



Model created in COMSOL Multiphysics 6.4

Vanadium Redox Flow Battery

Introduction

Redox flow batteries store energy in the liquid electrolytes, pumped through the cell and stored in external tanks, rather than in the porous electrodes like 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](#).

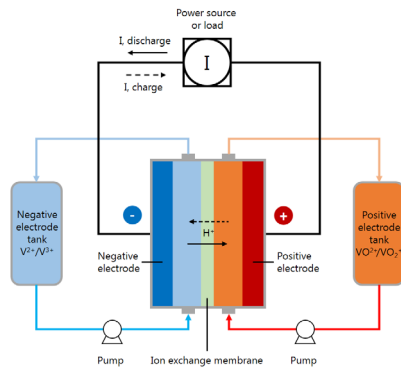


Figure 1: Schematic of a vanadium redox flow battery system.

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.

Model Definition

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.

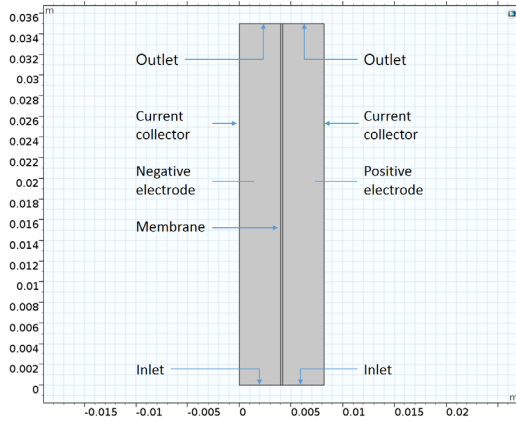


Figure 2: Model geometry. Three domains: negative electrode, membrane, positive electrode.

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 the bottom at a constant velocity in the y direction, corresponding to a flow rate of 30 ml/min at a 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 .

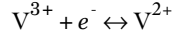
The models solves for a stationary case with a given set of inlet concentrations.

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



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

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

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:

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

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

where A is the specific surface area (SI unit: m²/m³) of the porous electrode, α_{neg} the transfer coefficient (dimensionless), and k_{neg} the rate constant.

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

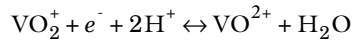
$$\eta = \phi_s - \phi_l - E_{\text{c}, \text{q}}$$

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⁺
- HSO₄⁻
- SO₄²⁻
- VO²⁺
- VO₂⁺

The positive electrode reaction is



with the equilibrium potential calculated according to

$$E_{\text{c}, \text{pos}} = E_{0, \text{pos}} + \frac{RT}{F} \ln \left(\frac{a_{\text{VO}_2^+} (a_{\text{H}^+})^2}{a_{\text{VO}^{2+}}} \right)$$

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

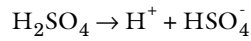
$$i_{0, \text{pos}} = F k_{\text{pos}} (a_{\text{VO}^{2+}})^{1 - \alpha_{\text{pos}}} (a_{\text{VO}_2^+})^{\alpha_{\text{pos}}}$$

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

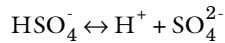
- H⁺
- HSO₄⁻
- SO₄²⁻
- V³⁺
- V²⁺
- VO²⁺
- VO₂⁺

SULFURIC ACID DISSOCIATION

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



whereas the second step



is described using a dissociation source term, r_d :

$$r_d = k_d \left(\frac{a_{\text{H}^+} - a_{\text{HSO}_4^-}}{a_{\text{H}^+} + a_{\text{HSO}_4^-}} - \beta \right)$$

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. The following equation describes the molar flux of species i , \mathbf{N}_i , due to diffusion, migration, and convection:

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

The first term is the diffusion flux and 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 $u_{\text{mob},i}$ (SI unit: $\text{s}\cdot\text{mol}/\text{kg}$) 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):

$$\mathbf{i}_l = F \sum_{i=1}^n z_i (-D_i \nabla c_i - z_i u_{\text{mob},i} F c_i \nabla \phi_l) \quad (1)$$

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:

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

The fixed space charge is prescribed in terms of the membrane charge concentration.

The checkbox Add Donnan shift to initial values, when enabled, shifts the initial values on the selection of the Ion-Exchange Membrane node in order to fulfill electroneutrality and compliance with the Donnan equilibria.

MEMBRANE — POROUS ELECTRODE BOUNDARY CONDITIONS

Donnan Conditions

The boundary conditions at the boundaries between the membrane and the porous electrode domains are set up as follows.

