Electrokinetic effects in the breakup of electrified jets: a Volume-Of-Fluid numerical study

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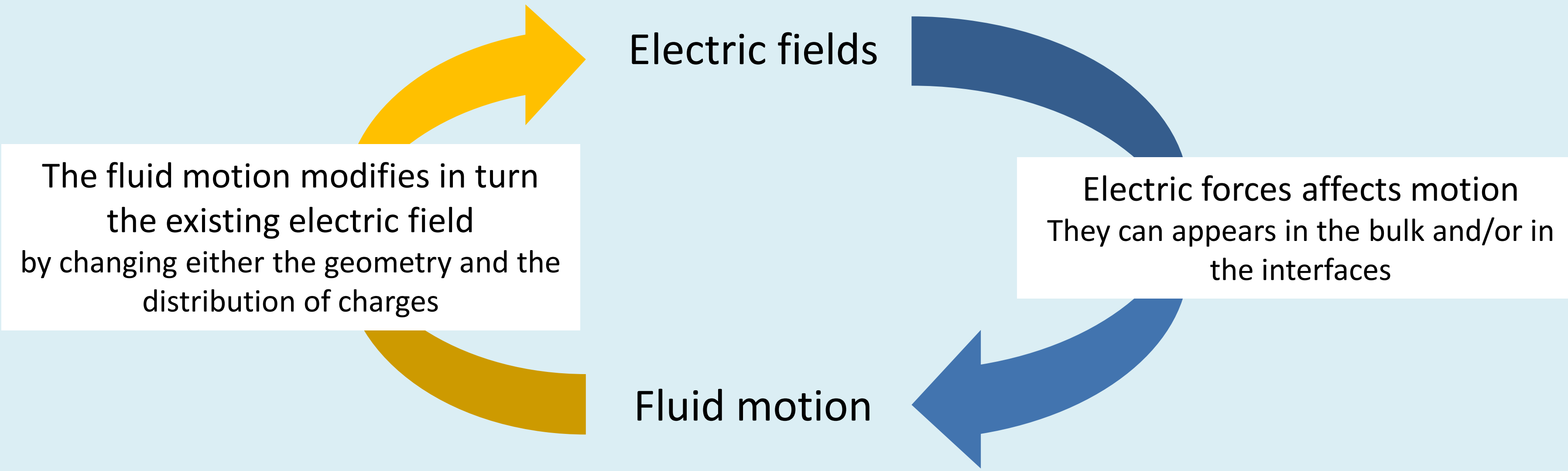
Introduction.

Electrohydrodynamics (EHD) deals with fluid motion induced by electric fields.



Fields:

Microfluidic devices
Electrospray
Electrified liquid bridges
…

Introduction. General EHD equations

Bulk equations

Maxwell Equations

$$\nabla \cdot (\varepsilon \mathbf{E}) = q$$
$$\nabla \times \mathbf{E} = 0$$
$$\frac{\partial q}{\partial t} + \nabla \cdot \mathbf{J} = 0$$

$\mathbf{E} = -\nabla\phi$ → $\nabla \cdot (\varepsilon \nabla \phi) = -q$

being $\mathbf{J} = q\mathbf{v} + k\mathbf{E}$

Navier-Stokes Equations

$$\nabla \cdot \mathbf{v} = 0$$
$$\rho \frac{D\mathbf{v}}{Dt} = -\nabla p + \nabla \cdot \left[\mu(\nabla \mathbf{v} + \nabla \mathbf{v}^T)\right] + \nabla \cdot \mathbf{T}_e$$

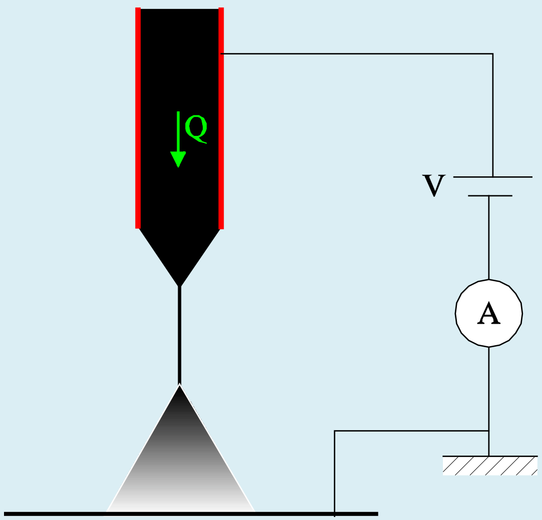
being

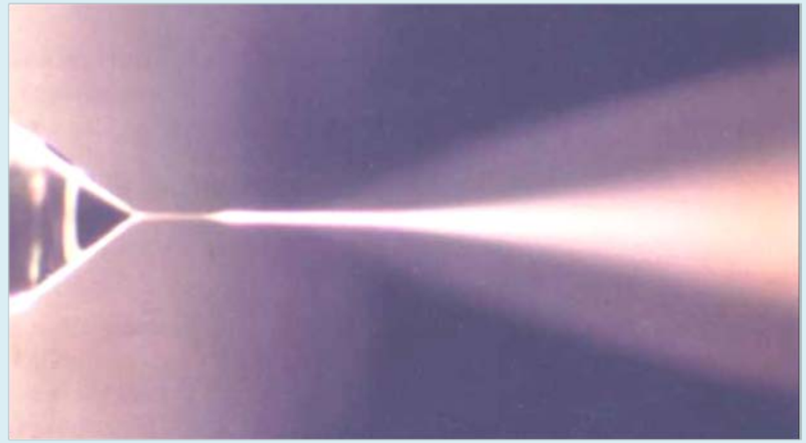
$$\mathbf{T}_e = \varepsilon \mathbf{E}\mathbf{E} - \frac{\varepsilon E^2}{2}\mathbf{I}$$

The EHD model assumes two main simplifications:

- Condense in q all the charged species.
  Is a more detailed description necessary?
- Conductivity k is homogeneous and constant.
  True?

