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ARTICLE

Supporting Information for

Modelling of redox flow battery electrode processes at a range of length scales: a review

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Table S1

Nomenclature for the symbols used in Table 5.

Symbol	Description
a_i	Activity of specie *i* (-)
A^v	Specific electrode/electrolyte area per unit volume (m^{-1})
c_i	Concentration of species *i* (mol m^{-3})
D_i	Diffusivity of species *i* (m^2 s^{-1})
E	Potential difference (V)
F	Faraday constant (C mol^{-1})
i^v	Current density per unit volume (A m^{-3})
k_s	Mass transfer coefficient (m s^{-1})
$\underline{N}_i$	Molar flux of species *i* (mol m^{-2} s^{-1})
OCV	Open circuit voltage (V)

P	Pressure (Pa)
r	Kinetic constant (mol m^{-2} s^{-1})
R	Universal gas constant (J mol^{-1} K^{-1})
$S_{C,i}^{v}$	Source term of species *i* due to capacitive contributions (mol m^{-3} s^{-1})
$S_{d,i}^{v}$	Source term of species *i* due to sulfuric acid dissociation kinetics (mol m^{-3} s^{-1})
t	Time (s)
T	Temperature (K)
$\underline{v}$	Molar average velocity (m s^{-1})
$\underline{w}$	Mass average velocity (m s^{-1})
z_i	Charge of species *i* (-)

Greek letters

α	First transfer coefficient (-)
β	Second transfer coefficient (-)
$\underline{\underline{B}}$	permeability tensor (m^2)
γ_i	Activity coefficient of species *i* (-)
ε_{ey}	Volume fraction of electrolyte phase (i.e., porosity) (-)
η	Overpotential (V)
$\underline{\underline{\kappa}}^{eff}$	effective conductivity factor tensor (-)
μ	Dynamic viscosity (kg m^{-1} s^{-1})
ν_i	Stoichiometric coefficient of species *i*
σ	Bulk conductivity (S m^{-1})
φ	Electric potential (V)

Subscripts

e	Electrons
ed	Electrode phase
ey	Electrolyte phase
i	Species in the electrolyte phase
$+$	Positive electrode
$-$	Negative electrode

Superscripts

eq	Local equilibrium conditions
IN	Inlet conditions
s	Surface (electrode/electrolyte interface)
$\circ$	Standard conditions

Table S2

Key governing equations and properties used for simulating electrode properties in VRFBs

Reference	Governing equations	Key properties used in simulation	Brief results
1	• *IR* drop including Bruggeman correction; • Inverted Butler-Volmer equation for activation overpotentials; • Effect on mass balance of vanadium species due to recirculation of electrolytes; • Mass balances of water and proton; • Reservoir concentrations of water and proton	• Reference rate constant for cathodic reaction at 293 K = 3.56×10^{-6} m/s; • Reference rate constant for anodic reaction at 293 K = 3×10^{-9} m/s; • Electronic conductivity of the graphite current collector = 9.1×10^{4} S/m; • Ionic conductivity of the electrolyte (both half cells) = 100 S/m; • Electrode width = 0.004 m; • Electrode breadth = 0.1 m; • Electrode height = 0.1 m;	The model is able to relate important characteristics of performance (such as the time to charge/discharge and the state of charge) to key system properties. Simulations have demonstrated that the model is able to capture the performance in practical systems to a high degree of accuracy.

