

Nucleation and Growth of Calcium Oxalate in an Electric Field

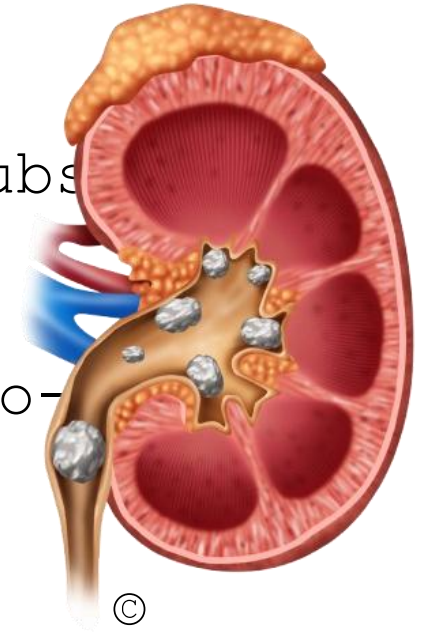
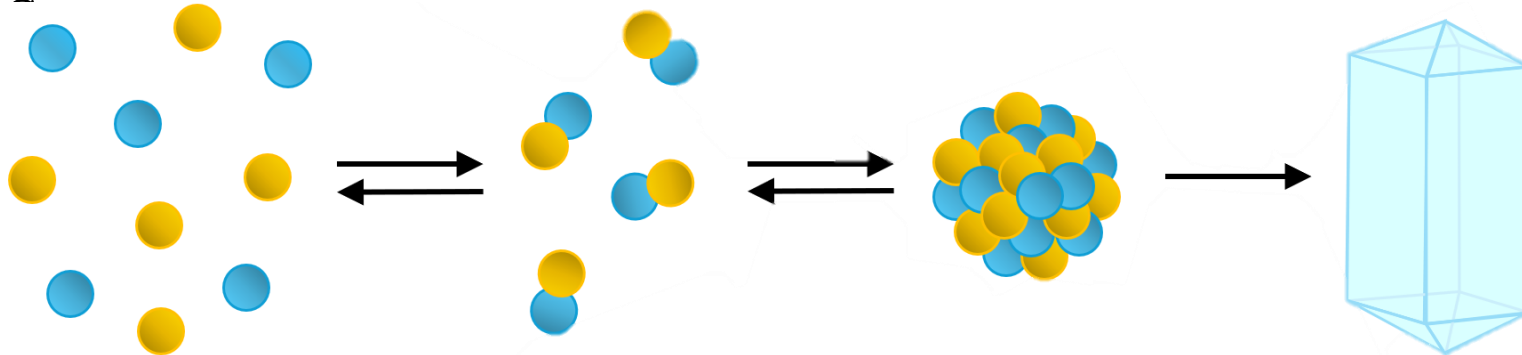
Kateřina Zedníčková, Michal Přibyl

