Modeling acid-base diodes using COMSOL with MATLAB

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1 The model

1.1 Acid-base diode

A gel or membrane connects an alkaline and an acidic reservoir with electric potential difference between them. The program computes in 1D the stationary concentration profiles of the ions, the potential profile in the gel/membrane and the current density.

In this model the diffusion (boundary) layers of the gel are neglected. The gel/membrane usually contains fixed (not mobile) ions, which results small jump in the concentrations at liquid-gel boundary. The applied boundary conditions (Dirichlet) are corrected with this jump regarding the Donnan equilibrium.

1.2 Equations

Poisson–Nernst–Planck (PNP) equations.

The PNP equations are selected in COMSOL using "Nernst–Planck equation without electroneutrality" in stationary mode and the "Poisson-equation".

1.3 Restrictions

The program can handle only one fixed cation and/or one fixed anion with charges $z = \pm 1$. The charge of the mobile ions should be $|z| < 3$.

2   Usage

2.1   Start

1. Start COMSOL with MATLAB (run `comsol matlab` in terminal emulator as user `matlab`; see the help of COMSOL and MATLAB for possible flags).

2. Change the current directory to the location of the acid-base diode program.

3. Run `start_acidbase();` to load the database of the existing computed models.

2.2   Select a model to calculate or to get the results

`[current,state,fem]=diode_fcn(mode,par,opts);`
   Type `help diode_fcn` for details.

2.3   Plot profiles

`p_plot(fem,data)`
   Type `help p_plot` for details.

2.4   Plot the current versus any parameter

`[X,Y]=c_plot(mode,par,var,side)`
   Type `help c_plot` for details.

2.5   Stop

Run `stop_acidbase();` to save the new or changed models. Then it is safe to type `exit` or close the MATLAB window.