		• Electrode porosity = 0.67; • Specific surface area for reaction = 420 m^{-1}; • Temperature = 297 K; • Initial [V(II)] = 60 mol/m^3; • Initial [V(III)] = 1140 mol/m^3; • Initial [V(IV)] = 1140 mol/m^3; • Initial [V(V)] = 60 mol/m^3; • Current density = 1000 A/m^2; • Initial proton concentration = 4200 mol/m^3; • Initial water concentration = 4.23×10^4 mol/m^3; • Linear electrolyte flow rate = 1 ml/s	
2	• Concentration change of ions governed by chemical reaction, flow rate of electrolysis solution and externally attached circuit behavior; • Concentration change by electrolysis circulation is governed by difference of concentration in tanks and cells, flow rate of electrolysis solution and volume of cell; • [V(II)] governed by cell current	• Constant flow rate = 3.5 L/min for all 12 cells; • Constant charge/discharge current = 35 A; • Constant temperature = 35 °C; • Initial [V(II)] = 1.7 mol/L during charging • Initial [V(II)] = 0 during discharging; • Threshold output voltage = 1.55 V; • Initial electrolyte concentration = 0.2 mol/L in cell.	The concentration change in electrolyte solution governed the dynamics of the battery dominantly. Substantial dynamics depend on the flow rate. Good correlation with experiments.
3	• Mass conservation in flow cell; • Equivalent circuit model; • Nernst equation; • uniform reaction along the entire porous electrode, which leads to the estimate of ohmic losses due to the electrolyte (using electrode thickness); • Dilute solution theory; • Bruggeman relationship; • Stokes-Einstein equation coupled with	• Width of electrode = 0.02 m; • Height of electrode = 0.05 m; • Thickness of electrode = 0.00425 m; • Porosity of the electrode = 0.929; • Specific surface area = 39000 m^{-1}; • Cathodic reaction rate constant = 8.7×10^{-6} m/s; • Anodic reaction rate constant = 1.6×10^{-5} m/s; • Applied charge/discharge current densities = 500 A/m^2; • Initial species concentration both electrodes =	Ohmic losses associated with electrolyte were dominating electrode losses. Thinner electrodes than the 4.5-mm-thick felt used in this study should reduce ohmic losses as well as pumping losses if the same space velocity is maintained.

	the Vogel-Taumman-Fulcher model; • Butler-Volmer equation	1250 mol/m^3; • Initial HCl concentration both electrodes = 2300 mol/m^3; • Beginning state of charge for charge = 0.025; • Beginning state of charge for discharge = 0.975; • Volumetric flow rate = 20 mL/min; • Pre Bruggeman factor = 2; • Non-ideal reactor factor = 2.	
4	• Nernst-Planck equation to express molar flux of ionic species in porous electrodes; • Bruggeman relation used to relate effective diffusion coefficient of active species to normal diffusion coefficient; • Volume-averaged differential material balance; • Charge balance between electrolyte and electrode; • Butler-Volmer for surface electrode reactions and charge/transfer overpotentials; • Darcy's law for velocities through electrode; • Incompressible flow	• Initial proton concentration = 1200 mol/m^3; • Initial $[HSO_4^-]$ = 1200 mol/m^3; • Initial $[V_2(SO_4)_3]$ = 1080 mol/m^3; • Initial $[VOSO_4]$ = 1080 mol/m^3; • Outlet pressure = 3×10^5 Pa; • Operating temperature = 300 K; • Specific electroactive area = 2×10^6 m^{-1}; • Carbon electrode fiber diameter = 1×10^{-5} m; • Thickness of carbon collectors = 6×10^{-3} m; • Thickness of carbon felt = 4×10^{-3} m; • Length of porous electrode = 0.1 m; • Porosity = 0.68; • Anodic reaction rate constant = 3×10^{-9} m/s; • Cathodic reaction rate constant = 1.75×10^{-7} m/s; • Kozeny-Carman constant for porous electrode = 5.55; • Electrolyte viscosity = 10^{-3} Pa-s; • Conductivity of solid parts of carbon felt = 500 S/m; • Conductivity of carbon current collector = 1000 S/m.	Successful reduction of a detailed multi-dimensional model to a set of 1-D convection-diffusion and charge conservation equations. This was achieved by a few simplifying assumptions, scaling and asymptotic analyses. The computational cost for solving the model is significantly reduced.
5	• Same as literature;[4] • Conservation equations;	• Electrode conductivity = 1000 S/m; • Mean pore diameter = 1.16×10^{-4} m;	The cell voltage prediction shows significant improvement over literature[4] and it also compares surprisingly well with other higher-