Lednice, 5/29 2026



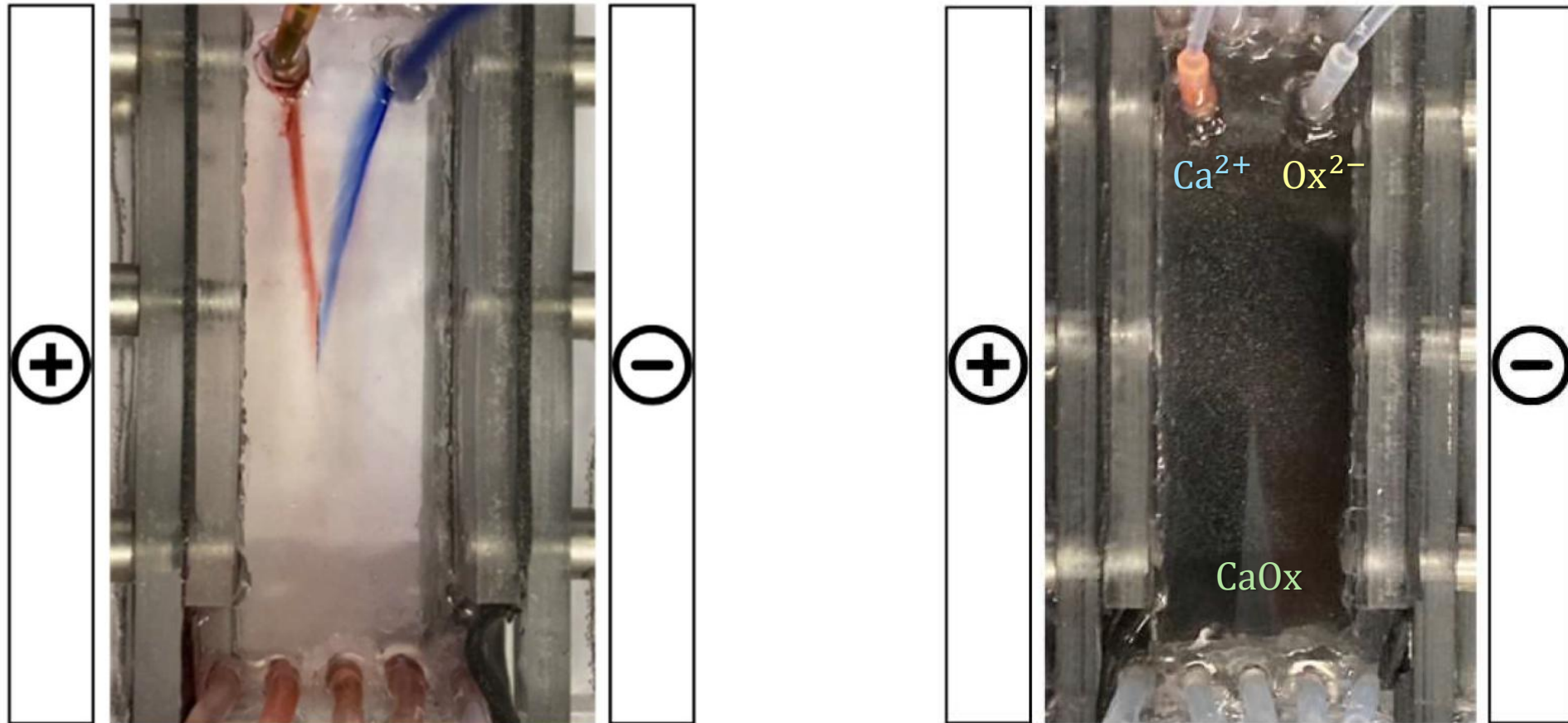
Introduction

- Electric field - controlled interaction and subsequent reaction of species
 - Fabrication of amorphous or crystalline nano-microparticles
 - Reaction of complementary molecules (e.g. antigen - antibody)
- Calcium oxalate (CaOx) - main component of kidney stone-



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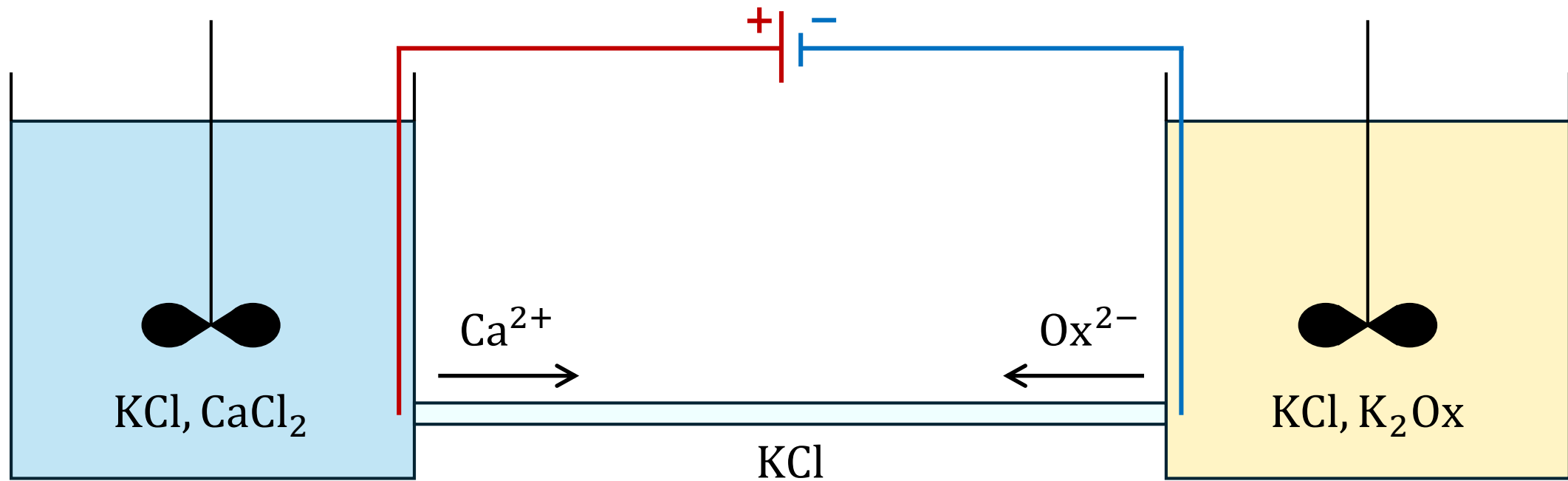
Experiments with Dyes and CaOx Precipitation (2D, Steady State)



Matouš Tůma. Studium transportu a chemických interakcí v zařízení pro elektroforézu s volným tokem. UCT Prague, 2025.

