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Unit cell model of a regenerative Hydrogen-Vanadium fuel cell

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REGENERATIVE HYDROGEN-VANADIUM FUEL CELL (RHVFC)

- A RHVFC that combines an aqueous vanadium electrolyte V(V)/V(IV) and hydrogen has been recently introduced[1],[2].

- During discharging, V(V) is reduced to V(IV) and hydrogen is oxidized, while the reverse process occurs in charging mode and hydrogen is stored.

- A better energy storage solution because of its fast hydrogen kinetics and reduced vanadium inventory, while any electrolyte cross-over that occurs to the hydrogen side can be readily collected and returned back to the catholyte tank.

Table 1. Comparison of electrochemical energy storage systems. Modified from [3].

ECES	Pb-A	Na-S	Zebra	Li-ion	H₂	H₂-V	FB
Scalability	Good	Good	Good	High	High	High	High
Flexibility	Good	Good	Good	Good	High	High	High
W-Wh independency	No	No	No	No	Yes	Yes	Yes
Environmental impact	Low	Low	Low	Low	Low	Low	Low
Safety	Low	Mild	Mild	Low	Mild	Mild	Low

ECES electrochemical energy storage; Pb-A advanced lead-acid; Na-S sodium-sulphur; Li-ion lithium-ion; H_2 electrolyzer/fuel cells; H_2-V hydrogen-vanadium fuel cell; FB flow battery.
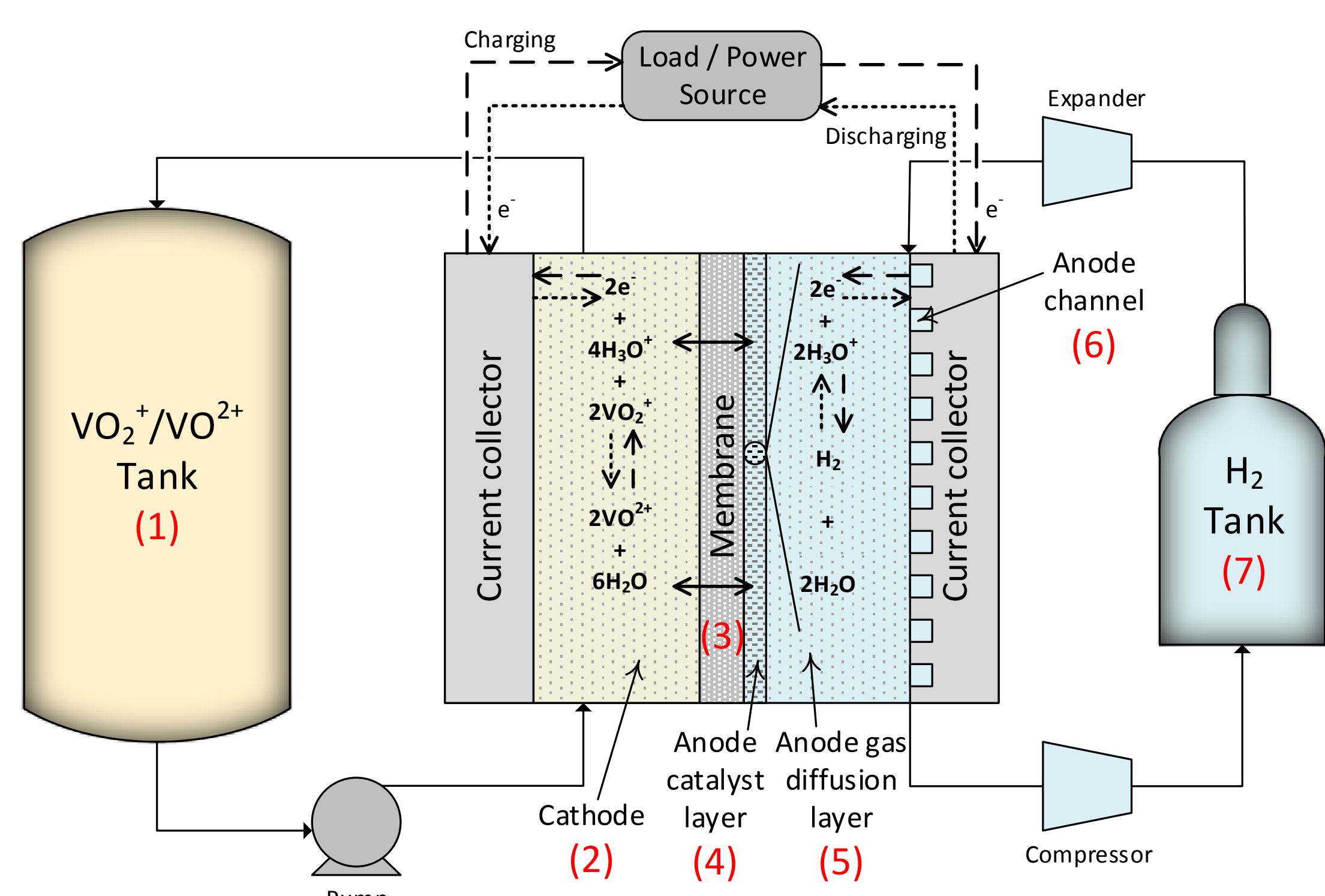