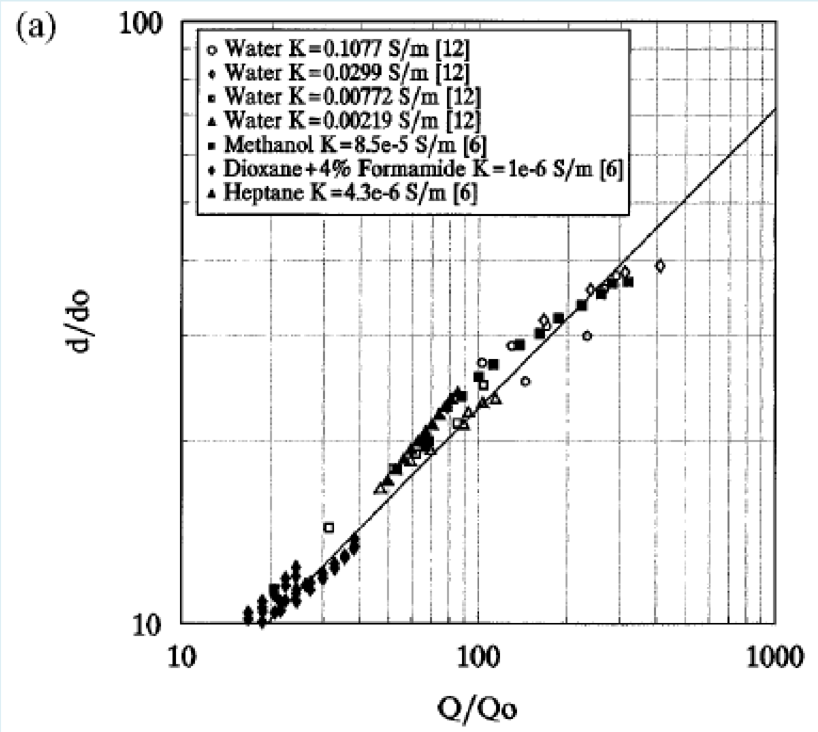
Depends on the problem. For example in cone-jet electrospraying

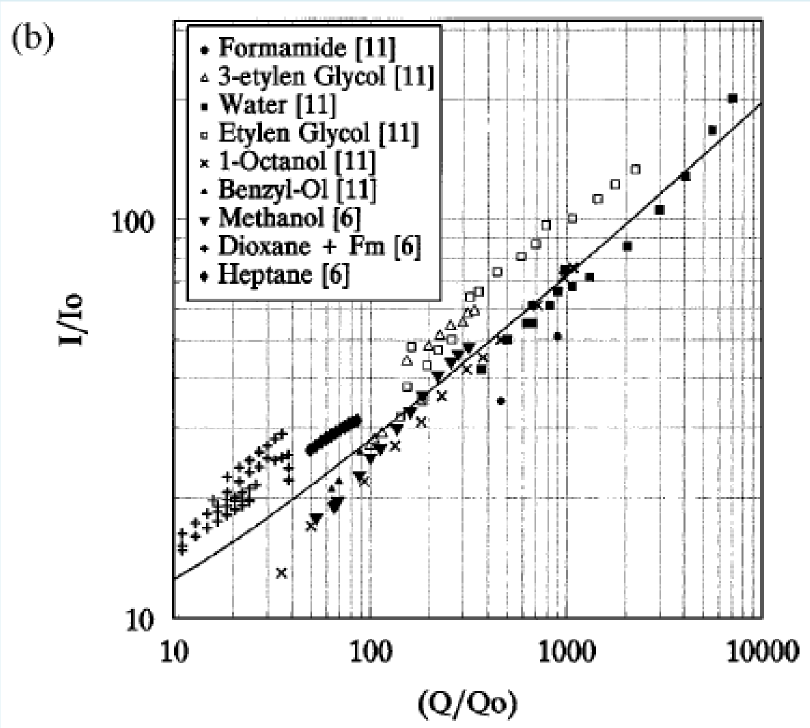




LIMITS. cone-jet electrospraying

EHD model has been used with success to develop scaling laws

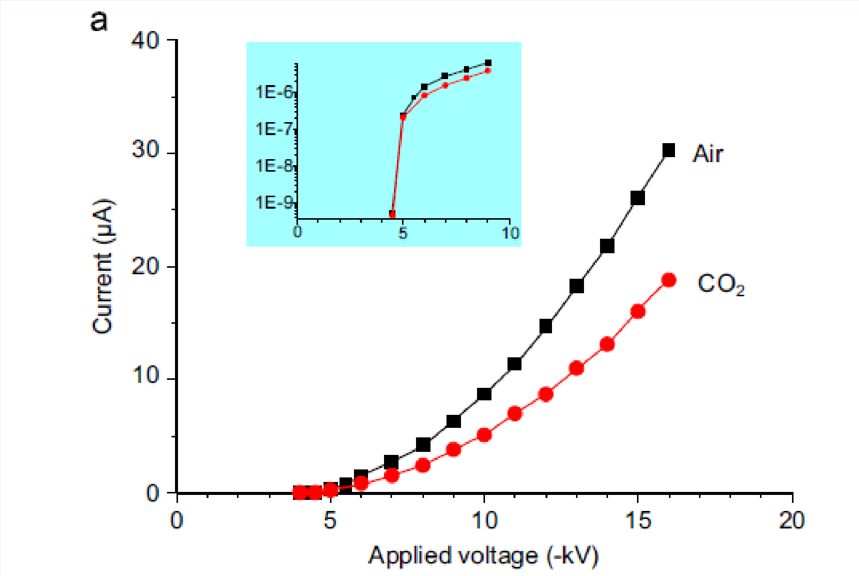


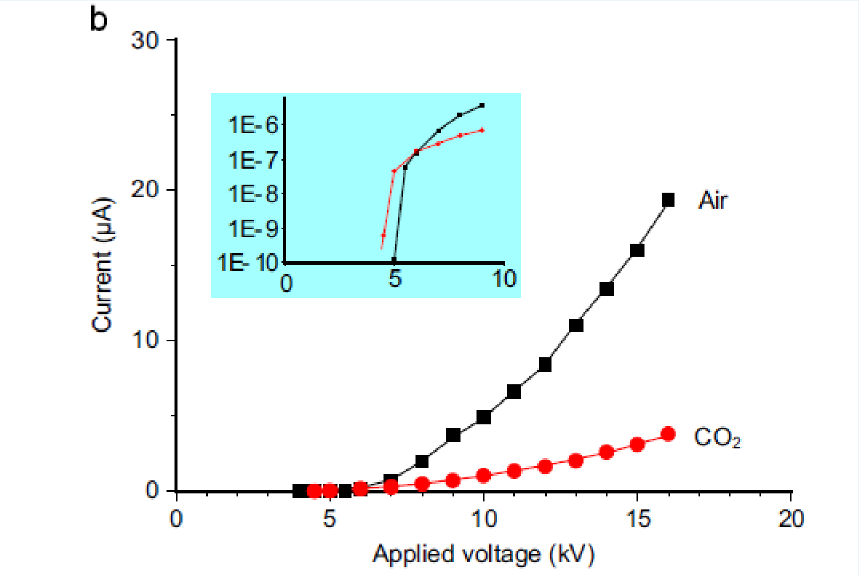


Gañan-Calvo PRL 79 (2) (1997)