Mathematical Model (1D, Time Dependent)

Illustrative scheme of modelled domain:



Component Concentrations and Electric Potential

Component balances:

$$\frac{\partial c_i}{\partial t} + \frac{\partial J_i}{\partial x} = \sum_k v_{ik} r_k \quad i = \text{K}^+, \text{Cl}^-, \text{Ca}^{2+}, \text{Ox}^{2-}, \text{CaOx}$$

$$J_i = -D_i \frac{\partial c_i}{\partial x} - \frac{z_i D_i F}{RT} c_i \frac{\partial \phi}{\partial x}$$

Diffusion

Electromigration

Electric charge balance:

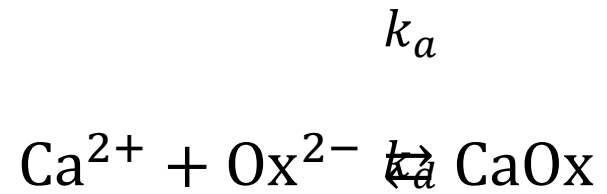
$$\frac{\partial i_s}{\partial x} = \frac{\partial}{\partial x} \left(F \sum_i z_i J_i \right) = 0$$

Electroneutrality:

$$F \sum_i z_i c_i = 0$$

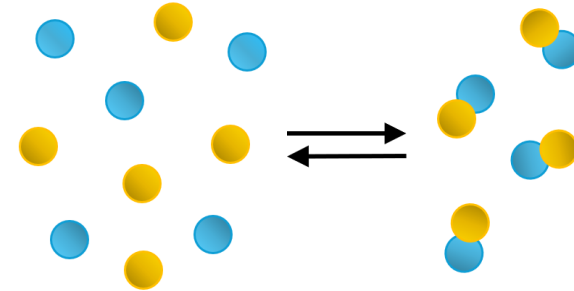
Ion Pair Formation

Fast reaction and establishment of equilibrium:



$$K_a = \frac{c_{\text{CaOx}}}{c_{\text{Ca}^{2+}} c_{\text{Ox}^{2-}}} = \frac{k_a}{k_d}$$

$$r_a = k_d (K_a c_{\text{Ca}^{2+}} c_{\text{Ox}^{2-}} - c_{\text{CaOx}})$$



Nucleation

Classical nucleation theory:

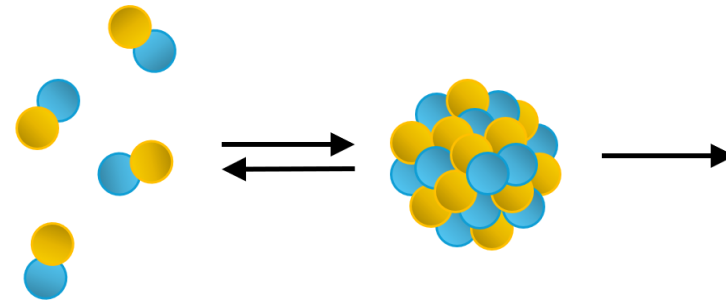
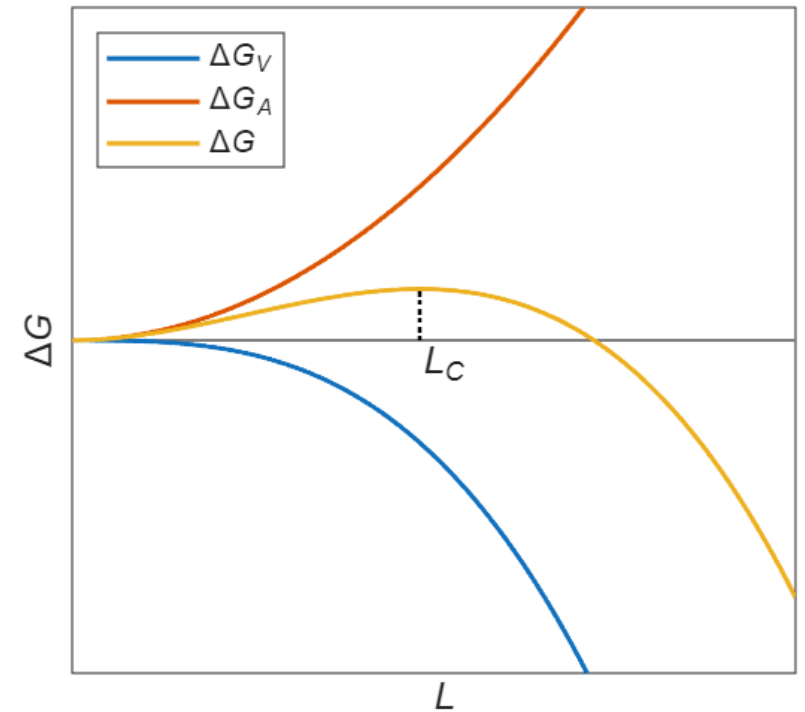
$$\Delta G = \Delta G_V + \Delta G_A = -\frac{kT k_V L^3 \ln S}{v_m} + \gamma k_A L^2$$

$$S = \frac{c_{Ca} c_{Ox}}{K_{sp}}$$

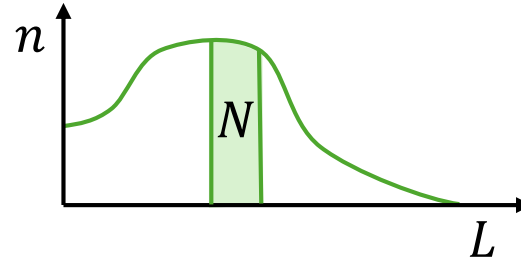
Nucleation rate:

$$J_{nuc} = k_J c_{CaOx}^{z_c} e^{-\frac{B}{(\ln S)^2}}$$

$$z_c = \frac{k_V L_C^3}{v_m} = \frac{2B}{(\ln S)^3}$$

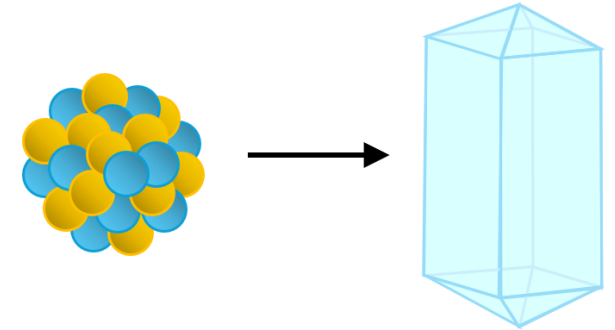


Crystal Growth



Population balance:

$$\frac{\partial n}{\partial t} = D_{ax} \frac{\partial^2 n}{\partial x^2} - G \frac{\partial n}{\partial L} + D_g \frac{\partial^2 n}{\partial L^2}$$



Axial
dispersion

Linear
growth:

Growth dispersion:

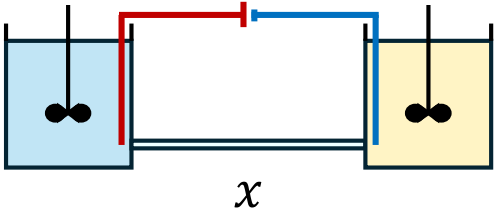
$$Pe_G = \frac{GL_{mean}}{D_g} \rightarrow D_g = \frac{GL_{mean}}{Pe_G}$$

Balance of CaO_x :

$$G = k_g(1 - S)^g$$

$$\frac{\partial c_{CaO_x}}{\partial t} = D_{CaO_x} \frac{\partial^2 c_{CaO_x}}{\partial x^2} + r_a - \frac{z_c}{N_A} J_{nuc} - \frac{\rho_{CaO_x}}{M_{CaO_x}} 3k_V \int_{L_c}^{\infty} \left(Gn - D_g \frac{\partial n}{\partial L} \right) L^2 dL$$

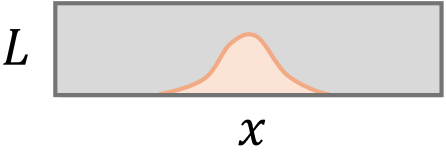
Nonlocal Coupling



1D domain (component concentrations, electric potential, nucleation rate)

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General Extrusion (supersaturation, nucleation rate)

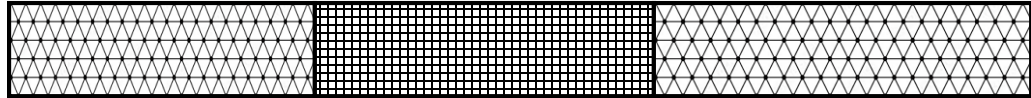


2D domain (population balance, crystal growth in L -axis)

Linear Projection (consumption in CaO_x balance)

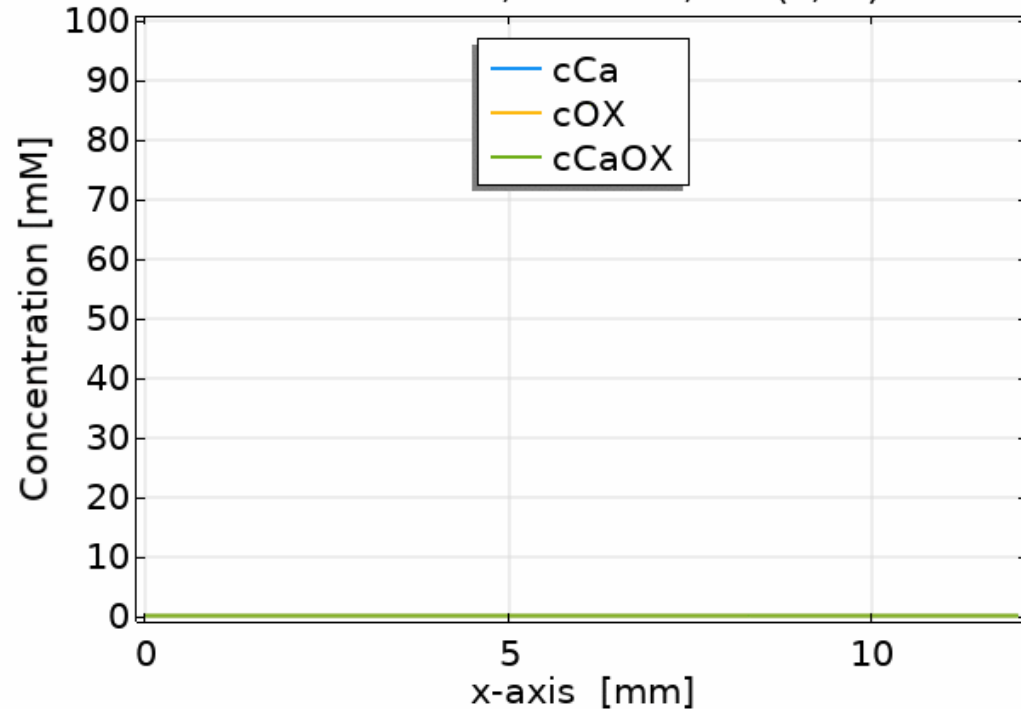
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Numerical Analysis