Figure 1. schematic diagram of a RHVFC, showing the model domains: (1) vanadium tank, (2) cathode, (3) membrane, (4) anode catalyst layer, (5) anode gas diffusion layer, (6) anode channel, and (7) hydrogen storage tank.

MODEL DEVELOPMENT

- A model has been developed by coupling mass transport and electrochemical phenomena, and is capable of predicting cell voltage under different operating conditions such as current, flow rate and state of charge.

- The approach is based on reported mathematical models for all-vanadium flow battery, polymer-electrolyte-membrane fuel cell and hydrogen-bromine fuel cell.

- Open Circuit Voltage (OCV) simulation considers the complete Nernst equation [4] using proton activity at each half-cell that is varying at the cathode and the anode, and the Donnan potential across the membrane.

- The time-dependant 0D model considers 7 domains, which are shown bellow together with the phenomena present at each one of them.
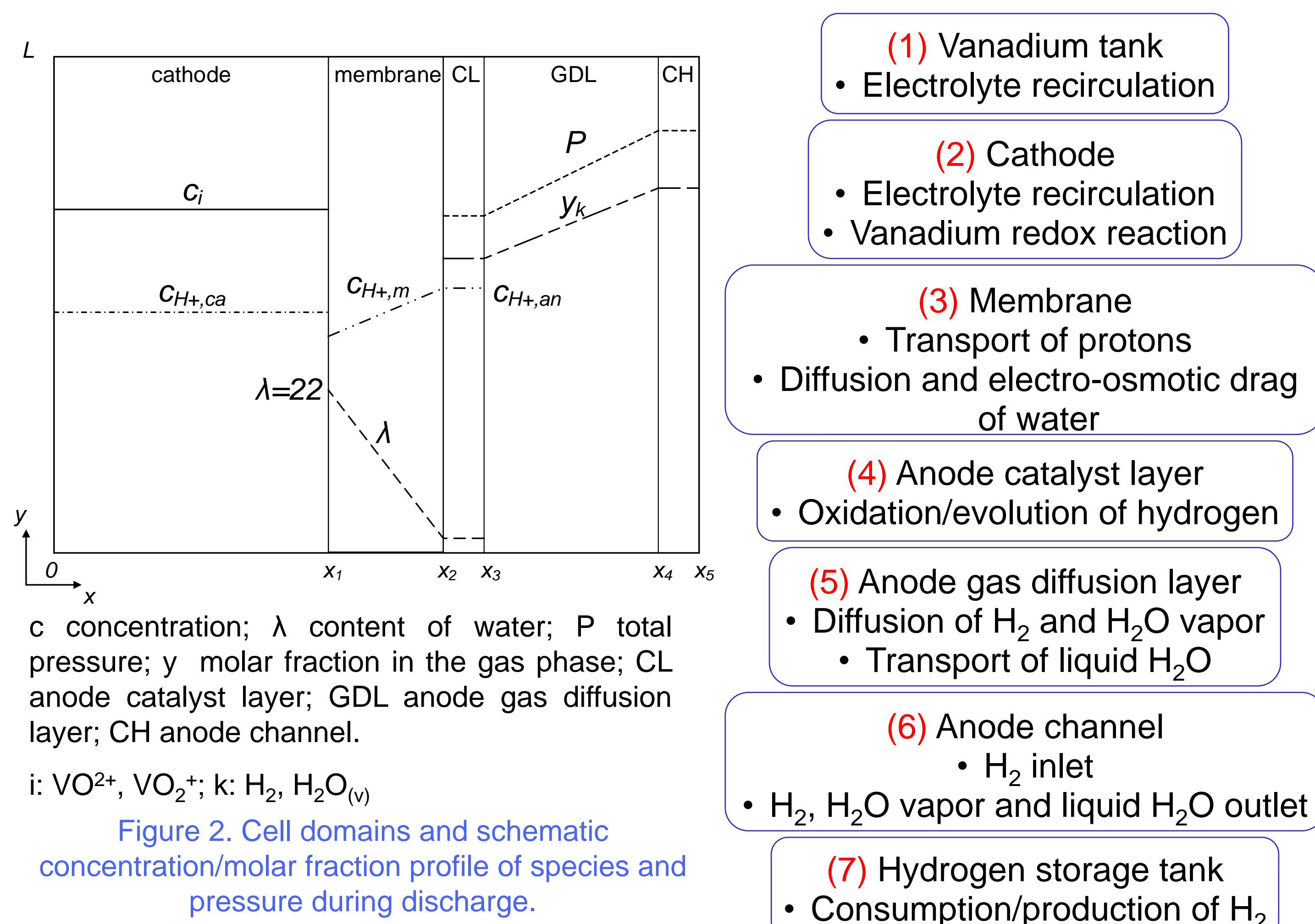
c concentration; λ content of water; P total pressure; y molar fraction in the gas phase; CL anode catalyst layer; GDL anode gas diffusion layer; CH anode channel.

