What matters most: AI × data driven R&D for corporate innovation

The reality and challenges of AI adoption in the materials industry: Barriers of data, talent, and organization

Mitsui Chemicals, Inc.

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Advancing human progress together

Mitsui Chemicals, Inc. is advancing R&D digitalization (DX) across a broad spectrum of activities centered on materials and advanced materials development, encompassing Materials Informatics (MI), computational chemistry, CAE (Computer-Aided Engineering)/fluid dynamics simulation, image analysis/AI application development and advanced analytical techniques including synchrotron radiation. The company has constructed the Digital Science Lab (DSL), introduced a new High Performance Computing (HPC) environment and consolidated R&D and process-side DX talent into a stand-alone organization reporting directly to the Head of the Research Division — marking a significant step forward in its research transformation.

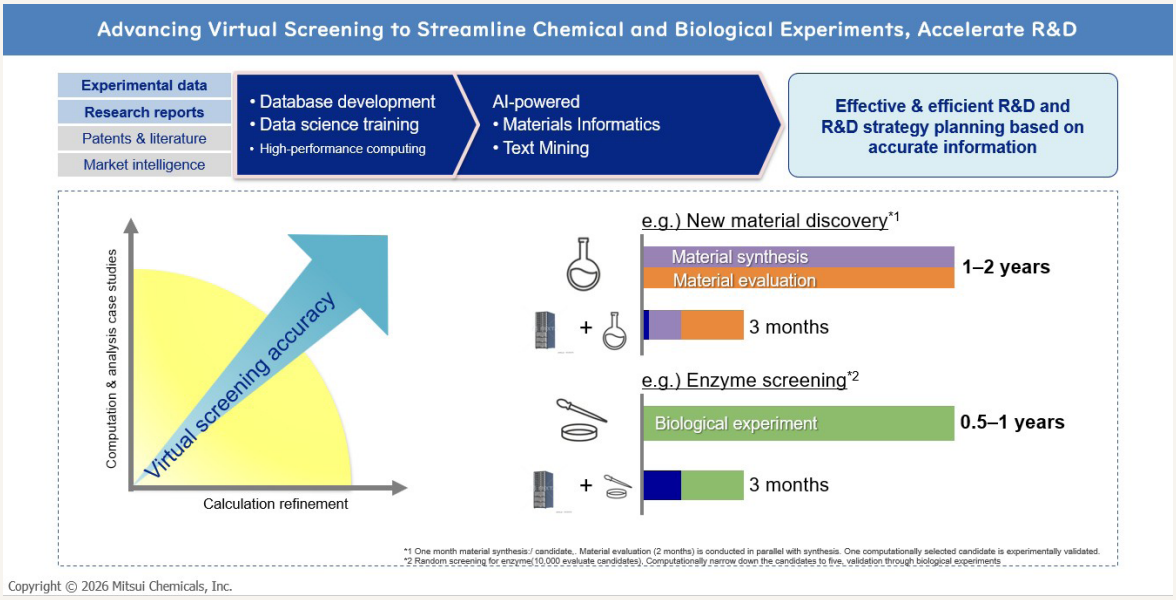
Challenges of AI adoption: Candidly identifying real-world barriers

- Low R&D expenditure ratio: ROI quantification and investment decision-making are inherently difficult
- Insufficient data literacy and cross-departmental data-sharing barriers: Organizational data silos exist across research, manufacturing, engineering, and planning functions
- Difficulty repurposing drug-development-oriented tools: Problem structures and data characteristics differ fundamentally
- Barrier to capturing negative data: failures and unsuccessful results are not accumulated as data

When data, people, and organizational structures operate in silos, DX risks remaining limited to **“siloed implementations”** rather than driving broader, organization-wide transformation.

