# A 3D Hydraulic Model for Flow Battery Stack Design Optimisation

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## Introduction

- A 3D hydraulic stack model has been developed in COMSOL Multiphysics. The model can simulate the electrolyte flow within active cell areas and the flow in the channels and manifolds of a battery stack.
- Ideally, the graphite felt should be isotropic and homogeneous, firmly attached to the cavity of the flow frame. However, a small bypass flow is usually inevitable in an actual battery cell due to the gaps between the felt and cavity walls, while the porosity of the felt can also be varied due to the thickness variations from manufacturing tolerances.
- This work evaluates the impact of the side gaps and porosity variations of felts by comparing the velocity and pressure distributions within cells, providing a potential countermeasure of applying dimples to control the bypass flow and maintain theoretical flow rates in active cell areas.

## Geometry

- A 3D parameterised stack geometry, as shown in Figure 1, has been built to simulate the hydraulic performance for the study.
- The assumed 1-mm side gaps on both sides of the felt from irregularities are undesirable, which can be mitigated by designing 2-mm dimples protruding from the flow frame into the felt.
- The felt segments with randomly distributed porosities from 0.87 to 0.89 [1] are assumed to estimate the porosity variations of a typical 4 ± 0.5 mm felt in a 3-mm cavity.

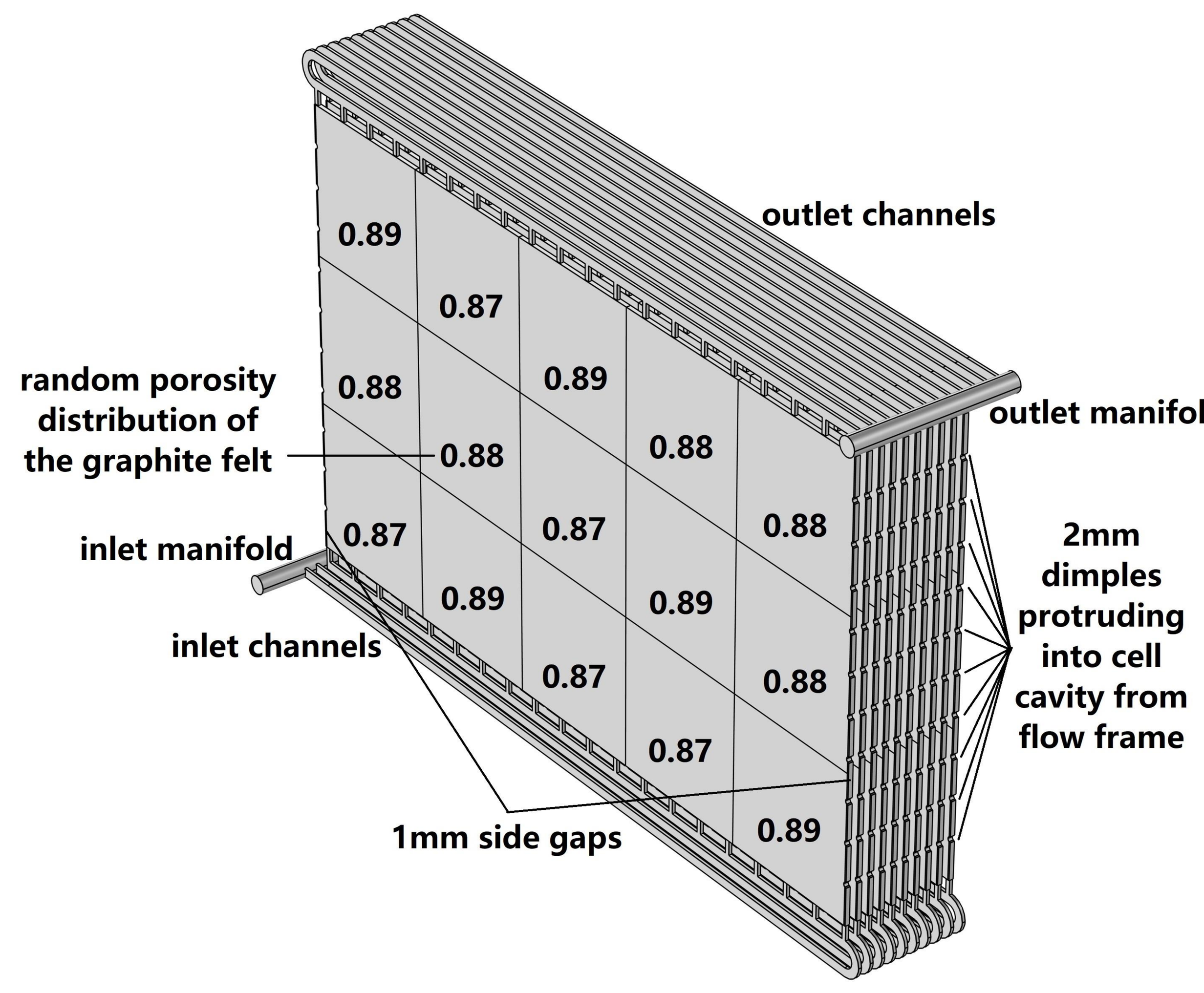


Figure 1. 3D parameterised geometry with the side gaps, porosity segments and dimples.

## Simulation Inputs

- Unless specified otherwise, the input parameters below in Table 1, mainly adapted from [2], are used to simulate the hydraulic performance of the negative half cells of the vanadium flow battery.

Table 1. Default input parameters for the simulations.

| Parameter | Value |
|---|---|
| fluid density | 1354 kg m$^{-3}$ |
| fluid viscosity | 4.928 mPa s |
| total vanadium concentration | 2 mol L$^{-1}$ |
| SOC upper limit of charging | 0.9 |
| charging current | 120 A |
| current density | 80 mA cm$^{-2}$ |
| ratio of applied flow rate to theoretical flow rate | 2 |
| felt size (high, wide, thick) | 300 x 500 x 3 mm |
| felt porosity | 0.88 |
| vertical channel length x width | 10 x 3 mm |
| horizontal channel width | 6 mm |
| channel depth | 2 mm |
| area ratio of manifold to channels | 1 |
| side gap width | 1 mm |
| dimple radius | 2 mm |
| fibre diameter | 17.6 μm |
| Kozeny-Carman constant | 4.28 |

## Simulation Results

- Figure 2 shows the velocity plot of an actual cell with side gaps and porosity segments, illustrating the preferential flow within the side gaps and low-resistance areas of the felt.

