BIOVIA

3DEXPERIENCE®

BATTERY CELL DESIGN AND OPTIMIZATION ACHIEVED VIA CONTRACT RESEARCH

Use Cases

As we aim to reduce CO_2 levels and achieve net-zero carbon emissions by 2050, batteries take the center stage. Battery manufacturers, niche cell designers, auto OEMs, eVTOL aircraft manufacturers, and materials companies are investing resources for ground-breaking innovations in battery technology. Batteries are complex systems of materials and their development requires skilled expertise and advanced digital solutions.

DASSAULT SYSTÈMES Contract Research team has been supporting industries such as automotive, aerospace, high technology, mining, energy, advanced materials, consumer packaged goods, Industrial equipment, healthcare, and medical devices for over 25+ years in various R&D areas. Contract Research's multidisciplinary domain experts have developed Advanced Technology Capability (ATC) using 3D chemistry-based software tools (mainly Materials Studio, COSMOtherm, and PipelinePilot). The proprietary ATCs include validated algorithms, content, models, methods, and workflows.

Contract Research offers flexible and collaborative engagements for battery cell design, sub-cell component optimization, manufacturing process improvements, and AI/machine learning-driven battery performance predictions. Working closely with industrial customers, the team provides significant new insights into processes, properties, and products. The Contract Research team helps customers improve their R&D productivity, accelerate their innovations, enable proactive failure remediation, empower them with capabilities for informed decision-making, and fast track their innovative products to market. The strict confidentiality and mutually beneficial IP terms, and timely delivery of goal-focused milestones by Contract Research are the perfect formula for a winning collaboration to create next-generation batteries which are lighter, faster, better, cheaper, safer, and also more easily recyclable.

Contract Research team has helped provide battery solutions to various industries. Due to the nature of the engagements, only high-level information is shared in the case studies.

DASSAULT SYSTEMES

CASE STUDY **1**

Focus Experiments Towards Success

CUSTOMER: A GLOBAL AUTOMOTIVE MANUFACTURER

"Modeling & Simulation results provided by CONTRACT RESEARCH experts enabled us to define and focus our experiments towards the most productive path cutting our time down by 30%"

— Director R&D, Automotive Manufacturer

Challenge

Experiments take too long and are too expensive to search a large chemical space of possible electrolyte alternatives for next-generation cells.

Solution

Contract Research team applied their expertise in building validated models of different electrolytes. Proprietary workflows were utilized for the simulations. The team then performed production runs and analyzed transport, thermal, and electrochemical behavior. The simulated properties were used to rapidly screen the different chemical systems using a "model-first" approach.
In addition, the validated workflows were delivered for further use by the customer.

Results

- 3D Chemistry based models validated against available experimental data
- Virtual twin models of numerous possibilities for electrolytes
- Key properties simulated using first-principles 3D Chemistry methods
- Safety considerations were taken into account by virtual screening of thermal properties
- Identified alternative electrolyte candidates to test in the lab

CASE STUDY **2**

Accelerate Innovation with Workflows

CUSTOMER: AN AUTOMOTIVE MANUFACTURER

"Strong partnership through CONTRACT RESEARCH makes all the difference. Our engineers now use workflows created by validated first-principles 3D Chemistry based modeling & simulations to innovate 40% faster."

— Manager, Cell Design Lab, Automotive Manufacturer

Challenge

Engineering models require experimental data which are sometimes time-consuming to obtain or hard to measure. Experimental data on localized phenomena such as swelling, dendrite growth, degradation, and aging are often impossible to obtain.

Solution

Contract Research team applied first-principles 3D chemistry-based modeling and simulation to obtain key properties in the absence of experimental data. The output from microscale simulations was used as input into engineering scale simulations. The resulting cell performance models were compared with measured data and were seen to perform well. Contract Research delivered validated models and workflows that could be used by cell design engineers.

Results

- Development of workflows for predicting properties; validated against measured experimental data
- Validated workflows for transport properties
- Validated workflows for electrochemical properties
- Validated workflows for local structural & mechanical properties
- Validated workflows for thermal properties

CASE STUDY **3**

Proactive Risk Reduction via Virtual Experiments

CUSTOMER: AN AEROSPACE CONTRACTOR

"The Battery Technology Center used battery materials modeling and simulations expertise of CONTRACT RESEARCH scientific team to save our company both time and money"

— Battery Risk Manager, Aerospace Contractor

Challenge

Batch-to-batch variation of battery materials supplied by a particular vendor resulted in drastic changes in cell performance.

Solution

Contract Research team modeled the material microstructure and simulated key electrochemical processes. Virtual twins of the electrode precursor revealed the source of structural and morphological inhomogeneity that caused variations in the cell performance. A series of "what/if" virtual experiments were conducted to model batch variations and test them with 3D chemistry-based first-principles simulations. From this exercise, the team was able to prescribe a proactive lab test of the material prior to building the cell. The vendor was informed to carry out this test for each batch.

