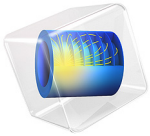


Vanadium Redox Flow Battery

Introduction

Redox flow batteries store the energy in the liquid electrolytes, pumped through the cell and stored in external tanks, rather than in the porous electrodes as for conventional batteries. This approach offers interesting solutions for low-cost energy storage, load leveling and power peak shaving.

The vanadium redox flow battery uses two different electrolyte solutions, one for the negative side of the cell and another for the positive side. The two solutions are kept separated in the cell by the use of an ion-exchange membrane that allows for transport of ions (primarily protons) between the two cell compartments. The principle of the vanadium redox flow battery is illustrated in Figure 1.

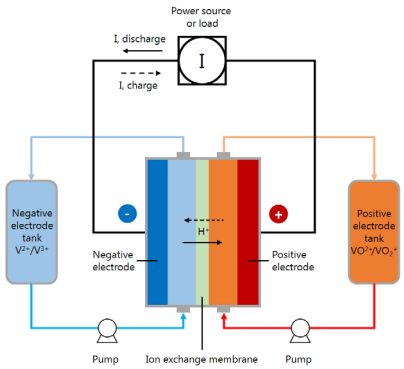


Figure 1: Schematic of a vanadium redox flow battery system.

This example demonstrates how to build a model consisting of two different cell compartments, with different ion compositions and electrode reactions, separated by an ion-exchange membrane. The model is a modified version of published works (Ref. 1 and Ref. 2).

See also the Application Libraries example Soluble Lead-Acid Redox Flow Battery for how to make a transient flow battery model by coupling the cell model to mass balances for the external storage tanks.

The cell geometry is shown in Figure 2. The model contains three domains, a negative porous electrode (4 mm thick), an ion-exchange membrane (203 µm thick) and a positive porous electrode (4 mm thick). The cell is 35 mm high.

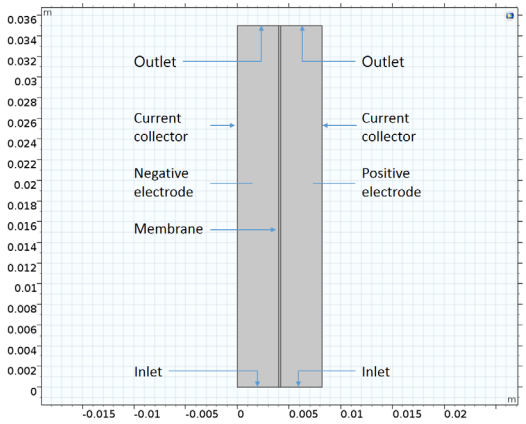


Figure 2: Model geometry. Three domains: negative electrode, membrane, positive electrode.

Each side of the cell is fed with an electrolyte containing sulfuric acid and a vanadium redox couple (see below), flowing through the porous electrodes. The liquid enters the cell from bottom at a constant velocity in the y-direction, corresponding to a flow rate of 30 ml/min at cell depth of 28.5 mm.

The left electrode is grounded, and the current leaves the cell over the rightmost boundary at an average current density of 100 mA/cm^2.

The models solves for a stationary case with a given set of inlet concentrations.

LIQUID ELECTROLYTE SPECIES AND ELECTRODE REACTIONS

The negative electrolyte contains the following ions:

- H^+
- HSO_4^-
- SO_4^{2-}
- V^{3+}
- V^{2+}

The negative electrode reaction is:

$$V^{3+} + e^- \leftrightarrow V^{2+}$$

The equilibrium potential for this reaction is calculated using Nernst equation according to

$$E_{\text{eq, neg}} = E_{0, \text{neg}} + \frac{RT}{F} \ln\left(\frac{a_{V^{3+}}}{a_{V^{2+}}}\right)$$

where $E_{0, \text{neg}}$ is the reference potential for the electrode reaction (SI unit: V), a_i is the chemical activity of species i (dimensionless), R is the molar gas constant (8.31 J/(mol·K)), T is the cell temperature (SI unit: K), and F is Faraday's constant (96,485 s·A/mol).

A Butler-Volmer type of kinetics expression is used for the negative electrode reaction according to:

$$i_{\text{neg}} = A i_{0, \text{neg}}\left(\exp\left(\left(\frac{(1-\alpha_{\text{neg}})F\eta_{\text{neg}}}{RT}\right) - \exp\left(\frac{-\alpha_{\text{neg}}F\eta_{\text{neg}}}{RT}\right)\right)\right)$$

$$i_{0, \text{neg}} = F k_{\text{neg}} (a_{V^{2+}})^{1-\alpha_{\text{neg}}} (a_{V^{3+}})^{\alpha_{\text{neg}}}$$

where A is the specific surface area (SI unit: m^2/m^3) of the porous electrode, α_{neg} the transfer coefficient (dimensionless), k_{neg} the rate constant.

The overpotential, η_{neg} (SI unit: V), is defined as

$$\eta = \phi_s - \phi_l - E_{\text{eq}}$$

where ϕ_s is the electric potential of the solid phase of the electrode (SI unit: V) and ϕ_l the electrolyte potential (SI unit: V).

The positive electrolyte contains the following ions:

- H^+
- HSO_4^-
- SO_4^{2-}
- VO^{2+}
- VO_2^+

The positive electrode reaction is:

$$VO_2^+ + e^- + 2H^+ \leftrightarrow VO^{2+} + H_2O$$

with the equilibrium potential calculated according to:

$$E_{\text{eq, pos}} = E_{0,\text{ pos}} + \frac{RT}{F}\ln\left(\frac{a_{VO_2^+}(a_{H^+})^2}{a_{VO^{2+}}}\right)$$

$$i_{\text{pos}} = Ai_{0,\text{ pos}}\left(\exp\left(\left(\frac{(1-\alpha_{\text{pos}})F\eta_{\text{pos}}}{RT}\right) - \exp\left(\frac{-\alpha_{\text{pos}}F\eta_{\text{pos}}}{RT}\right)\right)\right)$$

$$i_{0,\text{ pos}} = Fk_{\text{pos}}(a_{VO^{2+}})^{1-\alpha_{\text{pos}}}(a_{VO_2^+})^{\alpha_{\text{pos}}}$$

The ion exchange membrane accounts for transport of the following ions:

- H^+
- HSO_4^-
- SO_4^{2-}
- V^{3+}
- V^{2+}
- VO^{2+}
- VO_2^+

SULFURIC ACID DISSOCIATION

The first dissociation step of sulfuric acid is assumed to be complete

$$H_2SO_4 \rightarrow H^+ + HSO_4^-$$

whereas the second step

$$HSO_4^- \rightarrow H^+ + SO_4^{2-}$$

is described using a dissociation source term, r_d:

$$r_d = k_d\left(\frac{a_{H^+}a_{HSO_4^-}}{a_{H^+} + a_{HSO_4^-}} - \beta\right)$$

where k_d is a rate parameter, and β the degree of dissociation.

ION TRANSPORT EQUATIONS

In this model the Nernst–Planck equations are used for ion flux and charge transport by which the following equation describes the molar flux of species i, $\mathbf{N}_i$, due to diffusion, migration and convection:

$$\mathbf{N}_i = -D_i \nabla c_i - z_i u_{\mathrm{mob},i} F c_i \nabla \phi_l + c_i \mathbf{u}$$

The first term is the diffusion flux, D_i is the diffusion coefficient (SI unit: m^2/s). The migration term consists of the species charge number z_i, the species mobility $u_{\mathrm{mob},i}$ (SI unit: s·mol/kg) and the electrolyte potential (ϕ_l). In the convection term, $\mathbf{u}$ denotes the fluid velocity vector (SI unit: m/s).

The electrolyte current density is calculated using Faraday's law by summing up the contributions from the molar fluxes, multiplied by the species charges, with the observation that the convective term vanishes due to the electroneutrality condition (see the theory for the Tertiary Current Distribution, Nernst-Planck interface):

$$\mathbf{i}_l = F \sum_{i=1}^{n} z_i (-D_i \nabla c_i - z_i u_{\mathrm{m},i} F c_i \nabla \phi_l) \tag{1}$$

The conservation of charge is then used to calculate the electrolyte potential.

$$\nabla \cdot \mathbf{i}_l = F \sum_{i=1}^{n} z_i R_i$$

where the R_i terms are the reaction sources due the porous electrode reactions.