	• Electronic charge; • Ionic charge; • Fluid, electrolyte; • Species, electrolyte; • Electroneutrality	• Porosity = 0.929; • Specific surface area = 1.62×10^{4} m^{-1}; • Mean carbon-fibre diameter = 1.76×10^{-5} m; • Anodic and cathodic transfer coefficient = 0.5; • Anodic reaction rate constant = 6.8×10^{-7} m/s; • Cathodic reaction rate constant = 1.7×10^{-7} m/s; • Porous electrode length = 0.02 m; • Electrode width = 0.025 m; • Thickness = 0.003 m; • Kozeny-Carman constant = 4.28; • Electrolyte volumetric flow rate = 60 mL/min; • Dynamic viscosity of electrolytes = 4.928×10^{-3} Pa-s; • Initial proton concentration in anolyte = 6000 mol/m^{3}; • Initial catholyte proton concentration = 4500 mol/m^{3}; • Total vanadium ion concentration in both half cells = 1500 mol/m^{3}; • Operating temperature = 300 K; • Applied current density = 400 A/m^{2}.	dimensional models. This modified 1-D model is also capable of capturing the cell performance at different electrolyte flow rates, especially evidenced for the polarization curve.
6	A set of governing equations has been employed for the main domains (positive and negative electrodes, proton exchange membrane): • Continuity; • Momentum conservation; • Species conservation; • Charge conservation; • Butler-Volmer equation; • Nernst equation; • permeability of the porous media	• Same as literature;[5] • Operating temperature = 298 K; • Electrolyte volume = 30 mL; • Outlet pressure condition = 0; • Current = 0.2 – 0.4 A.	A decrease in electrode thickness ratio or porosity leads to a more rapid depletion of the reactant concentration, a higher integral average value of the transfer current density and a more uniform distribution of the over-potential. The mass transfer condition at the electrode surface only affects the value of the over-potential. The decrease in the local mass transfer coefficient leads to greater polarization and increased rate of side reactions.

	described by the Carman–Kozeny equation; - Bruggemann correction		
7	Similar to literature.[6]	Not provided in sufficient details.	(1) Enhancement in convective mass transport increases reaction rate in diminishing manner due to limited diffusion mass transfer; (2) lower ohmic resistance causes more uniform current density distribution; (3) decrease in diffusion rate increases the concentration polarization; (4) increase of local mass transfer coefficient raises reaction rate and makes effective reaction layer thinner; (5) bigger ratio of electrode length to thickness worsens concentration polarization.
8	Conservation principles of charge, mass and momentum	- Carbon electrode height = 10 cm - Thickness = 4 mm - Width = 10 cm - Collector thickness = 6 mm - Electrode porosity = 0.68 - Fiber diameter = 10 μm - Half-cell electrolyte volume = 250 mL - Specific surface area = 2×10^6 m^{-1} - Anodic reaction rate constant = 3×10^{-9} m/s; - Cathodic reaction rate constant = 1.75×10^{-7} m/s; - Kozeny-Carman constant: porous electrode = 5.55 - Electronic conductivity of porous electrode = 500 S/m - Conductivity of collectors = 1000 S/m.	Comparisons between the simulation results and experimental data have demonstrated a good degree of accuracy in predicting the trends observed in a laboratory test, with respect to variations in two key parameters (concentration and flow rate). Further simulations have predicted that decreasing the electrode porosity by a relatively small amount can lead to a substantial increase in coulombic efficiency and a decrease in the rates of hydrogen and oxygen evolution.
9	Same as literature.[6]	Including thermal parameters, the following were also considered: - Electrode height = 10 cm; - Electrode thickness = 4 mm; - Electrode width = 10 cm; - Collector thickness = 6.3 mm;	Heat is generated as a result of activation losses, electrochemical reaction and ohmic resistance. Numerical simulations demonstrate the effects of changes in the operating temperature on performance. It is shown that variations in the electrolyte flow rate and the magnitude of the applied current substantially alter the charge/discharge characteristics, the temperature rise and the distribution of temperature. The value of the applied current for