Results

- 3D Chemistry based validated models
- In-depth insights from 3D Chemistry virtual twins
- Output from a series of "what/if" virtual experiments to simulate variations
- Identification of the root cause of failure due to variation of the electrode precursor supplied by the vendor
- Prescription of remedial steps to the vendor to avoid future irregularities

CASE STUDY **4**

Failure Remediation Enabled by Virtual Twins

CUSTOMER: PERSONAL DEVICE MANUFACTURER

"Our company has manufacturing process 'know-how' for decades. CONTRACT RESEARCH team delivered critical process 'know-why' and enabled us to decrease failure rate from 9% to 1%."

— VP R&D, Device Manufacturer

Challenge

The manufacturing process of a particular device resulted in a high failure rate and while different process "knobs" were tweaked and tuned, the failure continued to persist.

Solution

The **Contract Research** team used their expertise in materials and process chemistry and came up with three hypotheses for the possible cause of failure. Using Advanced Technology Capability (ATC) modeling assets, each of the hypotheses was virtually tested. Atomistic and mesoscale models were built and the appropriate steps of the manufacturing process were simulated. Results from the virtual tests were compared with the observed behavior which revealed the reason for the persistent failure. Once the cause was identified, appropriate ATCs were used to formulate a fix to the problem.

Results

- 3D Chemistry based models for the three hypotheses
- In-depth insights from 3D Chemistry virtual twins revealing the cause of the failure from an unexpected source
- Appropriate change to the manufacturing process to remediate the failure

CASE STUDY **5**

Cycle Life Prediction using Machine Learning

CUSTOMER: DEVICE MANUFACTURER

"The CONTRACT RESEARCH team used their battery cell domain expertise combined with machine learning expertise to deliver predictive models for battery life"

— Manager, R&D, Device Manufacturer

Challenge

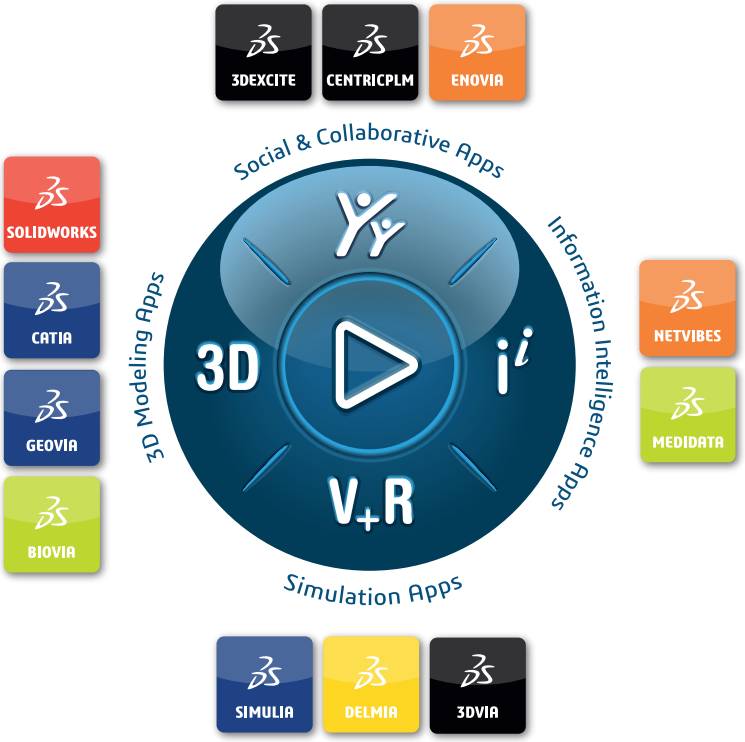
Warranty requirements to meet consumer satisfaction demand better and more accurate prediction of calendar life, cycle life, and operating temperature range which is extremely costly and time-consuming to obtain.

Solution

Customer provided relevant data on their battery cells of interest for a **Contract Research** engagement which rigorously respected the confidentiality agreement. Experts in the Contract Research team used the provided data and generated customer proprietary machine learning models using Pipeline Pilot as the main tool with other technology only available through a Contract Research engagement. The generated predictive models developed by the team was delivered to our customer.

Results

- Machine learning models to predict cycle life from the first few cycles of data
- Models designed to incorporate new data obtainable in the future
- Cost and time efficient methodology for replacing long-term experiments
- Decision-making tool for non-experts to use



Our **3D**EXPERIENCE® platform powers our brand applications, serving 11 industries, and provides a rich portfolio of industry solution experiences.

Dassault Systèmes, the **3D**EXPERIENCE Company, is a catalyst for human progress. We provide business and people with collaborative virtual environments to imagine sustainable innovations. By creating 'virtual experience twins' of the real world with our **3D**EXPERIENCE platform and applications, our customers push the boundaries of innovation, learning and production.

Dassault Systèmes' 20,000 employees are bringing value to more than 270,000 customers of all sizes, in all industries, in more than 140 countries. For more information, visit **www.3ds.com**.

Europe/Middle East/Africa
Dassault Systèmes
10, rue Marcel Dassault
CS 40501
78946 Vélizy-Villacoublay Cedex
France

Asia-Pacific
Dassault Systèmes K.K.
ThinkPark Tower
2-1-1 Osaki, Shinagawa-ku,
Tokyo 141-6020
Japan

Americas
Dassault Systèmes
175 Wyman Street
Waltham, Massachusetts
02451-1223
USA

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