LIMITS. cone-jet electrospraying

Classic EHD can not explain the different behavior observed when the polarity is changed





H.H. Kim *et al.* JAS 76 (2014)

LIMITS. Conclusions

- Therefore, to descend to a more detailed physical description of the charged species that form the electric charge is desirable.

- The study of the evolution, distribution, etc, of this charged species is the object of the **electrokinetic theory**.

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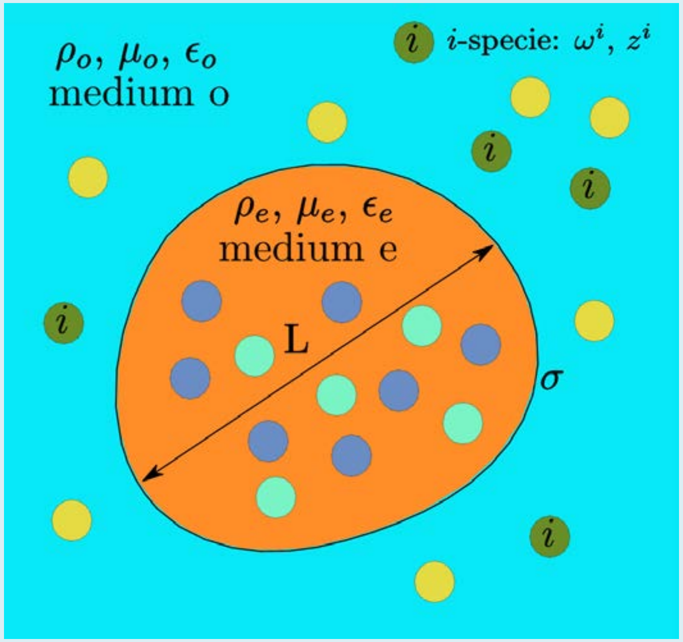
Electrokinetic equations



NERNST-PLANCK-POISSON (PNP) EQUATION

$$c_t^i + \nabla \cdot (c^i \mathbf{u}) = \nabla \cdot \left(\omega^i k_B T \nabla c^i - e \omega^i z^i \, c^i \mathbf{E} \right)$$

$$\nabla \cdot (\varepsilon \mathbf{E}) = \nabla \cdot (-\varepsilon \nabla \varphi) = q = \sum_i e z^i c^i$$

NAVIER-STOKES EQUATIONS

$$\nabla \cdot \mathbf{u} = 0,$$

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \nabla \cdot \mathbb{T}_v + \mathbf{F}_e + \sigma \kappa \delta_s \mathbf{n}$$

$$\mathbb{T}_v = 2\mu \mathbb{D} = \mu (\nabla \mathbf{u} + \nabla \mathbf{u}^T)$$

$$\mathbb{T}_e = \varepsilon \left(\mathbf{E}\mathbf{E} - \frac{E^2}{2} \mathbf{I} \right)$$

$$\mathbf{F}_e = \nabla \cdot \mathbb{T}_e = q\mathbf{E} - \frac{1}{2} E^2 \nabla \varepsilon.$$

Equations

Dimensionless parameter

Basis: ρ_e, c_o, L, σ and ε_o.

- Dimensionless ion diffusivities,
  $D^i = \frac{\omega^i k_B T}{L U_c}$ being $U_c = (\sigma/\rho_e L)^{1/2}$. $Pe^i = 1/D^i$.
- Ratio of characteristic electric fields,
  $\gamma^i = E_c L e z^i/(k_B T)$, with $E_c = (\sigma/\varepsilon_o L)^{1/2}$.
  ion specific conductivities, $\Lambda^i = D^i \gamma^i$.
- The Ohnesorge number,
  $C_\mu = \mu_e/\sqrt{\sigma L \rho_e}$.
- The dimensionless Debye parameter,
  $K_i = L/\lambda_D$, $\lambda_D = \sqrt{\frac{\varepsilon_e k_B T}{2e^2 (z^i)^2 c_o}}$ is the Debye length.
- Ratios of the relevant fluid properties,
  $R = \rho_o/\rho_e$; $M = \mu_o/\mu_e$ and $S = \varepsilon_e/\varepsilon_o$.

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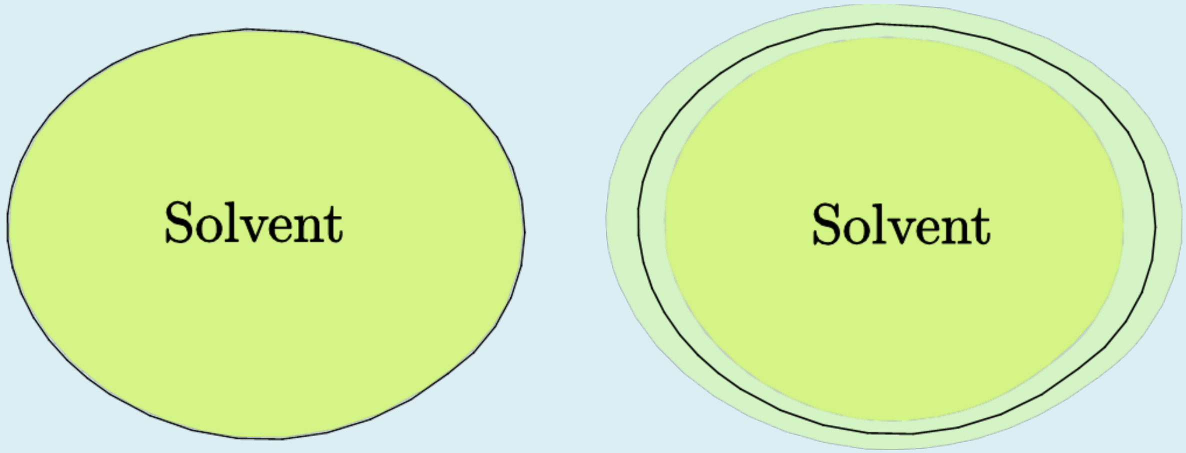
A VOF approach. Conservation of ionic species.