This model uses Equation 1 when solving for the electrolyte potential in the porous electrodes through the Tertiary Current Distribution, Nernst–Planck interface.

In the negative and positive porous electrode domains, where there is free electrolyte present, the concentrations for all the ions are of the same order of magnitude, and the gradients of c_i are not negligible. The membrane, however, consists of a polymer electrolyte, with additional negative ions fixed in the polymer matrix, implying that the concentration for this species is constant. In the ion-exchange membrane domain, a fixed space charge, ρ_{fix}, is added while calculating the sum of charges in the electroneutrality condition:

$$\rho_{\text{fix}} + F\sum_{i=1}^{n} z_i c_i = 0 \tag{2}$$

The fixed space charge is prescribed in terms of the membrane charge concentration which is varied using an auxiliary sweep in this model.

MEMBRANE — POROUS ELECTRODE BOUNDARY CONDITIONS

Donnan Conditions

The boundary conditions at the boundaries between the membrane and the porous electrode domains are set up in the following way.

For species existing on both sides of the membrane-electrode, we have the following relation between the potentials and the concentrations:

$$\phi_{l,m} = \phi_{l,e} - \frac{RT}{z_i F}\ln\left(\frac{c_{i,m}}{c_{i,e}}\right) \tag{3}$$

where $c_{i,m}$ is the species concentration in the membrane, and $c_{i,e}$ the species concentration in the free electrolyte and z_i the corresponding charge. The potential shift caused by Equation 3 is called Donnan potential (Ref. 3). The Ion Exchange Membrane Boundary feature in the Tertiary Current Distribution, Nernst–Planck interface is used to define the Donnan conditions.

Self-discharge Reactions

At the membrane-negative electrode boundary, the V^{3+} and V^{2+} are assumed to be immediately oxidized according to

$$V^{2+} \rightarrow V^{3+} + e^-$$

and

$$V^{3+} + 2H_2O \rightarrow VO^{2+} + 2H^+ + e^-$$

so that

$$c_{V^{3+}} = c_{V^{2+}} = 0 \tag{4}$$

Correspondingly, the VO^{2+} and VO_2^+ concentration are assumed to be zero at the membrane - positive electrode boundaries:

$$c_{VO^{2+}} = c_{VO_2^+} = 0 \tag{5}$$

as a result of the reduction reactions

$$VO_2^+ + e^- + 2H^+ \rightarrow VO^{2+} + H_2O$$

and

$$VO^{2+} + 2H^+ + e^- \rightarrow V^{3+} + 2H_2O$$

the fast oxidation/reduction reactions are implemented using the Fast Irreversible Reaction kinetics type of the Electrode Surface node.

Results and Discussion

Figure 3 shows the concentration of the V^{3+} and the VO^{2+} ions in the porous electrodes for the membrane charge concentration of –1900 mol/m^3. The ion concentration for these species is higher toward the current collectors and toward the outlets.

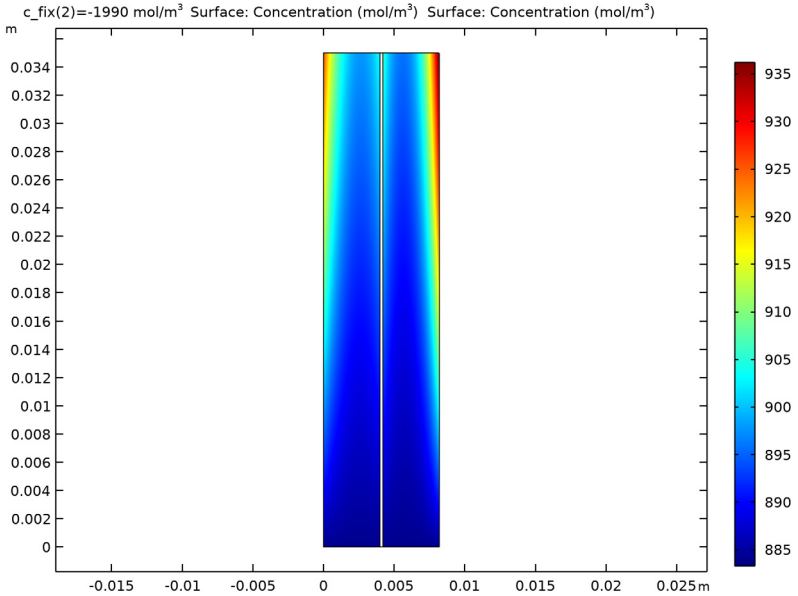


Figure 3: Concentration of the V^{3+} (left compartment) and the VO^{2+} (right compartment) ions for a membrane charge concentration of -1900 mol/m^3.

Figure 4 shows the concentration of the V^{2+} and the VO_2^+ ions for the membrane charge concentration of –1900 mol/m^3. Depletion occurs along the flow direction and also toward both the current collector and membrane sides of the electrodes.

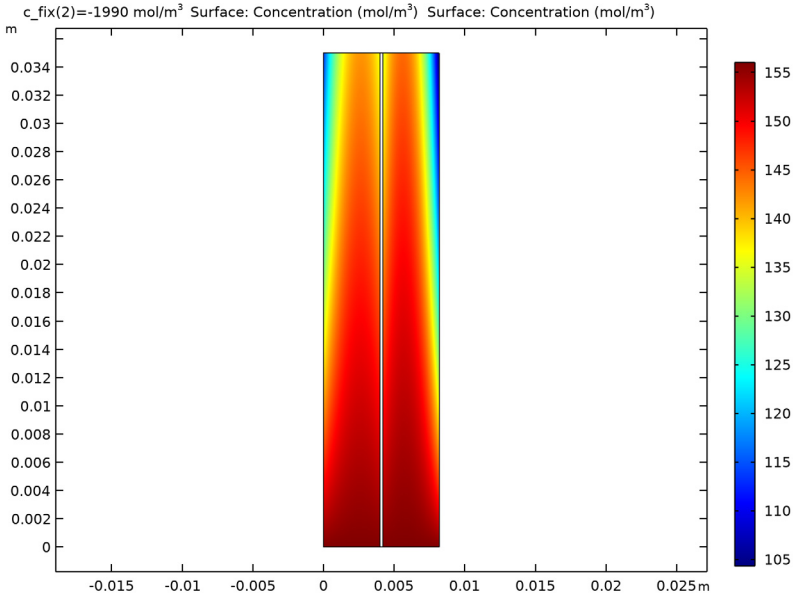


Figure 4: Concentration of the V^{2+} (left compartment) and the VO_2^+ (right compartment) ions for a membrane charge concentration of -1900 mol/m^3.

Figure 5 shows the electrolyte potential for the membrane charge concentration of -1900 mol/m^3, which decreases toward the positive current collector.

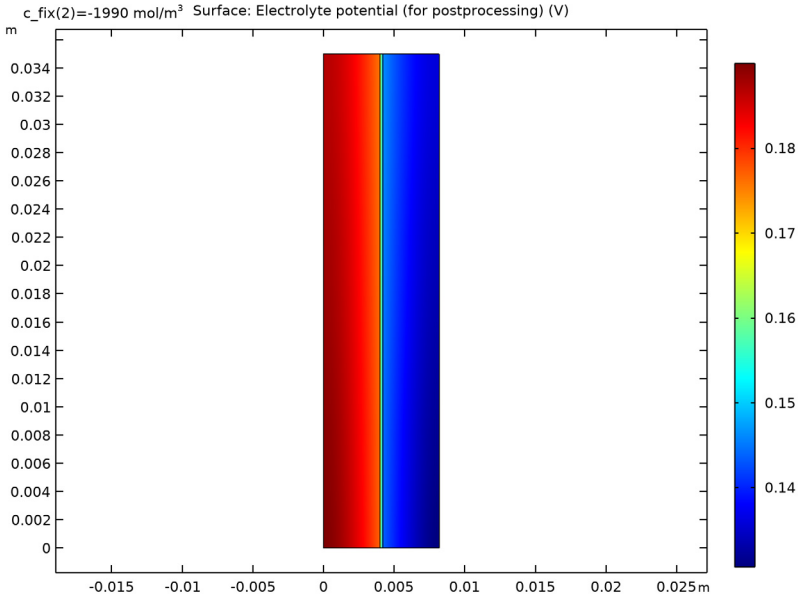


Figure 5: Electrolyte potential for a membrane charge concentration of -1900 mol/m^3.