i: VO^{2+}, VO_2^+; k: H_2, $H_2O_{(v)}$

Figure 2. Cell domains and schematic concentration/molar fraction profile of species and pressure during discharge.

(1) Vanadium tank
- Electrolyte recirculation

(2) Cathode
- Electrolyte recirculation
- Vanadium redox reaction

(3) Membrane
- Transport of protons
- Diffusion and electro-osmotic drag of water

(4) Anode catalyst layer
- Oxidation/evolution of hydrogen

(5) Anode gas diffusion layer
- Diffusion of H_2 and H_2O vapor
- Transport of liquid H_2O

(6) Anode channel
- H_2 inlet
- H_2, H_2O vapor and liquid H_2O outlet

(7) Hydrogen storage tank
- Consumption/production of H_2

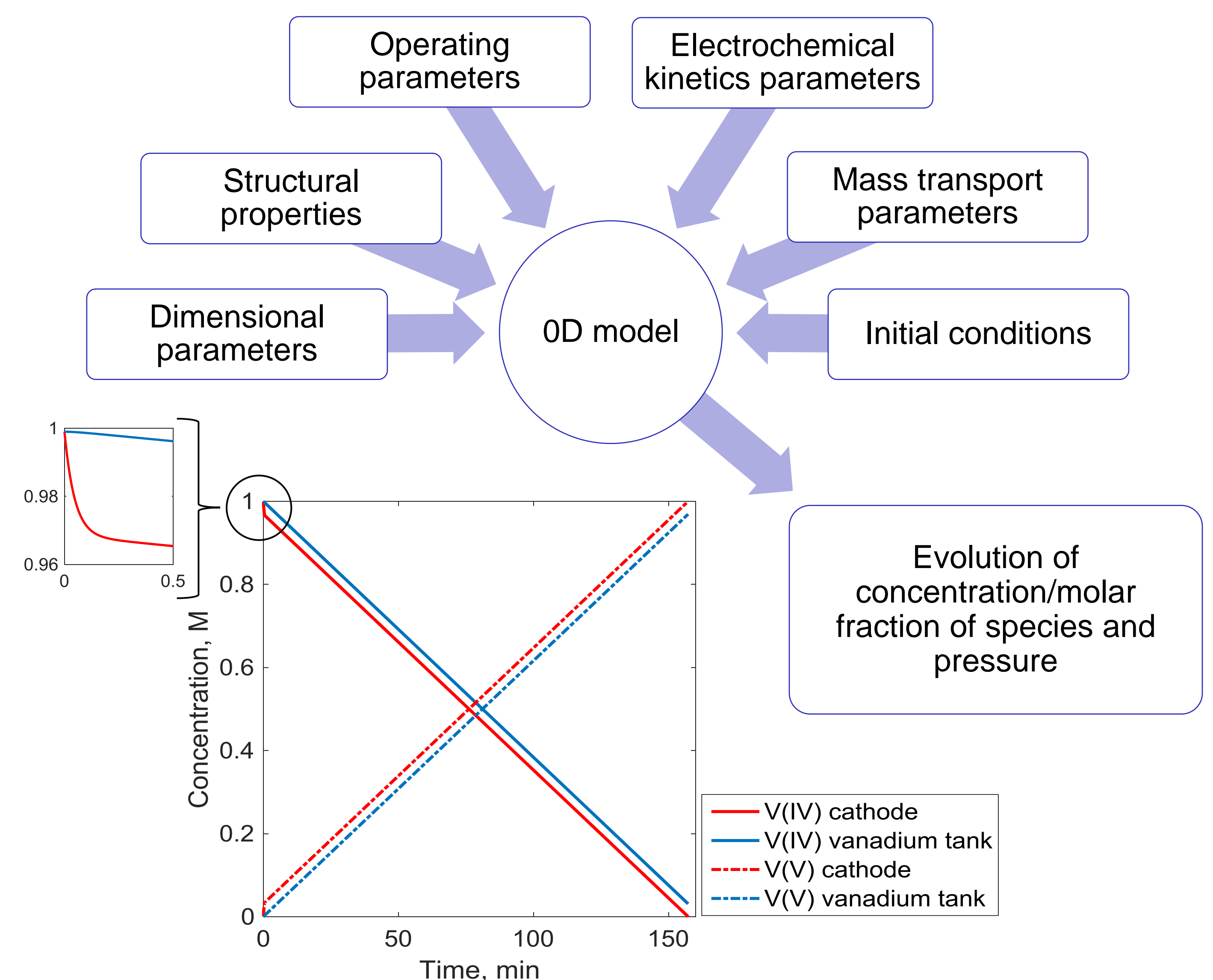- Inputs/outputs of the time-dependant 0D model

Figure 3. Evolution of V(IV) and V(V) concentration during charge.

EXPERIMENTAL & RESULT

In-house manufactured RHVFC

- Cross-sectional area of 131 cm².

- Catholyte (500 mL) 1M $VOSO_4$ dissolved in 5M H_2SO_4.

- Constant applied current density of 38 mA cm⁻².

