NIPPON SHOKUBAI R&D ACHIEVING SUSTAINABILITY GOAL WITH BIOVIA SOLVATION CHEMISTRY

Customer Story

Challenge:

Support the company's goal of achieving carbon neutrality by 2050 by increasing sustainability for its product lines, including the main business driver superabsorbent polymer and lithium battery electrolyte, at all stages of production, use, and disposal.

Solution:

Nippon Shokubai R&D leverages BIOVIA Solvation Chemistry and other modeling simulation tools to couple computational methods with laboratory analysis to discover more efficient catalysts and electrolytes.

Results:

- Expedite product development by reducing the number of laboratory experiments needed to discover new materials
- Improve process efficiency by cutting product development time and improved product performance.

CUSTOMER: A LEADING GLOBAL CHEMICAL COMPANY IN CATALYST TECHNOLOGY

Since 1941, NIPPON SHOKUBAI has grown up its business with unique catalyst technology.

The company has supplied, for example, Ethylene oxide, Acrylic acid, automobile catalyst, process catalyst and so on. Among all, their global market share of superabsorbent polymer comes up to No.1, now.

CHALLENGE:

Like many chemical companies around the world, Nippon Shokubai (Nippon Catalyst) is placing a growing emphasis on sustainability efforts, driven by stakeholder demands, government regulations, and a focus on the future. Techno Amenity, "providing affluence and comfort to people and society with our unique technology," features prominently in the company's mission.

The company aims to reduce CO_2 emissions by 30% by 2030 and to achieve carbon neutrality by 2050, in part by improving its production processes and making its catalysts more efficient. As a part of this effort, the company's European subsidiary NSE recently obtained certification for the biomass-derived propylene feedstock that it uses to make acrylic acid for its superabsorbent polymers, a key material in the production of disposable diapers.

Nippon Shokubai needed a more efficient, accurate way to acquire, analyze, and integrate data from laboratory experiments, modeling, and performance evaluations. Beginning in 2016, the company participated in a six-year research and development collaboration for basic material design technology, headed by Japan's New Energy and Industrial Technology Development Organization. The goal of this effort was to reduce the number of laboratory trials required for product and process development and to shorten the development period to 5% of that required by conventional material development that relies on experience and intuition.

SOLUTION:

Company researchers approached this challenge on multiple fronts. Modeling and simulation efforts focused on fundamental physics and chemistry help to identify promising materials and processes, pointing the way to the most likely solutions to the problems at hand. This allowed researchers to concentrate their efforts on the laboratory experiments that were most likely to yield useful results, which saves time and money, as well as reducing waste.

On the basic research front, the Nippon Shokubai team collaborated with the Institute of High Performance Computing in Singapore to study the reaction mechanism of acrolein oxidation to form acrylic acid. This oxidation is the final step in the transformation of propylene to the acrylic acid used in the industrial synthesis of the superabsorbent polymer that the company sells for use in disposable diaper production.

The complex oxidation reaction is affected by catalyst surface defects, hydrolysis, and re-oxidation of the catalyst surface, among other factors. The researchers performed a detailed reaction analysis using Turbomole to understand the role of water in their acrylic acid production process. The researchers found that water (a coproduct of propylene oxidation) plays an important role in accelerating acrolein oxidation. A follow-up study using isotopic labeling suggests that water may hydrolyze the catalyst surface (figure 1).

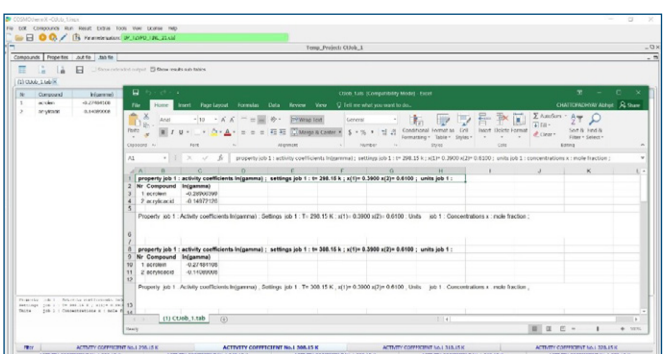


Figure 1. Activity coefficient for Acrolein and related molecule as from COSMOTHERM interface

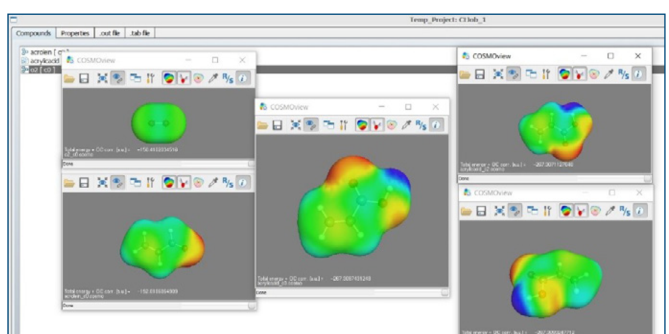


Figure 2. COSMO surface for the conformations of Acrolein, oxygen and the Acrylic acid as seen in COSMOVIEW

The orthorhombic MoVOx The orthorhombic MoVOx catalyst used in this study has shown outstanding performance because of the high inner surface area resulting from its large micropore volumes. The researchers used Solvation Chemistry package of BIOVIA to predict the catalyst's properties and optimize their acrylic acid production process. This software package performs quantum chemistry calculations for use in predicting thermodynamic properties, solubility, and phase equilibrium, as well as more computationally intensive tasks, such as predicting compounds whose molecular surfaces have similar charge density profiles (sigma profiles) as seen on figure 2.