$$c_i = \frac{\text{number of ions}}{\text{volume of solvent}} \qquad c_i\,\phi = \frac{\text{number of ions}}{\text{volume of space}}$$

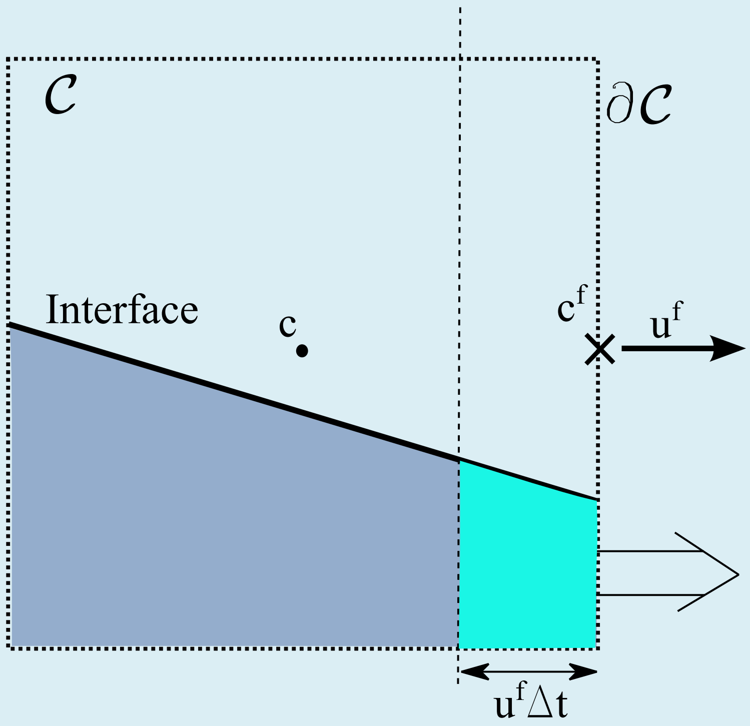
$$c^i_t + \nabla\cdot(c^i\mathbf{u}) = \nabla\cdot\left(D^i\nabla c^i + c^i\Lambda^i\nabla\varphi\right)$$

$$\phi_t + \nabla\cdot(\phi\mathbf{u}) = 0$$

$$(c^i\phi)_t + \nabla\cdot(c^i\phi\mathbf{u}) = \nabla\cdot\left(\phi D^i\nabla c^i\right) + \nabla\cdot\left(\Lambda^i\phi c^i\nabla\varphi\right)$$

A VOF approach. Conservation of ionic species.

$$(c^i\phi)_t + \nabla\cdot(c^i\phi\mathbf{u}) = \nabla\cdot\left(\phi D^i\nabla c^i\right) + \nabla\cdot\left(\Lambda^i\phi c^i\nabla\varphi\right)$$



- The concentration c^i is advected using the geometrical Volume-Of-Fluid technique.

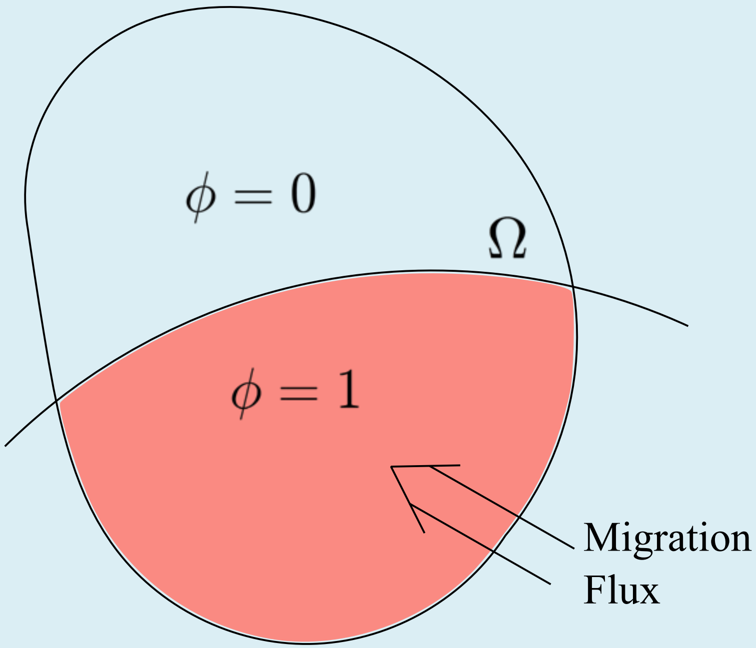
$$\mathrm{d}t\int_{\mathcal{C}}\nabla\cdot(\phi c^i\mathbf{u}) = \sum_{faces} c_f u_f\,\Delta t$$

- The concentration face value, c_f is calculated from cell concentration and slope-limited concentration gradients.
- Gerris wording: GfsVariableVOFConcentration

A VOF approach. Conservation of ionic species.

$$(c^i\phi)_t + \nabla\cdot(c^i\phi\mathbf{u}) = \nabla\cdot\left(\phi D^i\nabla c^i\right) + \nabla\cdot\left(\Lambda^i\phi c^i\nabla\varphi\right)$$

$\overline{\Lambda^i} = \phi\Lambda^i = 0\,;\ \overline{D^i} = \phi D^i = 0$



$\overline{\Lambda^i} = \phi\Lambda^i = \Lambda^i\,;\ \overline{D^i} = \phi D^i = D^i$

The factor ϕ in the migration terms is as a weighted diffusivity/conductivity ($\bar{D}^i$ $/\bar{\Lambda}^i$) that nullifies the migration fluxes across boundaries out of the solvent phase.

