural approach to the calculation:

- Define the mineral phases in the system and their chemistry
- Define mass, reactive surface area
- Define the solution circulating around it
- Let it react for some time …

Just like the real thing.

Drawbacks:

Need good data:

- mineralogical definition
- Surface area measurement
- Proportion of the different minerals

Which is not so simple when considering multi million tonne systems.

SRK database has 107 kinetic phases

Silicates

- Albite
- Andesine
- Anorthite
- Augite
- Biotite
- Epidote
- Fayalite
- Forsterite
- Hornblende
- K-Feldspar
- Muscovite
- Pyrophyllite
- SiO2
- Smectite

Ore Minerals

- Chalcopyrite
- Galena
- Orpiment
- Pyrite
- Pyrrhotite
- Realgar
- Sphalerite
- Uraninite

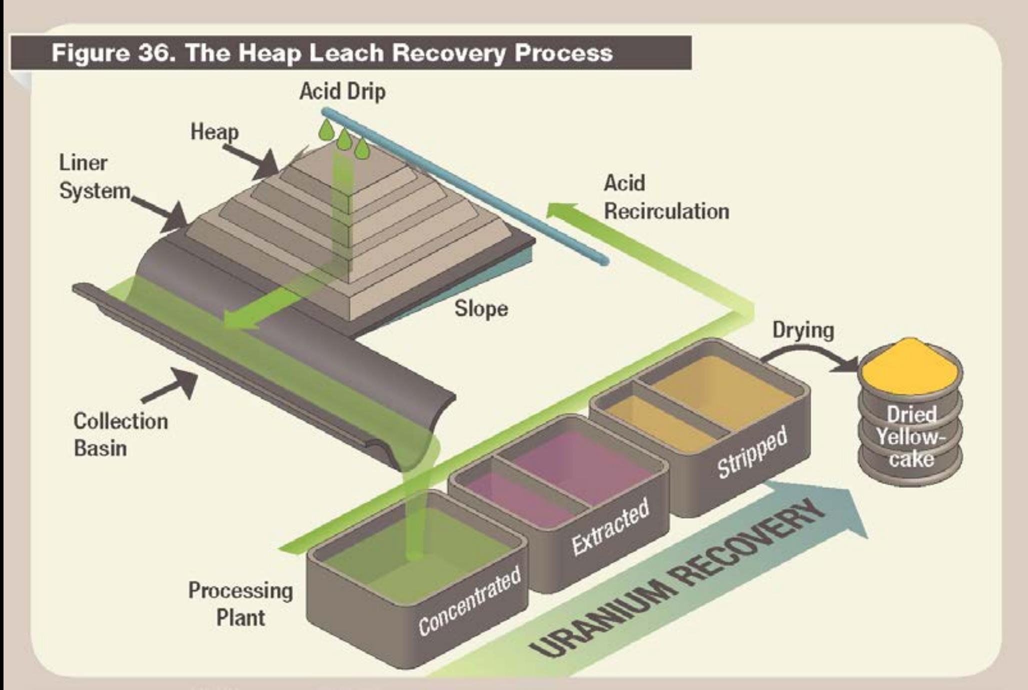
Carbonates, Sulfates, Oxides, etc

- Aragonite
- Barite
- Calcite
- Celestite
- Dawsonite
- Dolomite
- Fluorite
- Gibbsite
- Gypsum
- Goethite
- Halite
- Malachite
- Scorodite

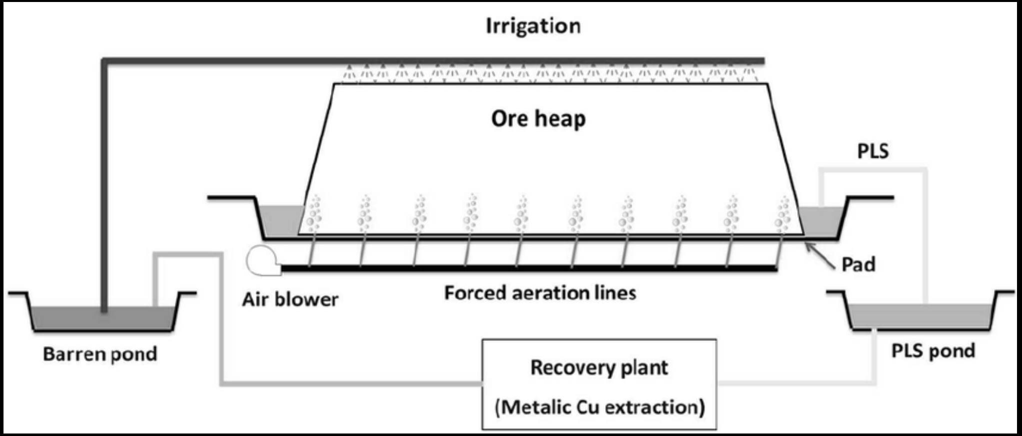
Heap Leach

Heap leaching :

- Common techniques used since the 15th century to recover metals
- 37 different heap leach mines in operation for gold, producing 7.4% of the world's gold
- Low capital cost (relative to other method)
- Usually used for low grade ore in oxidized host rock



Heap leach diagram (US NRC, 2015)
Uranium extraction



Heap leach schematic (Petersen, 2015)
Copper extraction

Cu HLP under construction in Arizona USA

Heap Leach Model – Assumptions and Hypothesis

For the purpose of the model the following assumptions were made:

- The system behaves like a 1-D column (a very large one); infiltrating solution percolates vertically downward
- 1-D downward flow with advection – dispersion
- Flowing – reacting system
- Both equilibrium chemistry and kinetic reactions
- The reactivity of the system is influenced by sulfide oxidation and carbonate / silicate buffering
- Additionally the kinetic model allows silicate buffering

Heap Leach Model – Mineralogical Assumptions

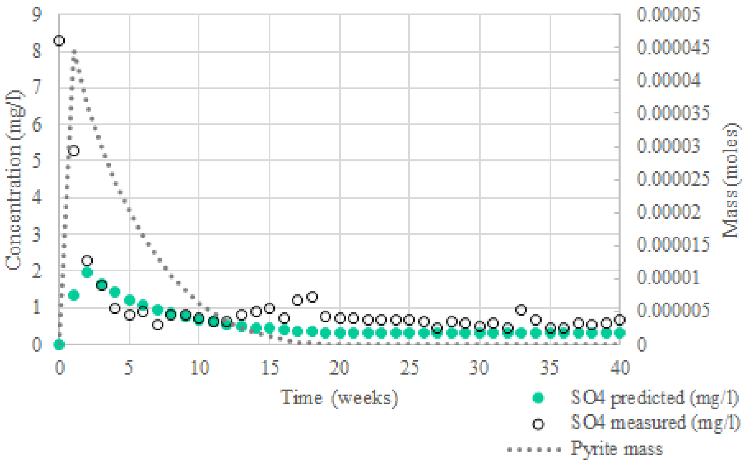
Assumed equilibrium controls

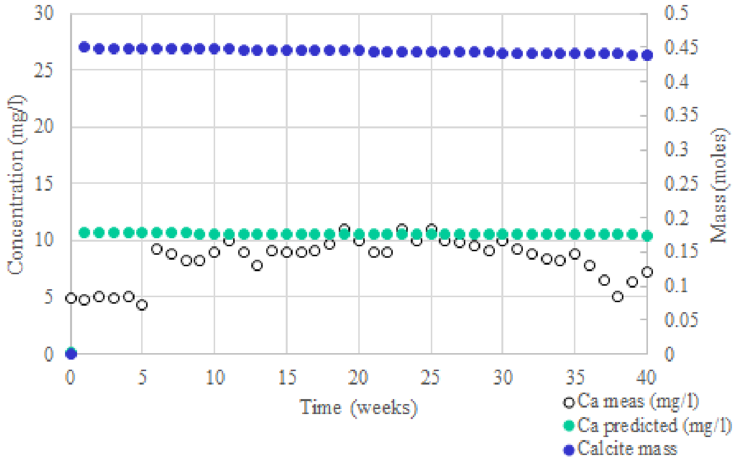
- Barite ($BaSO_4$)
- Epsomite ($MgSO_4:7H_2O$)
- Fluorite (CaF_2)
- Gibbsite ($Al[OH]_3$)
- Gypsum ($CaSO_4:2H_2O$)
- Amorphous Silica ($SiO_{2\ [a]}$)
- CO_2 and O_2 are unconstrained

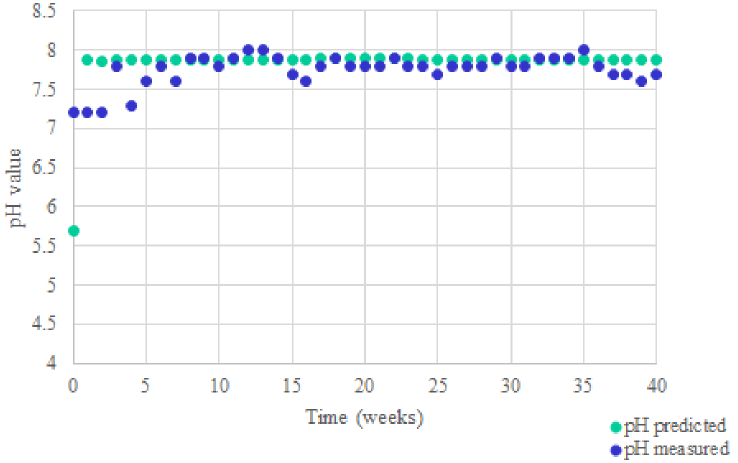
Assumed kinetic controls:

- Pyrite (FeS_2)
- Chalcopyrite ($CuFeS_2$)
- K-Feldspar ($KAlSi_3O_8$)
- Muscovite ($KAl_3Si_3O_{10}[OH]_{10}$)

It is reminiscent of a Humidity Cell….



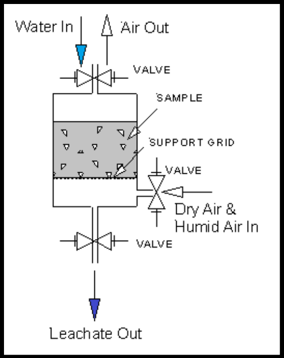




Kinetic model:

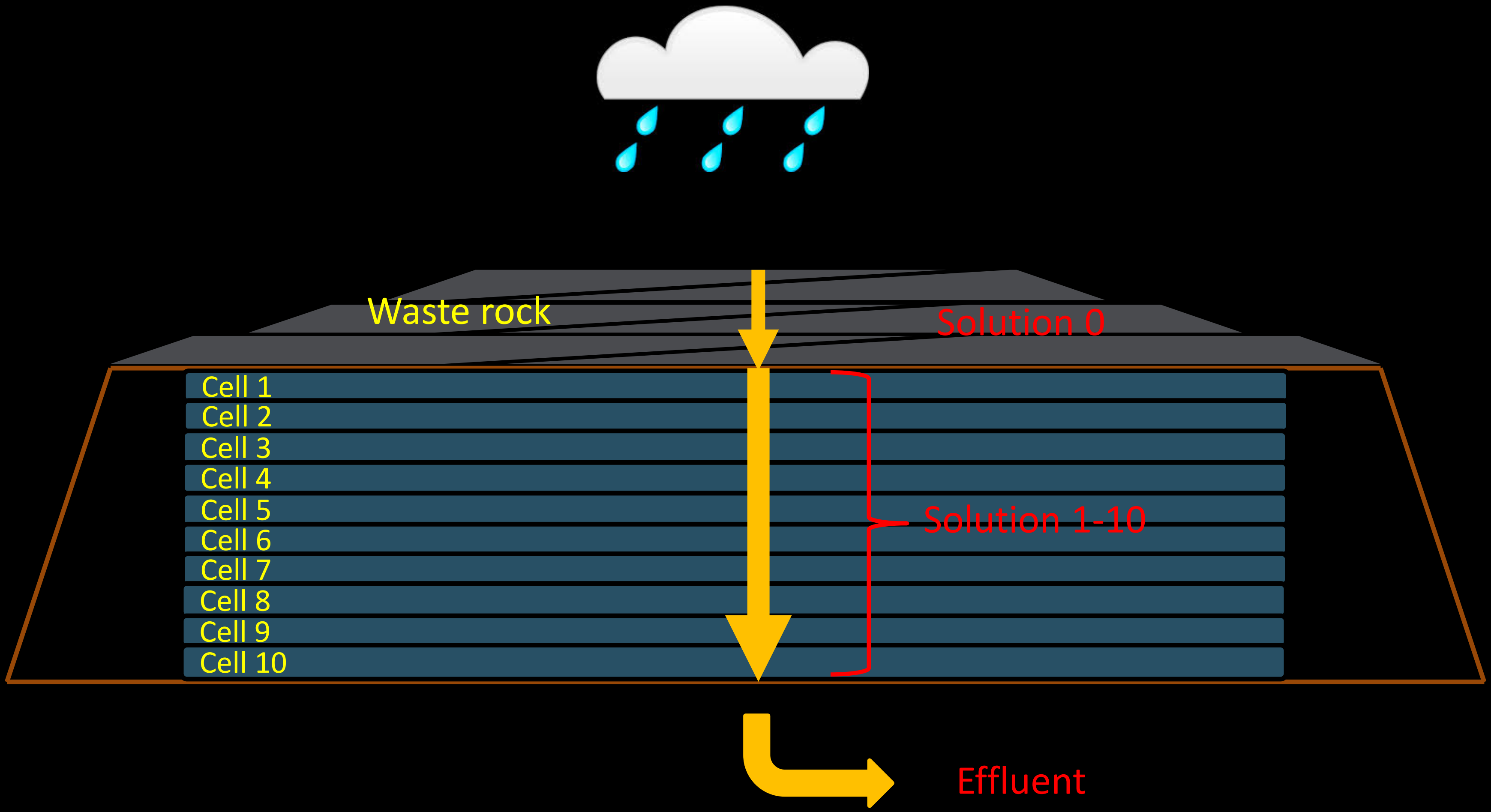
Reasonable fit for most samples over the long term.

Could not represent detailed/short-term variability of lab data.

