Selected Slides from Presentation at Simula Research Laboratory

Title Slide

Simulation of Membrane Potentials in Ion Selective Electrodes

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Oslo, Norway

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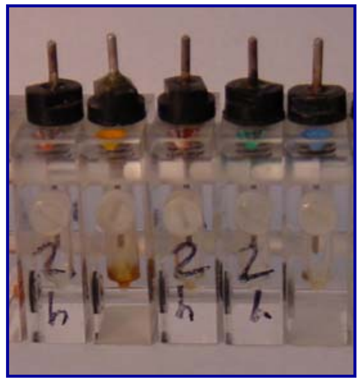
Åbo Academy / ProSense
Åbo (Turku), Finland

June 18, 2004

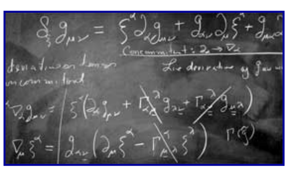


[ProSense]

Mapping Slide

This talk outlines a solver for coupled Nernst-Planck and Poisson equations

Ion selective electrodes (ISEs)



Mathematical model: Nernst-Planck and Poisson

Diffpack

Simulator design

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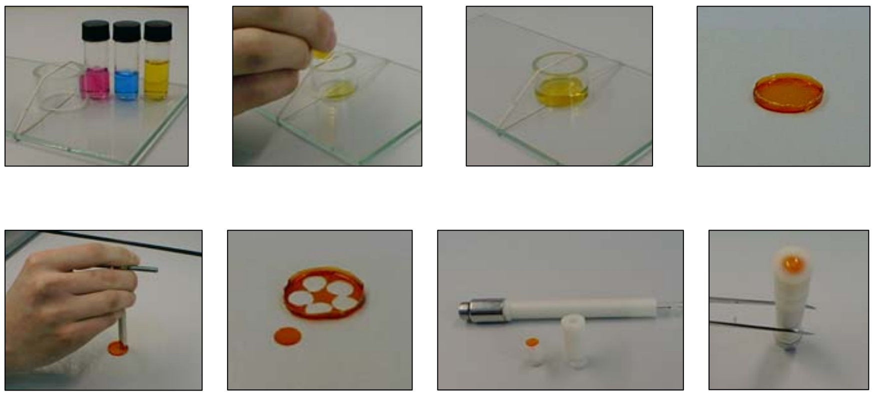
Slide from Section 1

Ion selective electrodes contain a PVC membrane saturated with a solvent



[ProSense, prototype in lab]

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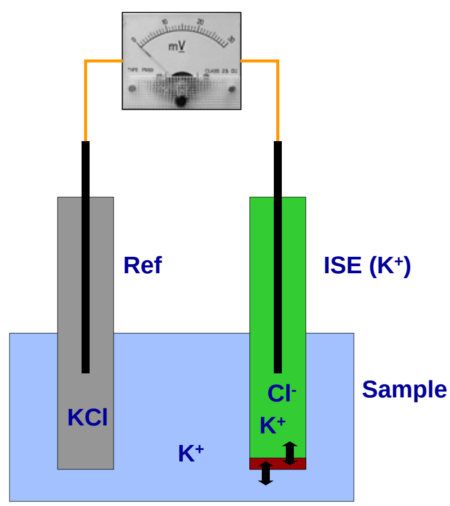
Slide from Section 1

The measured potential difference reflects the ionic activity in the sample solution

ISEs are selective and sensitive for target ion

Robust and low-cost devices, no maintenance

Can be miniaturized as solid state circuitry



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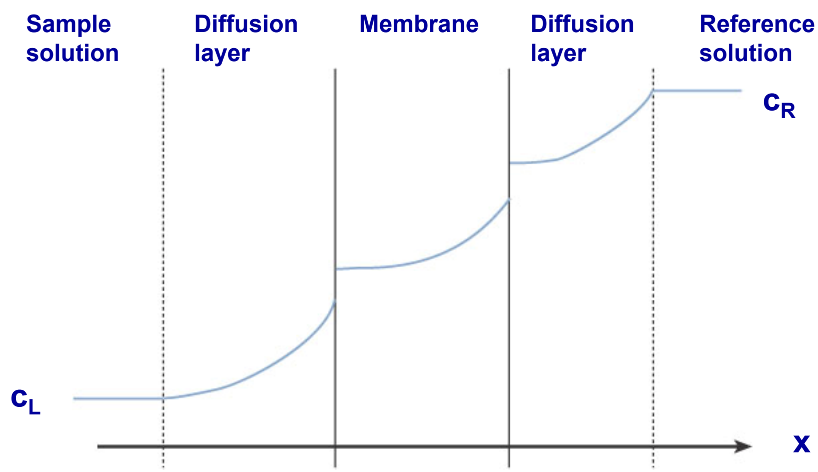
Slide from Section 2