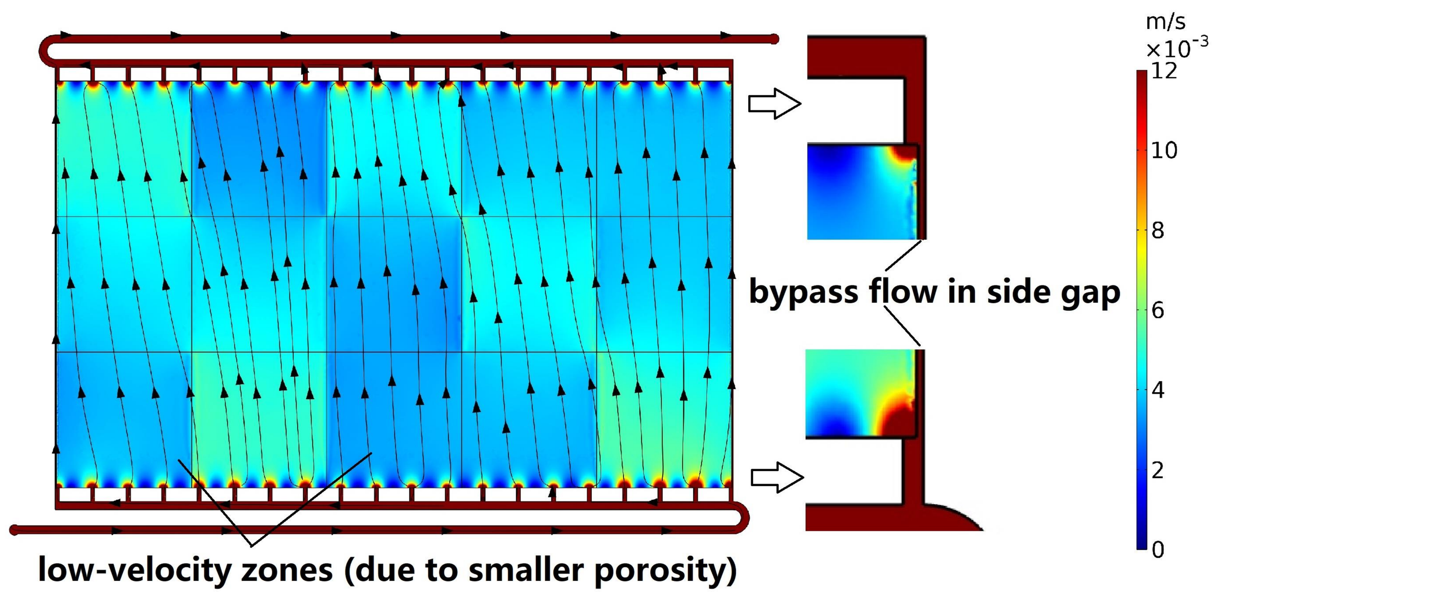


Figure 2. Flow velocity plot of an actual cell with porosity segments and side gaps (zoomed in).

- The actual flow rate in the active cell area is around 4 mm s-1, which is half the theoretical flow rate of approximately 8 mm s-1 as presented in Figure 3 (a).
- This lower flow rate can be alleviated by applying dimples protruding into the cell cavity to control the bypass flow in the side gaps as demonstrated in Figure 3 (b).