		- Electrode porosity = 0.68; - Electrode mean pore diameter = 10 μm; - Electrolyte half-cell volume = 250 mL; - Specific surface area = 2×10^6 m^{-1}; - Kozeny-Carman constant: porous electrode = 5.55 - Electrolyte viscosity = 10^{-3} Pa s; - Electrode conductivity = 500 S/m; - Collector conductivity = 1000 S/m; - Cathodic rate constant = 1.75×10^{-7} m/s; - Anodic reaction rate constant = 3×10^{-9} m/s; - Initial system temp. = 303 K; - Initial [V(III)] = 1053 mol/m^3; - Initial [V(II)] = 27 mol/m^3; - Initial [V(IV)] = 1053 mol/m^3; - Initial [V(V)] = 27 mol/m^3; - Initial [HSO_4^-] = 1200 mol/m^3; - Initial [H^+] = 1200 mol/m^3; - Volumetric flow rate = 1 mL/s; - Current = 10 A.	charge and discharge plays a crucial role in heat generation. The amount of heat generated and the timescale of the temperature rise do not increase linearly with the current. Regions of high temperature can form rapidly in the current collectors and electrodes due to large gradients in the electronic potential. Due to non-uniformities in the reactant concentrations and, therefore, potentials and transfer current densities, local maxima in temperature can develop. A large electrolyte flow rate, combined with regulation of the external temperature, could be used to avoid such hotspots by keeping the temperature distribution uniform. Moreover, such high flow rates increase the coulombic efficiency of the cell and lower the rates of hydrogen and oxygen evolution.
10	Same as literature.[9]	Same as literature.[9]	Bubble formation at the negative electrode is included in the model, taking into account the attendant reduction in the liquid volume and the transfer of momentum between the gas and liquid phases, using a modified multiphase-mixture approach. Numerical simulations are compared to experimental data for different vanadium concentrations and mean linear electrolyte flow rates, demonstrating good agreement. Comparisons to simulations with negligible hydrogen evolution demonstrate the effect of gas evolution on the efficiency of the battery. The effects of reactant concentration, flow rate, applied current density and gas bubble diameter on hydrogen evolution are investigated. Significant variations in the gas volume fraction and the bubble velocity are predicted, depending on the

			operating conditions.
11	Same as literature.[10]	Similar to the literature[10] but with following differences: - Electrode conductivity = 363 S/m; - Carbon collector conductivity = 5000 S/m; - Cathodic rate constant = 1.25×10^{-7} m/s; - Oxygen evolution exchange current density = 10^{-9} A/m^2; - Oxygen transfer coefficient = 0.3; - Electrode fibre diameter = 172 µm; - Oxygen bubble diameter = 50 µm; - Specific surface area = 3×10^6 m^{-1}; - Initial temp. = 298 K.	The multi-phase mixture model is used to describe the transport of oxygen in the form of gas bubbles. Numerical simulations are compared to experimental data, demonstrating good agreement. Parametric studies are performed to investigate the effects of changes in the operating temperature, electrolyte flow rate and bubble diameter on the extent of oxygen evolution. Increasing the electrolyte flow rate is found to reduce the volume of the oxygen gas evolved in the positive electrode. A larger bubble diameter is demonstrated to increase the buoyancy force exerted on the bubbles, leading to a faster slip velocity and a lower gas volume fraction. Substantial changes are observed over the range of reported bubble diameters. Increasing the operating temperature was found to increase the gas volume as a result of the enhanced rate of O_2 evolution. The charge efficiency of the cell drops markedly as a consequence.
12	- Charge conservation - Activation overpotential - Butler-Volmer - Fick's law of diffusion - Faraday's law	- Values are dependent on the compression rate which ranges from 0 to 63.6%; - The pressure at the outlets is arbitrarily set to 100 mbar; - Mass flow rate = 1.41×10^{-4} kg/s; - Current density = 400 A/m^2; - Rate constants = 1×10^{-8} m/s.	A reduction of the electrode thickness by compression lowers the area specific resistance (ASR), the porosity and the hydraulic permeability, which results in a better cell performance but also a higher pressure drop. The electrode compression mainly reduces the ohmic losses. Furthermore, the ASR has a high sensitivity to changes of the specific surface area and the reaction constant. These material parameters control the activation overpotentials of the reactions and are independent of the compression. High ohmic resistances are observed.
13	- Conservation of species; - Charge conservation; - Bruggemann correction; - Darcy's law; - Navier-Stokes equation;	- Porosity = 0.929; - Specific surface area = 1.62×10^4 m^2; - Electronic conductivity = 1000 S/m; - Carbon fiber diameter = 1.76×10^{-5} m; - Kozeny-Carman constant = 4.28;	It is shown that the velocity distribution in the given geometry of cell has a symmetric pattern in the electrode domain. The lower velocity in the electrode will cause the higher overpotential, which will result in the side reaction and corrosion of key materials locally. In the region closed to the inlet and outlet, transfer current density

