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2023年5月15日30

Report date

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1. Global Definitions

|  |  |
| --- | --- |
| Date | May 19, 2023 7:27:15 AM |

Global settings

|  |  |
| --- | --- |
| Name | 2023年5月15日30.mph |
| Path | E:\COMSOL\2023年5月15日30.mph |
| Version | COMSOL Multiphysics 5.6 (Build: 280) |

Used products

|  |
| --- |
| COMSOL Multiphysics |
| CAD Import Module |
| CFD Module |
| Chemical Reaction Engineering Module |
| Corrosion Module |
| Design Module |

Computer information

|  |  |
| --- | --- |
| CPU | AMD Ryzen 7 2700 Eight-Core Processor, 8 cores |
| Operating system | Windows 10 |

* 1. Parameters
     1. Geometric parameters

Geometric parameters

| **Name** | **Expression** | **Value** | **Description** |
| --- | --- | --- | --- |
| a\_ch | 0.4[mm] | 4E−4 m | Side length, micrometer |
| a\_Ch | 2[mm] | 0.002 m | Side length, millimetre |
| l | 20[mm] | 0.02 m | Reactor length |
| d\_GDL | 100[um] | 1E−4 m | Gas diffusion layer thickness |
| d\_CL | 50[um] | 5E−5 m | Catalyts layer thickness |
| d\_AEM | 30[um] | 3E−5 m | AEM layer thickness |
| S\_R | 4[cm^2] | 4E−4 m² | Aera of reactor |

* + 1. Basic setup parameters

Basic setup parameters

| **Name** | **Expression** | **Value** | **Description** |
| --- | --- | --- | --- |
| C0 | 1[M] | 1000 mol/m³ |  |
| E\_an | 0[V] | 0 V | AEM potential |
| E\_ca | -1.11[V] | −1.11 V | Cathode potential |
| E\_COeq | -0.11[V] | −0.11 V | Equilibrium potential, CO |
| E\_H2eq | 0[V] | 0 V | Equilibrium potential, H2 |
| E0 | 1[V] | 1 V |  |
| epsilon\_CL | 0.5 | 0.5 | Porosity, CL |
| epsilon\_GDL | 0.7 | 0.7 | Porosity, GDL |
| k | 1e-12[m^2] | 1E−12 m² | Permeability, estimated value |
| mu\_gas | 1e-5[Pa\*s] | 1E−5 Pa·s | Gas dynamic viscosity |
| p\_H2O | 3357[Pa] | 3357 Pa | Water vapor pressure |
| p0 | 1[atm] | 1.0133E5 Pa |  |
| Qm\_CO2 | Q\_in\*MCO2/V\_RT/a\_Ch^2\*w\_CO2 | 0.2374 kg/(m²·s) |  |
| Qm\_H2Og | Q\_in\*MH2O/V\_RT/a\_Ch^2\*w\_H2Og | 0.0033279 kg/(m²·s) |  |
| rho\_CO2 | MCO2/V\_RT | 1.9643 kg/m³ |  |
| rho\_in | ((MCO2\*w\_CO2 + MH2O\*w\_H2Og))/22.4[L/mol] | 1.9258 kg/m³ |  |
| S\_v | l^2\*d\_CL\*a\_v | 0.002 m² |  |
| S0 | 1[cm^2] | 1E−4 m² |  |
| sigma\_GDL | 222[S/m] | 222 S/m | Electrical conductivity, GDL |
| sigma\_m | 25[S/m] | 25 S/m | Electrical conductivity, AEM |
| T | 298.15[K] | 298.15 K | Temperature |
| v\_in\_ch | Q\_in/a\_ch/a\_ch | 3.125 m/s | Inlet velocity, micrometer |
| v\_in\_Ch | Q\_in/a\_Ch/a\_Ch | 0.125 m/s | Inlet velocity, millimetre |
| V\_RT | 22.4[L/mol] | 0.0224 m³/mol |  |
| w\_CO2 | 1 - w\_H2Og | 0.96687 |  |
| w\_H2Og | p\_H2O/p0 | 0.033131 |  |
| M\_in | w\_CO2\*MCO2 + w\_H2Og\*MH2O | 0.043139 kg/mol |  |
| R\_mcl | d\_CL\*epsilon\_CL/(sigma\_m\*epsilon\_CL)/S\_R + d\_AEM/sigma\_m/S\_R | 0.008 Ω |  |
| d\_SR | (d\_AEM + d\_CL)/S\_R | 0.2 1/m |  |
| sigma\_GDL\_m | 0.00001[S/m] | 1E−5 S/m | Electrical conductivity, GDL electrolyte |
| P\_ref | 1[atm] | 1.0133E5 Pa | Reference pressure |
| Q\_in | 30[ml/min] | 5E−7 m³/s | Inlet gas flow |
| a\_v | 1e5[1/m] | 1E5 1/m |  |
| Q\_V0 | 1[ml/min] | 1.6667E−8 m³/s |  |
| Q\_in\_num | Q\_in/Q\_V0 | 30 |  |