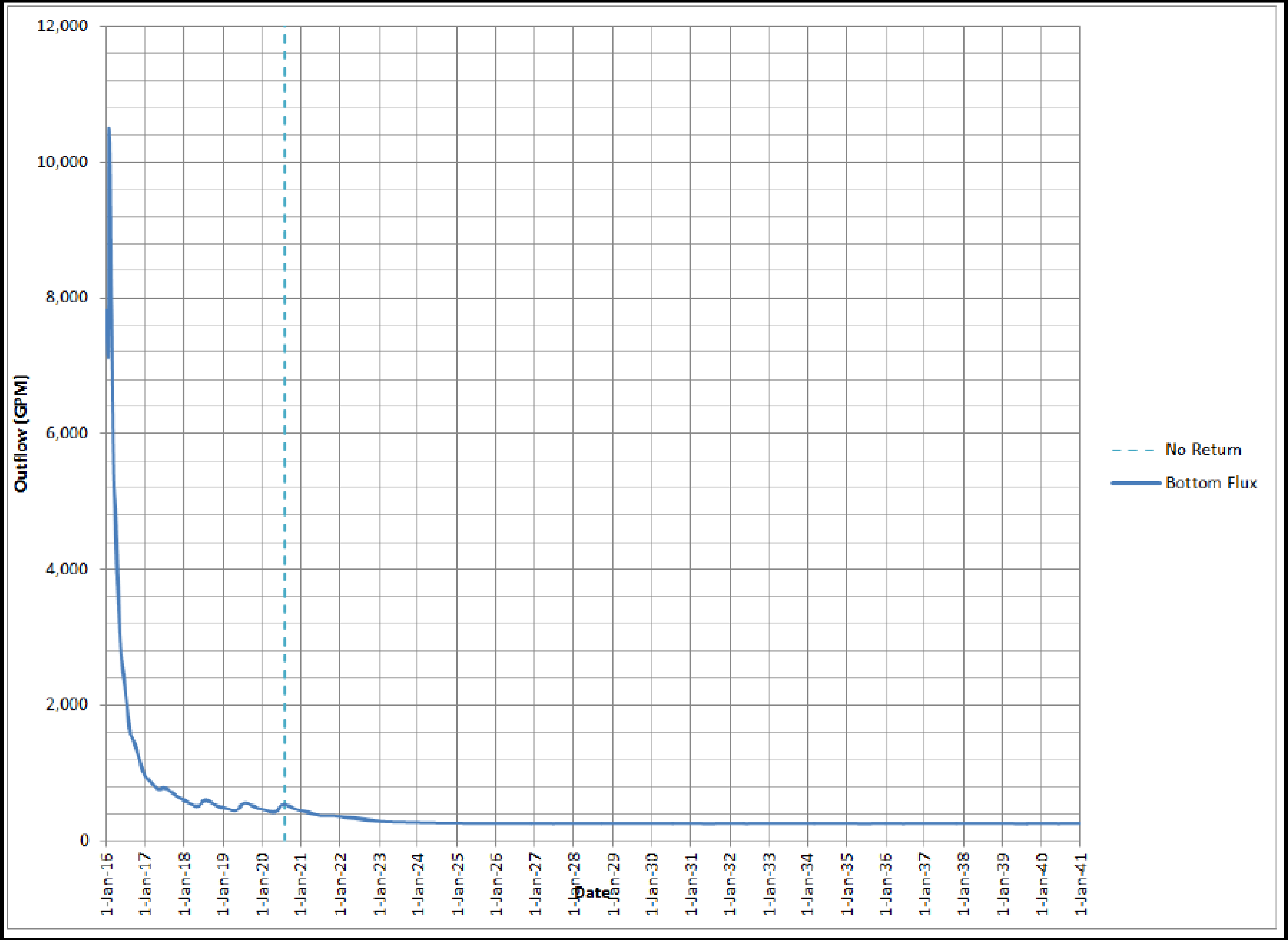


Please go and see the poster session for more info!

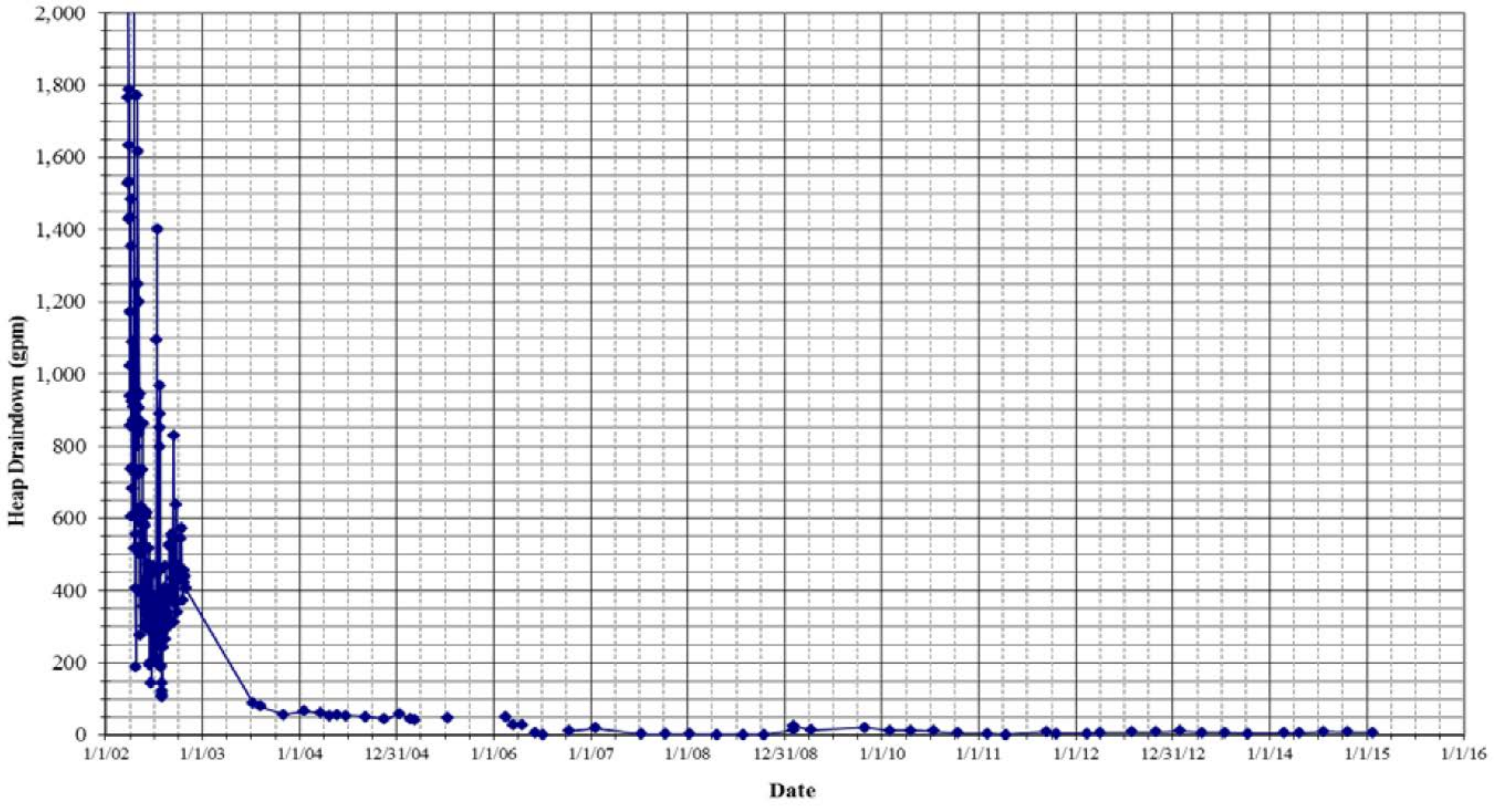
HLP Conceptual Model



Heap Leach Draindown Flow



Heap Leach Draindown Flow (Actual)