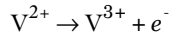
For species existing on both sides of the membrane-electrode, we have the following relation between the potentials and the concentrations:

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

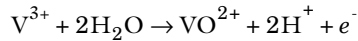
where $c_{i,m}$ is the species concentration in the membrane, and $c_{i,e}$ the species concentration in the free electrolyte and z_i the corresponding charge. The potential shift caused by [Equation 3](#) is called Donnan potential ([Ref. 3](#)). The Ion-Exchange Membrane Boundary feature in the Tertiary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

Self-discharge Reactions

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



and



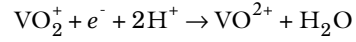
so that

$$c_{V^{3+}} = c_{V^{2+}} = 0 \quad (4)$$

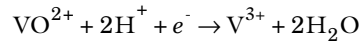
Correspondingly, the VO^{2+} and VO_2^+ concentrations are assumed to be zero at the membrane–negative electrode boundaries:

$$c_{\text{VO}^{2+}} = c_{\text{VO}_2^+} = 0 \quad (5)$$

as a result of the reduction reactions



and



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 a membrane negative charge concentration of 1990 mol/m^3 . The ion concentrations of these species are higher toward the current collectors and toward the outlets.

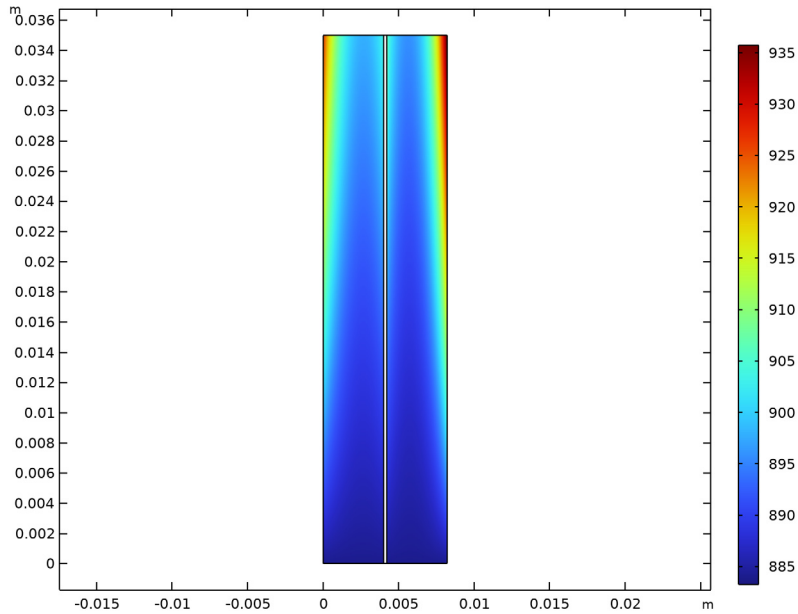


Figure 3: Concentration (mol/m^3) of the V^{3+} (left compartment) and the VO^{2+} (right compartment) ions for a membrane negative charge concentration of 1990 mol/m^3 .

Figure 4 shows the concentration of the V^{2+} and the VO_2^+ ions for the membrane negative charge concentration of 1990 mol/m^3 . Depletion occurs along the flow direction and also toward both the current collector and membrane sides of the electrodes.

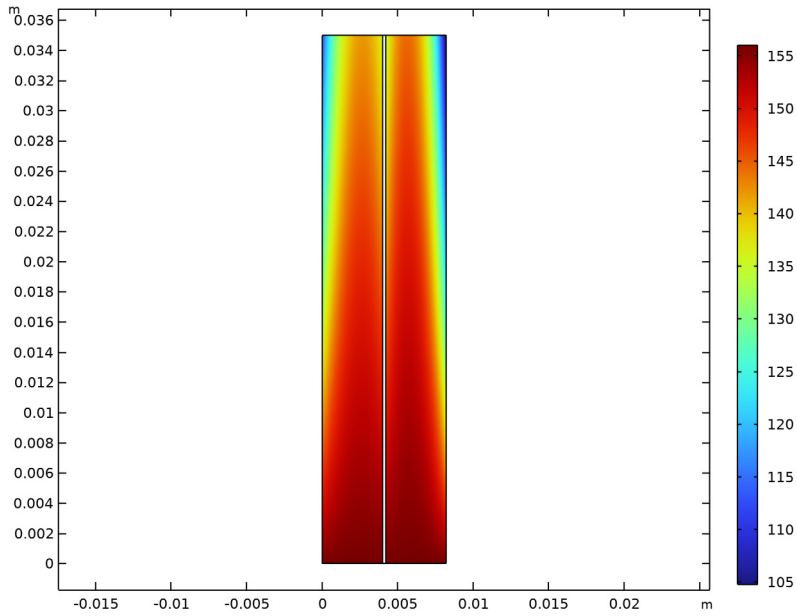


Figure 4: Concentration (mol/m^3) of the V^{2+} (left compartment) and the VO_2^+ (right compartment) ions for a membrane negative charge concentration of $1990 \text{ mol}/\text{m}^3$.

Figure 5 shows the electrolyte potential for the membrane negative charge concentration of $1990 \text{ mol}/\text{m}^3$, which decreases toward the positive current collector.