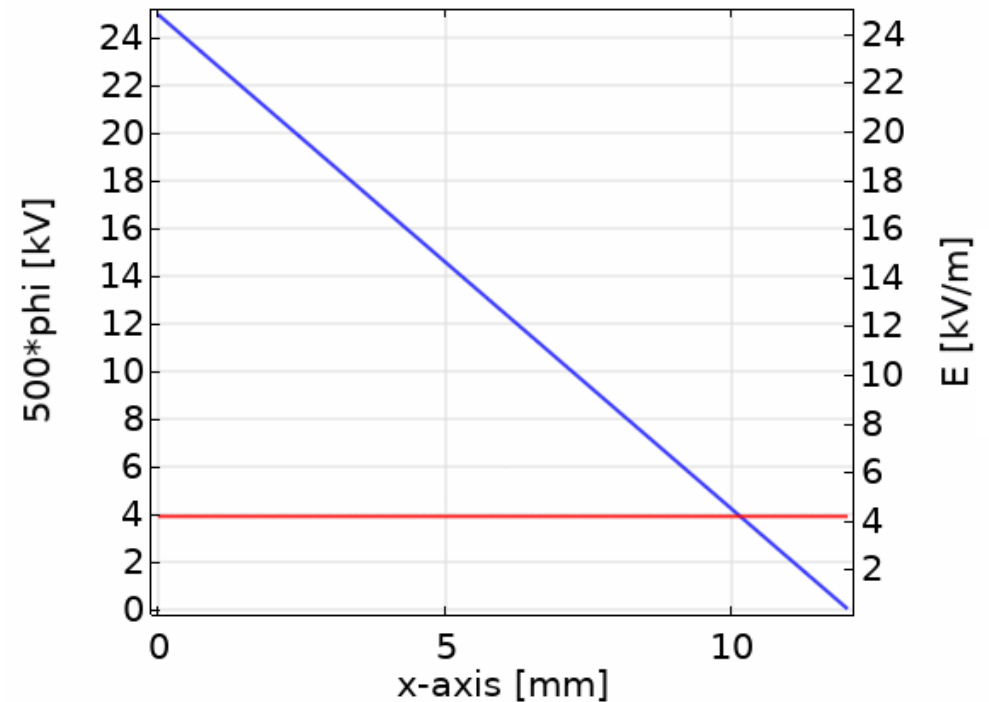
- 1D domain: 1×10^{-6} m elements in a 12 mm domain
- 2D domain: combination of mapped distributed and free triangular meshes
- BDF time dependent solver 
- Step function (0 to 1 s) applied to boundary conditions
- Boundary conditions: 100 mM CaCl_2 and K_2Ox
- Parametric studies:
 - Initial concentration of background electrolyte (KCl): 10, 100 and 1000 mM
 - Applied voltage: 40, 45 and 50 V

Component Concentrations and Electric Potential

Concentration of Ca, Ox and CaOX,
 $c_{in} = 100 \text{ mM}$, $U = 50 \text{ V}$, $t = (0,35) \text{ s}$



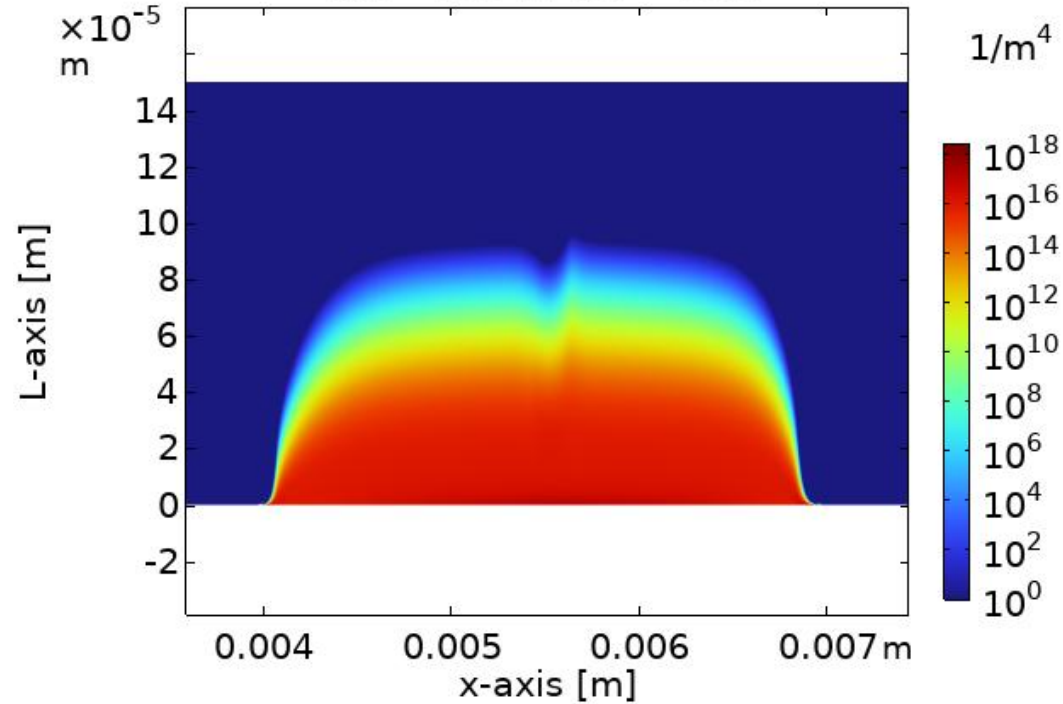
Electric potential ϕ and electric field strength E ,
 $c_{in} = 100 \text{ mM}$, $U = 50 \text{ V}$, $t = (0,35) \text{ s}$