* + 1. Gas constant parameters

Gas constant parameters

| **Name** | **Expression** | **Value** | **Description** |
| --- | --- | --- | --- |
| MO2 | 32[g/mol] | 0.032 kg/mol | Molar mass, O2 |
| MN2 | 28[g/mol] | 0.028 kg/mol | Molar mass, N2 |
| MH2O | 18[g/mol] | 0.018 kg/mol | Molar mass, H2O |
| MH2 | 2[g/mol] | 0.002 kg/mol | Molar mass, H2 |
| MCO2 | 44[g/mol] | 0.044 kg/mol | Molar mass，CO2 |
| MCO | 28[g/mol] | 0.028 kg/mol | Molar mass, CO |
| D\_eff\_H2\_H2O | 9.15e-5[m^2/s] | 9.15E−5 m²/s | 307.1K |
| D\_eff\_H2\_O2 | 8.91e-5[m^2/s] | 8.91E−5 m²/s | 316K |
| D\_eff\_H2\_N2 | 7.79e-5[m^2/s] | 7.79E−5 m²/s | 297.2K |
| D\_eff\_H2\_CO | 7.43e-5[m^2/s] | 7.43E−5 m²/s | 295.6K |
| D\_eff\_H2\_CO2 | 6.46e-5[m^2/s] | 6.46E−5 m²/s | 298.2K |
| D\_eff\_H2O\_N2 | 2.93e-5[m^2/s] | 2.93E−5 m²/s | 298.2K |
| D\_eff\_H2O\_O2 | 2.82e-5[m^2/s] | 2.82E−5 m²/s | 308.1K |
| D\_eff\_N2\_O2 | 2.20e-5[m^2/s] | 2.2E−5 m²/s | 293.2K |
| D\_eff\_H2O\_CO | 2.12e-5[m^2/s] | 2.12E−5 m²/s | 295.8K |
| D\_eff\_H2O\_CO2 | 2.02e-5[m^2/s] | 2.02E−5 m²/s | 307.4K |
| D\_eff\_CO\_CO2 | 1.85e-5[m^2/s] | 1.85E−5 m²/s | 315.4K |
| D\_eff\_N2\_CO2 | 1.65e-5[m^2/s] | 1.65E−5 m²/s | 298.2K |
| D\_eff\_O2\_CO2 | 1.56e-5[m^2/s] | 1.56E−5 m²/s | 296K |
| D\_eff\_CO\_N2 | 2.050e-5[m^2/s] | 2.05E−5 m²/s |  |

* + 1. Geometric parameters

Geometric parameters

| **Name** | **Expression** | **Value** | **Description** |
| --- | --- | --- | --- |
| a\_ch | 0.4[mm] | 4E−4 m | Side length, micrometer |
| a\_Ch | 2[mm] | 0.002 m | Side length, millimetre |
| l | 20[mm] | 0.02 m | Reactor length |
| d\_GDL | 100[um] | 1E−4 m | Gas diffusion layer thickness |
| d\_CL | 50[um] | 5E−5 m | Catalyts layer thickness |
| d\_AEM | 30[um] | 3E−5 m | AEM layer thickness |
| S\_R | 4[cm^2] | 4E−4 m² | Aera of reactor |

* + 1. Geometric parameters

Geometric parameters

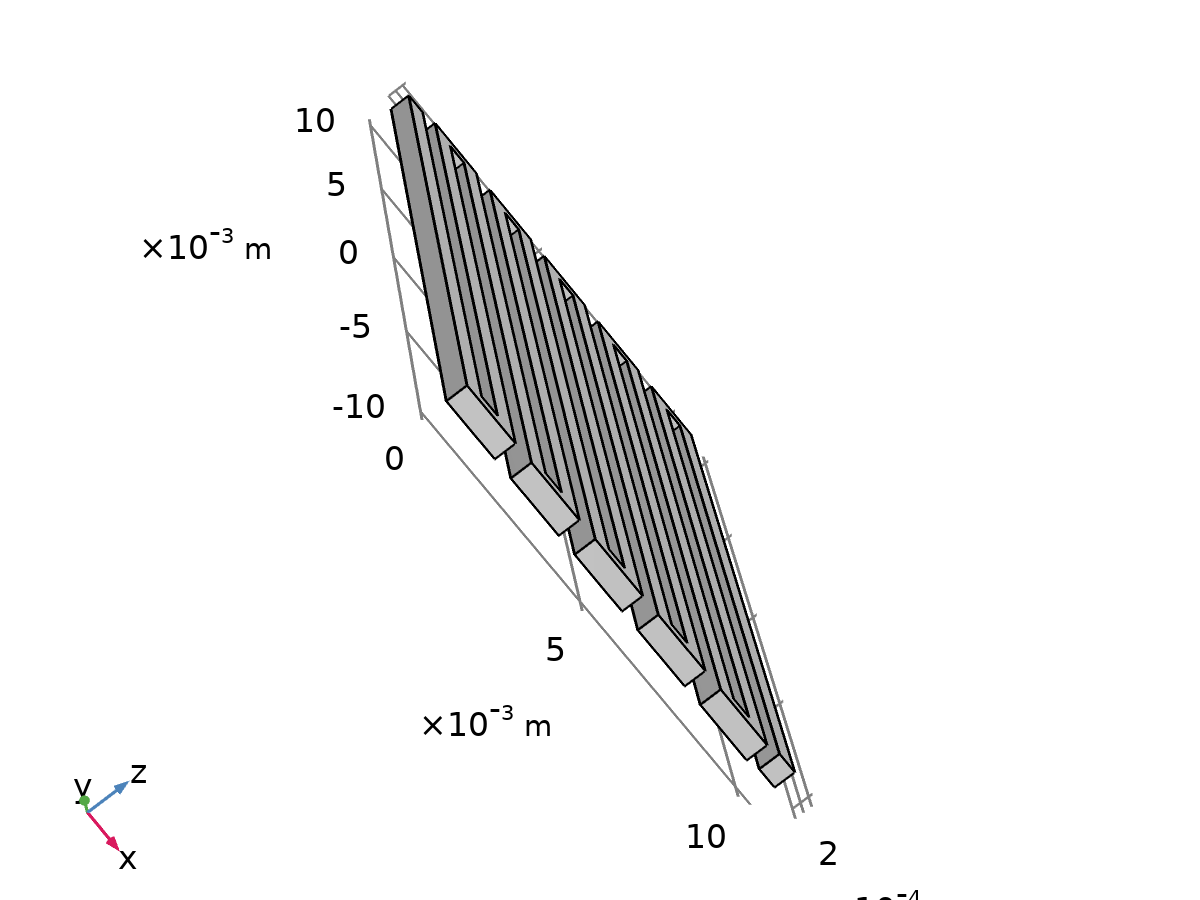
| **Name** | **Expression** | **Value** | **Description** |
| --- | --- | --- | --- |
| a\_ch | 0.4[mm] | 4E−4 m | Side length, micrometer |
| a\_Ch | 2[mm] | 0.002 m | Side length, millimetre |
| l | 20[mm] | 0.02 m | Reactor length |
| d\_GDL | 100[um] | 1E−4 m | Gas diffusion layer thickness |
| d\_CL | 50[um] | 5E−5 m | Catalyts layer thickness |
| d\_AEM | 30[um] | 3E−5 m | AEM layer thickness |
| S\_R | 4[cm^2] | 4E−4 m² | Aera of reactor |