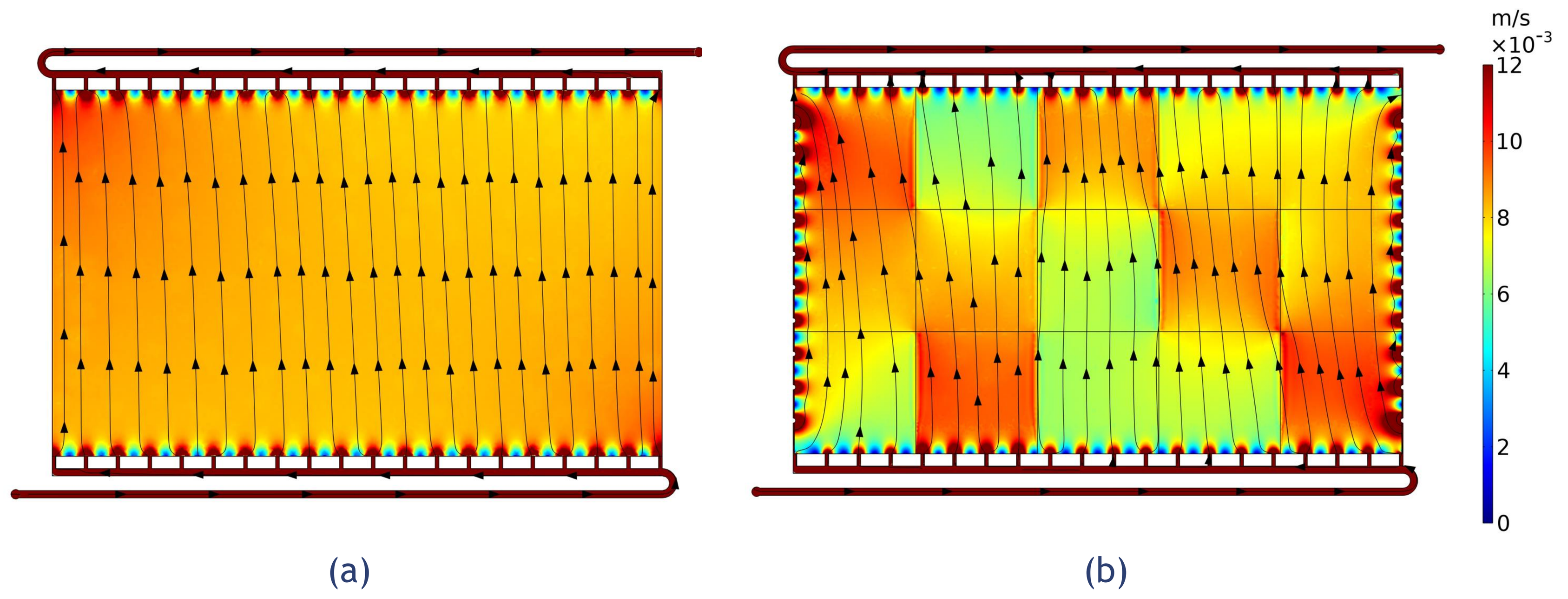


Figure 3. Flow velocity plots of (a) an ideal cell without side gaps and porosity segments; (b) an actual cell with porosity segments and dimples to control the bypass flow in the side gaps.

- As seen in Figure 4, the cell pressure loss significantly drops from the ideal 97.9 kPa to the actual 64.8 kPa with the consideration of side gaps and felt porosity variations.
- The cell pressure drop can be restored to 93.1 kPa by applying the dimples to control the bypass flow in the side gaps, which implies the predominant role of the side gaps towards the pressure difference.

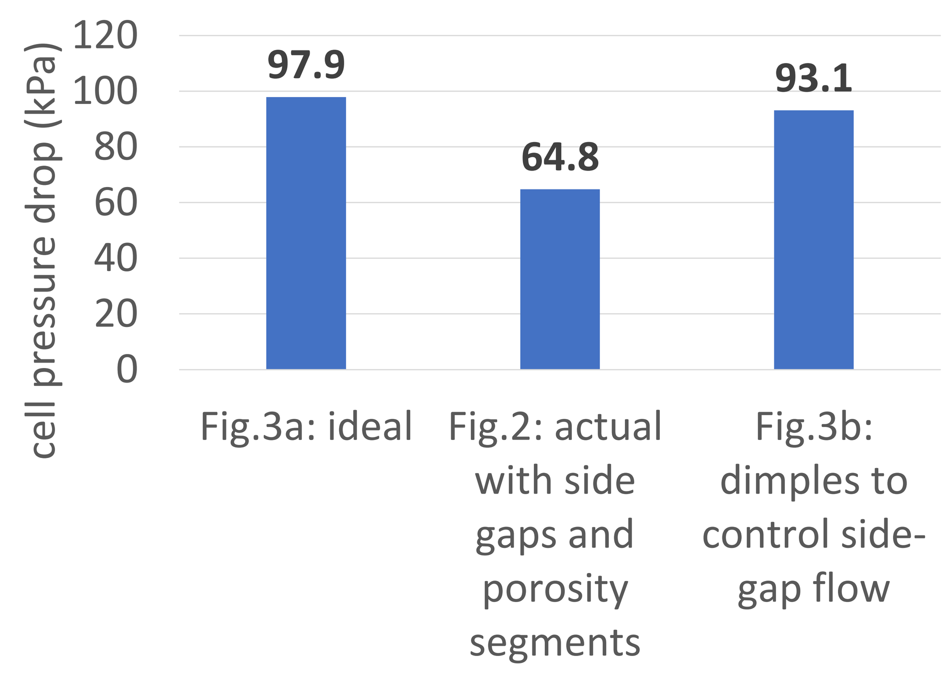


Figure 4. The cell pressure drops of the above cases.

## Conclusion

- The study shows a noticeable difference in the flow velocity and pressure drops between ideal cells without the undesirable side gaps and porosity variations and actual cells with those features.
- The side gaps tend to have a more considerable impact than the porosity segments on the flow velocity and cell pressure loss.
- The hydraulic model with the parameterised stack geometry includes an input interface, which allows the adaption to other chemistries/designs and can be a valuable tool for flow battery optimisation.

## Reference

1. N. Gurieff, V. Timchenko, and C. Menictas, "Variable porous electrode compression for redox flow battery systems," Batteries, vol. 4, no. 4, pp. 1-10, 2018, doi: 10.3390/batteries4040053
2. A. Tang, J. Bao, and M. Skyllas-Kazacos, "Studies on pressure losses and flow rate optimization in vanadium redox flow battery," Journal of Power Sources, vol. 248, pp. 154-162, 2014

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