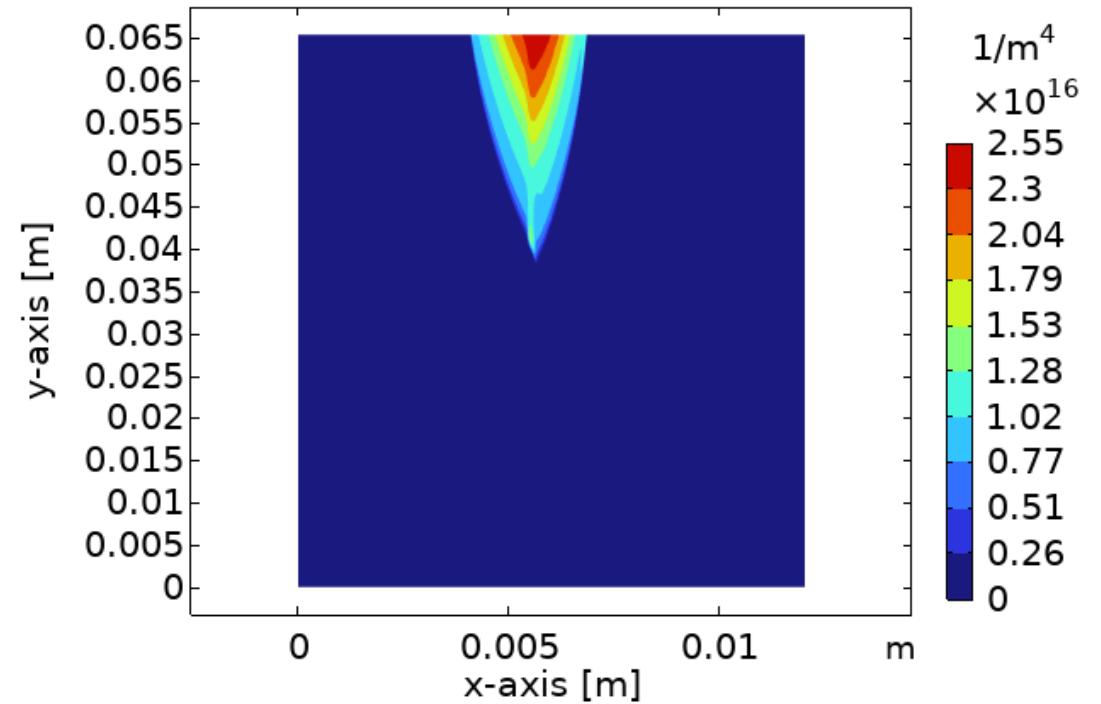
Calcium Oxalate Crystals (Population Density)