* + 1. Electrode kinetics

Electrode kinetics

| **Name** | **Expression** | **Value** | **Description** |
| --- | --- | --- | --- |
| Ac\_H2 | 1[V]/beta\_H2\_fitting | −0.26354 V |  |
| Ac\_CO | 1[V]/beta\_CO\_fitting | −0.48312 V |  |
| J0\_H2 | J0\_H2\_fitting/a\_v/d\_CL | −0.005762 A/m² |  |
| J0\_CO | J0\_CO\_fitting/a\_v/d\_CL | −1.645 A/m² |  |
| beta\_CO\_fitting | -4.76604/log(10) | −2.0699 | Fitting,CO |
| beta\_H2\_fitting | -8.737/log(10) | −3.7944 | Fitting,H2 |
| J0\_H2\_fitting | -0.002881[mA/cm^2] | −0.02881 A/m² | Current density,JH2 |
| J0\_CO\_fitting | -0.82252[mA/cm^2] | −8.2252 A/m² | Current density, JCO |
| alpha\_CO | -beta\_CO\_fitting\*R\_const\*T/F\_const\*log(10) | 0.12245 V |  |
| alpha\_H2 | -beta\_H2\_fitting\*R\_const\*T/F\_const\*log(10) | 0.22448 V |  |

* 1. Geometry Parts
     1. 蛇形通道（二维），方形回转，矩形横截面

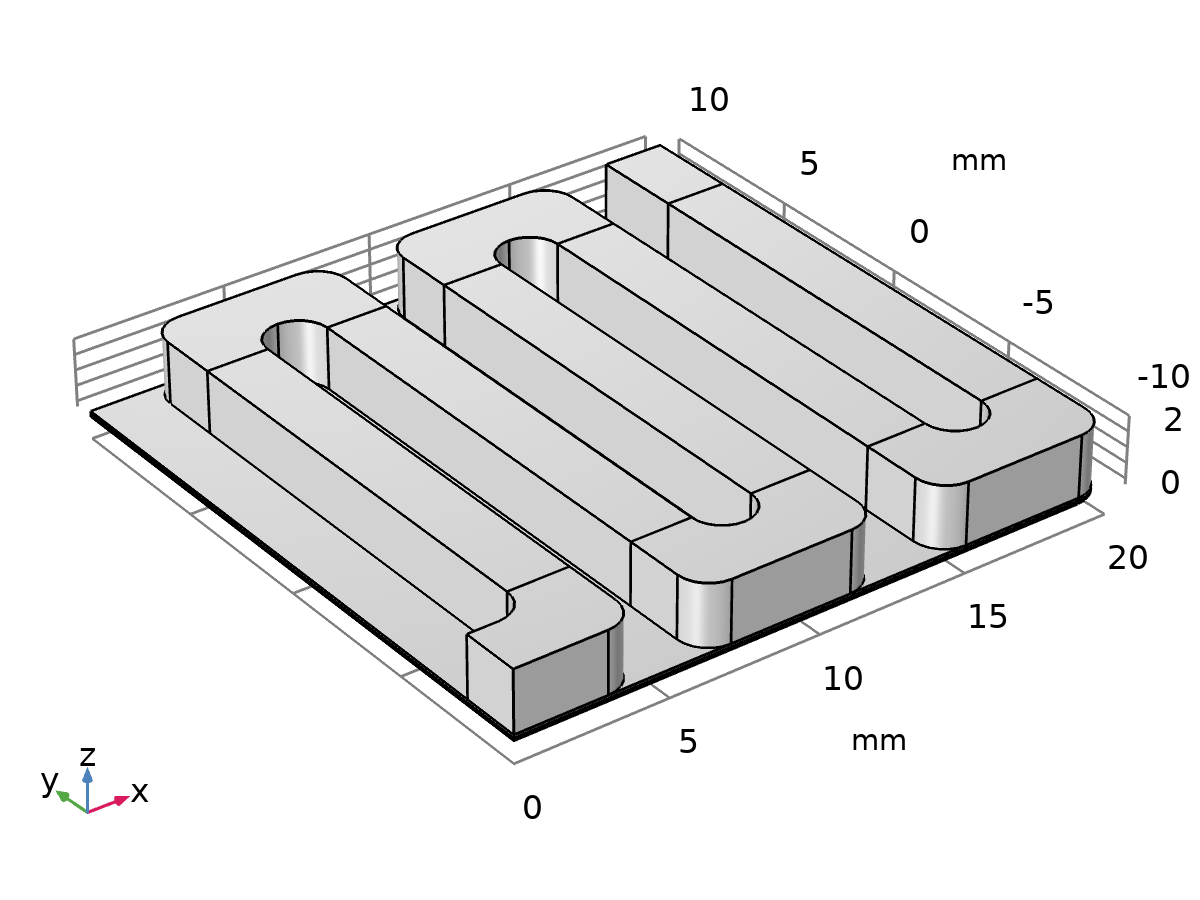


蛇形通道（二维），方形回转，矩形横截面

Units

|  |  |
| --- | --- |
| Length unit | m |
| Angular unit | deg |

1. 组件 1
   1. Geometry

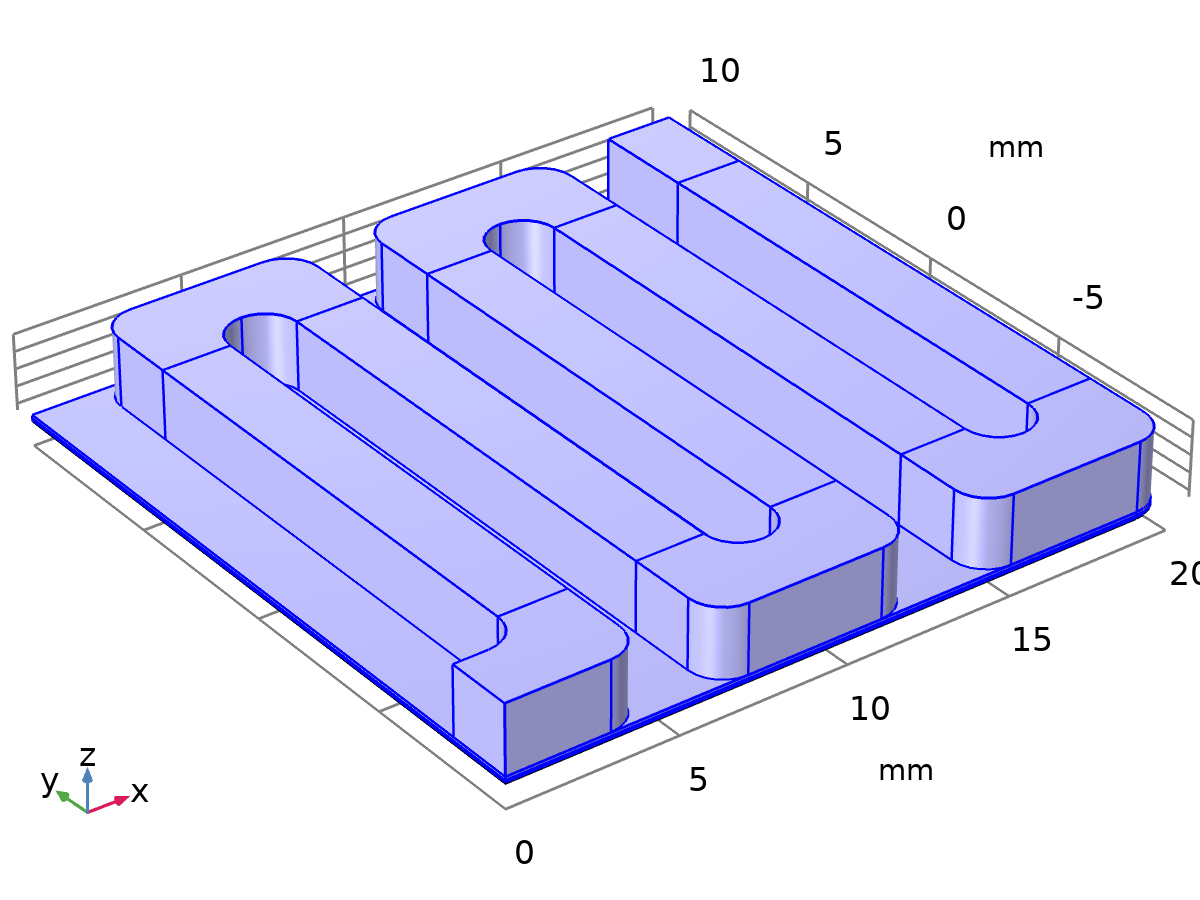


Geometry

Units

|  |  |
| --- | --- |
| Length unit | mm |
| Angular unit | deg |

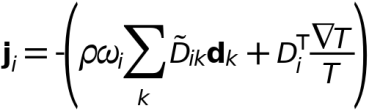
