

WHITEPAPER

BREATHE

HOW WE BUILT A PHYSICS-BASED
BATTERY MODEL PIPELINE

breathebatteries.com

Battery simulation drives battery innovation

Battery systems present an exceptionally complex design space, combining electrochemistry, thermodynamics and mechanics across multiple spatial and temporal scales. Traditional experimental approaches relying on time-intensive and costly empirical testing alone are becoming increasingly insufficient to manage this complexity, especially under the pressure of rapid development cycles and high performance demands. Simulation tools are therefore indispensable. But not all modelling paradigms are created equal.



A BATTERY HAS TWO CHARACTERISTICS NECESSITATING SIMULATION: IT'S COMPLEX, AND IT'S EXPENSIVE TO TEST. YOU CAN'T JUST TEST YOUR WAY OUT OF IT ANYMORE.

Dr Yan Zhao, CTO and Co-founder, Breathe



At Breathe, we anchor our software toolchain and approach to battery innovation in a physics-based modelling framework. Not because it's easier, but because it is fundamentally better suited for capturing the coupled phenomena that define real-world battery behaviour making it a more generalised and extrapolatable framework.

Crucially, we have industrialised our modelling approach to make it scalable, robust, and practical for commercial deployment. From our 7,500 sq ft battery laboratory in the heart of London, we delivered a fully parameterised model every 2.5 weeks in 2024, taking as little as 4-weeks from cell receipt to model delivery.

In this whitepaper, we'll deep dive into our approach to physics-based modelling, and how we developed an industrialised parameterisation process capable of delivering the accuracy, efficiency and scale required to meet our customer's battery development needs.

Why do we use physics-based modelling?

At Breathe we use physics-based models to power our software toolchain. Breathe Model, our cell simulation software, uses a customised SPMe (Single Particle Model with Electrolyte) - a light weight model able to deliver closed-loop control strategy design, providing insightful and accurate access to internal battery states.

Breathe Model is built to deliver an optimal balance between detailed insights, reliability, and computational efficiency. It offers a mechanism-informed approach that preserves fidelity across a broad range of conditions. This is especially critical for:

- Capturing internal states (e.g. anode potential, cathode potential)
- Predicting ageing under real-world duty cycles
- Designing for extrapolation where data is sparse or incomplete

Unlike empirical or data-driven models - which often break down without sufficient training data - physics-based models constrain outputs, with equations serving as robust "guardrails". This allows them to remain reliable even under extrapolated scenarios, such as extreme temperatures, high C-rates, or early failure diagnostics.



EQUATIONS ARE HELPFUL BECAUSE THEY REGULATE INTERACTIONS AND REDUCE THE AMOUNT OF DATA YOU NEED. BATTERIES ARE TOO COUPLED FOR DATA ALONE TO WORK.

Dr Yan Zhao, CTO and Co-founder, Breathe



We also develop our adapted SPMe model hand-in-hand with our parameterisation protocols - not after the fact. The interplay ensures, amongst other things, that the parameters of Breathe Model's equation set align with what is observable and measurable during the parameterisation process.

The Breathe Model pipeline: From physical cell to deployed model

Parameterisation - the process of translating physical battery measurements into usable model inputs - has traditionally been a bottleneck for deploying physics-based battery models at scale. Parameterising a single SPMe model could typically take months, due to:

Coupled physics:

Extracting 50–60 independent parameters (e.g. thermal, electrochemical, kinetic) requires isolating complex relationships.

Experimental barriers:

Obtaining open circuit voltage (OCV) curves, reaction kinetics, and temperature-coupled behaviour is slow, requires advanced and expensive equipment and is sometimes experimentally infeasible.

Estimation complexity:

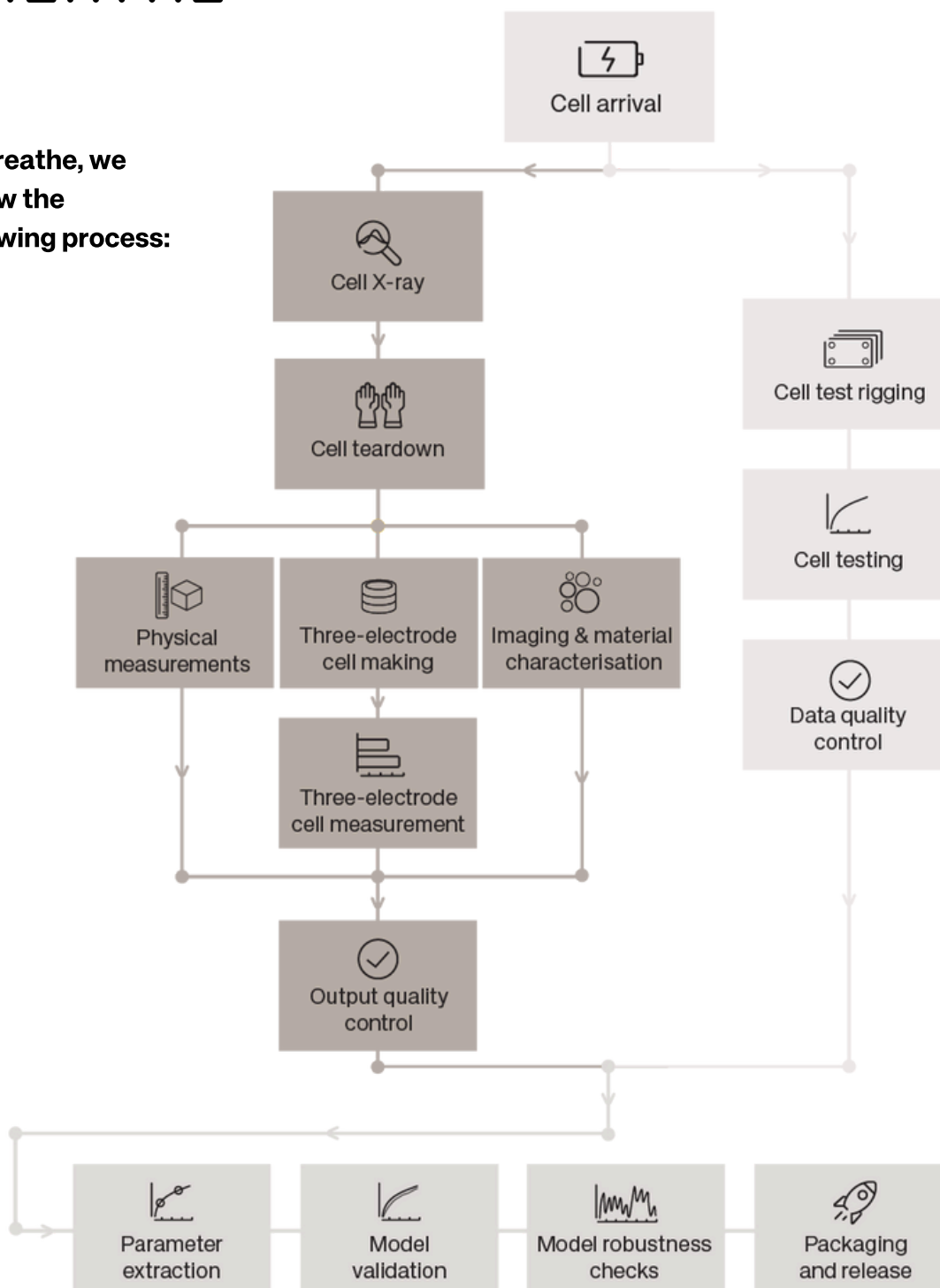
Even when data is available, reliably fitting the model is non-trivial. Early methods lacked robustness and clarity, requiring major manual input and iteration.



These are not just experience problems - they are organisational and interdisciplinary challenges.

At Breathe, we've transformed this bottleneck into a strength, establishing an industrialised pipeline capable of producing high-quality, reliable models in a matter of weeks rather than months.

At Breathe, we follow the following process:



KEY

Testing

Our testing team is responsible for cell-level tests, developing and maintaining our test infrastructure, receipt and safe storage of cells and maintaining testing quality.