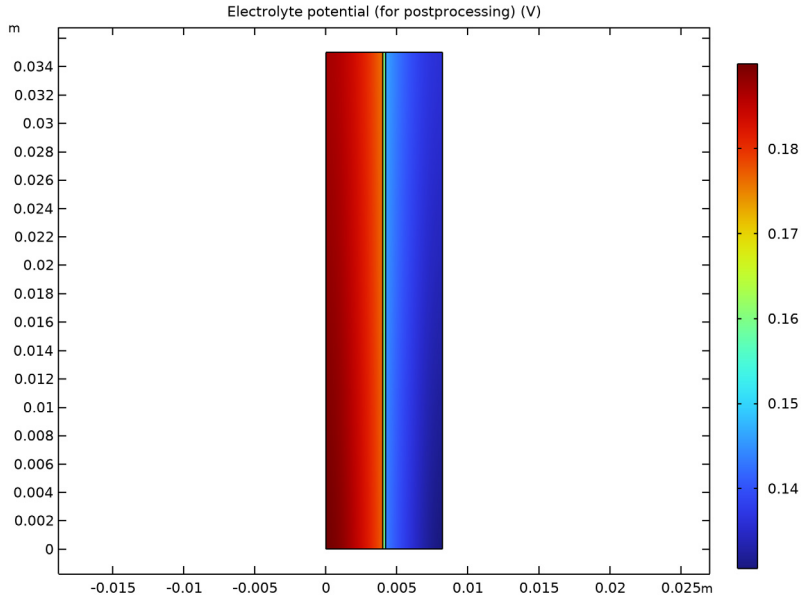


Figure 5: Electrolyte potential for a membrane negative charge concentration of 1990 mol/m^3 .

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.

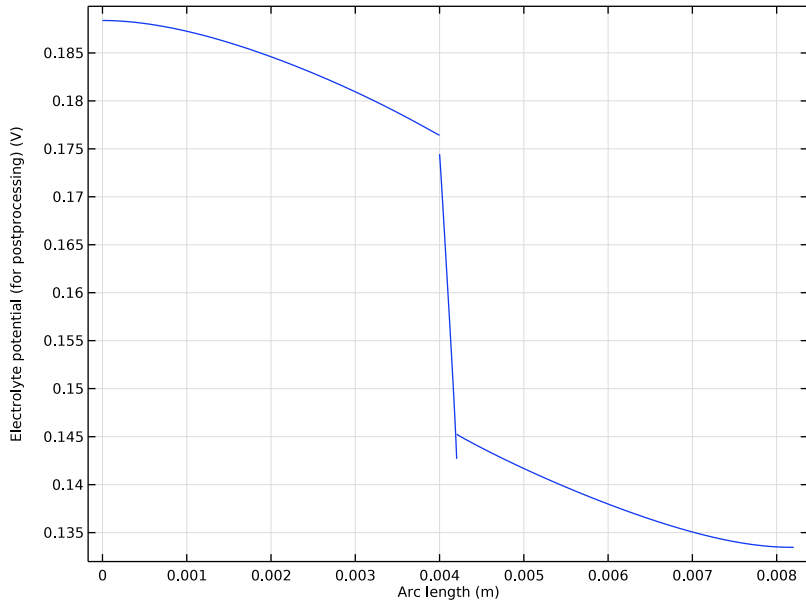


Figure 6: Electrolyte potential along a horizontal line placed at $y = h_{\text{cell}}/2$.

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.

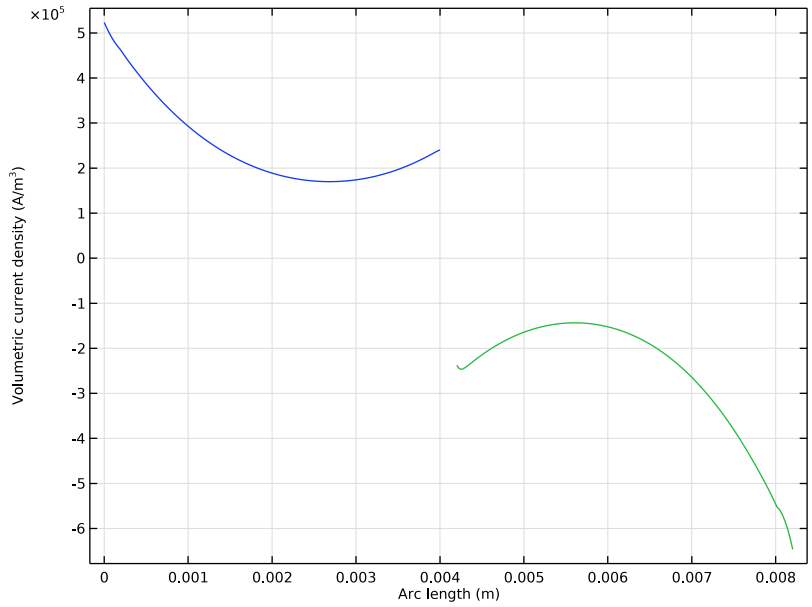


Figure 7: Electrode reaction source in the porous electrodes along a horizontal line placed at $y = h_{\text{cell}}/2$.