Specific Model Parameters

- Average HLP thickness = 150m
- Ten cells of equal thickness (15m)
- Cells are laterally continuous (1-D model)
- First pore volume cycles in 196 years
- Rock density = 2.96
- HLP porosity = 0.3
- HFO mass = 221.6 g/L
- Simulated 10 pore volumes (2,000 years)
- Chemistry of Solution 0 is constant through time

Chemistry of Model Inputs

Raffinate
Solution 1

pH	1.81
Al	6780
Be	1.32
Ca	493
Cd	1.8
Cu	15.4
Fe	671
F	1060
Mg	4940
SO4	66,600
U	24.8
Zn	364

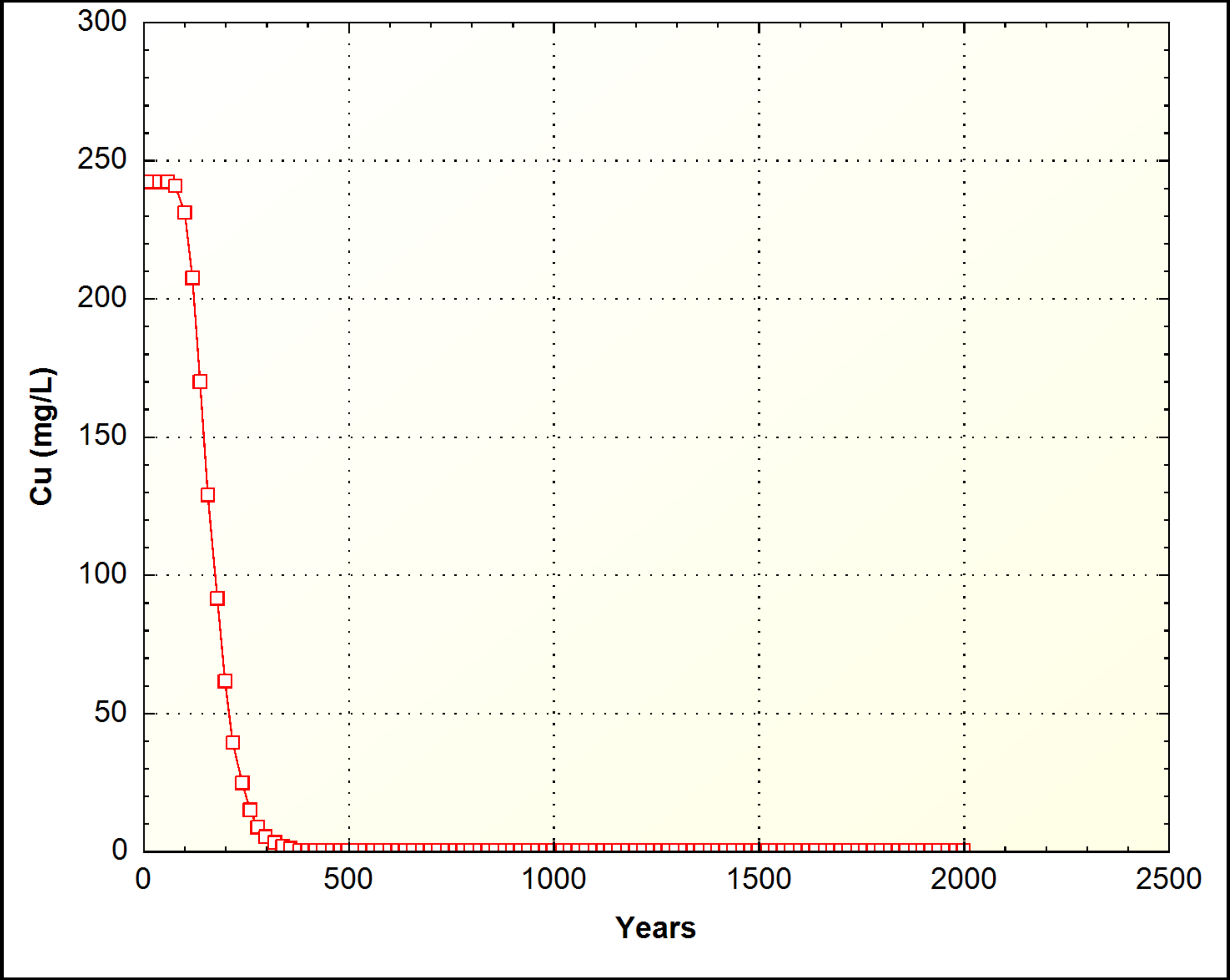
PLS
Solution 2-10

pH	2.19
Al	7300
Be	1.23
Ca	510
Cd	1.82
Cu	221
Fe	712
F	780
Mg	4740
SO4	71,500
U	25.5
Zn	356