	- Brinkman equation; - Carman-Kozeny equation; - Butler-Volmer	- Length = 0.046 m; - Width = 0.03 m; - Thickness = 0.003 m; - Electrolyte viscosity = 4.928×10^{-3} Pa s; - Initial vanadium concentration = 1500 mol/m^3; - Initial proton concentration = 4500 mol/m^3; - Cathodic rate constant = 1.7×10^{-7} m/s; - Volumetric flow rate = 27 mL/min; - Applied current density = 40-80 mA/cm^2	has relatively high value where high velocity occurs. The distributions of concentration, overpotential and transfer current density along electrode/current collector interface reveal the corresponding variational rules on the intersections of slices and interface. The uniformity of the distribution of velocity of electrolyte in the electrode is the key point to the optimal design of the vanadium redox flow battery.
14	- Transport in flow channel; - Transport through porous electrode (Nernst-Planck equation, Darcy's Law, Kozeny-Carman equation, electroneutrality and conservation of species and charge); - Transport through membrane; - Reaction kinetics	- Kozeny-Carman constant = 5.55; - Electrolyte viscosity = 1.07×10^{-6} m^2/s; - Electrolyte density = 1500 kg/m^3; - Electrode conductivity = 1000 S/m; - Cathodic rate constant = 1.75×10^{-7} m/s; - Anodic rate constant = 3×10^{-9} m/s; - Electrode thickness = 3 mm; - Electrode height = 10^{-1} m; - Electrode width = 10^{-1} m; - Temperature = 300 K; - Electrode porosity = 0.7; - Electrode fiber diameter = 17.6 µm; - Initial [V(II)] = 1200 mol/m^3; - Initial [V(III)] = 300 mol/m^3; - Initial [V(IV)] = 300 mol/m^3; - Initial [V(V)] = 1200 mol/m^3; - Initial proton concentration = 3000 mol/m^3; - Initial [HSO_4^-] = 3000 mol/m^3; - Current density = 400 A/m^2; - Volumetric electrolyte flow rate = 5 mL/s.	Results show that when a flow field is included a reduction in overpotentials depends not only on whether a flow field can ensure a more even distribution of electrolytes over the electrode surface, but also on whether the flow field can facilitate the transport of electrolytes from the flow field towards the membrane, improving the distribution uniformity in the through-plane direction. It is also shown that the pumping power varies with the selection of flow fields at a given flow rate. Results indicate that there is an optimal flow rate for each type of flow field at which the maximum power-based efficiency can be achieved. Also the cell with the serpentine flow field at the optimal flow rate shows the highest energy-based efficiency and round-trip efficiency (RTE).
15	- Navier-Stokes; - Electroneutrality;	This involves a pore-scaled resolved model with different path-lengths. However, some common data as for	The detailed geometry of the electrode is obtained using X-ray computed tomography (XCT) and calibrated against experimentally