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

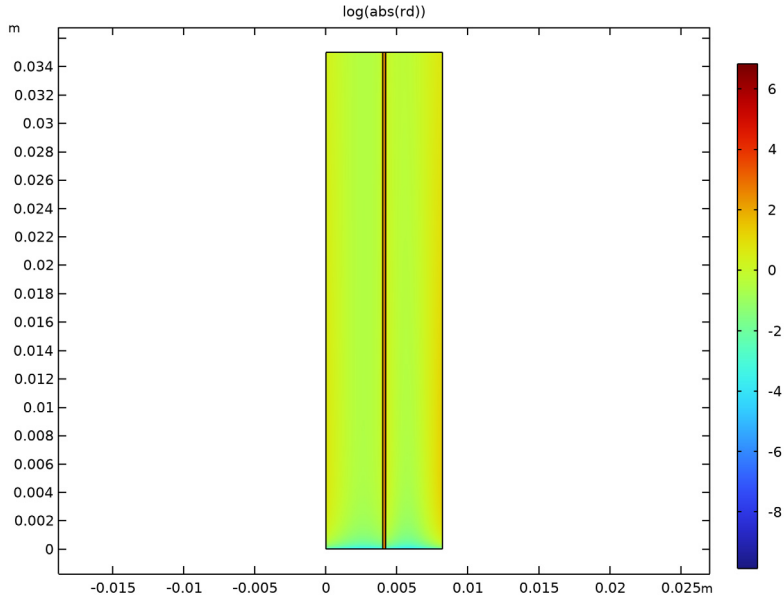


Figure 8: Sulfuric acid dissociation rate ($\text{mol}/(\text{m}^3\text{s})$) for a membrane negative charge concentration of $1990 \text{ mol}/\text{m}^3$.

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.

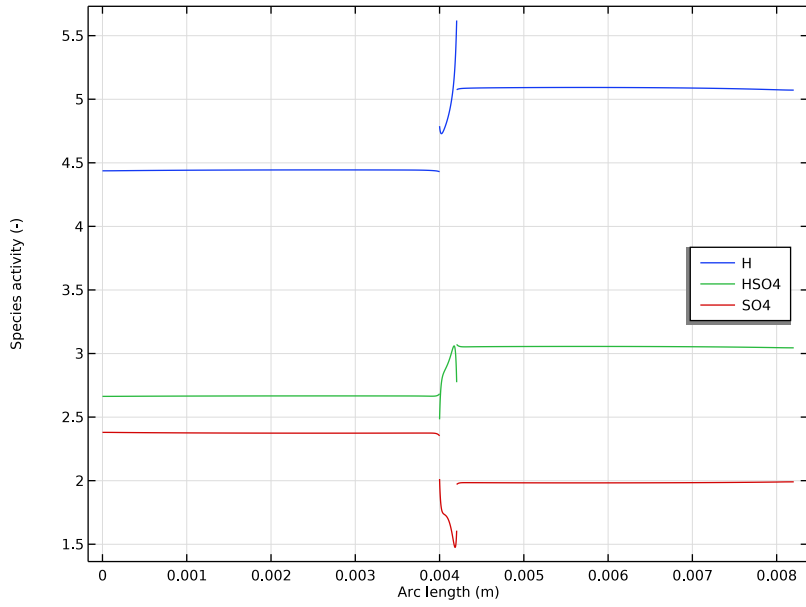


Figure 9: Sulfuric acid species along a horizontal line placed at $y = h_{\text{cell}}/2$.

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.

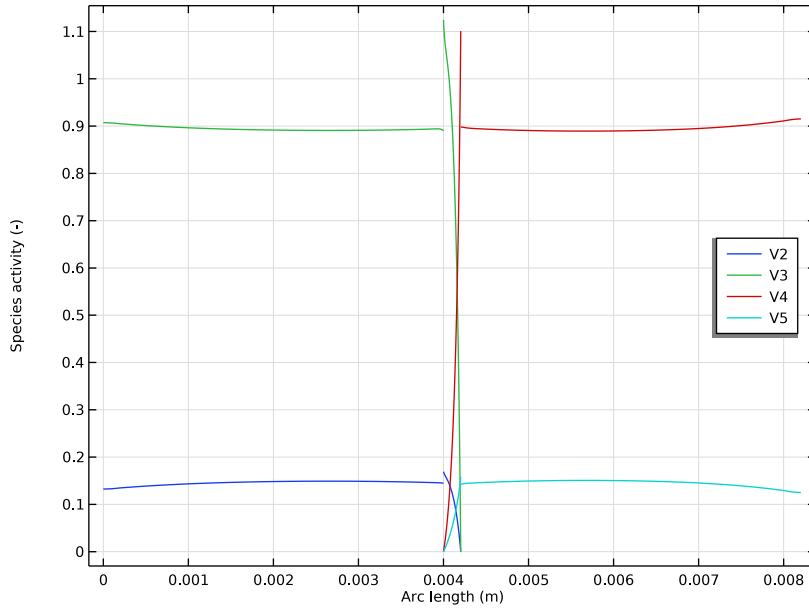


Figure 10: Vanadium species along a horizontal line placed at $y = h_{\text{cell}}/2$.