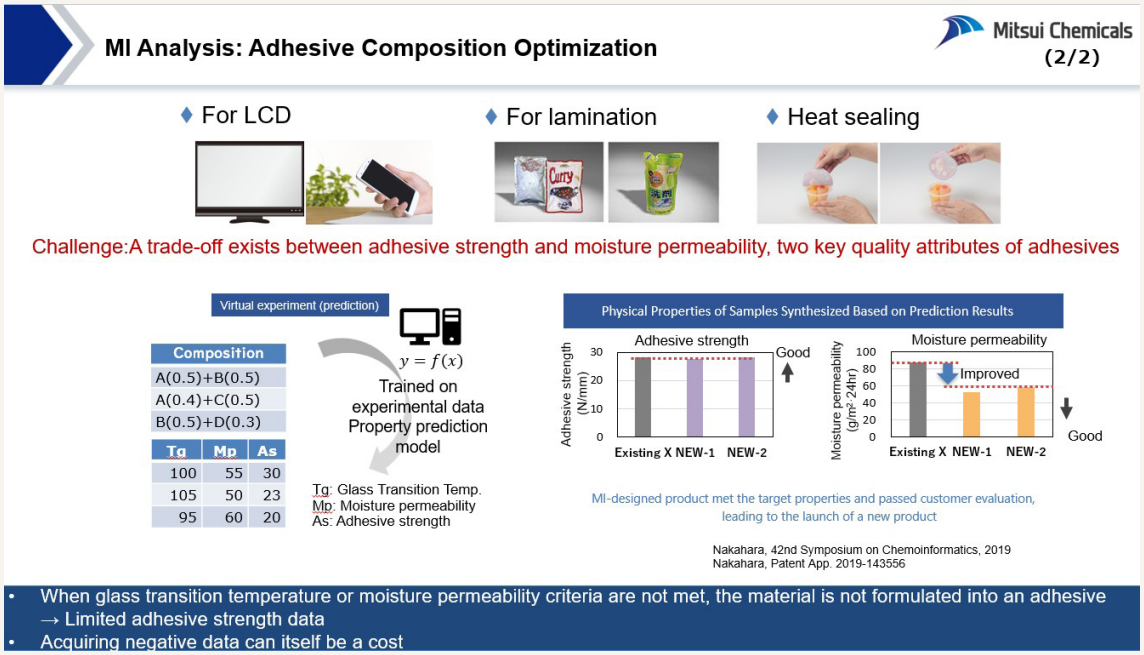
Mitsui Chemicals’ initiatives

1. Establishment of the Digital Science Lab (DSL): Bringing people and organizations together and designing an environment for “co-creation space”
2. Core technology portfolio: Integrating computational chemistry, MI, CAE, image analysis, and advanced analysis around HPC
3. Use of AI/MI and HPC: Shortening and streamlining the R&D process



Use case for MI

It was noted that without MI analysis, the development direction could not have been revised. At a time when investment decisions are difficult unless outcomes can be translated into cost terms, the fact that MI analysis enabled an earlier revision of the development direction represents a significant achievement. Because Mitsui Chemicals fully understands the reality that capturing negative data is costly and therefore tends to be approached cautiously, it is working to reduce wasted exploration and move more quickly toward promising candidates.



Importance of Scientific Data and Peer-Reviewed Literature: Data and information published in peer-reviewed literature are extremely important as reliable sources of evidence. Driven by advances in information technology, the volume of electronic publications has increased significantly, the predominant methods of accessing scientific literature have evolved and the number of academic journals themselves has grown rapidly. Furthermore, the research information landscape has changed dramatically over the past decade with the expansion of open-access journals and the emergence of preprint platforms. In response to these rapid changes, users themselves recognize the need to continuously make efforts to keep pace with the evolving environment.

Conclusion

In the materials industry, where many challenges such as molecular generation and property prediction remain difficult due to the diversity of materials and conditions, the key to successful AI utilization is not simply the adoption of AI models, but having the right combination of essential elements required for success.

Key Takeaway:

Dataset
Digitization and digitalization (development and expansion of research DB).

Skillset
Acquiring implementation and operational skills related to AI, MI, IT, and IoT.

Mindset
Fostering the awareness and culture needed to promote adoption and utilization, as part of organizational transformation.

In a constantly evolving environment, identifying a single “correct answer” is difficult. What is essential is to analyze the success and failure factors of leading cases and translate those insights into the company’s own context. Looking ahead to a future in which generative AI and automated or autonomous experimentation become standard practice, treating the organizational barriers that companies must overcome — data sharing, investment decision-making, and talent development — as part of the design of R&D DX may become a common factor in achieving meaningful outcomes.

People in this project:

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“It is through the co-creation of materials engineers and AI developers that a new culture of value creation — Materials DX — is born”