Development of SLL speciation, equilibrium and data fitting tool and its application to P recovery process from sludge

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agenda

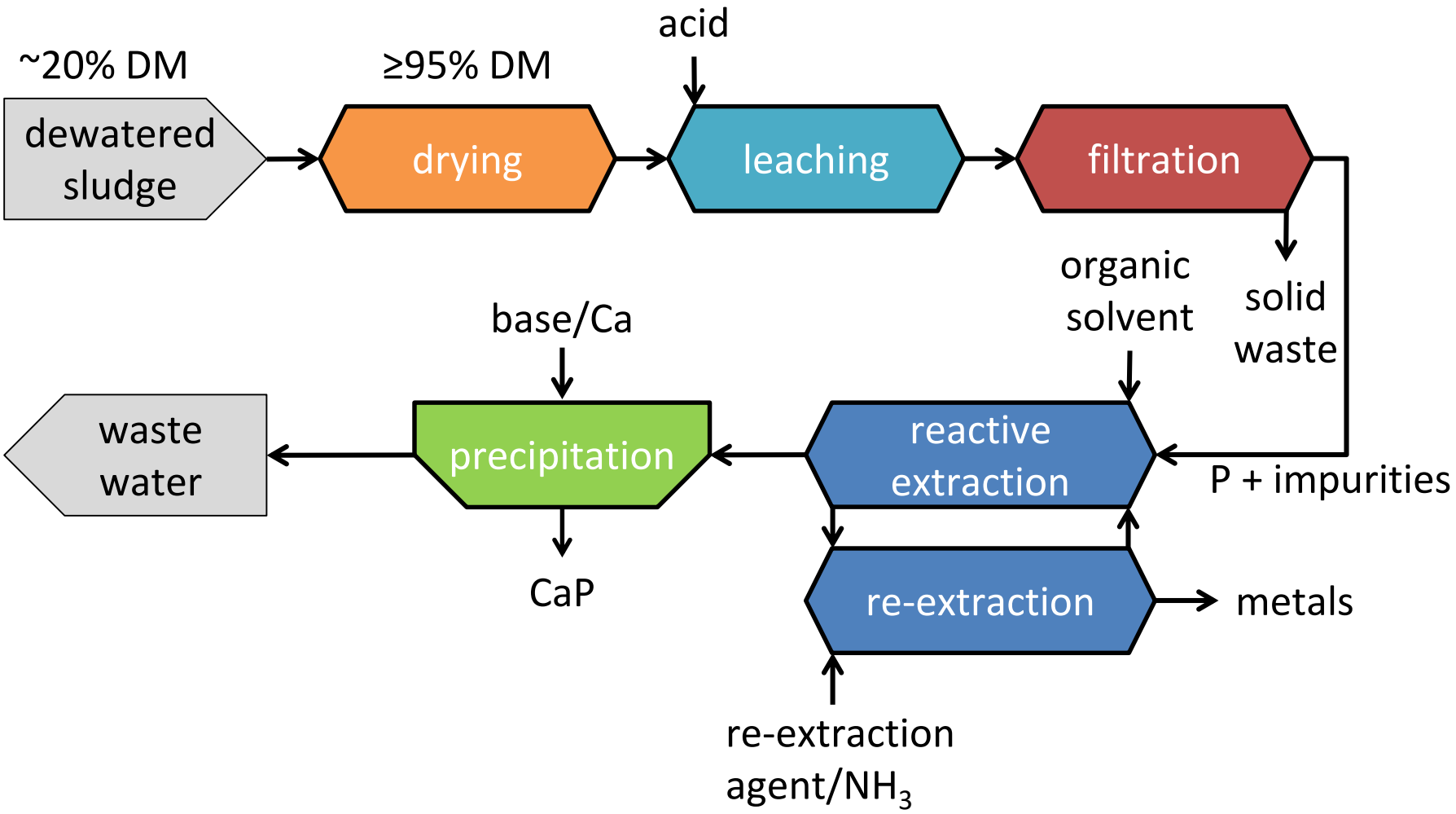
- Introduction to P recycling
- PULSE process
- why SLLE modelling
- SLLE tool
- results
- summary