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.

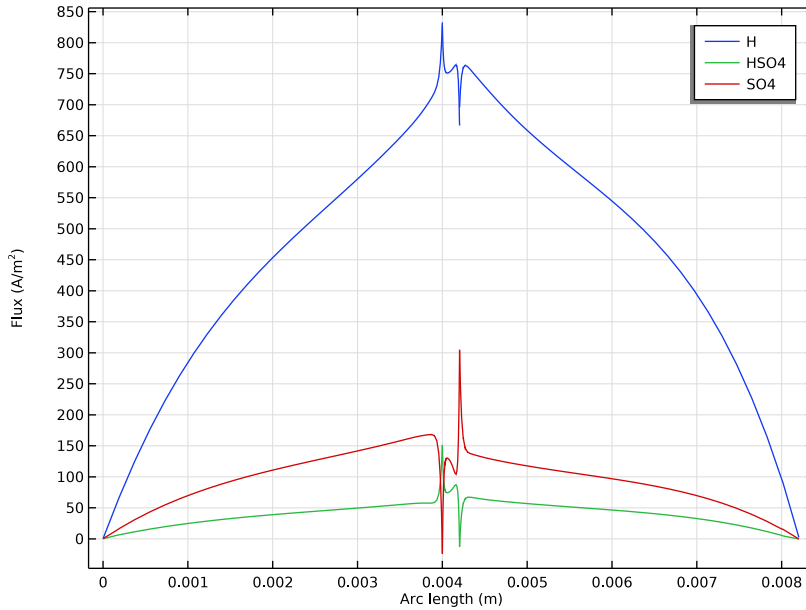


Figure 11: Sulfuric acid species fluxes along a horizontal line placed at $y = h_{\text{cell}}/2$.

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," *Electrochim. 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," *Electrochem. Commun.*, 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 (mol/m³)** table, enter the following settings:

cSO4_neg

cHSO4_neg

cH_neg

cV2

cV3

6 In the **Electrolyte potential (V)** text field, type `phi1_neg`.

7 In the **Electric potential (V)** 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 (mol/m³)** table, enter the following settings:

cSO4_mem

cHSO4_mem

cH_mem

cV2_mem

cV3_mem

cV4_mem

cV5_mem

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

13 In the **Electric potential (V)** 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 (mol/m³)** table, enter the following settings:

cSO4_pos

cHSO4_pos

cH_pos

cV4

cV5

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

19 In the **Electric potential (V)** 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 I

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** checkbox.
- 6 In the **Label** text field, type `Negative Electrode`.

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** checkbox.
- 7 In the **Label** text field, type `Membrane`.

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** checkbox.
- 7 In the **Label** text field, type `Positive Electrode`.

- 8 Click  **Build All Objects**.
- 9 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 **Definitions** toolbar, click  **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 In the **Label** text field, type Negative Electrode Variables.

Membrane Variables

- 1 In the **Definitions** toolbar, click  **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 In the **Label** text field, type Membrane Variables.

Positive Electrode Variables

- 1 In the **Definitions** toolbar, click  **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 In the **Label** text field, type Positive Electrode Variables.

TERTIARY CURRENT DISTRIBUTION, NERNST-PLANCK (NEGATIVE)


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

- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Tertiary Current Distribution, Nernst-Planck (tcd)**.
- 2 In the **Settings** window for **Tertiary Current Distribution, Nernst-Planck**, type Tertiary Current Distribution, Nernst-Planck (Negative) in the **Label** text field.
- 3 Locate the **Domain Selection** section. From the **Selection** list, choose **Negative Electrode**.
- 4 Locate the **Out-of-Plane Thickness** section. In the d_z text field, type `wCell`.

Species Charges 1

- 1 In the **Model Builder** window, under **Component 1 (comp1)** > **Tertiary Current Distribution, Nernst-Planck (Negative) (tcd)** click **Species Charges 1**.
- 2 In the **Settings** window for **Species Charges**, locate the **Charge** section.
- 3 In the z_{cSO4neg} text field, type -2.
- 4 In the z_{cHSO4neg} text field, type -1.
- 5 In the z_{cHneg} text field, type 1.
- 6 In the z_{cV2} text field, type 2.
- 7 In the z_{cV3} text field, type 3.

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 **Negative Electrode**.
- 4 Locate the **Convection** section. Specify the **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 **Porous Matrix Properties** section. In the ϵ_1 text field, type epsilon.
- 12 Locate the **Effective Transport Parameter Correction** section. From the **Electric conductivity** list, choose **No correction**.