Figure 6 shows a cut line plot of the electrolyte potential at half the cell height. The Donnan potential shifts at the membrane boundaries are clearly visible in the figure.

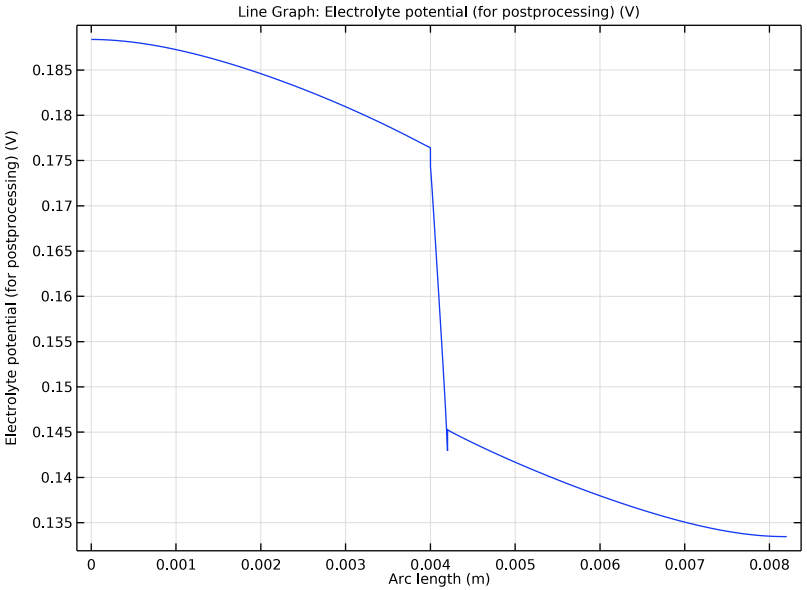


Figure 6: Electrolyte potential along a horizontal line placed at $y = h_{\text{cell}}/2$.

Figure 7 shows the electrode reaction source at half the cell height. The maximum is located toward the current collectors, with a minimum located in the middle of the electrodes. The reason for this phenomena is the similar conductivities of both phases (electrolyte and electrode) of the porous electrodes.

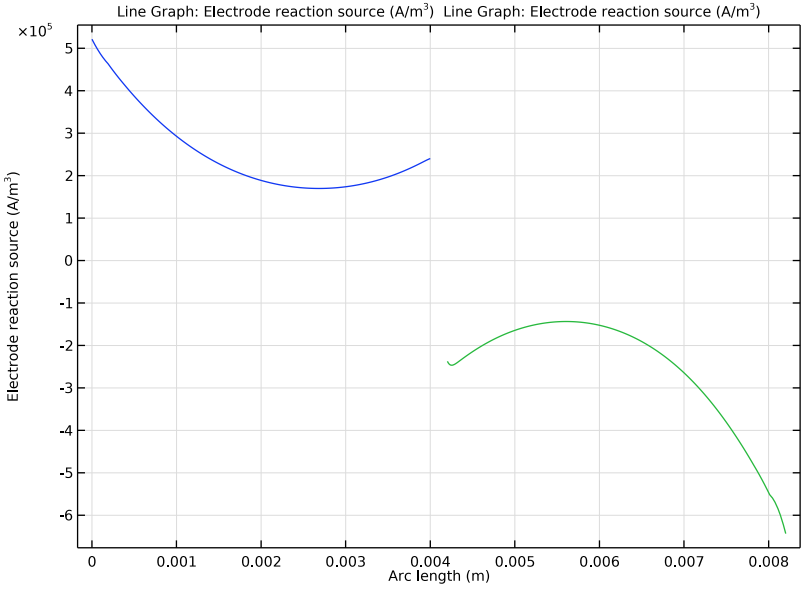


Figure 7: Electrode reaction source in the porous electrodes along a horizontal line placed at $y = h_{\text{cell}}/2$.

Figure 8 shows the logarithm of the absolute rate of the dissociation reaction. Except from very close to the boundaries, the rates are generally very low, indicating that equilibrium is reached swiftly.

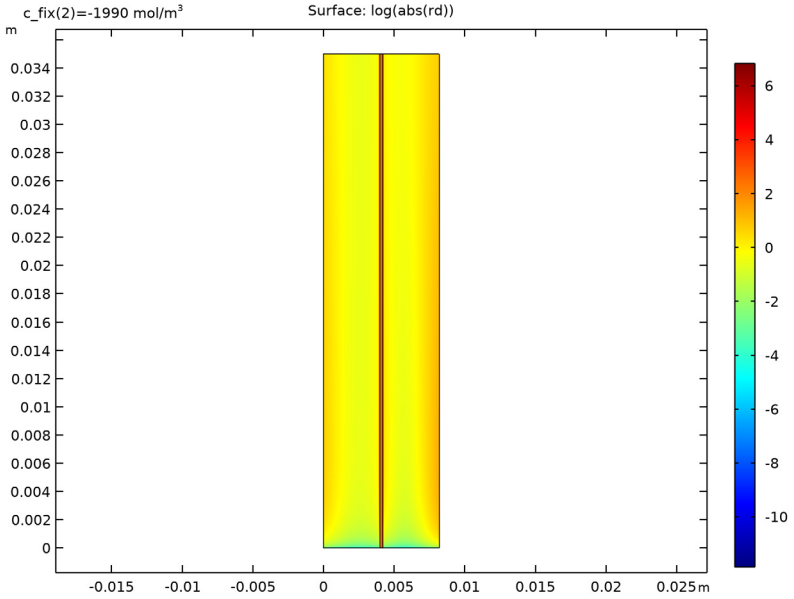


Figure 8: Sulfuric acid dissociation rate.

Figure 9 shows the local concentrations of the sulfuric acid species at half the cell height. In the electrodes, gradients are only seen close to the membrane; this is due to the influx and outflux of protons at the membrane boundaries in combination with the acid dissociation reaction.

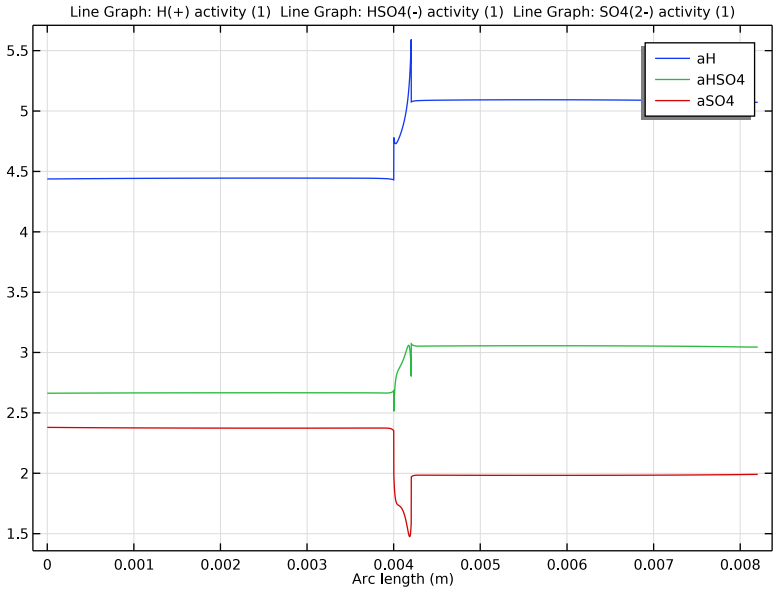


Figure 9: Sulfuric acid species along a horizontal line placed at $y = h_{\text{cell}}/2$.

Figure 10 shows the local concentrations of the vanadium species at half the cell height. The highest gradients of vanadium species is seen to be located in the ion exchange membrane.

