AI4X – Self Driving Discovery of Immersion Cooling Fluids for Data Center

Maryam Ebrahimiazar[1], Mahyar Rajabi-Kochi[2], Mohammad Zargartalebi[1*], Haoming Ye[1], Hanie Rezaei[1], Fernando Javier Carmona Esteva[2], Roozbeh Alishahian[1], Tarek Eid[1], Haoyang Deng[1], Seyed Mohamad Moosavi[2,3], David Sinton[1]

[1]Mechanical & Industrial Engineering, University of Toronto, Toronto, Ontario, Canada, [2]Chemical Engineering & Applied Chemistry, University of Toronto, Toronto, Ontario, Canada, [3]Vector Institute for Artificial Intelligence, Toronto, Ontario, Canada

Correspondence to: m.zargartalebi@utoronto.ca, Mohamad.moosavi@utoronto.ca, dave.sinton@utoronto.ca

1. Introduction

As artificial intelligence and other compute-intensive workloads continue to scale, the energy required to operate and cool data centers is becoming an increasing concern. In the United States, data centers already consume about 4% of total electricity, a figure projected to rise to roughly 12% by 2030, with cooling responsible for nearly 40% of this demand[1]. Immersion cooling—where servers are submerged in engineered dielectric fluids—offers a promising route to reducing cooling energy to as little as 5%[2]. Achieving this potential, however, requires discovering thermal fluids that satisfy both thermal and electrical constraints.

Heat-transfer performance in immersion cooling is governed by thermal conductivity, viscosity, density, thermal expansion, and specific heat capacity, yet optimizing these properties simultaneously remains difficult. Cooling performance is determined using a figure of merit (FOM)[3],

$$FOM = k\left(\frac{\beta C_p \rho^2}{\mu k}\right)^{0.2813} \qquad \text{Eq. 1}$$

where β is the thermal expansion coefficient, c_p the specific heat capacity, ρ the density, μ the dynamic viscosity, and k the thermal conductivity. In addition to good cooling performance, thermal fluids must maintain excellent electrical insulation, including low electrical conductivity and high dielectric strength, to ensure safe and reliable operation in direct contact with electronic components.

Thermal fluid discovery is constrained by both experimental and combinatorial challenges. Measuring a complete set of thermophysical and electrical properties for a single formulation can require nearly a full working day, with specific heat capacity measurements alone taking several hours and other properties requiring tens of minutes each. At the same time, the design space is vast: although there are an estimated 10^{60} candidate organic molecules, no single fluid meets all thermal and electrical requirements in practice, necessitating mixtures and additives that expand the formulation space by orders of magnitude[4–6]. Mixture properties are often highly non-linear and non-ideal due to complex intermolecular interactions, making performance difficult to predict. While computational models provide faster screening, their accuracy is limited for novel chemistries and multi-component systems.

These challenges motivate self-driving labs that integrate high-throughput experimentation with machine-learning (ML)–driven decision making. We introduce an autonomous platform that combines rapid thermophysical and electrical characterization, adaptive machine learning, and on-demand molecular dynamics simulations to accelerate the discovery of high-performance thermal fluids. By linking molecular representations to mixture-level thermal and electrical behavior, the platform identifies non-intuitive mixtures and reveals interaction patterns governing key properties. Additionally, networked platforms can communicate and operate in parallel—each running complementary experiments while sharing insights.

2. Methodology

We developed an integrated experimental/ML platform (see figure 1) for rapid characterization of key thermal fluid properties. Microfluidic devices[7,8] were designed in-house to enable high-throughput measurements of specific heat capacity and thermal conductivity, while a commercial instrument was adapted for automated viscosity and density characterization. In addition, custom in-house devices were developed to measure electrical properties relevant to im-

mersion cooling, including electrical conductivity and dielectric behavior. Together, these sensors along with an automated flow handling system, allow autonomous evaluation of multiple formulations at a throughput approximately 100X higher than conventional methods and using 10X lower sample.

To efficiently explore the large chemical design space, an ML-based pre-screening model was first applied to a candidate pool exceeding 100 million structures, removing invalid molecules such as metals, salts, highly reactive functional groups, and other undesirable chemistries. The remaining candidates were explored using in-house Feature Adaptive Mixture Bayesian optimization (FAMBO), which adaptively guided the self-driving lab toward promising formulations by maximizing the FOM. At each iteration, new formulations were proposed by balancing exploration of under-sampled regions with exploitation of high-performing candidates.