Conservation of ionic species: A VOF approach (IV)

$$\nabla \cdot (\phi D^i \nabla c^i) = \nabla \cdot [D^i \nabla (c^i \phi)] - \nabla \cdot (D^i c^i \nabla \phi)\,,$$

$$(c^i\phi)_t + \nabla \cdot (c^i \phi \mathbf{u}) = \underbrace{\nabla \cdot [D^i \nabla (c^i \phi)]}_{\text{term A}} - \underbrace{\nabla \cdot (D^i c^i \nabla \phi)}_{\text{term B}} \mp \underbrace{\nabla \cdot \left(\Lambda^i \phi c^i \mathbf{E}\right)}_{\text{term C}},$$

$$h \int_{\mathcal{C}} \nabla \cdot [D^i \nabla (c^i \phi)] = \int_{\partial \mathcal{C}} D^i \nabla (c^i \phi) \cdot \mathbf{n} = \sum_f (D^i)^f \nabla^f (c^i \phi),$$

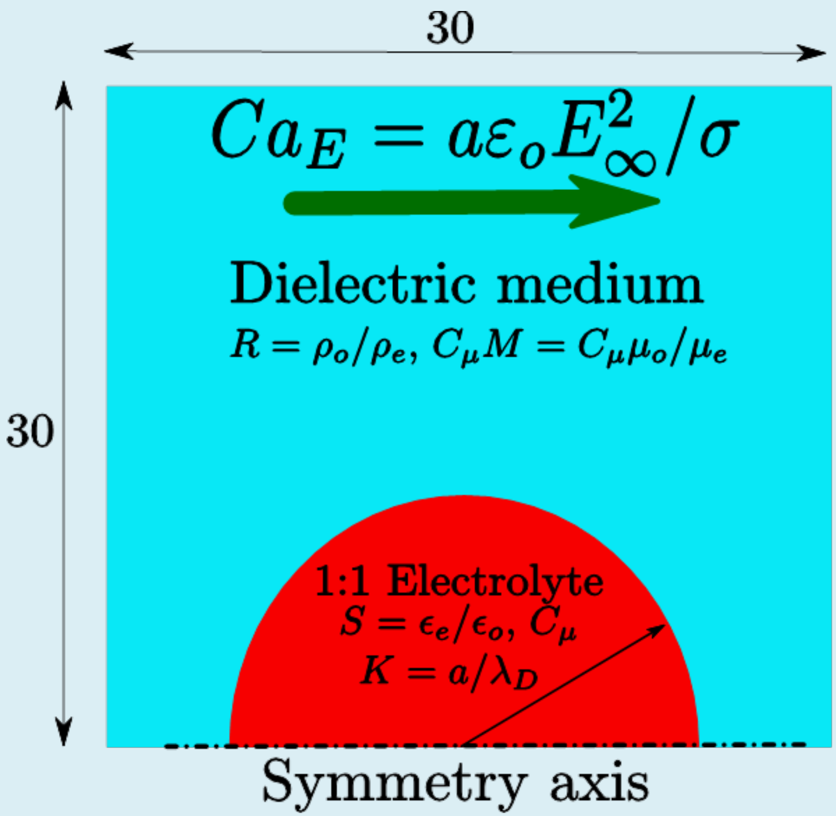
GERRIS wording:

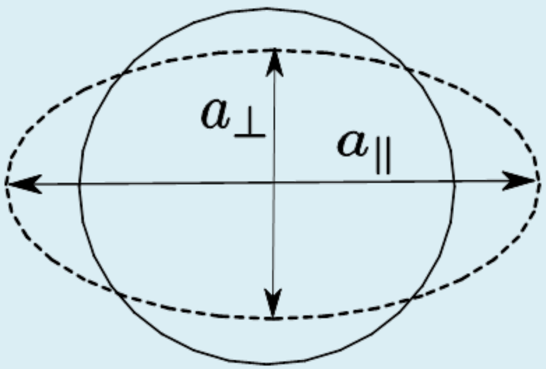
term A: SourceDiffusion c^i D^i

term B: SourceDiffusionExplicit c^i $-c^i D^i$ ϕ

term C: SourceDiffusionExplicit c^i $-c^i D^i \gamma^i$ φ

Validation



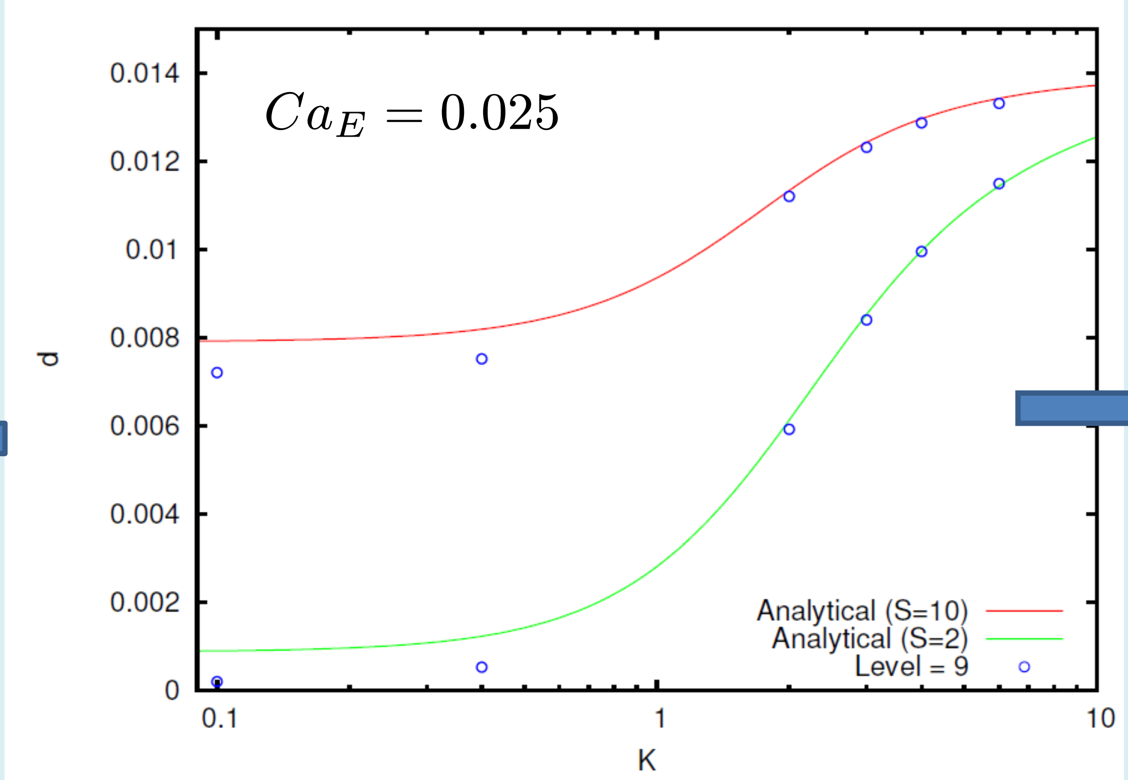


$$d = \frac{a_\parallel - a_\perp}{a_\parallel + a_\perp}$$

BC: Slip velocity

Validation

To the dielectric limit



To the leaky-dielectric limit

$$\frac{d}{Ca_E} = \frac{9}{16} \times \frac{(S-1)\left\{S\left[2 - K^2/(K\coth K - 1)\right]^2 - 1\right\} + K^2 S}{\left[2(S-1) + SK^2/(K\coth K - 1)\right]^2}$$

corresponds to $R = 1,\ C_\mu = 1,\ M = 1,\ D^+ = D^- = 1$

Zholkovskij *et al.*
J. Fluid Mech. 472 (2002)

Validation

Level	d	rate of convergence	relative error (%)
$K = 0.1$			
8	0.00531	–	33.03
9	0.00721	$1.9\ 10^{-3}$	9.04
10	0.00736	$1.5\ 10^{-4}$	7.21
$K = 6$			
8	0.01223	–	10.44
9	0.01332	$1.1\ 10^{-3}$	2.47
10	0.01365	$3.4\ 10^{-4}$	0.0

- The rate of convergence with the grid is similar for $K = 0.1$ and $K = 6$.
- The relative error is larger for lower K values, Artifact due to very low value of d for $K = 0.1$ ($d|_{K=0.1} = 7.93\ 10^{-3}$).

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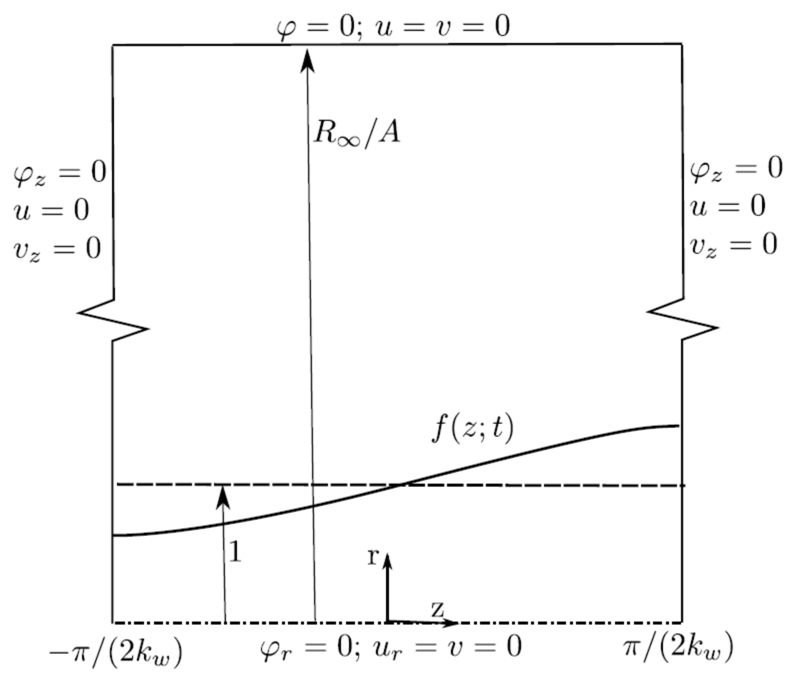
DESCRIPTION OF THE PROBLEM

Breakup of a liquid charged capillary column



Initial conditions

$$f(z;0) = 1 + \epsilon \sin(\kappa_w z)$$
$$c^+(z,r;0) = B^+$$
$$c^-(z,r;0) = B^-$$

Dimensionless governing parameters

(1) for the perturbation, ϵ and κ_w;

(2) for the charged species, D^+, D^-, γ and K;

(3) for the electrical conditions, B^+, B^- and R_∞/A; and

(4) for the fluid properties, C_μ, S, R and M.

$$Ca_E = \frac{A\varepsilon_o E_o^2}{\sigma} = \frac{K^4 S^2}{16\gamma^2}(B^+ - B^-)^2$$

RESULTS

Breakup of a liquid charged capillary column

- We focus mainly in electrokinetic effects. So the following parameters are kept fixed.

$$\epsilon = 0.1,\ \kappa_w = 0.6283,\ C_\mu = 0.05,\ R = M = 10^{-2} \text{ and } S = 10.$$

- In order to have a more pronounced effect cation is smaller than anion

$$D^+ = 7 \text{ and } D^- = 1.$$

- We investigate the influence of polarity,

$$\text{Positive polarity: } B^+ = 1.01 \text{ and } B^+ = 0.99$$
$$\text{Negative polariy: } B^+ = 0.99 \text{ and } B^+ = 1.01.$$