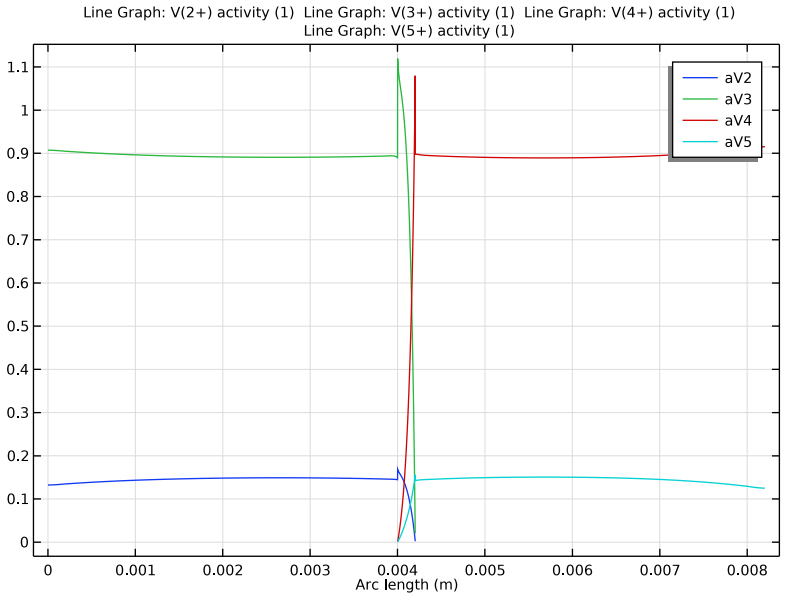


Figure 10: Vanadium species along a horizontal line placed at $y = h_{\text{cell}}/2$.

Figure 11 shows the local fluxes of the sulfuric acid species at half the cell height. The fluxes are seen to be the maximum close to the ion exchange membrane.

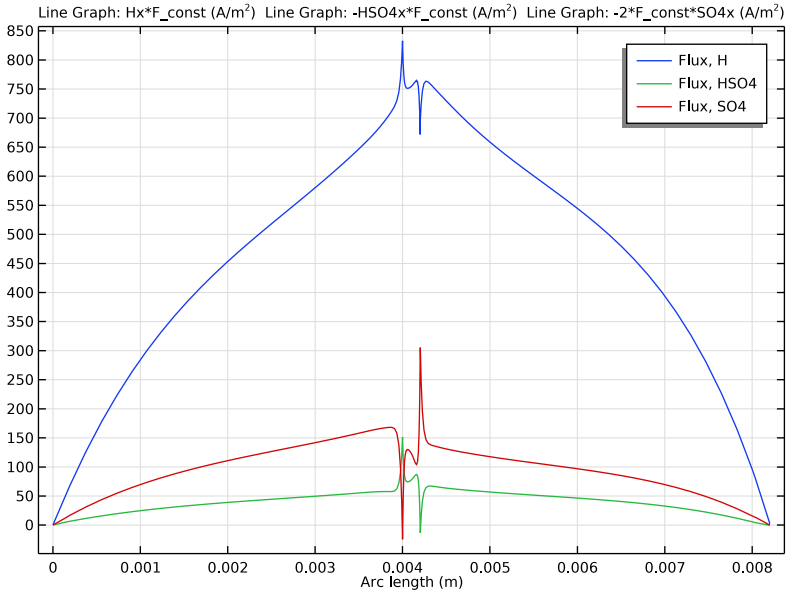


Figure 11: Sulfuric acid species fluxes along a horizontal line placed at $y = h_{cell}/2$.

References

1. K. Knehr, E Agar, C. Dennison, A. Kalidindi, and E. Kumbur, "A Transient Vanadium Flow Battery Model Incorporating Vanadium Crossover and Water Transport through the Membrane", *J. Electrochem. Soc.*, vol. 159, no. 9, pp A1446–A1459, 2012.

2. A.A. Shah, M.J. Watt-Smith, and F.C. Walsh "A dynamic performance model for redox-flow batteries involving soluble species", *Electrochimica Acta* vol. 53, pp 8087–8100, 2008.

3. K.W. Knehr and E.C. Kumbur, "Open circuit voltage of vanadium redox flow batteries: Discrepancy between models and experiments", *Electrochemistry Communications*, vol. 13, pp 342–345, 2011

Application Library path: `Battery_Design_Module/Flow_Batteries/v_flow_battery`

Modeling Instructions

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **2D**.

Add three Tertiary Current Distribution, Nernst Planck interfaces to your model. They will represent the physics for the two porous electrodes and the membrane.

2 In the **Select Physics** tree, select **Electrochemistry>Tertiary Current Distribution, Nernst-Planck>Tertiary, Electroneutrality (tcd)**.

3 Click **Add**.

4 In the **Number of species** text field, type `5`.

5 In the **Concentrations** table, enter the following settings:

`cSO4_neg`
`cHSO4_neg`
`cH_neg`
`cV2`
`cV3`

6 In the **Electrolyte potential** text field, type `phil_neg`.

7 In the **Electric potential** text field, type `phis_neg`.

8 In the **Select Physics** tree, select **Electrochemistry>Tertiary Current Distribution, Nernst-Planck>Tertiary, Electroneutrality (tcd)**.

9 Click **Add**.

10 In the **Number of species** text field, type `7`.

11 In the **Concentrations** table, enter the following settings:

cSO4_mem
cHSO4_mem
cH_mem
cV2_mem
cV3_mem
cV4_mem
cV5_mem

12 In the **Electrolyte potential** text field, type `phil_mem`.

13 In the **Electric potential** text field, type `phis_mem`.

14 In the **Select Physics** tree, select **Electrochemistry>Tertiary Current Distribution, Nernst-Planck>Tertiary, Electroneutrality (tcd)**.

15 Click **Add**.

16 In the **Number of species** text field, type `5`.

17 In the **Concentrations** table, enter the following settings:

cSO4_pos
cHSO4_pos
cH_pos
cV4
cV5

18 In the **Electrolyte potential** text field, type `phil_pos`.

19 In the **Electric potential** text field, type `phis_pos`.

20 Click **Study**.

21 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces> Stationary with Initialization**.

22 Click **Done**.

GLOBAL DEFINITIONS

Add the model parameters from a text file.

Parameters 1

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

2 In the **Settings** window for **Parameters**, locate the **Parameters** section.

3 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `v_flow_battery_parameters.txt`.

GEOMETRY 1

Draw the geometry as a union of three rectangles (the two porous electrodes and the membrane domains).

Negative Electrode

1 In the **Geometry** toolbar, click **Rectangle**.

2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.

3 In the **Width** text field, type `L_e`.

4 In the **Height** text field, type `H_cell`.

5 Locate the **Selections of Resulting Entities** section. Select the **Resulting objects selection** check box.

6 Right-click **Rectangle 1 (r1)** and choose **Rename**.

7 In the **Rename Rectangle** dialog box, type `Negative Electrode` in the **New label** text field.

8 Click **OK**.

Membrane

1 In the **Geometry** toolbar, click **Rectangle**.

2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.

3 In the **Width** text field, type `L_m`.

4 In the **Height** text field, type `H_cell`.

5 Locate the **Position** section. In the **x** text field, type `L_e`.

6 Locate the **Selections of Resulting Entities** section. Select the **Resulting objects selection** check box.

7 Right-click **Rectangle 2 (r2)** and choose **Rename**.

8 In the **Rename Rectangle** dialog box, type `Membrane` in the **New label** text field.

9 Click **OK**.

Positive Electrode

1 In the **Geometry** toolbar, click **Rectangle**.

2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.

3 In the **Width** text field, type `L_e`.

4 In the **Height** text field, type `H_cell`.

5 Locate the **Position** section. In the **x** text field, type `L_e+L_m`.

6 Locate the **Selections of Resulting Entities** section. Select the **Resulting objects selection** check box.

7 Right-click **Rectangle 3 (r3)** and choose **Rename**.

8 In the **Rename Rectangle** dialog box, type `Positive Electrode` in the **New label** text field.

9 Click **OK**.

10 In the **Settings** window for **Rectangle**, click **Build All Objects**.

11 Click the **Zoom Extents** button in the **Graphics** toolbar.

Compare the geometry with Figure 2.

DEFINITIONS

Add domain specific variables.