Porous Electrode Reaction 1

- 1 In the **Model Builder** window, click **Porous Electrode Reaction 1**.
- 2 In the **Settings** window for **Porous Electrode Reaction**, locate the **Stoichiometric Coefficients** section.
- 3 In the v_{cV2} text field, type 1.
- 4 In the v_{cV3} text field, type -1.
- 5 Locate the **Equilibrium Potential** section. In the $E_{eq,ref}(T)$ text field, type E0_neg.
- 6 Locate the **Electrode Kinetics** section. In the $i_{0,ref}(T)$ 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 $c_{0,cHSO4neg}$ text field, type cHSO4_0_neg.
- 5 In the $c_{0,cHneg}$ text field, type cH_0_neg.


- 6 In the $c_{0,cV2}$ text field, type $cV2_0$.
- 7 In the $c_{0,cV3}$ text field, type $cV3_0$.
- 8 Locate the **Boundary Condition Type** section. From the list, choose **Flux (Danckwerts)**.

Outflow I

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Outflow**.
- 2 Select Boundary 3 only.


Ion-Exchange Membrane Boundary I

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 $c_{mem,cSO4neg}$ text field, type $cSO4_mem$.
- 7 Select the **Species cHSO4_neg** checkbox.
- 8 In the $c_{mem,cHSO4neg}$ text field, type $cHSO4_mem$.
- 9 Select the **Species cH_neg** checkbox.
- 10 In the $c_{mem,cHneg}$ text field, type cH_mem .
- 11 Select the **Species cV2** checkbox.
- 12 In the $c_{mem,cV2}$ text field, type $cV2_mem$.
- 13 Select the **Species cV3** checkbox.
- 14 In the $c_{mem,cV3}$ text field, type $cV3_mem$.

Electrode Current Density I

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 $i_{n,s}$ text field, type -tcd2.itot.

Initial Values I

- 1 In the **Model Builder** window, click **Initial Values I**.
- 2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.
- 3 In the $cHSO_{4,neg}$ 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_z text field, type wCell.

Species Charges I


- 1 In the **Model Builder** window, under **Component 1 (comp1)** > **Tertiary Current Distribution, Nernst-Planck (Ion Exchange Membrane) (tcd2)** click **Species Charges I**.
- 2 In the **Settings** window for **Species Charges**, locate the **Charge** section.
- 3 In the $z_{cSO_{4mem}}$ text field, type -2.
- 4 In the $z_{cHSO_{4mem}}$ text field, type -1.
- 5 In the z_{cHmem} text field, type 1.
- 6 In the $z_{cV_{2mem}}$ text field, type 2.
- 7 In the $z_{cV_{3mem}}$ text field, type 3.
- 8 In the $z_{cV_{4mem}}$ text field, type 2.
- 9 In the $z_{cV_{5mem}}$ text field, type 1.

Ion-Exchange Membrane I

- 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 -cHm*F_const.
- 5 Locate the **Diffusion** section. In the D_{cSO4mem} text field, type DS04.
- 6 In the D_{cHSO4mem} text field, type DHS04.
- 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 **Porous Matrix Properties** section. In the ϵ_1 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, 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 v_{cHmem} text field, type -2.
- 4 In the v_{cV4mem} text field, type 1.
- 5 In the v_{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, 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 v_{cHmem} text field, type -2.
- 6 In the v_{cV3mem} text field, type 1.
- 7 In the v_{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 v_{cV2mem} text field, type 1.
- 6 In the v_{cV3mem} text field, type -1.

Initial Values 1

- 1 In the **Model Builder** window, under **Component 1 (comp1)** > **Tertiary Current Distribution, Nernst-Planck (Ion Exchange Membrane) (tcd2)** click **Initial Values 1**.
- 2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.
- 3 In the $c_{\text{HSO4}_{\text{mem}}}$ text field, type cHSO4_0_mem.
- 4 In the $c_{\text{H}_{\text{mem}}}$ text field, type cH_0_mem.
- 5 In the $c_{\text{V2}_{\text{mem}}}$ text field, type cV2_0_mem.
- 6 In the $c_{\text{V3}_{\text{mem}}}$ text field, type cV3_0_mem.
- 7 In the $c_{\text{V4}_{\text{mem}}}$ text field, type cV4_0_mem.
- 8 In the $c_{\text{V5}_{\text{mem}}}$ text field, type cV5_0_mem.
- 9 In the $phil_{\text{mem}}$ text field, type -E0_neg.

TERTIARY CURRENT DISTRIBUTION, NERNST-PLANCK (POSITIVE)

Finish the physics settings by setting up the tertiary 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_z text field, type wCell.