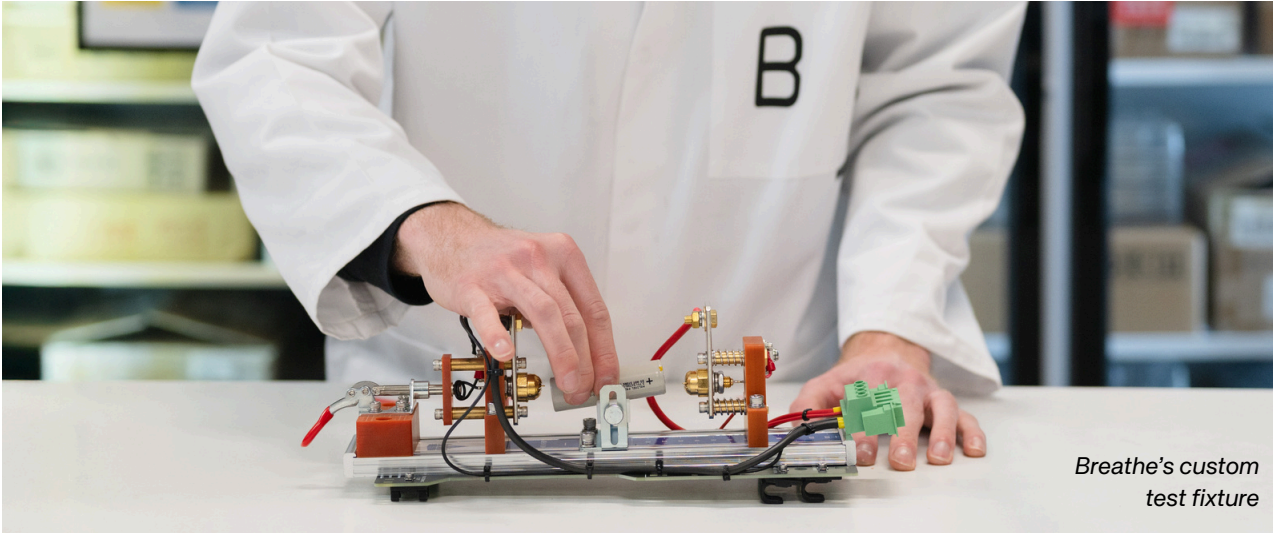
Cell chemistry

Our cell chemistry team is responsible for our glovebox environment, sub-cell testing and characterisation, cell teardown and identifying the most robust methods of parameter extraction.

Modelling

Our modelling team is responsible for building and delivering the model, including robustness checks, validation and delivery.

Testing



*Breathe's custom
test fixture*

ACTIVITY	OUTPUT	TOOLS
Cell arrival	Cell weight, cell health measurements	Scale, handheld battery tester
Cell test rigging	Quality controlled test environment	Custom cell test fixture
Cell testing	Cell capacity, OCV, constant current, kinetic test data, model validation data	Battery cyclers and thermal chambers



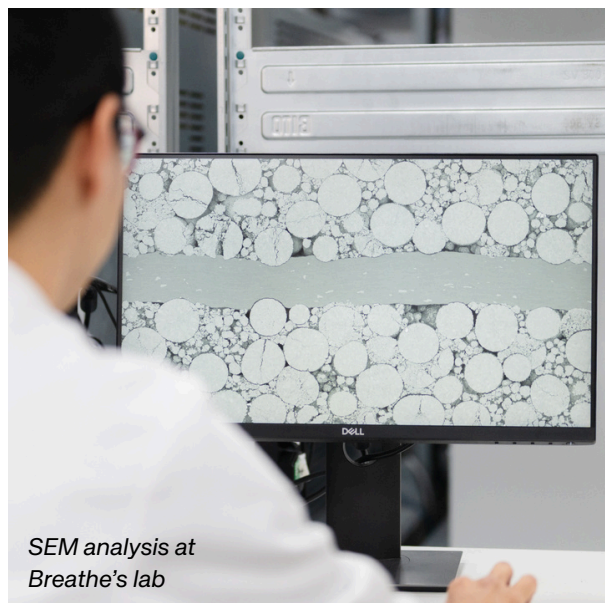
*Breathe lab with Keysight, Arbin
and Binder equipment*

Cell chemistry

ACTIVITY	OUTPUT	TOOLS
X-ray	X-ray to support safe teardown	X-ray service
Cell teardown	Cell components for analysis	Glovebox, custom cell cutting rig
Physical measurements	Length, width, thickness, area of electrode / separator / current collectors, mass and thickness of electrodes, electrode conductivity	Ruler, calliper, thickness gauge, microbalance and electrode resistance measurement system
Three-electrode cell measurements	Electrode OCVs, hysteresis and stoichiometric limits, electrode capacity	High-precision three-electrode battery cycler
Imaging & material characterisation	Porosity and volume ratio binder, active material(s) of electrodes	Scanning electron microscopy, energy-dispersive X-ray spectroscopy, mercury intrusion porosimetry