Negative Electrode Variables

1 In the **Home** toolbar, click **Variables** and choose **Local Variables**.

2 In the **Settings** window for **Variables**, locate the **Geometric Entity Selection** section.

3 From the **Geometric entity level** list, choose **Domain**.

4 From the **Selection** list, choose **Negative Electrode**.

5 Locate the **Variables** section. Click **Load from File**.

6 Browse to the model's Application Libraries folder and double-click the file `v_flow_battery_negative_variables.txt`.

7 Right-click **Variables 1** and choose **Rename**.

8 In the **Rename Variables** dialog box, type `Negative Electrode Variables` in the **New label** text field.

9 Click **OK**.

Membrane Variables

1 In the **Home** toolbar, click **Variables** and choose **Local Variables**.

2 In the **Settings** window for **Variables**, locate the **Geometric Entity Selection** section.

3 From the **Geometric entity level** list, choose **Domain**.

4 From the **Selection** list, choose **Membrane**.

5 Locate the **Variables** section. Click **Load from File**.

6 Browse to the model's Application Libraries folder and double-click the file `v_flow_battery_membrane_variables.txt`.

7 Right-click **Variables 2** and choose **Rename**.

8 In the **Rename Variables** dialog box, type `Membrane Variables` in the **New label** text field.

9 Click **OK**.

Positive Electrode Variables

1 In the **Home** toolbar, click **Variables** and choose **Local Variables**.

2 In the **Settings** window for **Variables**, locate the **Geometric Entity Selection** section.

3 From the **Geometric entity level** list, choose **Domain**.

4 From the **Selection** list, choose **Positive Electrode**.

5 Locate the **Variables** section. Click **Load from File**.

6 Browse to the model's Application Libraries folder and double-click the file `v_flow_battery_positive_variables.txt`.

7 Right-click **Variables 3** and choose **Rename**.

8 In the **Rename Variables** dialog box, type `Positive Electrode Variables` in the **New label** text field.

9 Click **OK**.

TERTIARY CURRENT DISTRIBUTION, NERNST-PLANCK (NEGATIVE)

Now start defining the current distribution models. Start with the negative porous electrode.

1 In the **Settings** window for **Tertiary Current Distribution, Nernst-Planck**, type `Tertiary Current Distribution, Nernst-Planck (Negative)` in the **Label** text field.

2 Locate the **Domain Selection** section. From the **Selection** list, choose **Negative Electrode**.

3 Locate the **Out-of-Plane Thickness** section. In the d text field, type `wCell`.

Porous Electrode 1

1 Right-click **Component 1 (comp1)>Tertiary Current Distribution, Nernst-Planck (Negative)** and choose **Porous Electrode**.

2 In the **Settings** window for **Porous Electrode**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Negative Electrode**.

4 Locate the **Convection** section. Specify the $\mathbf{u}$ vector as

0	x
v	y

5 Locate the **Electrode Current Conduction** section. From the σ_s list, choose **User defined**. In the associated text field, type `sigma_e`.

6 Locate the **Diffusion** section. In the D_{cSO4neg} text field, type `DSO4`.

7 In the D_{cHSO4neg} text field, type `DHSO4`.

8 In the D_{cHneg} text field, type `DH`.

9 In the D_{cV2} text field, type `DV2`.

10 In the D_{cV3} text field, type `DV3`.

11 Locate the **Migration in Electric Field** section. In the z_{cSO4neg} text field, type `-2`.

12 In the z_{cHSO4neg} text field, type `-1`.

13 In the z_{cHneg} text field, type `1`.

14 In the z_{cV2} text field, type `2`.

15 In the z_{cV3} text field, type `3`.

16 Locate the **Porous Matrix Properties** section. In the ε_l text field, type `epsilon`.

17 Locate the **Effective Transport Parameter Correction** section. From the **Electrical conductivity** list, choose **No correction**.

Porous Electrode Reaction 1

1 In the **Model Builder** window, expand the **Porous Electrode 1** node, then click **Porous Electrode Reaction 1**.

2 In the **Settings** window for **Porous Electrode Reaction**, locate the **Stoichiometric Coefficients** section.

3 In the ν_{cV2} text field, type `1`.

4 In the ν_{cV3} text field, type `-1`.

5 Locate the **Equilibrium Potential** section. In the $E_{\mathrm{eq,ref}}(T)$ text field, type `E0_neg`.

6 Locate the **Electrode Kinetics** section. In the $i_{0,\mathrm{ref}}(T)$ text field, type `i0ref_neg`.

7 In the α_a text field, type `alpha_neg`.

8 Locate the **Active Specific Surface Area** section. In the a_v text field, type `a`.

Reactions 1

1 In the **Physics** toolbar, click **Domains** and choose **Reactions**.

2 In the **Settings** window for **Reactions**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Negative Electrode**.

4 Locate the **Reaction Rates** section. In the R_{cSO4neg} text field, type `-rd`.

5 In the R_{cHSO4neg} text field, type `rd`.

6 In the R_{cHneg} text field, type `-rd`.

Electric Ground 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Electric Ground**.

2 Select Boundary 1 only.

Inflow 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Inflow**.

2 Select Boundary 2 only.

3 In the **Settings** window for **Inflow**, locate the **Concentration** section.

4 In the $c_{0,\text{cHSO4neg}}$ text field, type `cHSO4_0_neg`.

5 In the $c_{0,\text{cHneg}}$ text field, type `cH_0_neg`.

6 In the $c_{0,\text{cV2}}$ text field, type `cV2_0`.

7 In the $c_{0,\text{cV3}}$ text field, type `cV3_0`.

8 Locate the **Boundary Condition Type** section. From the list, choose **Flux (Danckwerts)**.

Outflow 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Outflow**.

2 Select Boundary 3 only.

Ion Exchange Membrane Boundary 1

The electrolyte potential and species concentration in the membrane and in the porous electrodes are coupled by the use of Donnan potential expression on the boundary between the membrane and the porous electrode.

1 In the **Physics** toolbar, click **Boundaries** and choose **Ion Exchange Membrane Boundary**.

2 Select Boundary 4 only.

3 In the **Settings** window for **Ion Exchange Membrane Boundary**, locate the **Ion Exchange Membrane Boundary** section.

4 From the ϕ_{m} list, choose **Electrolyte potential (tcd2)**.

5 From the **Ion exchange membrane transport model** list, choose **Multiple ions**.

6 In the $c_{\text{mem,cSO4neg}}$ text field, type `cSO4_mem`.

7 Select the **Species cHSO4_neg** check box.

8 In the $c_{\mathrm{mem,cHSO4neg}}$ text field, type `cHSO4_mem`.

9 Select the **Species cH_neg** check box.

10 In the $c_{\mathrm{mem,cHneg}}$ text field, type `cH_mem`.

11 Select the **Species cV2** check box.

12 In the $c_{\mathrm{mem,cV2}}$ text field, type `cV2_mem`.

13 Select the **Species cV3** check box.

14 In the $c_{\mathrm{mem,cV3}}$ text field, type `cV3_mem`.

Electrode Current Density 1

Add the electrode current density for the current balance.

1 In the **Physics** toolbar, click **Boundaries** and choose **Electrode Current Density**.

2 Select Boundary 4 only.

3 In the **Settings** window for **Electrode Current Density**, locate the **Electrode Current Density** section.

4 In the $i_{n,\mathrm{s}}$ text field, type `-tcd2.itot`.

Initial Values 1

1 In the **Model Builder** window, click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the $cHSO4_{\mathrm{neg}}$ text field, type `cHSO4_0_neg`.

4 In the cH_{neg} text field, type `cH_0_neg`.

5 In the $cV2$ text field, type `cV2_0`.

6 In the $cV3$ text field, type `cV3_0`.

TERTIARY CURRENT DISTRIBUTION, NERNST-PLANCK (ION EXCHANGE MEMBRANE)

Now set up the Tertiary Current Distribution model for the membrane.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Tertiary Current Distribution, Nernst-Planck 2 (tcd2)**.

2 In the **Settings** window for **Tertiary Current Distribution, Nernst-Planck**, type `Tertiary Current Distribution, Nernst-Planck (Ion Exchange Membrane)` in the **Label** text field.

3 Locate the **Domain Selection** section. From the **Selection** list, choose **Membrane**.

4 Locate the **Out-of-Plane Thickness** section. In the d text field, type `wCell`.

Ion Exchange Membrane 1

1 In the **Physics** toolbar, click **Domains** and choose **Ion Exchange Membrane**.

2 In the **Settings** window for **Ion Exchange Membrane**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Membrane**.