Species Charges 1

- 1 In the **Model Builder** window, under **Component 1 (comp1)** > **Tertiary Current Distribution, Nernst-Planck (Positive) (tcd3)** click **Species Charges 1**.
- 2 In the **Settings** window for **Species Charges**, locate the **Charge** section.
- 3 In the $z_{\text{cSO4}_{\text{pos}}}$ text field, type -2.
- 4 In the $z_{\text{cHSO4}_{\text{pos}}}$ text field, type -1.

- 5 In the z_{cHpos} text field, type 1.
- 6 In the z_{cV4} text field, type 2.
- 7 In the z_{cV5} text field, type 1.

Porous Electrode I

- 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 **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 DS04.
- 7 In the D_{cHSO4pos} text field, type DHS04.
- 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 **Porous Matrix Properties** section. In the ϵ_1 text field, type epsilon.
- 12 Locate the **Effective Transport Parameter Correction** section. From the **Electric conductivity** list, choose **No correction**.


Porous Electrode Reaction I

- 1 In the **Model Builder** window, click **Porous Electrode Reaction I**.
- 2 In the **Settings** window for **Porous Electrode Reaction**, locate the **Stoichiometric Coefficients** section.
- 3 In the v_{cHpos} text field, type -2.
- 4 In the v_{cV4} text field, type 1.
- 5 In the v_{cV5} text field, type -1.
- 6 Locate the **Equilibrium Potential** section. In the $E_{\text{eq,ref}}(T)$ text field, type E0_pos.
- 7 Locate the **Electrode Kinetics** section. In the $i_{0,\text{ref}}(T)$ 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 I

- 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 I

- 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 $i_{\text{s,average}}$ text field, type i_avg.

Inflow I


- 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 $c_{0,\text{cHSO4pos}}$ text field, type cHSO4_0_pos.
- 5 In the $c_{0,\text{cHpos}}$ text field, type cH_0_pos.
- 6 In the $c_{0,\text{cV4}}$ text field, type cV4_0.
- 7 In the $c_{0,\text{cV5}}$ text field, type cV5_0.
- 8 Locate the **Boundary Condition Type** section. From the list, choose **Flux (Danckwerts)**.

Outflow I

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Outflow**.
- 2 Select Boundary 9 only.

Ion-Exchange Membrane Boundary I


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 $c_{mem,cSO4pos}$ text field, type cSO4_mem.
- 7 Select the **Species cHSO4_pos** checkbox.
- 8 In the $c_{mem,cHSO4pos}$ text field, type cHSO4_mem.
- 9 Select the **Species cH_pos** checkbox.
- 10 In the $c_{mem,cHpos}$ text field, type cH_mem.
- 11 Select the **Species cV4** checkbox.
- 12 In the $c_{mem,cV4}$ text field, type cV4_mem.
- 13 Select the **Species cV5** checkbox.
- 14 In the $c_{mem,cV5}$ text field, type cV5_mem.

Electrode Current Density I

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 $i_{n,s}$ text field, type -tcd2.itot.

Initial Values I

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

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** checkbox.


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.

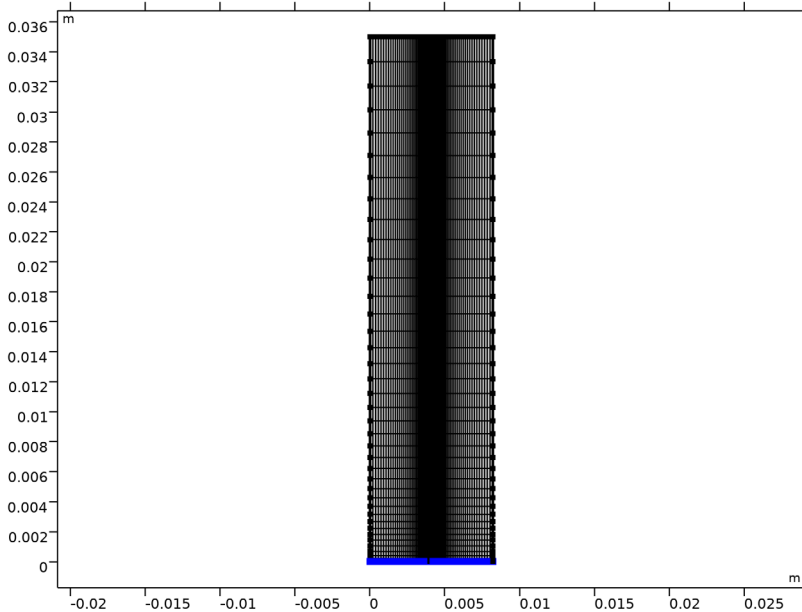
Boundary Layers 1

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

The problem is now 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** checkbox.


Step 2: Stationary

In the **Study** toolbar, click  **Compute**.

RESULTS

Reproduce the plots from the [Results and Discussion](#) section in the following way:


2D Plot Group 1

- 1 In the **Results** toolbar, click  **2D Plot Group**.
- 2 In the **Settings** window for **2D Plot Group**, click to expand the **Title** section.
- 3 From the **Title type** list, choose **None**.