* 1. Transport of Concentrated Species

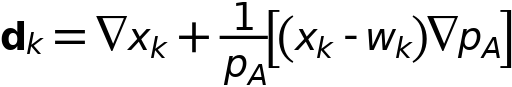


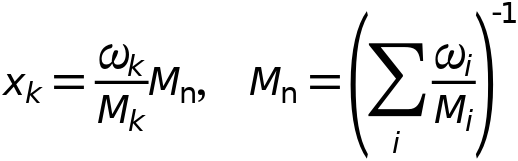
Transport of Concentrated Species

Equations





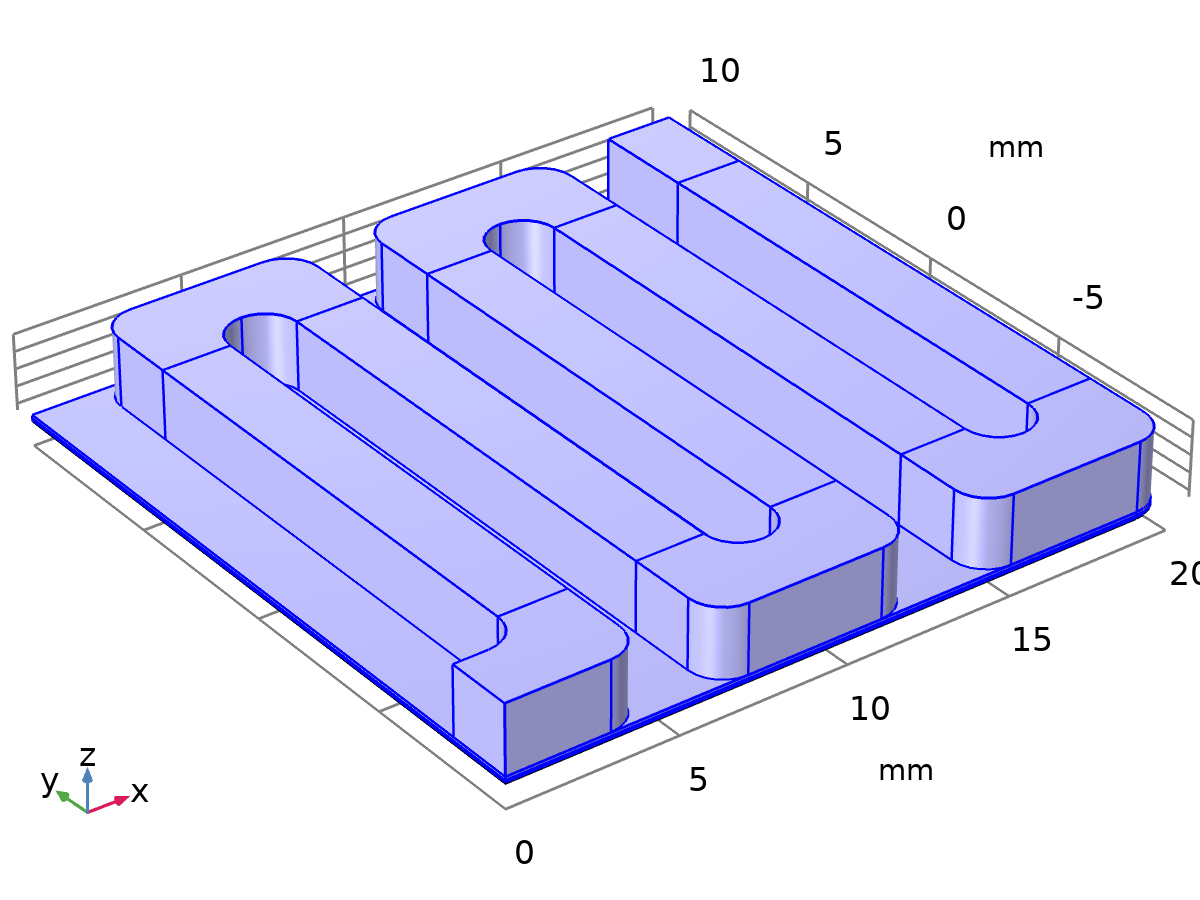




Features

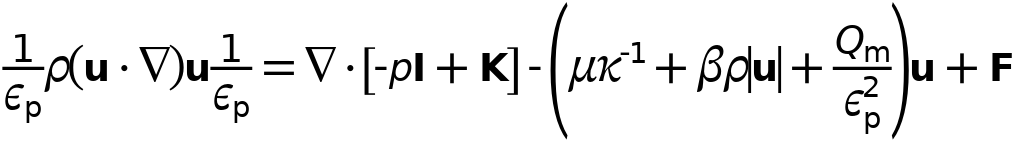
| **Name** | **Level** |
| --- | --- |
| Transport Properties | Domain |
| Initial Values | Domain |
| No Flux | Boundary |
| Porous Media Transport Properties1 | Domain |
| Porous Media Transport Properties2 | Domain |
| Outflow | Boundary |
| Porous Electrode Coupling | Domain |
| Flux | Boundary |