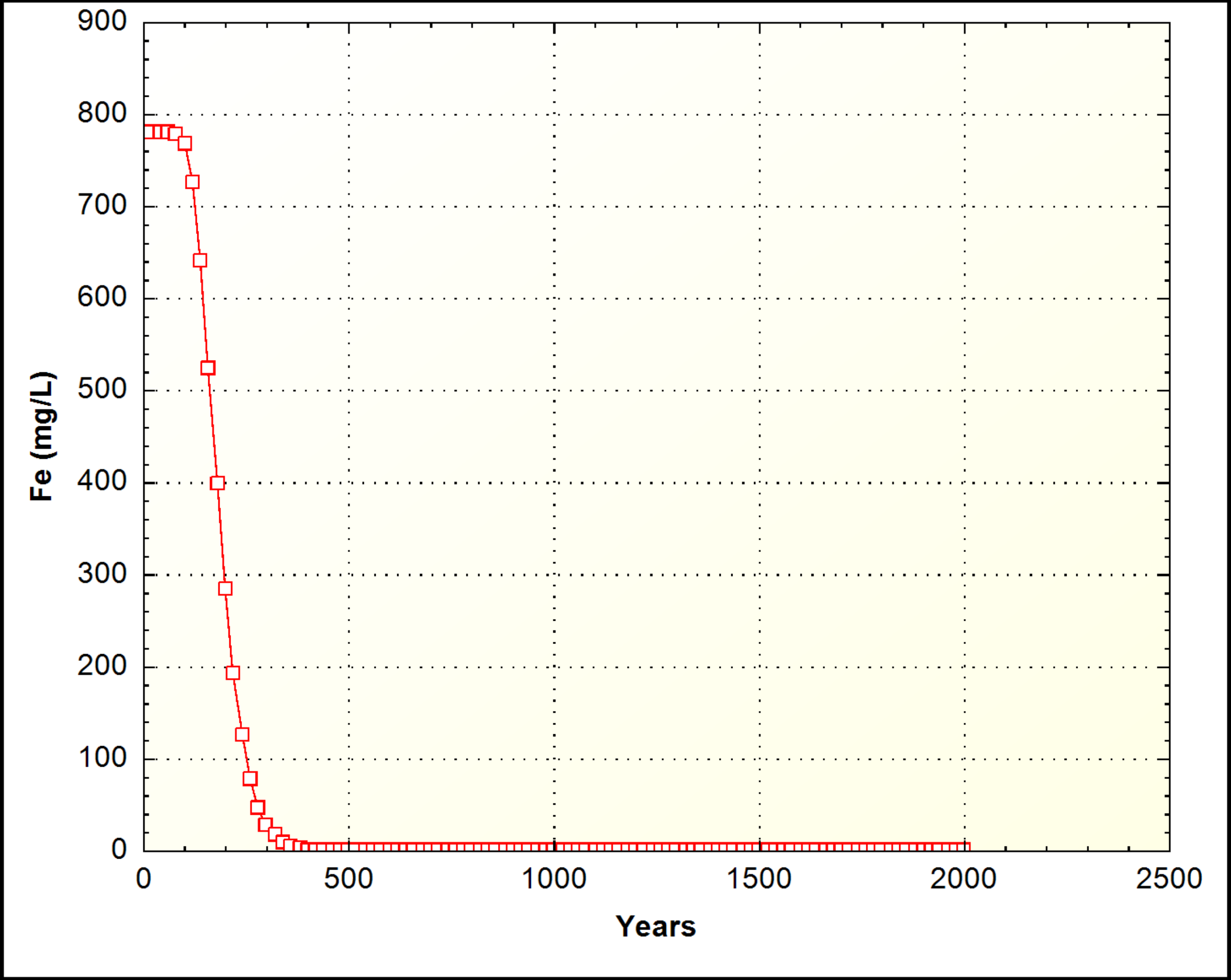
Waste Rock Cover (predicted)
Solution 0

pH	7.2
Al	0.003
Be	0.00005
Ca	70.1
Cd	0.0002
Cu	0.02
Fe	0.002
F	2.11
Mg	14.8
SO4	256
U	0.081
Zn	0.08