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, under **Results** click **2D Plot Group 1**.
- 2 In the **Settings** window for **2D Plot Group**, type **V3/V4 Species Concentration** in the **Label** text field.

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 In the **Settings** window for **2D Plot Group**, type *V2/V5 Species Concentration* in the **Label** text field.

2D Plot Group 3

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

Surface 1

1 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, 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 Click to expand the **Title** section. From the **Title type** list, choose **None**.


Line Graph 1

- 1 Right-click **ID 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 **ID Plot Group 4** toolbar, click  **Plot**.


Electrolyte potential

- 1 In the **Model Builder** window, right-click **ID Plot Group 4** and choose **Rename**.
- 2 In the **Rename ID Plot Group** dialog, type Electrolyte potential in the **New label** text field.
- 3 Click **OK**.


ID Plot Group 5

- 1 In the **Results** toolbar, click  **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Title** section.
- 3 From the **Title type** list, choose **None**.

Line Graph 1

- 1 Right-click **ID 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 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 - Volumetric current density - A/m³**.
- 5 In the **ID 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 **ID Plot Group 5** toolbar, click  **Plot**.

Electrode reaction current densities


- 1 In the **Model Builder** window, right-click **ID Plot Group 5** and choose **Rename**.
- 2 In the **Rename ID Plot Group** dialog, type Electrode reaction current densities in the **New label** text field.

3 Click **OK**.

2D Plot Group 6

In the **Results** toolbar, click  **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 $\log(\text{abs}(\text{rd}))$.
- 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, type **Dissociation rate** in the **New label** text field.
- 3 Click **OK**.

ID Plot Group 7

- 1 In the **Results** toolbar, click  **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Cut Line 2D 1**.
- 4 Locate the **Title** section. From the **Title type** list, choose **None**.
- 5 Locate the **Plot Settings** section.
- 6 Select the **y-axis label** checkbox. In the associated text field, type **Species activity (-)**.
- 7 Locate the **Legend** section. From the **Position** list, choose **Middle right**.

Line Graph 1

- 1 In the **Model Builder** window, expand the **ID Plot Group 7** node.
- 2 Right-click **ID Plot Group 7** and choose **Line Graph**.
- 3 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
- 4 In the **Expression** text field, type **aH**.
- 5 Click to expand the **Legends** section. Select the **Show legends** checkbox.
- 6 From the **Legends** list, choose **Manual**.

7 In the table, enter the following settings:

Legends

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 aHSO4.
- 4 Locate the **Legends** section. In the table, enter the following settings:

Legends

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 aSO4.
- 4 Locate the **Legends** section. In the table, enter the following settings:


Legends

SO4

Sulfuric acid species

- 1 In the **Model Builder** window, click **ID Plot Group 7**.
- 2 In the **ID Plot Group 7** toolbar, click  **Plot**.
- 3 In the **Settings** window for **ID Plot Group**, type Sulfuric acid species in the **Label** text field.

ID Plot Group 8

- 1 In the **Results** toolbar, click  **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Cut Line 2D 1**.
- 4 Locate the **Title** section. From the **Title type** list, choose **None**.
- 5 Locate the **Plot Settings** section.
- 6 Select the **y-axis label** checkbox. In the associated text field, type Species activity (-).

7 Locate the **Legend** section. From the **Position** list, choose **Middle right**.

Line Graph 1

- 1 Right-click **ID 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** checkbox.
- 5 From the **Legends** list, choose **Manual**.
- 6 In the table, enter the following settings:

Legends

V2

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

V3

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

V4

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

V5

V2/V3/V4/V5

- 1 In the **Model Builder** window, click **ID Plot Group 8**.
- 2 In the **ID Plot Group 8** toolbar, click  **Plot**.
- 3 In the **Settings** window for **ID Plot Group**, type V2/V3/V4/V5 in the **Label** text field.

ID Plot Group 9

- 1 In the **Results** toolbar, click  **ID Plot Group**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Cut Line 2D 1**.
- 4 Locate the **Title** section. From the **Title type** list, choose **None**.
- 5 Locate the **Plot Settings** section.
- 6 Select the **y-axis label** checkbox. In the associated text field, type Flux (A/m²</sup>).

Line Graph 1

- 1 Right-click **ID 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 $Hx \cdot F_{\text{const}}$.
- 4 Locate the **Legends** section. Select the **Show legends** checkbox.
- 5 From the **Legends** list, choose **Manual**.
- 6 In the table, enter the following settings:

Legends

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 $-HSO_4x \cdot F_{\text{const}}$.

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

Legends

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

SO4

Fluxes

- 1 In the **Model Builder** window, click **ID Plot Group 9**.
- 2 In the **ID Plot Group 9** toolbar, click  **Plot**.
- 3 In the **Settings** window for **ID Plot Group**, type Fluxes in the **Label** text field.