- Catholyte flow rate of 100 mL min⁻¹.
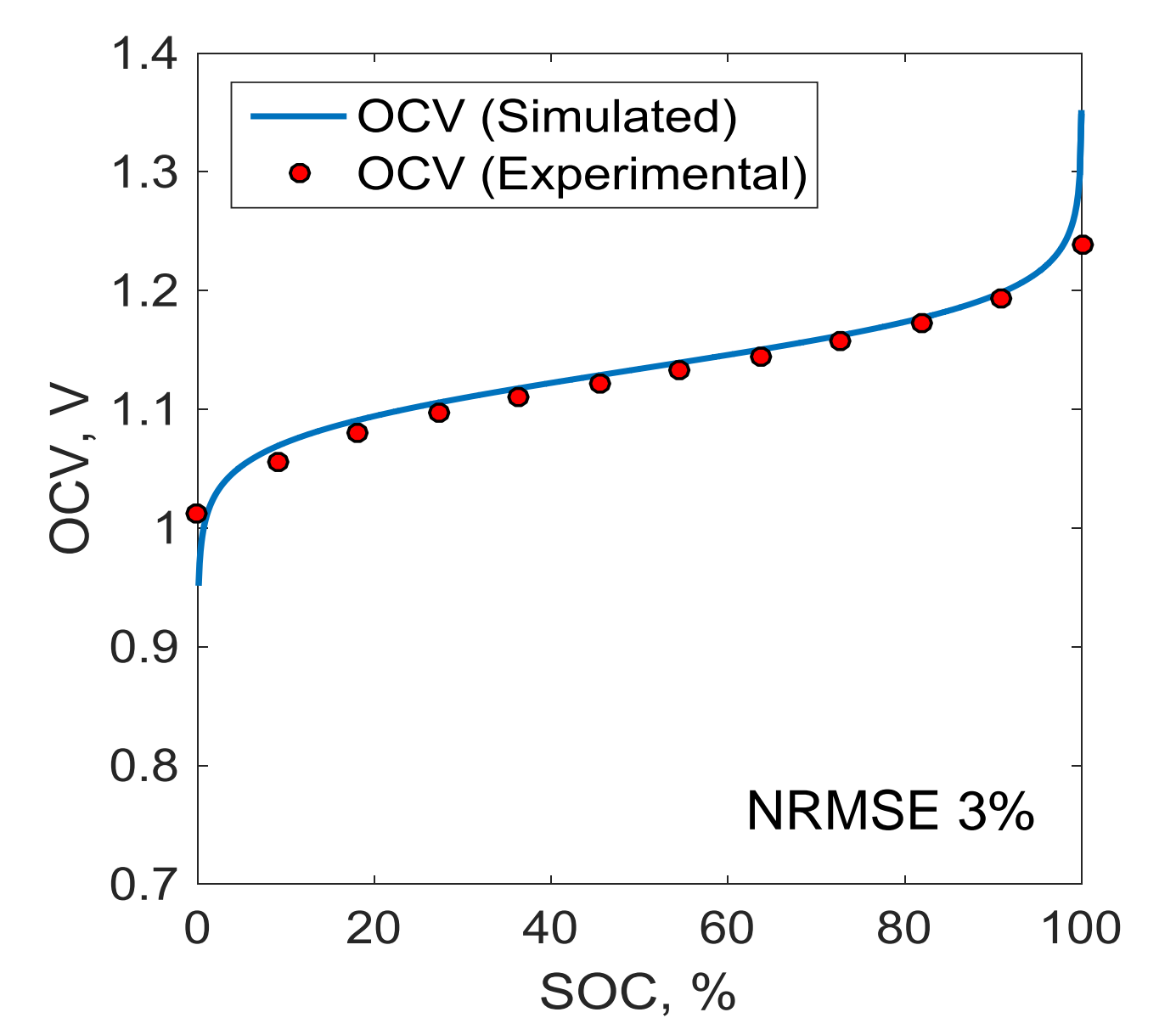
- Hydrogen flow rate of 600 mL min⁻¹.

Figure 4. Comparison of simulated and experimental values: OCV vs SOC.

$$E_{OCV} = E_{cell}^0 + \frac{RT}{F} \ln\left(\frac{[VO_2^+][H^+]_{ca}^2 \left(p_{H_2}\right)^{0.5}}{[VO^{2+}][H^+]_{an}} \right), \quad E_{cell}^0 = 0.99V$$

CONCLUSIONS & FURTHER WORK

- An accurate model of a RHVFC is essential for system performance evaluation and optimisation.

- A time-dependent 0D model has been developed, using the complete Nernst equation to predict OCV.

- Simulated OCV shows a good fit to the experimental data with a NRMSE of 3% which responds mainly to the difference at 0% and 100% of SOC. Agreement of experimental and simulation results demonstrates the model fidelity.

- Further work will use the model as the basis for RHVFC stack and system performance evaluation.

ACKNOWLEDGEMENTS

REFERENCES

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[3] P. Alotto, M. Guarnieri, and F. Moro, "Redox flow batteries for the storage of renewable energy: A review," Renew. Sustain. Energy Rev., vol. 29, pp. 325–335, 2014.

[4] K. W. Knehr and E. C. Kumbur, "Open circuit voltage of vanadium redox flow batteries: Discrepancy between models and experiments," Electrochem. commun., vol. 13, no. 4, pp. 342–345, Apr. 2011.