introduction

- essential element for all forms of life
- finite resource
- EU imports more than 90% of P
- sewage has potential to cover more than 20% of P demand in North-West Europe

rock phosphate

PULSE (Phosphorus University of Liege Sludge Extraction) process



PULSE process

- leaching of P and metals from sludge

$$FePO_4 + 3HCl \rightarrow Fe^{3+} + H_3PO_4 + 3Cl^-$$

- Reactive extraction of metals with organic solvent

$$\mathrm{Fe^{3+} + 4Cl^- \leftrightarrow FeCl_4^-}$$

$$\overline{R_3NHCl} + FeCl_4^- \leftrightarrow \overline{FeCl_4R_3NH} + Cl^-$$

- Precipitation of CaP

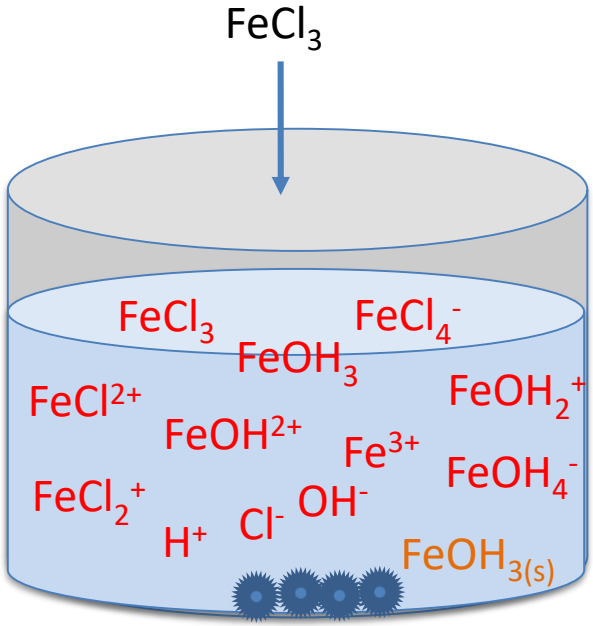
$$Ca^{2+} + HPO_4^{2-} \rightarrow CaH(PO_4)$$

why equilibrium (SLLE) modelling

- process development
  - evaluation of unit operations
- deeper understanding
- process optimization
- minimize experimental work

liquid phase speciation

- charge balance (CB)
  - $0 = \sum_{i=0}^{n} c_i z_i$
- mass balance (MB)
  - $Ctot_j = \sum_{i=0}^{n} \nu_{i,j} c_i$
- law of mass action (LMA)
  - $logK_m = \sum_{i=0}^{n} \nu_{i,r}\, log\, a_i$