Empirical potential expressions are to be replaced by more accurate models



Concentration profile, ion #i

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Slide from Section 2 (Animation)

Operator splitting gives a sequence of PDEs—and one ODE per spatial point

$$\frac{\partial c_i(x,t)}{\partial t} = -\frac{\partial}{\partial x}[f_i(x,t)] \quad \text{for } x \in \Omega$$

Concentration c_i of specie #i, i=1,…,n_{ion}

$$f_i(x,t) = -D_i(x,t)\frac{\partial c_i(x,t)}{\partial x} - K_i(x,t)c_i(x,t),$$
$$K_i(x,t) = -D_i(x,t)z_i\frac{F}{RT}E(x,t)$$

Unknowns c_i and E

$$\varepsilon\frac{\partial E(x,t)}{\partial t} = I - F\sum_{i=1}^{n_{ion}} z_i f_i(x,t) \quad \text{for } x \in \Omega$$

Electrical field E

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Slide from
Section 2
(Animation)

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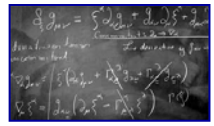

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Slide from
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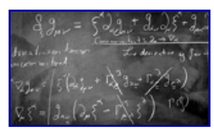

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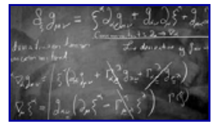
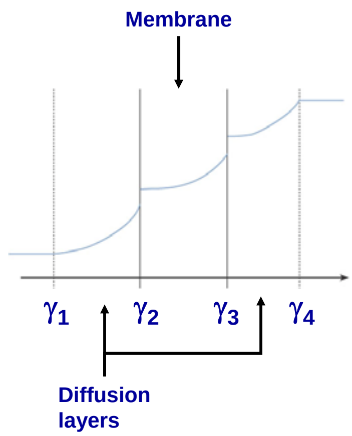
Selected Slides from Presentation at Simula Research Laboratory

Slide from Section 2 (Animation)

Flux conditions are present at the boundaries of the membrane





Slide from Section 2 (Animation)

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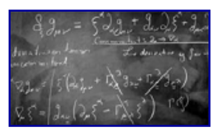

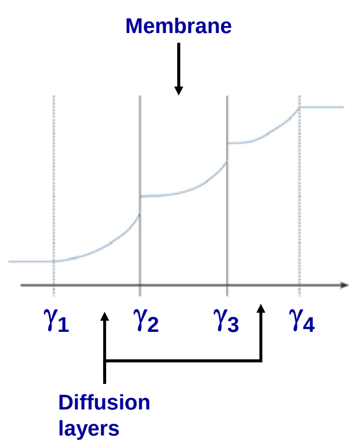

$$c_i(\gamma_1, t) = c_{i,L}(t)$$
$$c_i(\gamma_4, t) = c_{i,R}(t)$$

$$f_i(\gamma_2, t) = \overrightarrow{k}_{i,2} c_i^-(\gamma_2, t) - \overleftarrow{k}_{i,2} c_i^+(\gamma_2, t)$$
$$f_i(\gamma_3, t) = -\overrightarrow{k}_{i,3} c_i^+(\gamma_3, t) + \overleftarrow{k}_{i,3} c_i^-(\gamma_3, t)$$

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Slide from Section 2 (Animation)

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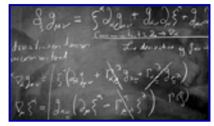

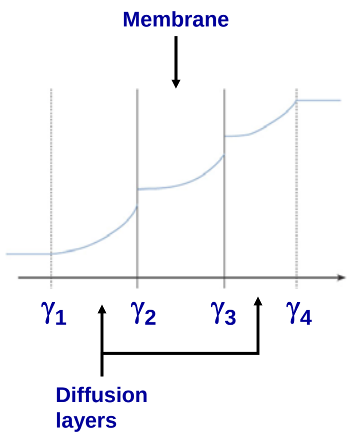

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Membrane only

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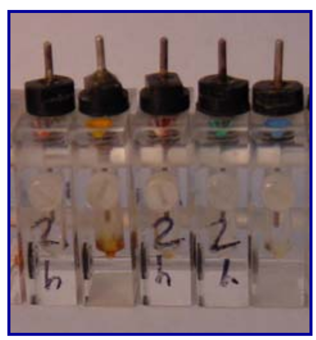
Conclusion Slide

In summary, PDE-based models offer more versatile simulations of ionic activity

Computational use of PDEs in this context is novel

Good match between computations and experiments is observed

Use of finite elements allows models to capture ignored effects



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