* 1. Brinkman Equations



Brinkman Equations

Equations

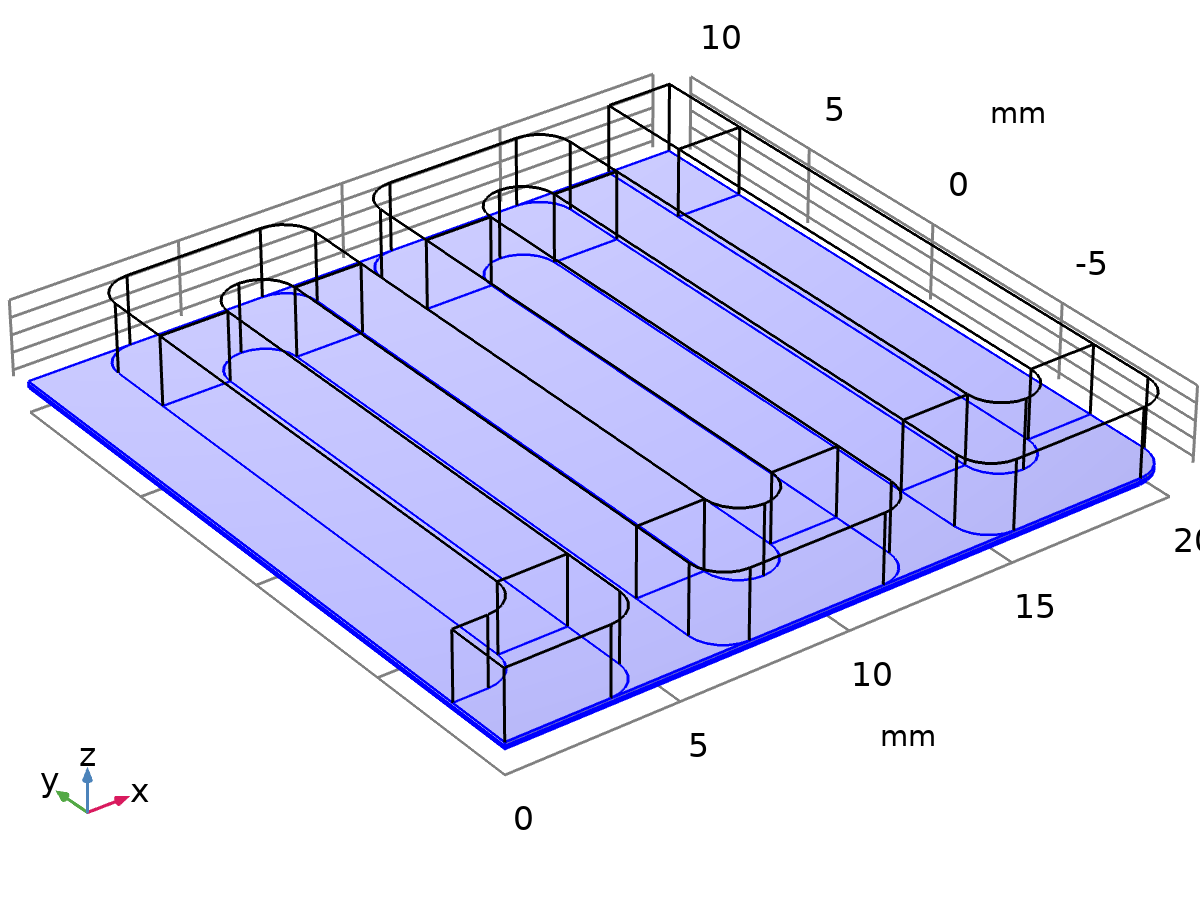




Features

| **Name** | **Level** |
| --- | --- |
| Fluid and Matrix Properties | Domain |
| Initial Values | Domain |
| Wall | Boundary |
| Fluid Properties1 | Domain |
| Fluid and Matri Properties | Domain |
| Inlet | Boundary |
| Outlet | Boundary |
| Wall2 | Boundary |