Time=35 s

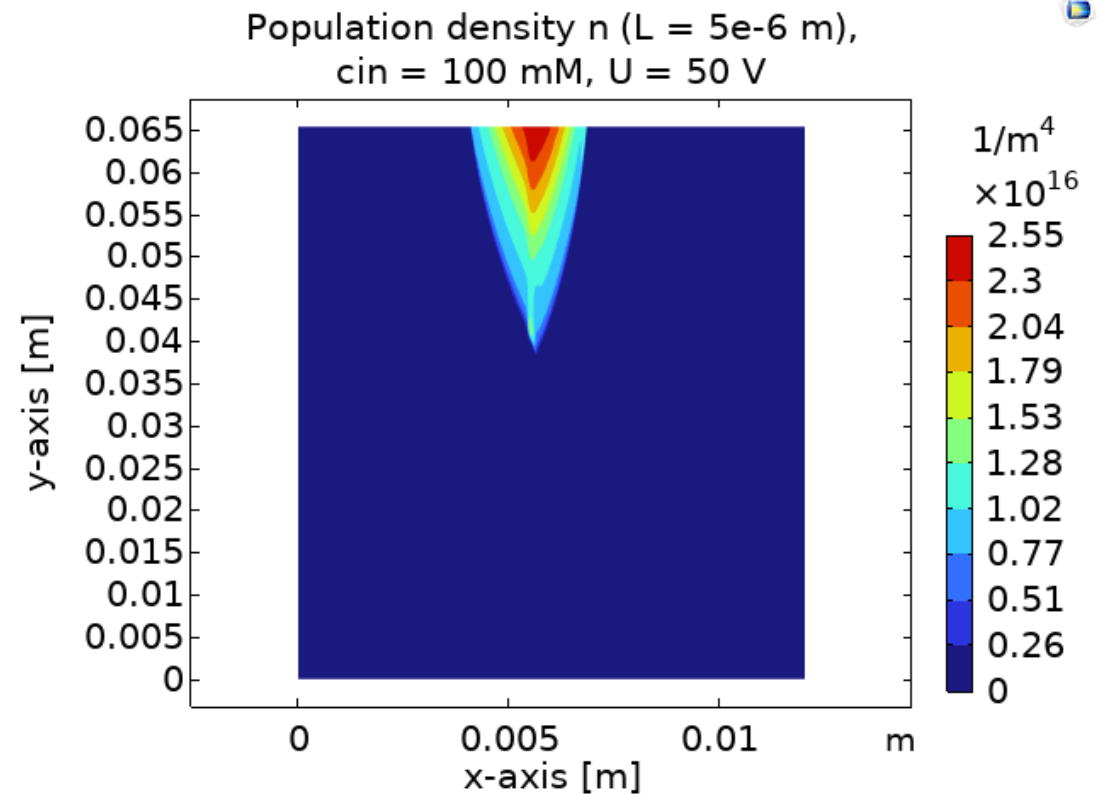
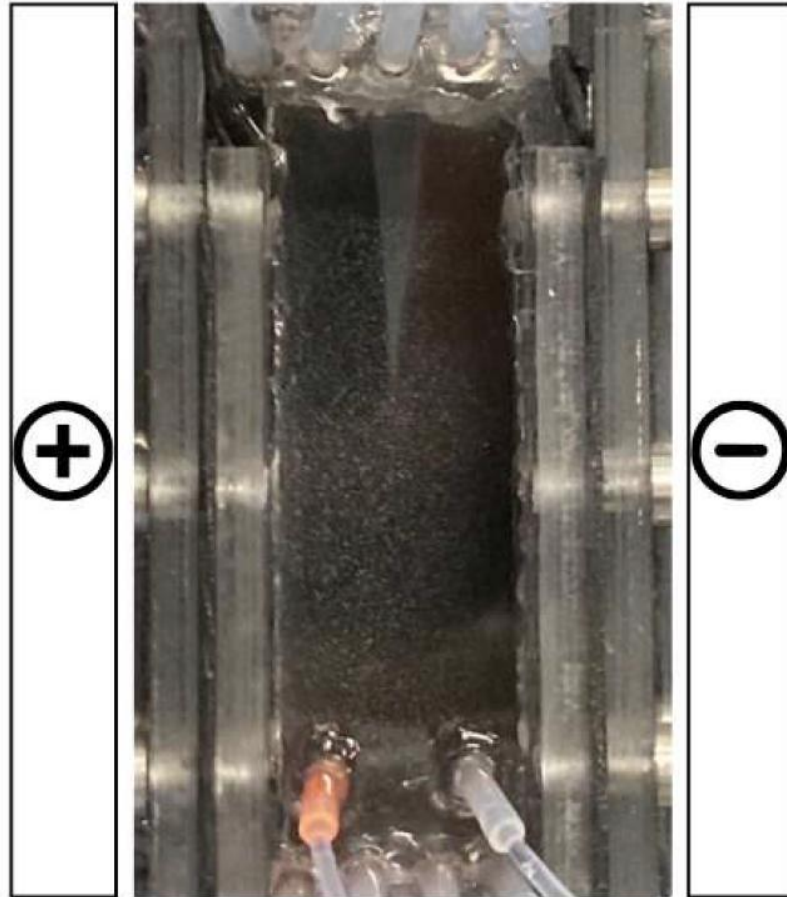
Population density n ,
 $c_{in} = 100 \text{ mM}$, $U = 50 \text{ V}$



Population density n ($L = 5e-6 \text{ m}$),
 $c_{in} = 100 \text{ mM}$, $U = 50 \text{ V}$

