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# Mitsui Chemicals and Hitachi Start Demonstration Test for Practical Application of MI Technology to Speed Up Materials Development

*Realizing DX in new materials development; Established AI technology to reduce the number of experiments for organic material development by about 1/4*

**Tokyo, June 28, 2021** --- Mitsui Chemicals, Inc. (TSE: 4183, Mitsui Chemicals) and Hitachi, Ltd. (TSE: 6501, Hitachi) today announced that they have begun a practical demonstration test of materials informatics (MI) technology developed by Hitachi that utilizes artificial intelligence (AI) for actual development of new materials. Prior to the demonstration test, Hitachi's technology has been verified by using past organic material development records provided by Mitsui Chemicals, and it was confirmed that the number of experimental trials required to develop new high-performance compounds can be reduced to about 1/4 compared with that for conventional MI, shortening the development period.
This technology will be presented at the conference "DICOMO2021" (1) to be held on June 30, 2021.

In the future, Hitachi aims to establish this MI technology as a practical method for the "Materials Development Solution," (2) which is one of Hitachi's "Lumada" solutions with advanced technologies, to reduce time and costs for customers' and partners' development processes, and to strengthen their competitiveness. Mitsui Chemicals will continuously create innovative products, services, and business models in an agile manner to solve social issues through DX. Both companies will continue to promote collaborative creation (3) on materials development and contribute to realization of a sustainable society.

## Merits for Mitsui Chemicals

Development of new products is one of the most crucial activities in Mitsui Chemicals' business. However, it reluctantly spends significant time and incurs significant costs on processes such as problem setting, basic research, and scale-up experiments. At this time, combining the vast knowledge of Mitsui Chemicals obtained through its past new materials development with digital technologies provided by Hitachi will lead to a drastic reduction in the time and cost needed for new materials development.

## MI Technologies developed by Hitachi

Hitachi developed a new deep-learning technology to suggest chemical formulas expected to have characteristics better than existing chemical compounds as an advanced MI, which is a technology to develop new materials with AI and simulation technologies. The new technology, even in an organic material development that requires a huge experimental dataset, enables chemical formula suggestion without

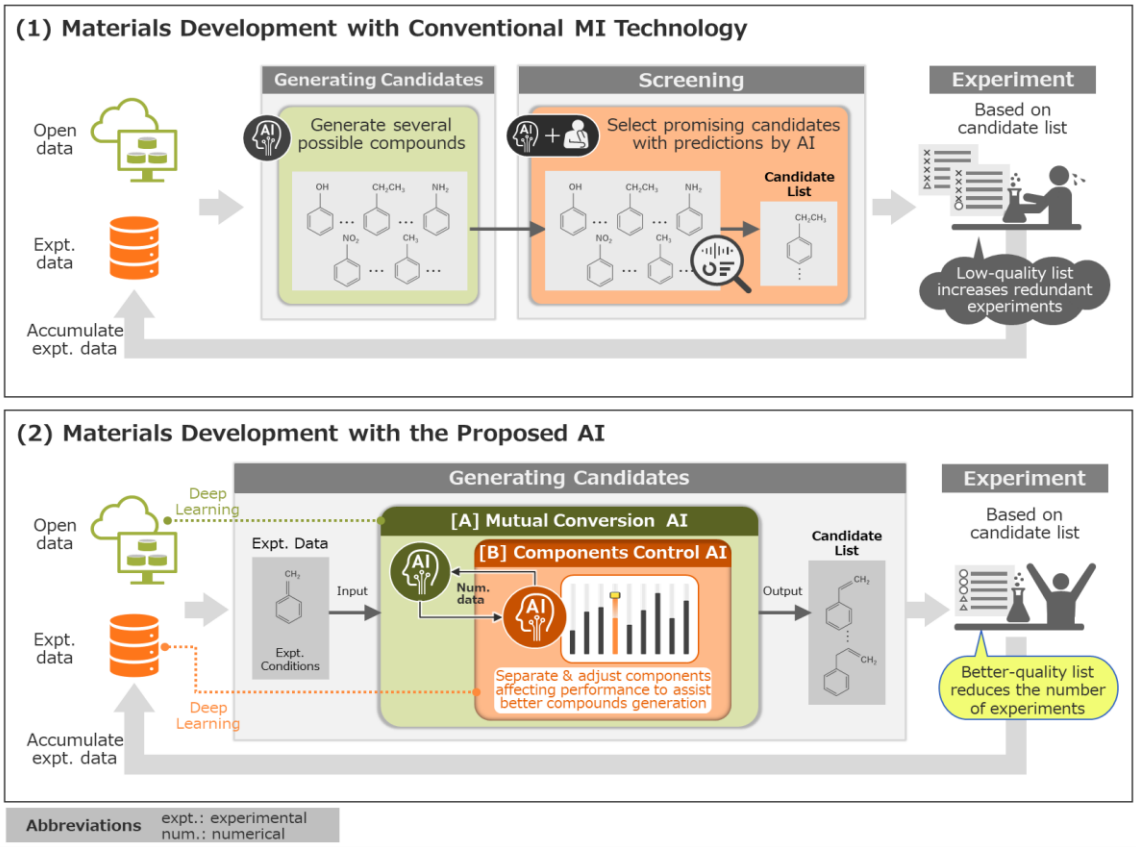
such a dataset.
Features of the technology are as follows.