$a_i = \gamma_i c_i$

a_i = activity of ith species

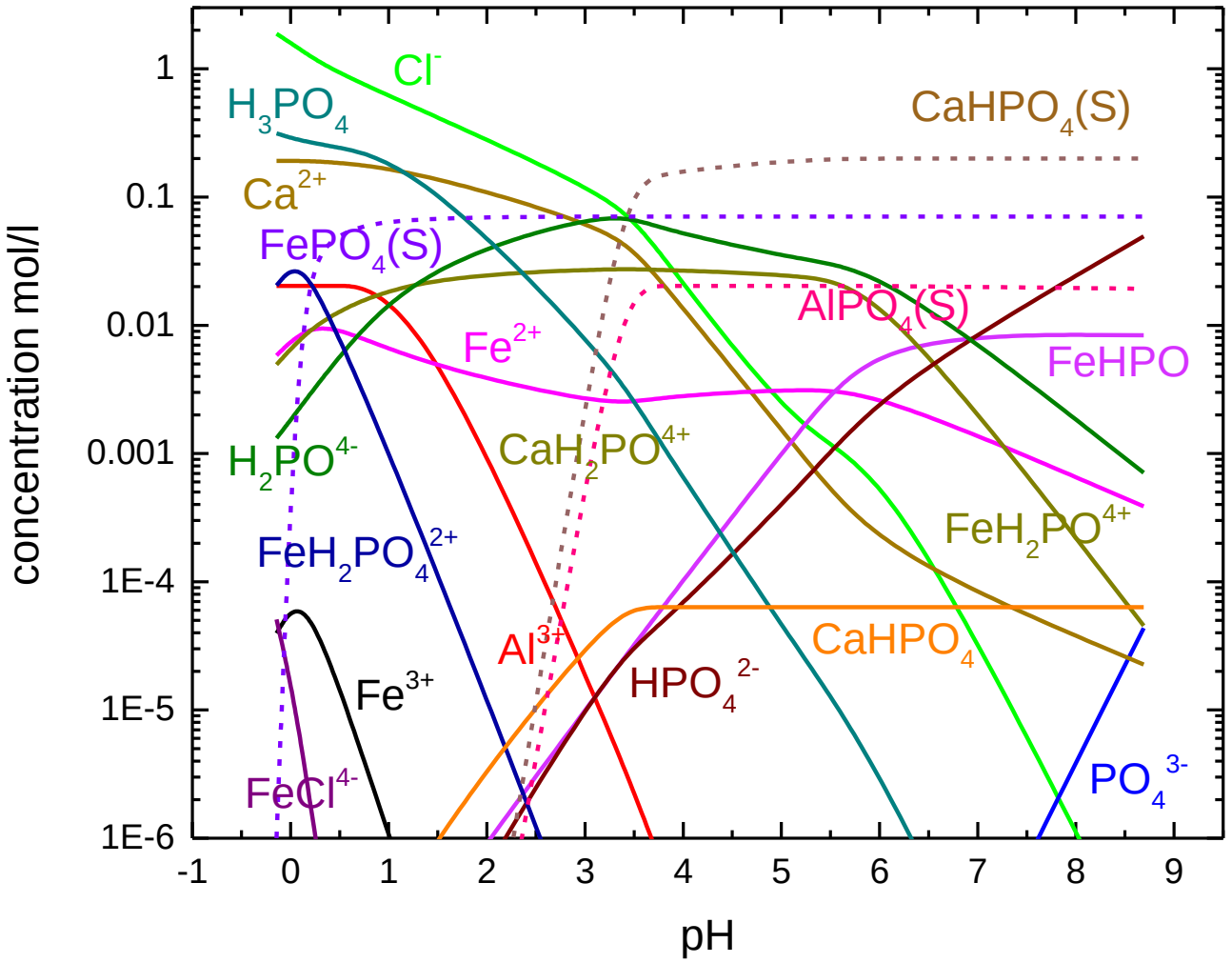
γ_i = activity coefficient

c_i = concentration

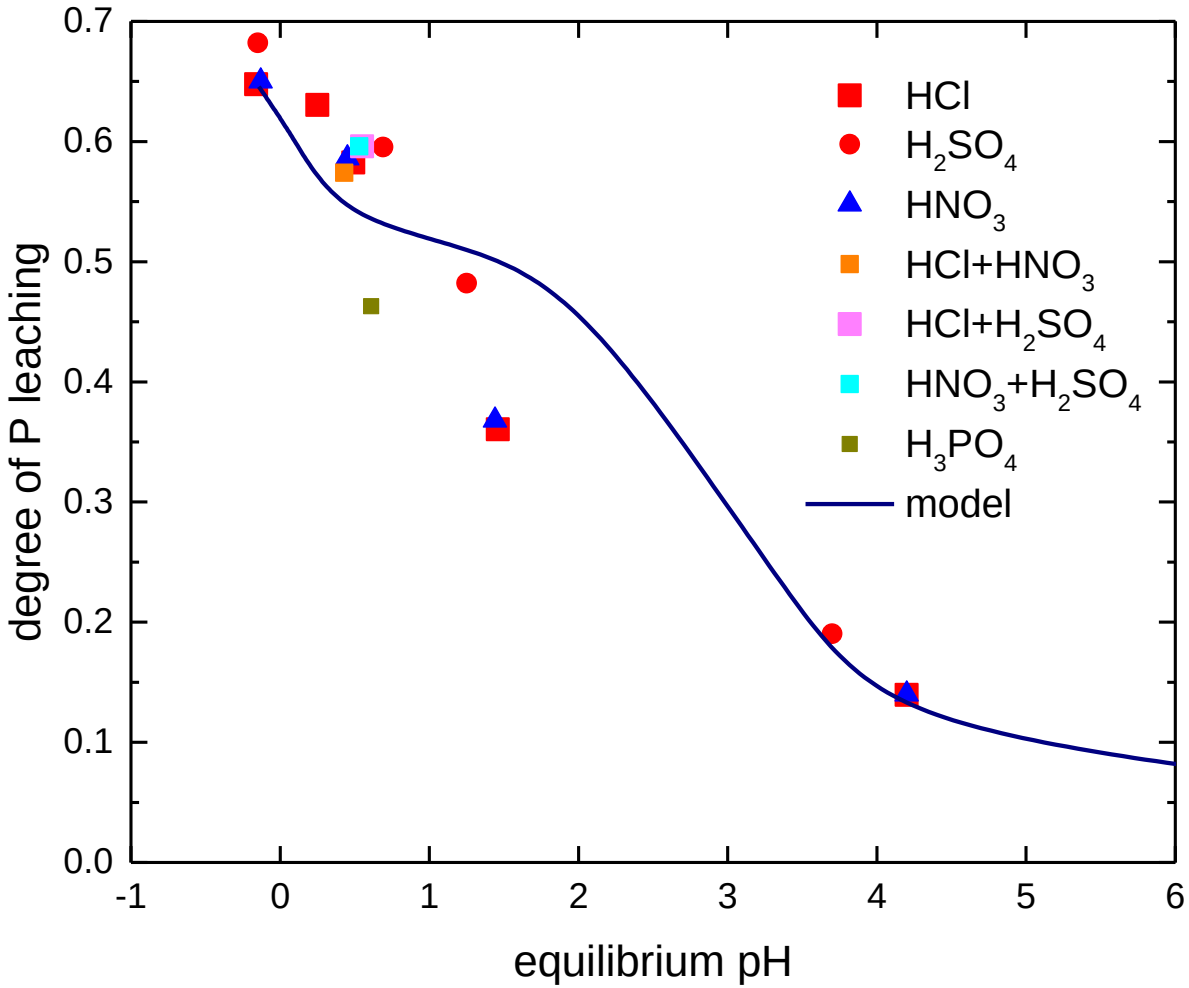
solid-liquid equilibrium

- $AB_{solid} \leftrightarrow \nu_1 A + \nu_2 B$
- from LMA
  - $K_{sp} = a_{A0}^{\nu_1} a_{B0}^{\nu_2}$
- Ion Activity product: $IAP = a_A^{\nu_1} a_B^{\nu_2}$
- Saturation Index: $SI = \log IAP - log\ K_{sp}$
- $SI = 0$: $IAP = K_{sp} \rightarrow$ equilibrium
- $SI < 0$: $IAP < K_{sp} \rightarrow$ undersaturated (dissolution)
- $SI > 0$: $IAP > K_{sp} \rightarrow$ supersaturated (precipitation)