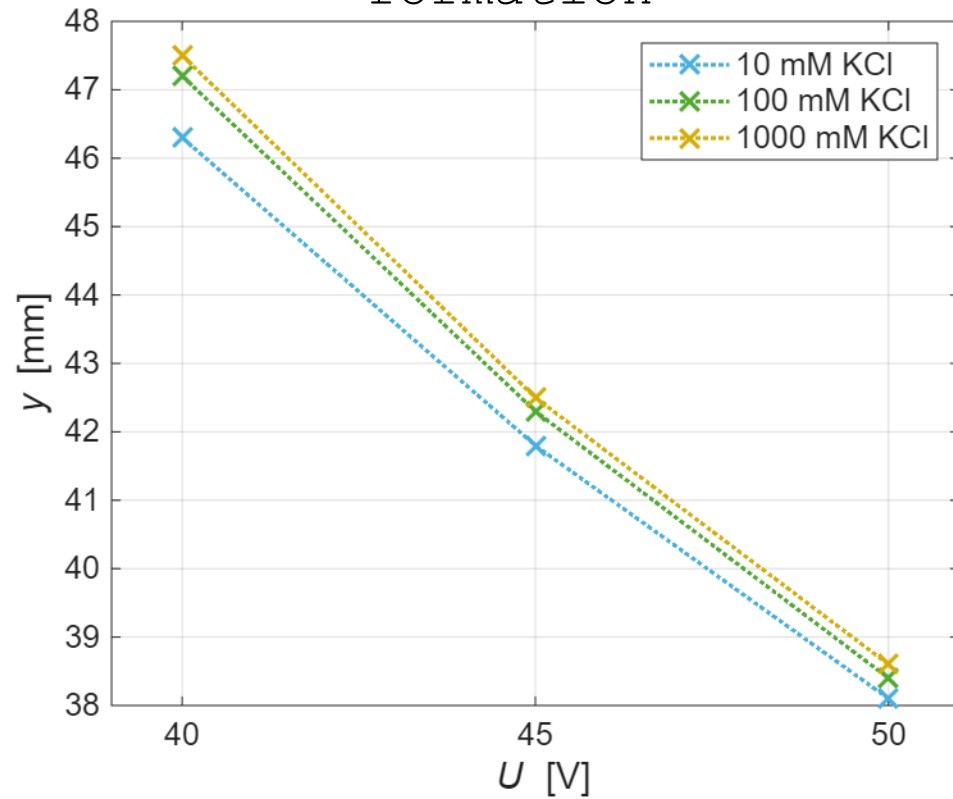


Calcium Oxalate Crystals (Population Density)

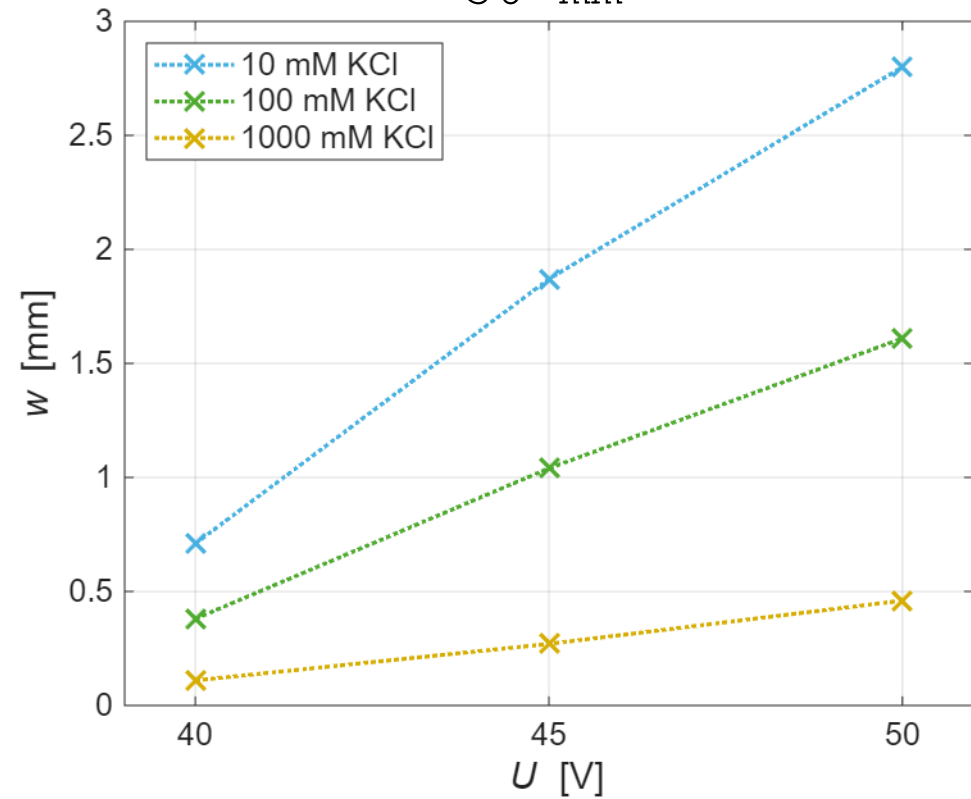


Parametric Studies

Distance needed for crystals formation



Width of crystal zone at y = 50 mm



Conclusions



- Mathematical model of ion pair formation, nucleation, and crystal growth of calcium oxalate in an electric field



- Good qualitative agreement with experiments



- Preparation of well-defined amorphous and crystalline products (e.g. in pharmaceutical industry)

- Provides insights into the mechanism of kidney stone formation

Thank you for your attention!