**1. "Nested" AIs that utilize large open data**
**2. Component adjustment to improve the generation probability of high-performance compounds**

1. Hitachi adopted a nested structure of two independently trained AIs.[4] The inner AI is trained with experimental data and the outer AI is trained with large, open data.[5] Due to the structure, this technology is applicable for development of new materials even when only a small amount of experimental data[6] is available.

2. In this method, the outer AI transforms the chemical formulas given as text into numerical data. The inner AI extracts and adjusts the components[7] of the numerical data affecting the performance to create new numerical data representing high-performance compounds. By inversely transforming such numerical data into a chemical formula, high-performance compounds are suggested with higher probability. Accordingly, the number of experiments will be reduced.

## Comparison with Conventional MI Technology




Deep-learning technology that can automatically generate chemical formulas for high-performance materials even with small amounts of experimental data

**About Mitsui Chemicals, Inc.**
For more information, please visit Mitsui Chemicals' website (https://jp.mitsuichemicals.com/en/index.htm).

**About Hitachi, Ltd.**
For more information, please visit Hitachi's website (https://www.hitachi.com/).

**Supplementary Information (Backgrounds)**
In the field of materials science, MI with advanced technologies such as AI and simulation is expected to improve the efficiency of R&D to meet the diversifying demand for materials such as plastic materials with low environmental impact. For example, AI is applied to analyzing data such as material blend ratios and manufacturing conditions (temperature, pressure, etc.) to estimate the optimal blend amounts and manufacturing conditions for creating high-performance materials.
In a general case of MI applied to the development of organic materials, AI is required to handle chemical formulas in textual format (e.g., ethanol ($CH_3CH_2OH$)), but this is not an easy task. Therefore, as a known approach, the structure and properties of compounds are expressed numerically as descriptors,(8) and AI can predict performance from such descriptors. However, these descriptors cannot be easily inversely transformed into chemical formulas. In the conventional method, experts manually identify the chemical formulas of new materials by selecting from a large number of chemical formulas based on the predicted performance values of AI, and then evaluate their actual performance through real experiments (see Figure (1)).
In recent years, with advances in deep learning, AIs that can directly generate and suggest chemical formulas have been developed. However, such AI requires a large amount of experimental data which contains chemical formulas, experimental conditions, and their performance-index values (9) to learn the relationship between chemical structures and performance. Due to this requirement, the number of experiments needed to obtain training data increases.

(1) Information Processing Society of Japan, “Multimedia, Distributed, Cooperative and Mobile (DICOMO2021) Symposium,”
(2) “Materials Development Solution” is one of Hitachi's “Lumada” solutions that accelerate DX, and is a service supporting the development of new materials for customers through MI. It mainly includes two services; (1) “Materials Data Analysis Environment Provision Service” -- a cloud service that enables easy visualization and high-speed analysis of huge amounts of simulation data and experimental data related to materials development, and (2) “Materials Data Analysis Service” -- Hitachi receives customer’s materials data and develops optimal AI and other analytics tools for their R&D to perform analysis on behalf of the customer.
(3) Mitsui Chemicals and Hitachi have been collaborating on materials development using MI since 2017.
(4) Patent pending.
(5) A group of data in a format called SMILES (Simplified Molecular Input Line Entry System), in which existing chemical formulas are expressed as character strings. There are approximately 500,000 entries.
(6) Data of chemical formulas and their material property values on a scale of 100 to 1,000.
(7) Patent pending.

(8) A numerical representation of the chemical characteristics of a compound, called a “fingerprint.”
(9) A numerical value that quantitatively evaluates the functions and properties of a material, such as viscosity and solubility.

For more information regarding this release,
please contact the Research & Development Group, Hitachi, Ltd.
https://www8.hitachi.co.jp/inquiry/hqrd/news/en/form.jsp

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