Breathe's laboratory tooling

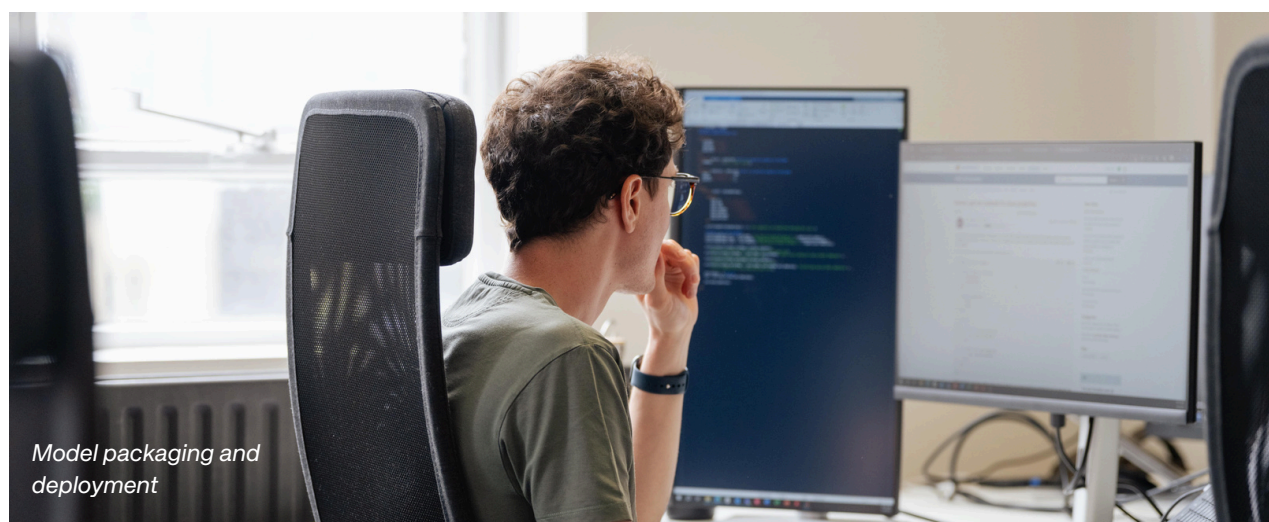


SEM analysis at Breathe's lab

Modelling



ACTIVITY	OUTPUT	TOOLS
Parameter extraction	Thermodynamic and kinetic parameters	Python, Matlab, CASADI
Model validation	Model validation data	Matlab, Simulink
Model robustness check	Stress-test results	Matlab, Simulink
Packaging and release	Final model delivery	DevOps tools



Quality assurance: Validation and robustness testing

Every model is subjected to a number of validation and robustness procedures to ensure its accuracy across use cases. We perform cell level tests in the lab and compare the simulated results to cell level results. Testing includes:

- **Validation against held-out experiments:** This ensures predicted outputs align with unseen physical behaviour.
- **Robustness checks:** We systematically exercise the model across extreme and corner cases to test for divergence or instability.
- **Deployment constraints:** The final model is bounded with metadata describing its valid operating domain - temperature, C-rate, SoC window - ensuring reliable use in different scenarios.

We also maintain a policy of transparency in model capability, allowing customers to know where the model excels and where it may require caution. This ensures battery engineers have full confidence and trust in the model and its ability to answer their most critical questions.



ONCE WE DO THE PARAMETERISATION, WE VALIDATE IT, THEN DO ROBUSTNESS CHECKING - CAN THE MODEL BREAK, DIVERGE, OR FAIL UNDER DIFFERENT CONDITIONS? THAT'S THE FINAL STEP BEFORE WE DEPLOY. THEN WE'RE TRANSPARENT WITH THE CUSTOMER ON WHERE THE MODEL IS STRONG OR NOT SO STRONG. ENGINEERS CAN USE THE MODEL TO SOLVE QUESTIONS STRIAHT AWAY, RATHER THAN SPENDING CYCLES FIGURING OUT HOW TO BUILD AN ACCURATE MODEL INTERNALLY.



Dr Dhammika Widanalage, Head of Battery Modelling, Breathe



Operational scale: Industrialising for volume and variability

Breathe's pipeline has evolved beyond lab-scale prototyping, drawing from our experience supporting Breathe Charge - our embedded adaptive charge control software - where we have been parameterising physics-based models annually for embedded applications since 2019 to deliver superior charging experiences.

The shift from hand-crafted to industrial parameterisation is not merely one of automation - it's one of culture, process and resilience.

We've gone from calibrating a few models per year to delivering over 40+ high-fidelity embedded models annually. The future target is even more ambitious: producing multiple models per week with robust repeatability across chemistries, formats, and suppliers.

To achieve operational scale to date, we've invested in the highest quality equipment and the world's best battery talent. It has enabled us to build the following:

- **Standardised processes for multi-chemistry compatibility** - we are form factor and chemistry agnostic.
- **Cross-disciplinary workflows** that span experimentalists, modellers, and software engineers.
- **Repeatable instrumentation and automation** to handle diverse cell geometries and conditions.

This allows us to not only serve bespoke projects but also create a high-throughput environment, delivering validated models weekly rather than annually.