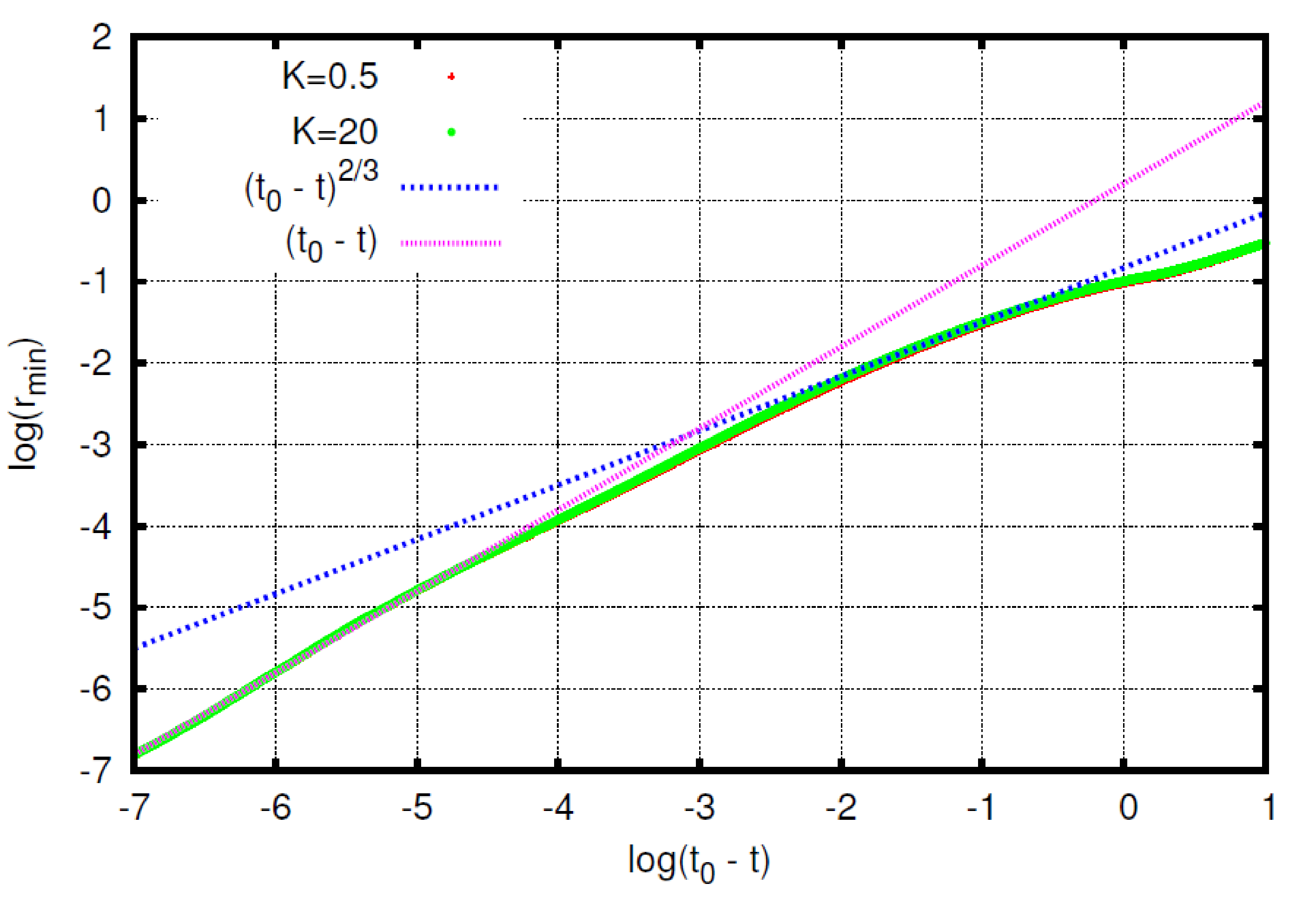
- The only free parameter is K= L/λ_D.

- The level of electrification is kept fixed, Ca_E = 0.125

- Then γ is calculated from $Ca_E = \dfrac{A\varepsilon_o E_o^2}{\sigma} = \dfrac{K^4 S^2}{16\gamma^2}(B^+ - B^-)^2$

RESULTS

Breakup of a liquid charged capillary column



Results

The validity of the homogeneous conductivity assumption

Classic EHD Model:

$$q_t + \nabla \cdot (q\mathbf{u}) = -\nabla \cdot (\alpha\, S\mathbf{E})$$

→ Dimensionless homogeneous conductivity

From PNP equation:

$$q = \frac{SK^2}{2\gamma}(c^+ - c^-)$$

$$c_t^+ + \nabla \cdot (c^+\mathbf{u}) = \nabla \cdot \left(D^+\nabla c^+ - D^+\gamma\mathbf{E}\right)$$

$$c_t^- + \nabla \cdot (c^-\mathbf{u}) = \nabla \cdot \left(D^-\nabla c^- + D^-\gamma\mathbf{E}\right)$$

$$q_t + \nabla \cdot (q\mathbf{u}) = \frac{K^2 S}{2\gamma}\nabla \cdot (D^+\nabla c^+ - D^-\nabla c^-) - \nabla \cdot \left(\frac{D^+c^+ + D^-c^-}{2}K^2 S\mathbf{E}\right)$$

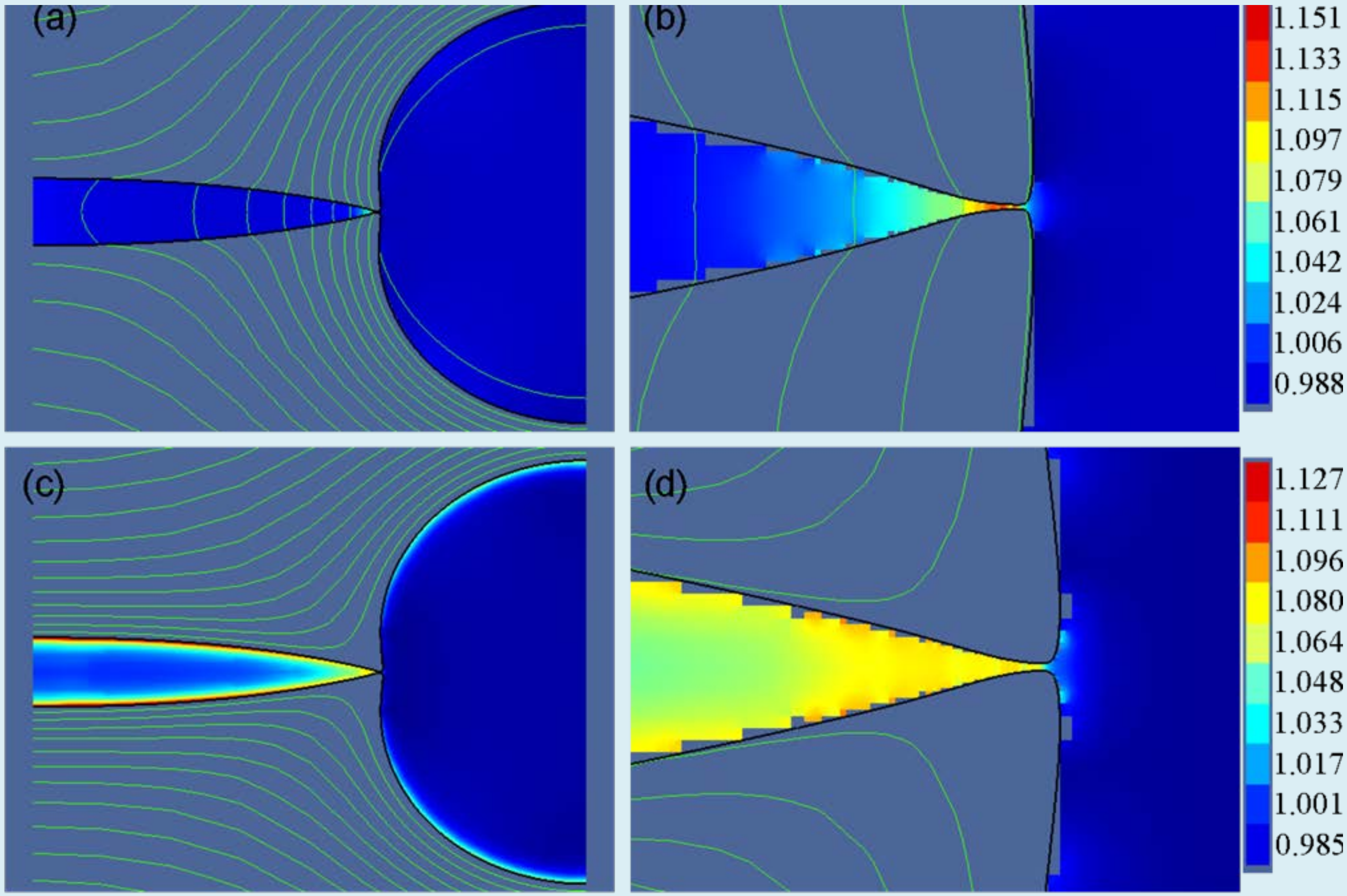
$$\alpha = \frac{K^2 S}{2}(D^+c^+ + D^-c^-)$$