SLE modelling results



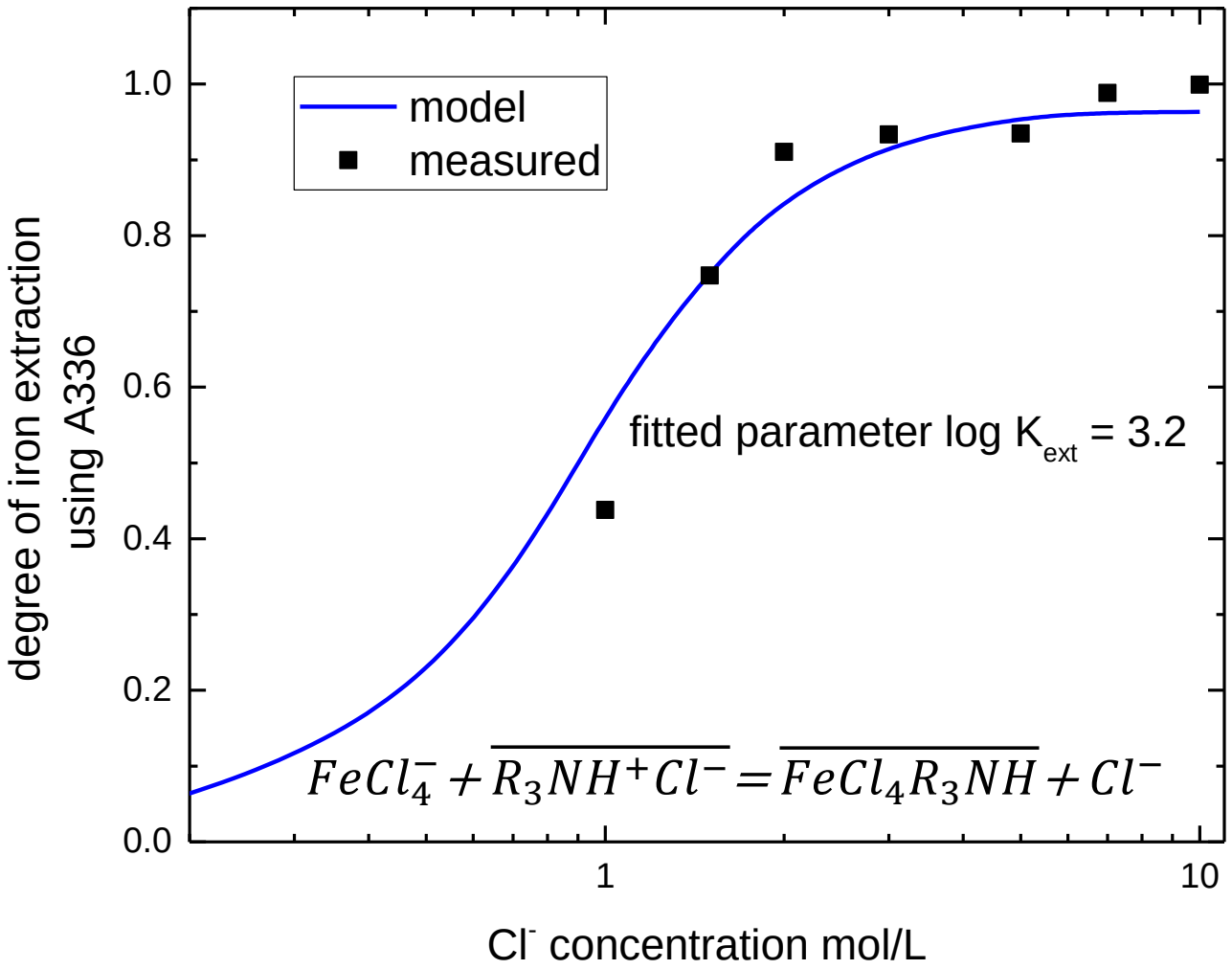
experimental v/s SLE speciation results



non-linear data fitting

- deviation of modelling results
  - complex nature of sludge
  - P and metals bound to organic matter
- lack of thermodynamic data
- fitting of multiple parameters - equilibrium constants and reaction stoichiometry

LLE - non-linear data fitting



summary

- MATLAB tool for simulation of SLLE with precipitation of multiple solid phases
- good correlation between model and experimental data
- data fitting – lack thermodynamic data and nature of sludge
- further development of the model
  - incorporate activity models for IS>1 mol/L
  - incorporate temperature dependence for logK
  - tool to simulate the entire pulse process

Interreg North-West Europe
Phos4You
European Regional Development Fund

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