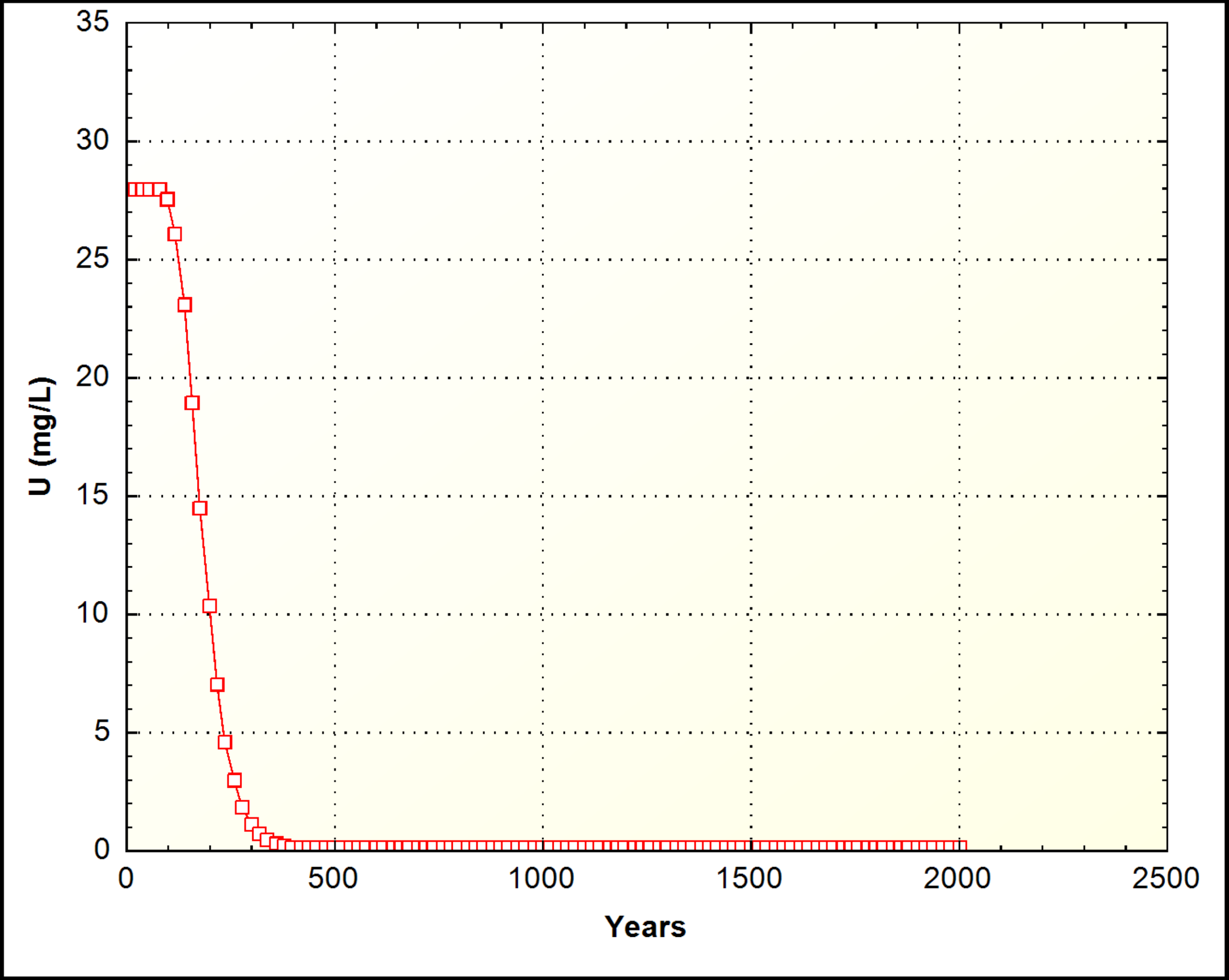
Predictive Model Results (Cu)



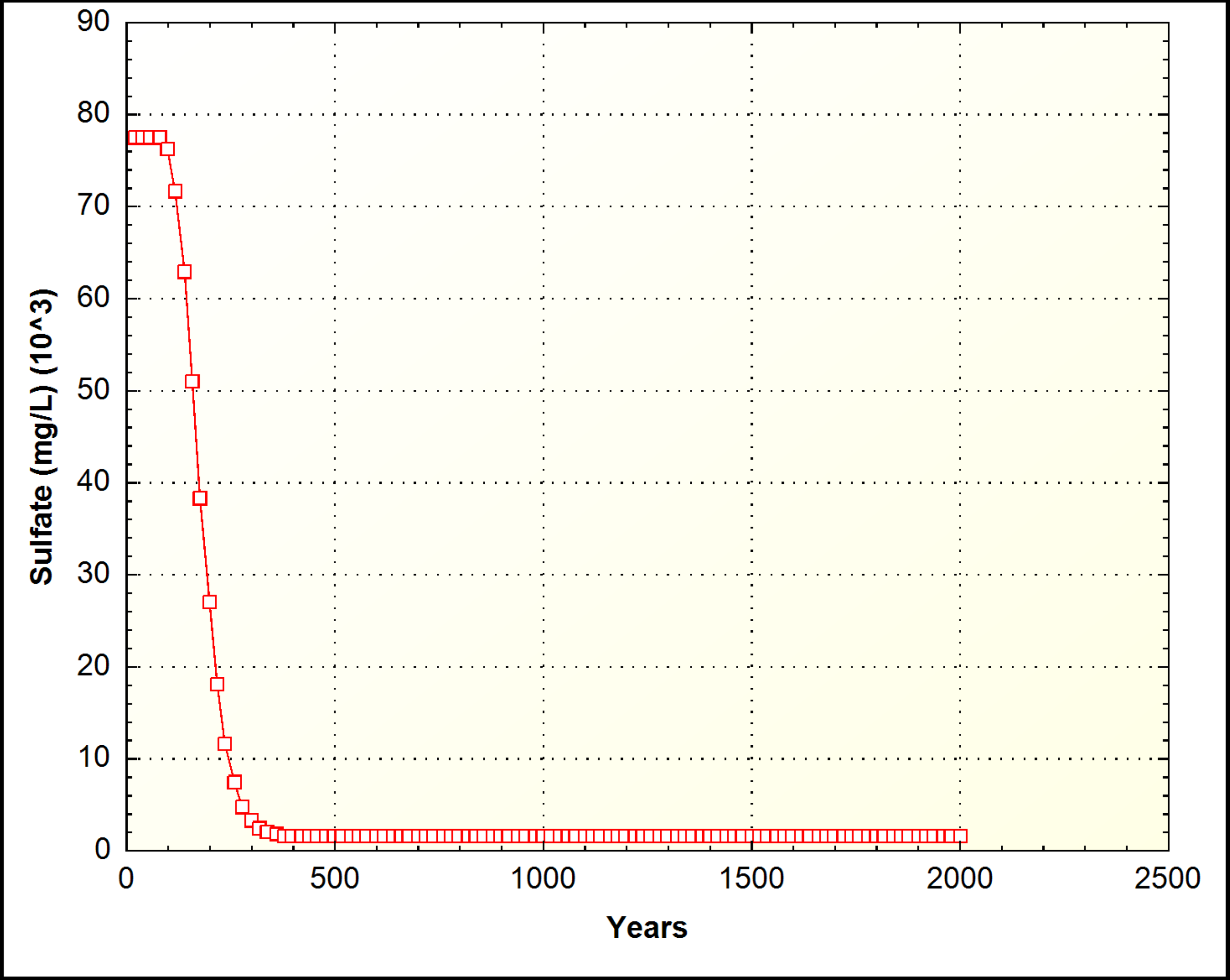
Predictive Model Results (Fe)