Results

The validity of the homogeneous conductivity assumption

Positive polarity

Relative bulk conductivity = $\dfrac{D^+c^+ + D^-c^-}{D^+B^+ + D^-B^-}$

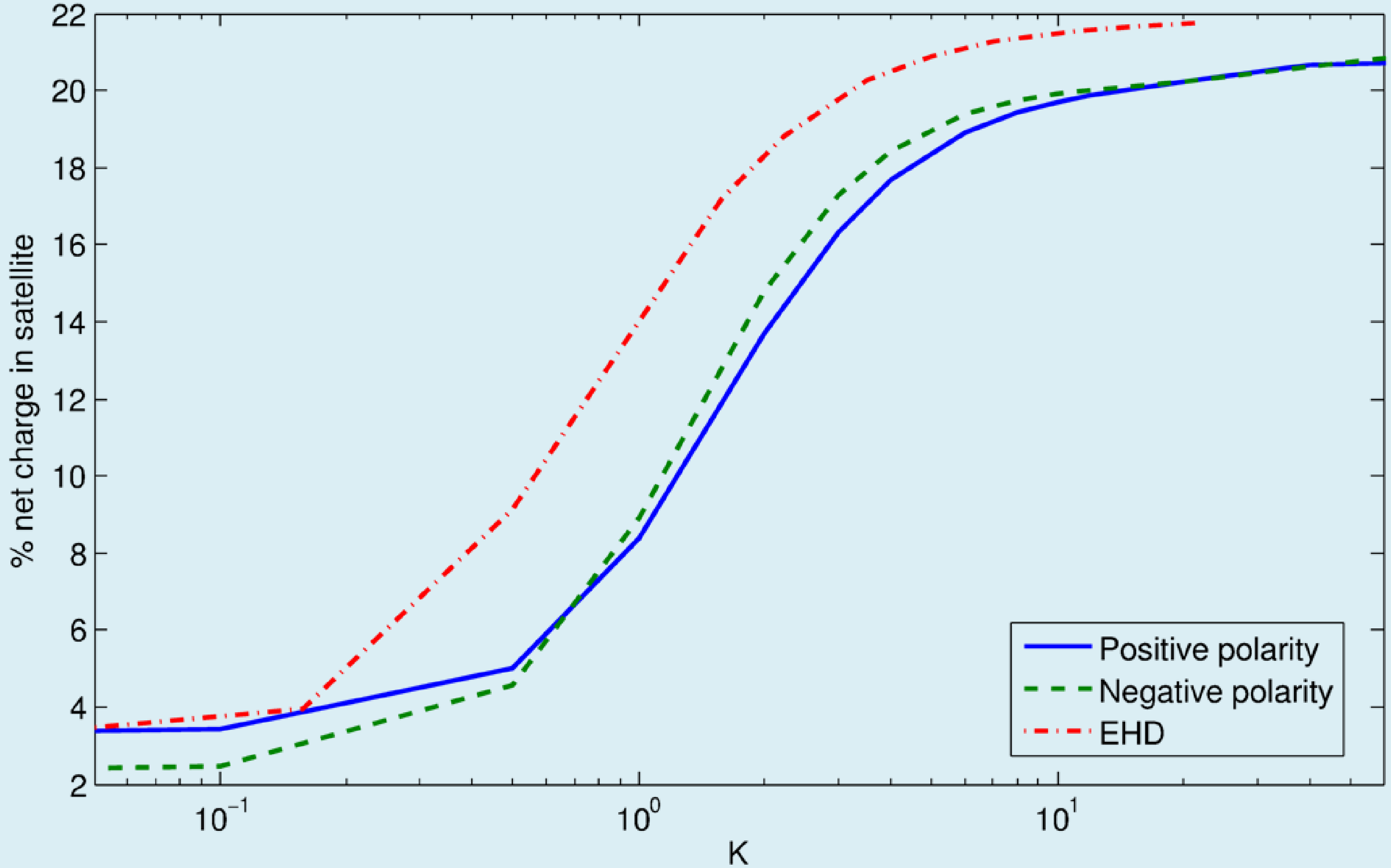


K=0.5

K=20

Results

The validity of the homogeneous conductivity assumption



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Conclusions

1. A general electrokinetic model and numerical scheme has been presented and validated.

2. The numerical scheme is available through GERRIS.

3. In the cases when thermal diffusion, electrosmotic motion and singularities compete EHD model can yield different results than the present electrokinetic model.

4. Method can be improved restricting the resolution of the diffusion term to the domain of interest.

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