"By leveraging BIOVIA modelling and simulation tools, Nippon Shokubai researchers have been able to expedite product development and improve process efficiency significantly."

— Satoshi Ishida, Strategy & Planning Group Leader at Nippon Shokubai

Nippon Shokubai also uses Solvation Chemistry to optimize production and performance for several of its product lines, including its Ionel-brand lithium bis (flourosulfonyl) imide electrolyte for lithium batteries, and to screen compounds that are not already in the company's database.

Various physical properties can be calculated as numerical values familiar to experimenters, such as prediction of solubility and phase equilibrium using the results of quantum chemical calculations, and prediction of similarity of compounds using σ profiles. BIOVIA's quantum chemistry calculation tools like DMol^3 and Solvation Chemistry are utilized for this LiFSI patenting and process optimization.

RESULT:

Nippon Shokubai improved its production process using machine learning-driven performance prediction technology to screen catalysts and more fully understand the reaction mechanism for acrylic acid production. The result was a superabsorbent polymer with an absorption volume and rate that is more than 10% greater than its conventional counterparts.

By leveraging modeling and simulation, researchers expect to at least double the speed of development for all of the company's product lines, not only its polymers and batteries. By reducing the number of laboratory experiments needed to evaluate material compositions and processing parameters, they can focus on the experiments that are most likely to yield useful results. This not only saves time and money, but it reduces waste as well.

FUTURE:

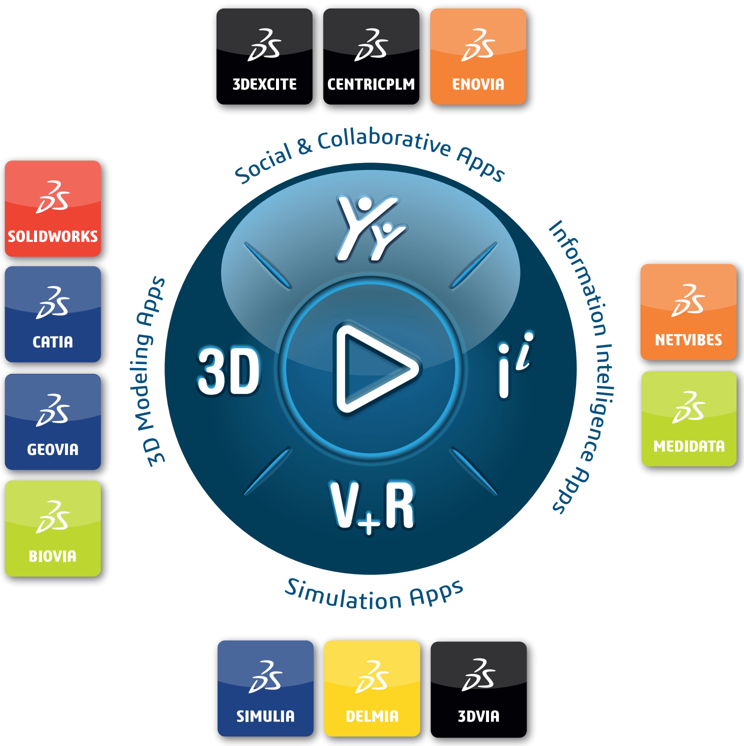
Nippon Shokubai researchers are working to create a centralized database that manages data from the automatic synthesis robot, the automatic evaluation device, and the results of their simulations to further shorten development periods. A thorough analysis of reaction mechanisms will require acquiring and integrating experimental, modeling, and performance evaluation data without losing information or introducing errors.

Under ideal conditions, data obtained from modeling could be used in the same fashion as experimental data for input to calculations. The ability to easily digitize the electronic states of key catalyst molecules, rather than manually collecting calculation results one by one, will be key in developing this capability.

The results of this effort can be used to optimize the manufacturing equipment that produces water-absorbent resin and speed up production. Data science also contributes to optimizing the composition and molecular weight of the polymer builders used for laundry detergents and other products. Such efforts help Nippon Shokubai to balance and optimize the many interacting factors that go into the products that meet their customers' needs.

REFERENCES

1. Torstein Fjermestad, Wen-qing Li, Graham Rugg, Satoshi Ishida, Masaaki Okuno, Kazuo Sagi, Alexander Genest, and Notker Rösch. *Acrolein oxidation to acrylic acid over the MoVOx material. Insights from DFT modeling.* Appl. Catal. A, 2018, 565, pp. 68–75.



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

DASSAULT SYSTEMES | The **3D**EXPERIENCE® Company