* 1. Secondary Current Distribution



Secondary Current Distribution

Equations



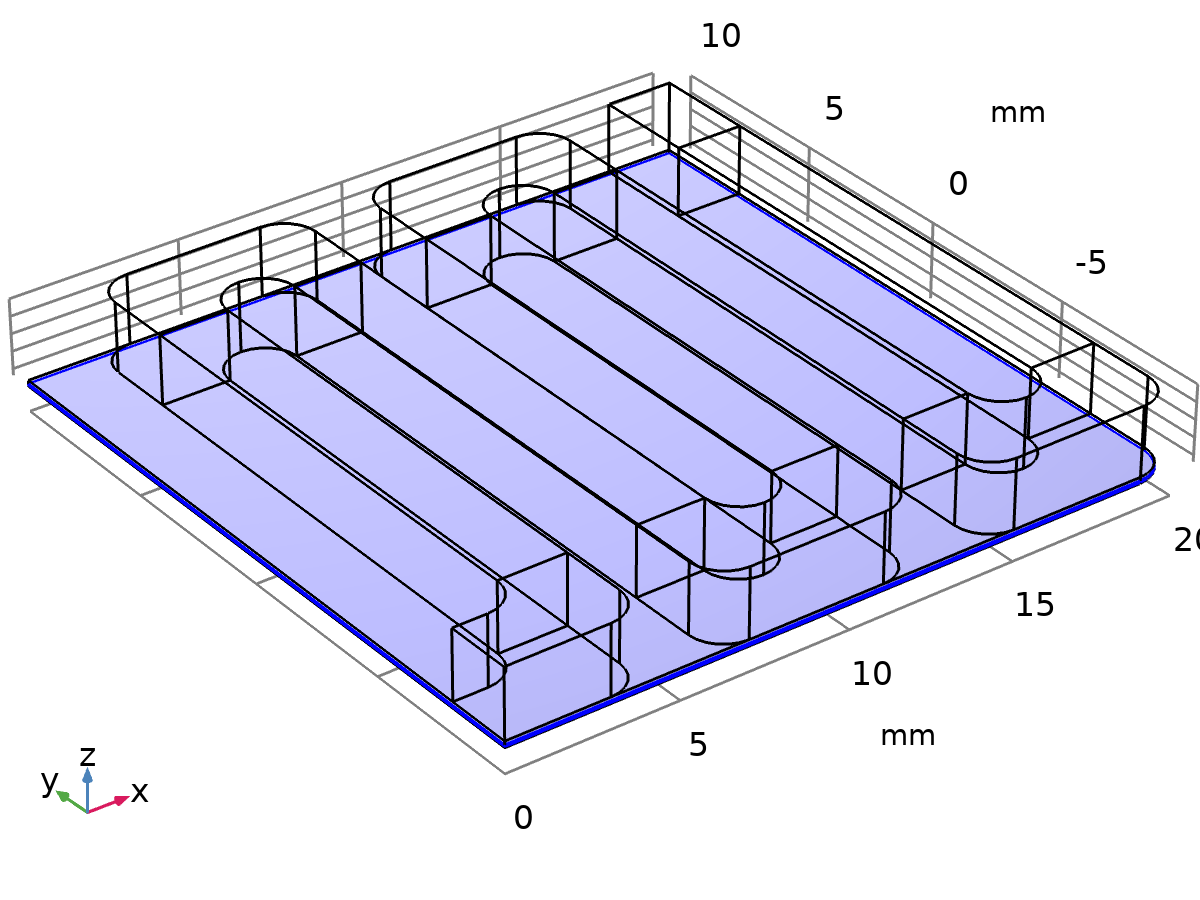




Features

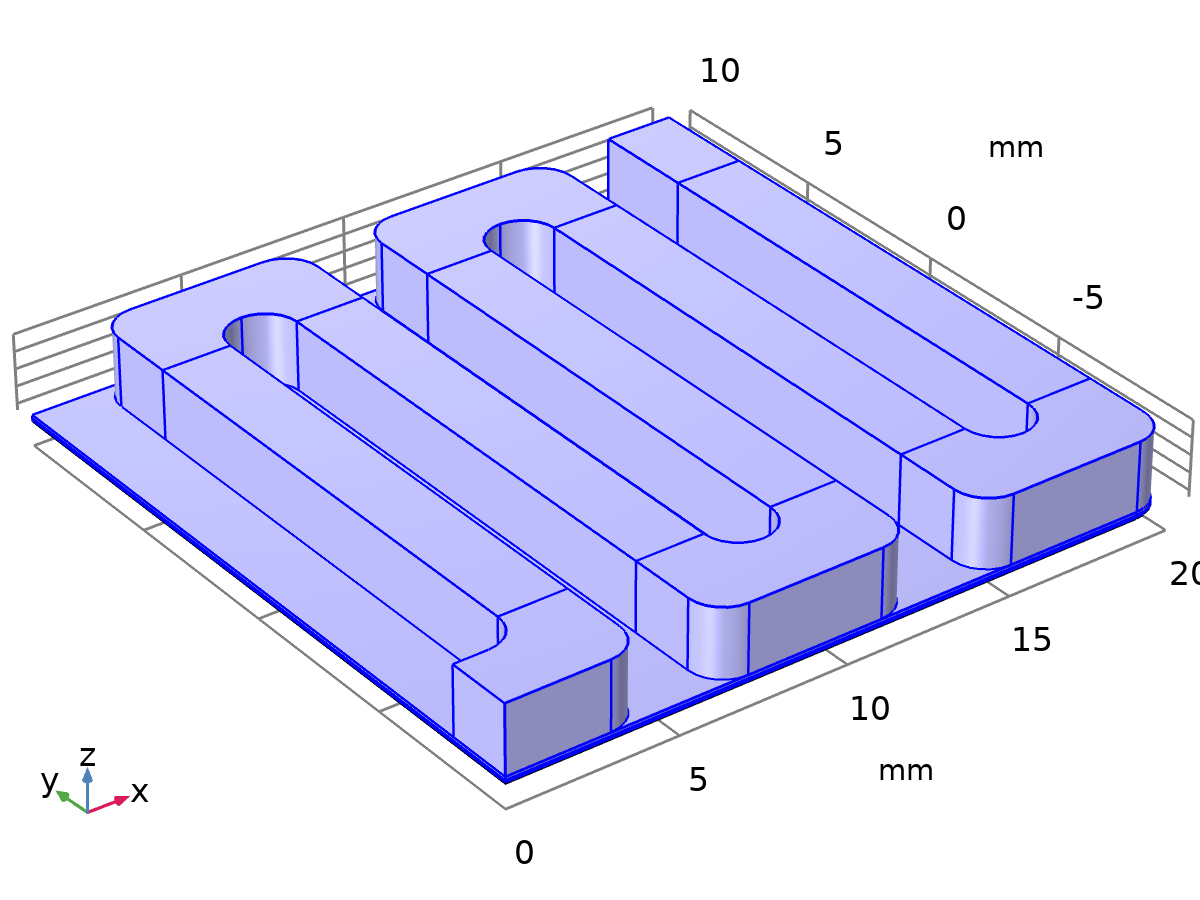
| **Name** | **Level** |
| --- | --- |
| AEM | Domain |
| 绝缘 1 | Boundary |
| Initial Values | Domain |
| GDL | Domain |
| CL | Domain |
| Electric Potential | Boundary |
| Electrolyte Potential | Boundary |