4 Locate the **Ion Exchange Membrane Properties** section. In the ρ_{fix} text field, type `c_fix*F_const`.

5 Locate the **Diffusion** section. In the $D_{cSO4mem}$ text field, type `DSO4`.

6 In the $D_{cHSO4mem}$ text field, type `DHSO4`.

7 In the D_{cHmem} text field, type `DH`.

8 In the D_{cV2mem} text field, type `DV2`.

9 In the D_{cV3mem} text field, type `DV3`.

10 In the D_{cV4mem} text field, type `DV4`.

11 In the D_{cV5mem} text field, type `DV5`.

12 Locate the **Migration in Electric Field** section. In the $z_{cSO4mem}$ text field, type `-2`.

13 In the $z_{cHSO4mem}$ text field, type `-1`.

14 In the z_{cHmem} text field, type `1`.

15 In the z_{cV2mem} text field, type `2`.

16 In the z_{cV3mem} text field, type `3`.

17 In the z_{cV4mem} text field, type `2`.

18 In the z_{cV5mem} text field, type `1`.

19 Locate the **Porous Matrix Properties** section. In the ε_l text field, type `0.1`.

Reactions 1

1 In the **Physics** toolbar, click **Domains** and choose **Reactions**.

2 In the **Settings** window for **Reactions**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Membrane**.

4 Locate the **Reaction Rates** section. In the $R_{cSO4mem}$ text field, type `-rd`.

5 In the $R_{cHSO4mem}$ text field, type `rd`.

6 In the R_{cHmem} text field, type `-rd`.

Electrode Surface 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Electrode Surface**.

2 Select Boundary 4 only.

Electrode Reaction 1

1 In the **Model Builder** window, expand the **Electrode Surface 1** node, then click **Electrode Reaction 1**.

2 In the **Settings** window for **Electrode Reaction**, locate the **Stoichiometric Coefficients** section.

3 In the ν_{cHmem} text field, type `-2`.

4 In the ν_{cV3mem} text field, type `1`.

5 In the ν_{cV4mem} text field, type `-1`.

6 Locate the **Equilibrium Potential** section. From the E_{eq} list, choose **User defined**. Locate the **Electrode Kinetics** section. From the **Kinetics expression type** list, choose **Fast irreversible electrode reaction**.

7 From the c_{lim} list, choose **cV4_mem**.

Electrode Surface 1

In the **Model Builder** window, click **Electrode Surface 1**.

Electrode Reaction 2

1 In the **Physics** toolbar, click **Attributes** and choose **Electrode Reaction**.

2 In the **Settings** window for **Electrode Reaction**, locate the **Stoichiometric Coefficients** section.

3 In the ν_{cHmem} text field, type `-2`.

4 In the ν_{cV4mem} text field, type `1`.

5 In the ν_{cV5mem} text field, type `-1`.

6 Locate the **Equilibrium Potential** section. From the E_{eq} list, choose **User defined**. Locate the **Electrode Kinetics** section. From the **Kinetics expression type** list, choose **Fast irreversible electrode reaction**.

7 From the c_{lim} list, choose **cV5_mem**.

Electrode Surface 2

1 In the **Physics** toolbar, click **Boundaries** and choose **Electrode Surface**.

2 Select Boundary 7 only.

Electrode Reaction 1

1 In the **Model Builder** window, expand the **Electrode Surface 2** node, then click **Electrode Reaction 1**.

2 In the **Settings** window for **Electrode Reaction**, locate the **Equilibrium Potential** section.

3 From the E_{eq} list, choose **User defined**. Locate the **Electrode Kinetics** section. From the **Kinetics expression type** list, choose **Fast irreversible electrode reaction**.

4 From the c_{lim} list, choose **cV2_mem**.

5 Locate the **Stoichiometric Coefficients** section. In the ν_{cHmem} text field, type `-2`.

6 In the ν_{cV3mem} text field, type `1`.

7 In the ν_{cV4mem} text field, type `-1`.

Electrode Surface 2

In the **Model Builder** window, click **Electrode Surface 2**.

Electrode Reaction 2

1 In the **Physics** toolbar, click **Attributes** and choose **Electrode Reaction**.

2 In the **Settings** window for **Electrode Reaction**, locate the **Equilibrium Potential** section.

3 From the E_{eq} list, choose **User defined**. Locate the **Electrode Kinetics** section. From the **Kinetics expression type** list, choose **Fast irreversible electrode reaction**.

4 From the c_{lim} list, choose **cV3_mem**.

5 Locate the **Stoichiometric Coefficients** section. In the ν_{cV2mem} text field, type `1`.

6 In the ν_{cV3mem} text field, type `-1`.

Initial Values 1

1 In the **Model Builder** window, click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the $cHSO4_{mem}$ text field, type `(cHSO4_0_pos+cHSO4_0_neg)/2`.

4 In the cH_{mem} text field, type `(cH_0_pos+cH_0_neg)/2`.

5 In the $cV2_{mem}$ text field, type `cV2_0/2`.

6 In the $cV3_{mem}$ text field, type `cV3_0/2`.

7 In the $cV4_{mem}$ text field, type `cV4_0/2`.

8 In the $cV5_{mem}$ text field, type `cV5_0/2`.

9 In the $phil_{mem}$ text field, type `-E0_neg`.

TERTIARY CURRENT DISTRIBUTION, NERNST-PLANCK (POSITIVE)

Finish the physics settings by setting up the tertary current distribution model for the positive porous electrode.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Tertiary Current Distribution, Nernst-Planck 3 (tcd3)**.

2 In the **Settings** window for **Tertiary Current Distribution, Nernst-Planck**, type `Tertiary Current Distribution, Nernst-Planck (Positive)` in the **Label** text field.

3 Locate the **Domain Selection** section. From the **Selection** list, choose **Positive Electrode**.

4 Locate the **Out-of-Plane Thickness** section. In the d text field, type `wCell`.

Porous Electrode 1

1 In the **Physics** toolbar, click **Domains** and choose **Porous Electrode**.

2 In the **Settings** window for **Porous Electrode**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Positive Electrode**.

4 Locate the **Convection** section. Specify the $\mathbf{u}$ vector as

0	x
v	y

5 Locate the **Electrode Current Conduction** section. From the σ_s list, choose **User defined**. In the associated text field, type `sigma_e`.

6 Locate the **Diffusion** section. In the D_{cSO4pos} text field, type `DSO4`.

7 In the D_{cHSO4pos} text field, type `DHSO4`.

8 In the D_{cHpos} text field, type `DH`.

9 In the D_{cV4} text field, type `DV4`.

10 In the D_{cV5} text field, type `DV5`.

11 Locate the **Migration in Electric Field** section. In the z_{cSO4pos} text field, type `-2`.

12 In the z_{cHSO4pos} text field, type `-1`.

13 In the z_{cHpos} text field, type `1`.

14 In the z_{cV4} text field, type `2`.

15 In the z_{cV5} text field, type `1`.

16 Locate the **Porous Matrix Properties** section. In the ε_l text field, type `epsilon`.

17 Locate the **Effective Transport Parameter Correction** section. From the **Electrical conductivity** list, choose **No correction**.

Porous Electrode Reaction 1

1 In the **Model Builder** window, expand the **Porous Electrode 1** node, then click **Porous Electrode Reaction 1**.

2 In the **Settings** window for **Porous Electrode Reaction**, locate the **Stoichiometric Coefficients** section.

3 In the ν_{cHpos} text field, type `-2`.

4 In the ν_{cV4} text field, type `1`.

5 In the ν_{cV5} text field, type `-1`.

6 Locate the **Equilibrium Potential** section. In the $E_{eq,ref}(T)$ text field, type `E0_pos`.

7 Locate the **Electrode Kinetics** section. In the $i_{0,ref}(T)$ text field, type `i0ref_pos`.

8 In the α_a text field, type `alpha_pos`.

9 Locate the **Active Specific Surface Area** section. In the a_v text field, type `a`.

Reactions 1

1 In the **Physics** toolbar, click **Domains** and choose **Reactions**.

2 In the **Settings** window for **Reactions**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Positive Electrode**.

4 Locate the **Reaction Rates** section. In the $R_{cSO4pos}$ text field, type `-rd`.

5 In the $R_{cHSO4pos}$ text field, type `rd`.

6 In the R_{cHpos} text field, type `-rd`.

Electrode Current 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Electrode Current**.

2 In the **Settings** window for **Electrode Current**, locate the **Electrode Current** section.

3 From the list, choose **Average current density**.

4 Select Boundary 10 only.

5 In the $i_{s,average}$ text field, type `i_avg`.

Inflow 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Inflow**.