Our operational capability is further enhanced through our choice of partners, with our laboratory operating with best-in-class equipment. We buy battery cyclers primarily to parameterise and validate physics-based battery models. We, and our customers, then use those models to generate the data that drives early, impactful decision making, ultimately enabling faster development of lower-cost, higher-performing battery systems.

Choosing reliable partners, such as Keysight, Arbin and Binder, to support our battery model parameterisation and validation efforts ensures we can deliver the quality, speed and level of industrialisation that our customers expect.

Cross-functional specialisation: Building a world-class team

The pipeline integrates contributions across our team, which comprises 20+ PhDs, 20+ nationalities and more than 190 years of battery engineering experience. To deliver our industrialised process, we combine a range of specialisms which include:

- **Cell teardown technicians:** To safely disassemble cells and prepare electrodes.
- **Electrochemical analysts:** To run specialised experiments (three-electrode setups, thermal cycling).
- **Material scientists:** To analyse SEM and porosimetry measurements, even navigating hazardous methods like mercury intrusion.
- **Model developers and validation engineers:** To translate measurement into parameters and validate models under diverse operating conditions.

This enables a seamless loop from lab to model to deployment.



Strategic advantage: Why industrialisation matters

Physics-based modelling is no longer just a research activity constrained to laboratories, unable to be deployed in real-world applications. It is now a strategic differentiator for charge control, cell design, and aging prediction. Our approach to physics-based modelling provides our customers with a unique advantage thanks to:

- **Accurate and stable models** grounded in the real physics of the system with unrivalled visibility and understanding of a cell's internal states.
- **Operational efficiency** that reduces time-to-model from months to weeks, delivering cost savings by reducing the reliance on expensive, resource heavy empirical testing.
- **Model reuse and adaptability** across platforms and use-cases including different cell form factors, chemistries and product applications.

We believe this ability to translate physics into meaningful improvements to battery design, validation and optimisation is the foundation for accelerating battery innovation across sectors - from OEMs to cell designers to integrators.



The journey toward accelerated battery development and a predictive future

The ability to deliver an industrialised modelling pipeline is not only a technical achievement - it's a critical enabler for smarter, faster battery development.

With experience across hundreds of cells - from coin cells to large-format commercial packs, we've codified:

- How to **optimise trade-offs** between test effort and model robustness.
- How to structure team workflows that **maximise insight velocity** while minimising rework.

By combining deep domain expertise in physics-based modelling with scalable infrastructure and workflows, we offer our customers a predictive, cost-effective foundation for both today's decisions - and tomorrow's breakthroughs.



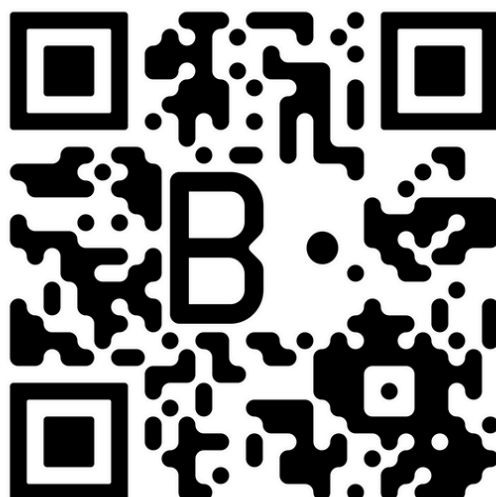
See our parametisation pipeline in action

Download a free Breathe Model instance for Molicel P45B

We're offering an exclusive opportunity for you to try Breathe Model, our cell simulation software, for free.

Get started with a **free Molicel P45B cell instance**. Ready-to-run, so you can get to know Breathe Model.

Simply scan the QR code (or [click here](#)) and fill out the form to receive instant access to your model:



Requirements:

- MATLAB, Simulink & Simscape version R2023a or newer

Features:

- Operating C-rate range of 10C discharge to 5C charge
- Operating temperature range of 0 °C to 50 °C
- Fully validated accuracy
- Transparent performance
- Expertly parameterised
- Instant access to key battery states
- Out-of-the-box worked examples

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About Breathe

Your battery partner

Breathe is more than a battery performance company.

Since being spun out of Imperial College in 2019, our focus has been on building battery technology to accelerate sustainable electrification. Today, we provide a software toolchain for batteries that encompasses the full battery development lifecycle to enable the design, validation and optimisation of better batteries.

Our dream is that one day everyone will breathe clean air. That's why we makes batteries better.

[breathebatteries.com](https://www.breathebatteries.com)

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