* 1. Multiphysics
     1. Potential Coupling



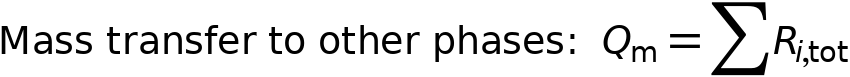
Potential Coupling

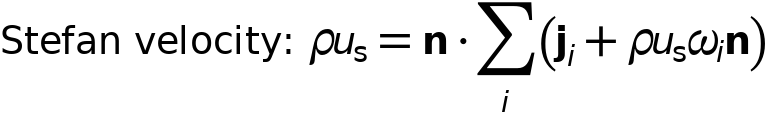
* + 1. Reaction Flow



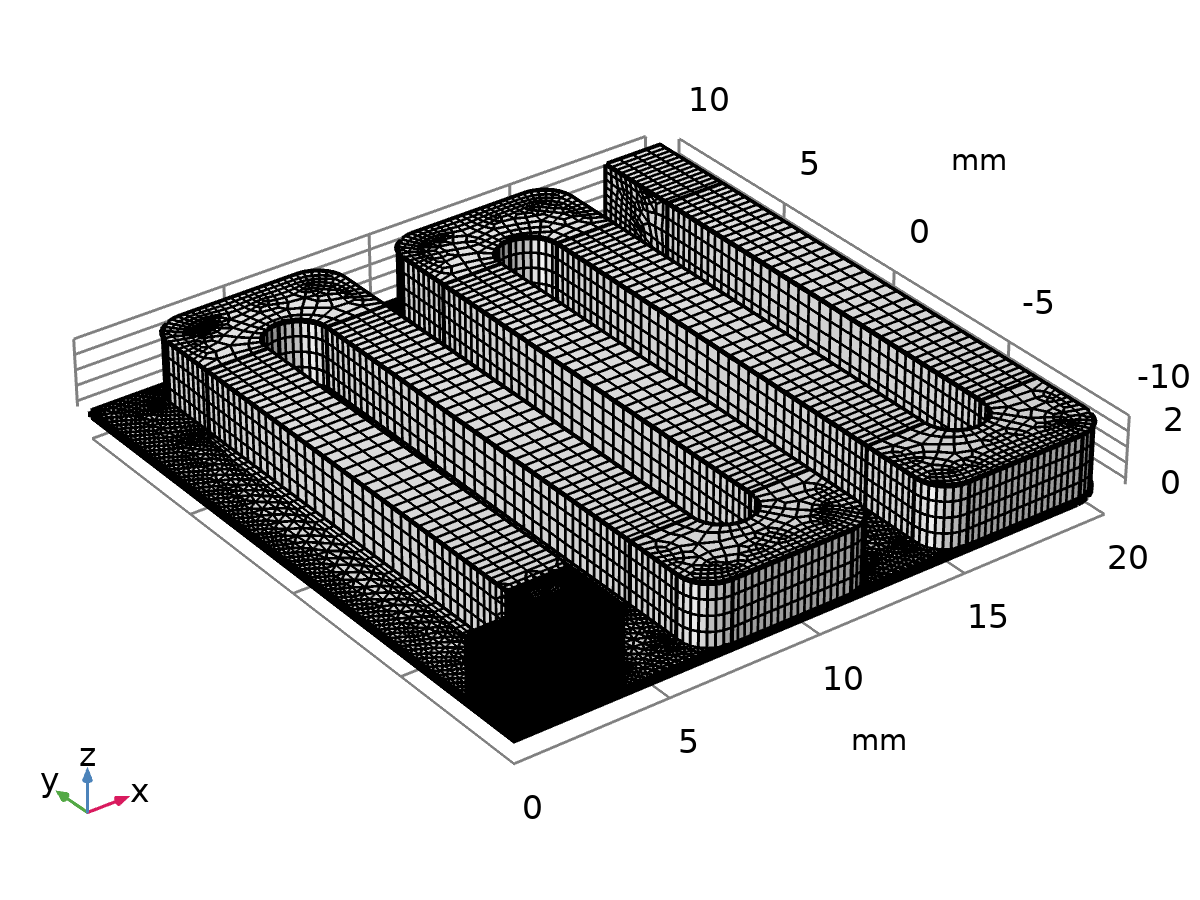
Reaction Flow

Equations





* 1. Mesh



Mesh