2 Select Boundary 8 only.

3 In the **Settings** window for **Inflow**, locate the **Concentration** section.

4 In the $c_{0,cHSO4pos}$ text field, type `cHSO4_0_pos`.

5 In the $c_{0,cHpos}$ text field, type `cH_0_pos`.

6 In the $c_{0,cV4}$ text field, type `cV4_0`.

7 In the $c_{0,cV5}$ text field, type `cV5_0`.

8 Locate the **Boundary Condition Type** section. From the list, choose **Flux (Danckwerts)**.

Outflow 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Outflow**.

2 Select Boundary 9 only.

Ion Exchange Membrane Boundary 1

The boundary condition for the membrane boundary is set as before. The electrolyte potential and species concentration in the membrane and in the porous electrode are coupled by the use of Donnan potential expressions on the boundary between the membrane and the porous electrode.

1 In the **Physics** toolbar, click **Boundaries** and choose **Ion Exchange Membrane Boundary**.

2 Select Boundary 7 only.

3 In the **Settings** window for **Ion Exchange Membrane Boundary**, locate the **Ion Exchange Membrane Boundary** section.

4 From the ϕ_m list, choose **Electrolyte potential (tcd2)**.

5 From the **Ion exchange membrane transport model** list, choose **Multiple ions**.

6 In the $c_{\mathrm{mem,cSO4pos}}$ text field, type `cSO4_mem`.

7 Select the **Species cHSO4_pos** check box.

8 In the $c_{\mathrm{mem,cHSO4pos}}$ text field, type `cHSO4_mem`.

9 Select the **Species cH_pos** check box.

10 In the $c_{\mathrm{mem,cHpos}}$ text field, type `cH_mem`.

11 Select the **Species cV4** check box.

12 In the $c_{\mathrm{mem,cV4}}$ text field, type `cV4_mem`.

13 Select the **Species cV5** check box.

14 In the $c_{\mathrm{mem,cV5}}$ text field, type `cV5_mem`.

Electrode Current Density 1

Add the electrode current density for the current balance.

1 In the **Physics** toolbar, click **Boundaries** and choose **Electrode Current Density**.

2 Select Boundary 7 only.

3 In the **Settings** window for **Electrode Current Density**, locate the **Electrode Current Density** section.

4 In the $i_{n,\mathrm{s}}$ text field, type `-tcd2.itot`.

Initial Values 1

1 In the **Model Builder** window, click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the $cHSO4_{pos}$ text field, type `cHSO4_0_pos`.

4 In the cH_{pos} text field, type `cH_0_pos`.

5 In the $cV4$ text field, type `cV4_0`.

6 In the $cV5$ text field, type `cV5_0`.

GLOBAL DEFINITIONS

Default Model Inputs

Set up the temperature value used in the entire model.

1 In the **Model Builder** window, under **Global Definitions** click **Default Model Inputs**.

2 In the **Settings** window for **Default Model Inputs**, locate the **Browse Model Inputs** section.

3 In the tree, select **General>Temperature (K) - minput.T**.

4 Find the **Expression for remaining selection** subsection. In the **Temperature** text field, type `T`.

MESH 1

Create a mapped mesh with higher resolution in the porous electrodes toward the membrane and with a boundary layer mesh at the fluid inlet.

Mapped 1

In the **Mesh** toolbar, click  **Mapped**.

Distribution 1

1 Right-click **Mapped 1** and choose **Distribution**.

2 Select Boundaries 5 and 6 only.

3 In the **Settings** window for **Distribution**, locate the **Distribution** section.

4 From the **Distribution type** list, choose **Predefined**.

5 In the **Number of elements** text field, type `20`.

6 In the **Element ratio** text field, type `2`.

7 Select the **Symmetric distribution** check box.

Distribution 2

1 In the **Model Builder** window, right-click **Mapped 1** and choose **Distribution**.

2 Select Boundaries 2 and 3 only.

3 In the **Settings** window for **Distribution**, locate the **Distribution** section.

4 From the **Distribution type** list, choose **Predefined**.

5 In the **Number of elements** text field, type 40.

6 In the **Element ratio** text field, type 20.

Distribution 3

1 Right-click **Distribution 2** and choose **Duplicate**.

2 In the **Settings** window for **Distribution**, locate the **Boundary Selection** section.

3 Click  **Clear Selection**.

4 Select Boundaries 8 and 9 only.

5 Locate the **Distribution** section. Select the **Reverse direction** check box.

Distribution 4

1 In the **Model Builder** window, right-click **Mapped 1** and choose **Distribution**.

2 Select Boundaries 1, 4, 7, and 10 only.

3 In the **Settings** window for **Distribution**, locate the **Distribution** section.

4 From the **Distribution type** list, choose **Predefined**.

5 In the **Number of elements** text field, type 40 .

6 In the **Element ratio** text field, type 20.

Boundary Layers 1

In the **Mesh** toolbar, click  **Boundary Layers**.

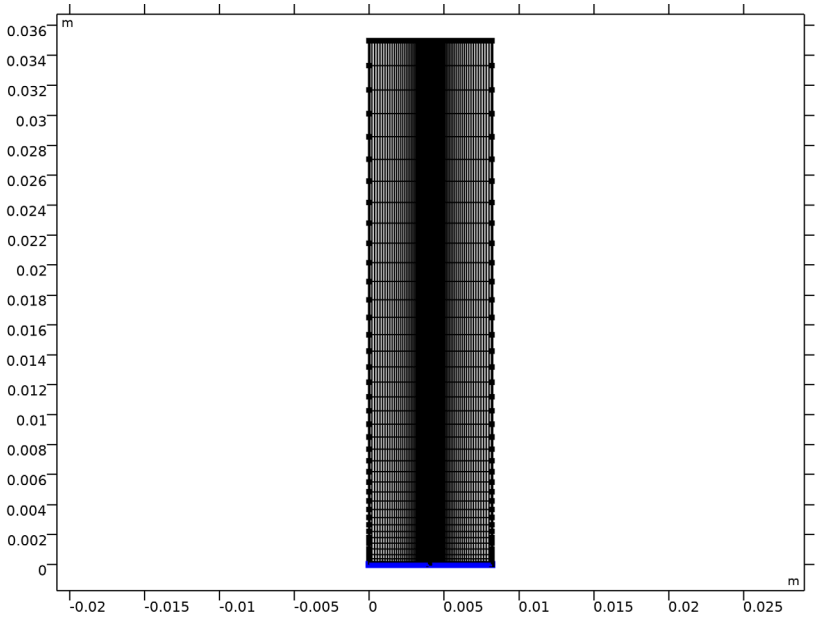
Boundary Layer Properties

1 In the **Model Builder** window, click **Boundary Layer Properties**.

2 Select Boundaries 2 and 8 only.

3 In the **Settings** window for **Boundary Layer Properties**, click **Build All**.

Your mesh should now look like this:



STUDY 1

Run the model for two values of membrane charge concentration using an auxiliary sweep. The problem is then ready for solving.

1 In the **Model Builder** window, click **Study 1**.

2 In the **Settings** window for **Study**, locate the **Study Settings** section.

3 Clear the **Generate default plots** check box.

Step 2: Stationary

1 In the **Model Builder** window, under **Study 1** click **Step 2: Stationary**.

2 In the **Settings** window for **Stationary**, click to expand the **Study Extensions** section.

3 Select the **Auxiliary sweep** check box.

4 Click **Add**.

5 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
c_fix ((0[M] used during Current Distribution Initialization, -cHm used after Auxiliary sweep))	`0 -cHm`	`mol/m^3`

6 In the **Home** toolbar, click **Compute**.

RESULTS

Reproduce the plots from the Results and Discussion section in the following way:

2D Plot Group 1

In the **Home** toolbar, click **Add Plot Group** and choose **2D Plot Group**.

Surface 1

1 Right-click **2D Plot Group 1** and choose **Surface**.

2 In the **Settings** window for **Surface**, locate the **Expression** section.

3 In the **Expression** text field, type `cV3`.

Surface 2

1 Right-click **Surface 1** and choose **Duplicate**.

2 In the **Settings** window for **Surface**, locate the **Expression** section.

3 In the **Expression** text field, type `cV4`.

4 Click to expand the **Inherit Style** section. From the **Plot** list, choose **Surface 1**.

5 In the **2D Plot Group 1** toolbar, click **Plot**.

V3/V4 Species Concentration

1 In the **Model Builder** window, right-click **2D Plot Group 1** and choose **Rename**.

2 In the **Rename 2D Plot Group** dialog box, type `V3/V4 Species Concentration` in the **New label** text field.

3 Click **OK**.

V3/V4 Species Concentration 1

1 Right-click **V3/V4 Species Concentration** and choose **Duplicate**.

Now modify the plot group that was created by the duplicate operation.