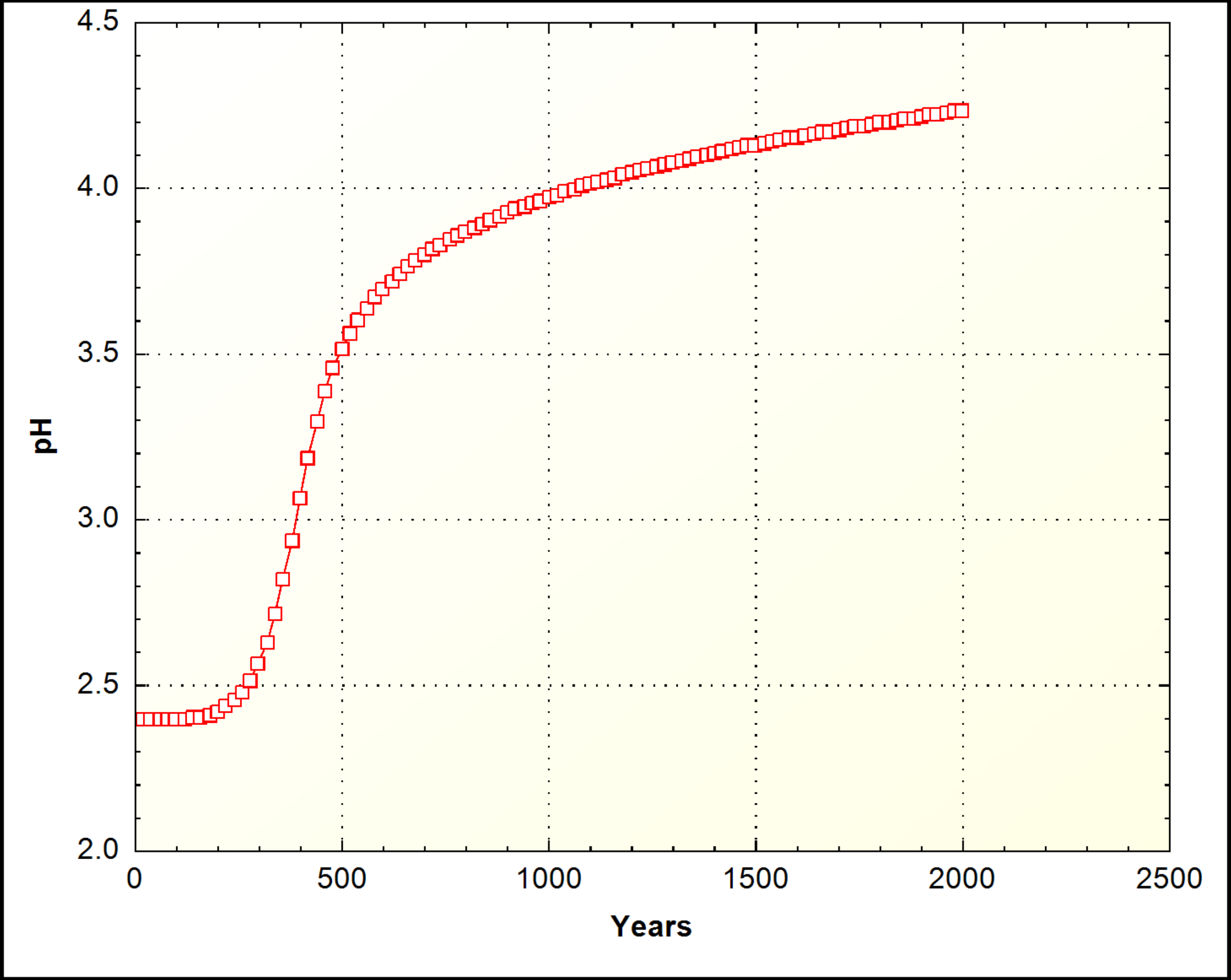
Predictive Model Results (U)



Predictive Model Results (Sulfate)



Predictive Model Results (pH)



Predictive Model Results

Mass Transfer (g/L)

Pyrite	0.0000075
Chalcopyrite	0.0000012
K-Feldspar	0.17
Muscovite	0.00015

Summary of Predictions

- HLP Draindown modelling requires flow estimation
  - 1 PV ~200 years
  - Draindown attains steady state ± 8 years
- Solute attenuation controlled by PV displacement (100’s of years)
- Metals flushed out within 2 PVs
- pH below 4 for 5 PVs
- Sulfides and silicates are reactive at acidic pH