	• Charge conservation; • Butler-Volmer; • Nernst equation; • Mass and momentum balance; • Species balance; • Charge conservation; • Lattice Boltzmann method for fluid flow; • Finite volume method for charge and species transport	continuum models involve: • Porosity = 0.9256; • Specific surface area = 41.9 mm^{-1}; • Mean pore diameter = 115.5 µm; • Mean fibre diameter = 15.16 µm; • Solid conductivity = 1000 S/m; • External current density = 400 A/m^2; • Transfer coefficient (for all electrodes and states) = 0.5; • Cathodic rate constant = 1.7×10^{-7} m/s; • Anodic rate constant = 6.8×10^{-7} m/s; • Operating temperature = 298 K; • Total [vanadium] = 2000 mol/m^3; • Initial $[H^+]^{+ve\ electrode}$ = 4000 mol/m^3; • Initial $[H^+]^{-ve\ electrode}$ = 6000 mol/m^3; • Initial [water] = 4200 mol/m^3; • [Fixed charge site] = 1200 mol/m^3.	determined pore-scale characteristics (e.g., pore and fiber diameter, porosity, and surface area). The processed XCT data is then used as geometry input for modeling of the electrochemical processes in the VRFB. The flow of electrolyte through the pore space is modeled using the lattice Boltzmann method (LBM) while the finite volume method (FVM) is used to solve the coupled species and charge transport and predict the performance of the VRFB under various conditions. An electrochemical model using the Butler–Volmer equations is used to provide species and charge coupling at the surfaces of the carbon fibers. The cell voltage and overpotential for idealized geometries as a function of the active surface area and the state of charge (SOC) are examined first and the results are compared with a simplified model based on charge conservation, as well as those obtained using volume-averaged models. The pore-scale model is then used to study the averaged and local species concentration, overpotential, and current density based on detailed XCT geometries. The performance predictions from the present model show good agreement with macroscopic models and experimental observations.
16	Same as literature.[15]	Same as literature[15] except a few changes: • Porosity = 0.929; • Specific surface area = 16200 m^{-1}; • Half-cell width = 0.003 m; • Average velocity = 0.014 m/s; • Initial [vanadium] = 1500 mol/m^3.	Localized, averaged and statistical distributions of concentration, overpotential and current density fields across the tested 3D electrode domains are determined to identify the key parameters affecting the electrolyte flow and utilization. The results show that overall cell voltage increases with increasing flow rate for the investigated electrode morphologies and SOCs as a result of decreasing concentration gradients. However, the marginal gain in cell voltage diminishes once the concentration field approaches uniformity at sufficiently high flow rates. It is also observed that cell performance improves for denser electrode structures with more active surface area, as a result of more uniform and lower absolute current density and overpotential fields. Finally, the simulations suggest that a significant detriment to the performance of a VRFB

			occurs in the event of fuel starvation for low electrolytic concentrations and low flow rates.
17	• Butler-Volmer kinetics; • Tafel equation; • Arrhenius form of exchange current density; • Nernst equation; • Gibbs free energy; • Peclet and Sherwood numbers; • Species conservation; • Nernst-Planck equation; • Bruggeman relation; • Stokes-Einstein equation; • MacMullin number; • Charge conservation equation (Phase potential equation); • Ohm's law; • Conservation of mass and momentum; • Darcy's Law; • Carman-Kozeny model; • Energy conservation eq.	Including thermal parameters, following considered: • Electrode height = 10 cm; • Width = 10 cm; • Thickness = 0.4 cm; • Collector thickness = 6.3 mm; • Electrode mean pore size = 0.02 mm; • Electrolyte volume in tank = 250 mL; • Electrode transfer coefficient = 0.5; • Electrode conductivity = 500 S/m; • Collector conductivity = 1000 S/m; • Temperature = 298 K; • Inlet flow rate to electrode = 1 mL/s; • Pressure = 3 atm.; • Current = 10 A; • Cathodic rate constant = 1.7×10^{-7} m/s; • Anodic rate constant = 6.8×10^{-7} m/s; • Contact resistance between electrode and collector = 50 Ω m^2; • Electrode volumetric porosity = 0.8 • [V(II)] = [V(V)] = 27 mol/m^3; • [V(III)] = [V(IV)] = 1053 mol/m^3; • $[H^+] = [HSO_4^-]$ = 1200 mol/m^3; • $[SO_4^{2-}]^{positive}$ = 2174 mol/m^3; • $[SO_4^{2-}]^{negative}$ = 1607 mol/m^3.	At pore level, the diffusion timescale and Peclet number are dependent on pore dimension, and were found to be around 1 second and 1,000, respectively, in the case of study. Analysis also indicated that electrolyte pumping power accounts for a very small portion of RFB power product (<0.1% in the case of study). It was observed that peak temperature appears near the separator initially, and then shifts to downstream for both charging and discharging operations. It takes about 60 s for temperature to be stabilized, which is consistent with the timescale analysis on heating (~10 s) and convective cooling (~40 s). The V(V) concentration at the outlet shows a rapid change in the initial seconds when switching operation. Most transfer current production occurs near the separator. The Damköhler (Da) number indicated that the macroscopic diffusive resistance is significant in the transverse direction, relative to the reaction kinetics. The transfer current changes little from the upstream to downstream during the initial periods of charging and discharging.
18	Same as literature.[15]	• Reservoir electrolyte volume = 2.232×10^{-4} m^3; • Electrode volume = 4×10^{-5} m^3; • Porosity = 0.67; • Electrode width = 0.004 m;	The simulation results reveal that the mass transfer and cross over effects, which were not captured by other continuum models in the literature, can have a significant impact on the voltage response. Mass transfer effects increase the overpotential and thus reduce the