Surface 1

1 In the **Model Builder** window, expand the **V3/V4 Species Concentration 1** node, then click **Surface 1**.

2 In the **Settings** window for **Surface**, locate the **Expression** section.

3 In the **Expression** text field, type `cV2`.

Surface 2

1 In the **Model Builder** window, click **Surface 2**.

2 In the **Settings** window for **Surface**, locate the **Expression** section.

3 In the **Expression** text field, type `cV5`.

V2/V5 Species Concentration

1 In the **Model Builder** window, click **V3/V4 Species Concentration 1**.

2 In the **V3/V4 Species Concentration 1** toolbar, click **Plot**.

3 Right-click **V3/V4 Species Concentration 1** and choose **Rename**.

4 In the **Rename 2D Plot Group** dialog box, type `V2/V5 Species Concentration` in the **New label** text field.

5 Click **OK**.

2D Plot Group 3

In the **Home** toolbar, click **Add Plot Group** and choose **2D Plot Group**.

Surface 1

1 In the **Model Builder** window, right-click **2D Plot Group 3** and choose **Surface**.

2 In the **2D Plot Group 3** toolbar, click **Plot**.

Electrolyte potential 2D

1 In the **Model Builder** window, right-click **2D Plot Group 3** and choose **Rename**.

2 In the **Rename 2D Plot Group** dialog box, type `Electrolyte potential 2D` in the **New label** text field.

3 Click **OK**.

Cut Line 2D 1

1 In the **Results** toolbar, click **Cut Line 2D**.

2 In the **Settings** window for **Cut Line 2D**, locate the **Line Data** section.

3 In row **Point 1**, set **Y** to `H_cell/2`.

4 In row **Point 2**, set **X** to `L_e*2+L_m` and **y** to `H_cell/2`.

1D Plot Group 4

1 In the **Results** toolbar, click **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

3 From the **Dataset** list, choose **Cut Line 2D 1**.

4 From the **Parameter selection (c_fix)** list, choose **Last**.

Line Graph 1

1 Right-click **1D Plot Group 4** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Definitions> Variables>phil - Electrolyte potential (for postprocessing) - V**.

3 In the **1D Plot Group 4** toolbar, click **Plot**.

Electrolyte potential

1 In the **Model Builder** window, right-click **1D Plot Group 4** and choose **Rename**.

2 In the **Rename 1D Plot Group** dialog box, type `Electrolyte potential` in the **New label** text field.

3 Click **OK**.

1D Plot Group 5

In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

Line Graph 1

1 Right-click **1D Plot Group 5** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, locate the **Data** section.

3 From the **Dataset** list, choose **Cut Line 2D 1**.

4 From the **Parameter selection (c_fix)** list, choose **Last**.

5 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Tertiary Current Distribution, Nernst-Planck (Negative)>Electrode kinetics>tcd.ivtot - Electrode reaction source - A/m³**.

6 In the **1D Plot Group 5** toolbar, click **Plot**.

Line Graph 2

1 Right-click **Line Graph 1** and choose **Duplicate**.

2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `tcd3.ivtot`.

4 In the **1D Plot Group 5** toolbar, click **Plot**.

Electrode reaction current densities

1 In the **Model Builder** window, right-click **1D Plot Group 5** and choose **Rename**.

2 In the **Rename 1D Plot Group** dialog box, type `Electrode reaction current densities` in the **New label** text field.

3 Click **OK**.

2D Plot Group 6

In the **Home** toolbar, click **Add Plot Group** and choose **2D Plot Group**.

Surface 1

1 Right-click **2D Plot Group 6** and choose **Surface**.

2 In the **Settings** window for **Surface**, locate the **Expression** section.

3 In the **Expression** text field, type `log(abs(rd))`.

4 In the **2D Plot Group 6** toolbar, click **Plot**.

Dissociation rate

1 In the **Model Builder** window, right-click **2D Plot Group 6** and choose **Rename**.

2 In the **Rename 2D Plot Group** dialog box, type `Dissociation rate` in the **New label** text field.

3 Click **OK**.

1D Plot Group 7

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

3 From the **Dataset** list, choose **Cut Line 2D 1**.

4 From the **Parameter selection (c_fix)** list, choose **Last**.

Line Graph 1

1 Right-click **1D Plot Group 7** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `aH`.

4 Click to expand the **Legends** section. Select the **Show legends** check box.

5 From the **Legends** list, choose **Manual**.

6 In the table, enter the following settings:

Legends
aH

Line Graph 2

1 Right-click **Line Graph 1** and choose **Duplicate**.

2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `aHSO4`.

4 Locate the **Legends** section. In the table, enter the following settings:

Legends
aHSO4

Line Graph 3

1 Right-click **Line Graph 2** and choose **Duplicate**.

2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `aSO4`.

4 Locate the **Legends** section. In the table, enter the following settings:

Legends
aSO4

Sulphuric acid species

1 In the **Model Builder** window, click **1D Plot Group 7**.

2 In the **1D Plot Group 7** toolbar, click **Plot**.

3 Right-click **1D Plot Group 7** and choose **Rename**.

4 In the **Rename 1D Plot Group** dialog box, type `Sulphuric acid species` in the **New label** text field.

5 Click **OK**.

1D Plot Group 8

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

3 From the **Dataset** list, choose **Cut Line 2D 1**.

4 From the **Parameter selection (c_fix)** list, choose **Last**.

Line Graph 1

1 Right-click **1D Plot Group 8** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `aV2`.

4 Locate the **Legends** section. Select the **Show legends** check box.

5 From the **Legends** list, choose **Manual**.

6 In the table, enter the following settings:

Legends
aV2

Line Graph 2

1 Right-click **Line Graph 1** and choose **Duplicate**.

2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `aV3`.

4 Locate the **Legends** section. In the table, enter the following settings:

Legends
aV3

Line Graph 3

1 Right-click **Line Graph 2** and choose **Duplicate**.

2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `aV4`.

4 Locate the **Legends** section. In the table, enter the following settings:

Legends
aV4

Line Graph 4

1 Right-click **Line Graph 3** and choose **Duplicate**.

2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `aV5`.

4 Locate the **Legends** section. In the table, enter the following settings:

Legends
aV5

V2/V3/V4/V5

1 In the **Model Builder** window, click **1D Plot Group 8**.

2 In the **1D Plot Group 8** toolbar, click  **Plot**.

3 Right-click **1D Plot Group 8** and choose **Rename**.

4 In the **Rename 1D Plot Group** dialog box, type `V2/V3/V4/V5` in the **New label** text field.

5 Click **OK**.

1D Plot Group 9

1 In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, locate the **Data** section.

3 From the **Dataset** list, choose **Cut Line 2D 1**.

4 From the **Parameter selection (c_fix)** list, choose **Last**.

Line Graph 1

1 Right-click **1D Plot Group 9** and choose **Line Graph**.

2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `Hx*F_const`.

4 Locate the **Legends** section. Select the **Show legends** check box.

5 From the **Legends** list, choose **Manual**.

6 In the table, enter the following settings:

Legends
`Flux, H`

Line Graph 2

1 Right-click **Line Graph 1** and choose **Duplicate**.

2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `-HSO4x*F_const`.

4 Locate the **Legends** section. In the table, enter the following settings:

Legends
`Flux, HSO4`

Line Graph 3

1 Right-click **Line Graph 2** and choose **Duplicate**.

2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.

3 In the **Expression** text field, type `-2*F_const*SO4x`.

4 Locate the **Legends** section. In the table, enter the following settings:

Legends
`Flux, SO4`

Fluxes

1 In the **Model Builder** window, click **1D Plot Group 9**.

2 In the **1D Plot Group 9** toolbar, click  **Plot**.

3 Right-click **1D Plot Group 9** and choose **Rename**.

4 In the **Rename 1D Plot Group** dialog box, type `Fluxes` in the **New label** text field.

5 Click **OK**.