		Current collector width = 0.005 m; Electrode breadth = 0.1 m; Electrode height = 0.1 m; Specific surface area for reaction = 420 m^{-1}; Collector conductivity = 9.1×10^4 S/m; Electrode conductivity = 100 S/m.	battery output voltage during discharge. Vanadium crossover causes a concentration imbalance between the two half-cells that negatively affects the voltage response particularly after long term cycling.
19	As in literature[18] and also including the determination of: distribution of the pressure and of the flow velocity in cell; distribution of the chemical species in the cell taking into account electrochemical interaction; distribution of the electric field and of the current density in the cell.	Carman-Kozeny constant = 4.28; Electrode width = 52×10^{-3} m; Electrode length = 77×10^{-3} m; Electrode thickness = 3×10^{-3} m; Porosity = 0.929; Specific surface area = 1.62×10^4 m^2; Fiber diameter = 17.2×10^{-6} m. Electrolyte viscosity = 4.928×10^{-3} Pa s; Initial [vanadium] = 0.5 mol/L; Initial [proton] = 5 mol/L; Cathodic rate constant = 1.7×10^{-7} m/s; Anodic rate constant = 6.8×10^{-7} m/s; Temperature = 300 K; Electrolyte volume in each tank = 0.1 L; Volumetric flow rate = 1.67×10^{-6} m^3/s.	The numerical solution of equations of fluid dynamics and of electrochemistry is carried out by means of the method of coarse particles combined by the iteration process. The analysis of the calculation results combined with experimental data allows to obtain the main characteristics of the VFB—the voltage, the current and the internal resistance. Numerical results are found to be consistent with experimental values.
20	Open circuit voltage by Nernst equation; Temperature prediction; Thermal effect on voltage; Concentration overpotential unit involving Fick's first law; Internal resistance; State space model; Extended Kalman filter method	Electrolyte density = 1400 kg/m^3; [Vanadium] = 1.5 M; Electrode area = 875 cm^2; Specific heat of electrolyte = 3200 J/kg-K; Charging resistance = 0.015 Ω; Discharging resistance = 0.024 Ω; Electrolyte flow rate = 125 cm^3/s; Initial SOC = 0.1; Operating temp. = 298 K; Current density = 50 mA/cm^2.	Extended Kalman filter (EKF) method is proposed for SOC estimation for VRBs. By measuring the stack terminal voltages and applied currents, SOC can be predicted with a state estimator instead of an additional open circuit flow cell. To implement EKF estimator, an electrical model is required for battery analysis. A thermal-dependent electrical circuit model is proposed to describe the charge/discharge characteristics of the VRB. Two scenarios are tested for the robustness of the EKF. For lab testing scenarios, the filtered stack voltage tracks the experimental data despite the model errors. For the online operation, the simulated temperature rise is

			observed and the maximum SOC error is within 5.5%. It is concluded that EKF method is capable of accurately predicting SOC using stack terminal voltages and applied currents in the absence of an open flow cell for OCV measurement.
21	• Modified Nernst–Planck equation; • Darcy's law; • Butler-Volmer; • Species and material balances; • Mass flux from flow channel to catalyst layer (limiting current density); • Relation between diffusivity and Peclet number; • Relation between mass flux and mass transfer coefficient	• Electrolyte volume in each half cell = 20 mL; • Initial proton concentration = 3 M; • Commercial graphite felt used with physical properties given in corporate website (SGL Carbon).	It is found that the effect of flow dispersion becomes more significant with an increase in flow rates. The pore-level mass-transfer coefficient is found to be independent of current density and the correlation equation in terms of Reynolds number and the intrinsic diffusivity has been proposed.

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