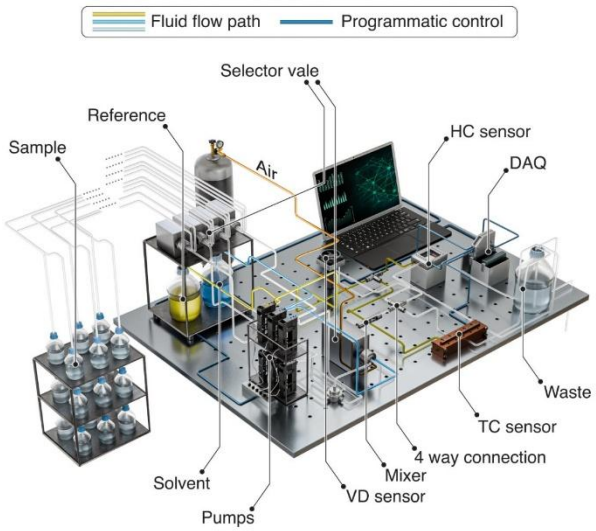

Fig. 1: Self-driving thermal fluid discovery platform for immersion cooling

3. Results

Across a 200-iteration FAMBO campaign, we identified more than 30 previously unexplored fluid mixtures whose performance exceeded that of the best-performing thermal fluids. All of these formulations surpassed the benchmark FOM, with the top-performing mixture delivering more than a 20% improvement. This enhancement was driven by a combination of favorable property shifts, including an approximately 70% increase in specific heat capacity, and a ~25% reduction in viscosity at 40 °C. These gains cannot be explained by ideal mixing rules and instead arise from excess contributions associated with non-ideal molecular interactions.

The sampling efficiency of FAMBO is enabled by its feature-adaptive molecular representation. It selects an orthogonal subset of descriptors at each optimization cycle to capture independent thermophysical dimensions contributing to the FOM. This adaptive strategy allows the optimizer to navigate high-dimensional mixture space and identify steep performance gradients that would be difficult to detect using fixed representations.

Robustness of the top six mixtures was evaluated through validation experiments using independent instruments, operators, and randomized measurement sequences, confirming reproducibility of the observed improvements. Long-term thermal aging at 40 °C for 1,000 h showed no statistically significant degradation in viscosity, thermal conductivity, or heat capacity for the top six mixtures.

Acknowledgments

The authors would like to acknowledge funding and technical support from bp applied sciences through bp Technology Ventures Ltd. The authors acknowledge the support of the Natural Sciences and Engineering Research Council of Canada (NSERC). This research was undertaken, in part, thanks to funding from the Canada Research Chairs Program. This research is part of the University of Toronto's Acceleration Consortium, which receives funding from the Canada First Research Excellence Fund (CFREF).

References

1. Chen S. How much energy will AI really consume? The good, the bad and the unknown. *Trends in Chemistry*. 2021;3(2):133-145. doi:10.1016/j.trechm.2020.11.004

2. Zhou K, Yu X, Xie B, Xie H, Fu W. Immersion cooling technology development status of data center. Rui-ming F, Liao Q, eds. *Sci Tech Energ Transition*. 2024;79:41. doi:10.2516/stet/2024022

3. Brink R. Base Specification for Immersion Fluids.

4. Fallani A, Medrano Sandonas L, Tkatchenko A. Inverse mapping of quantum properties to

structures for chemical space of small organic molecules. *Nat Commun.* 2024;15(1):6061. doi:10.1038/s41467-024-50401-1

5. Coley CW. Defining and Exploring Chemical Spaces. *Trends in Chemistry.* 2021;3(2):133-145. doi:10.1016/j.trechm.2020.11.004

6. Westermayr J, Gilkes J, Barrett R, Maurer RJ. High-throughput property-driven generative design of functional organic molecules. *Nat Comput Sci.* 2023;3(2):139-148. doi:10.1038/s43588-022-00391-1

7. Kazemi A, Zargartalebi M, Sinton D. Differential microthermometry enables high-throughput calorimetry. *Energy Environ Sci.* 2024;17(2):813-823. doi:10.1039/D3EE03865C

8. Kazemi A, Zargartalebi M, Sinton D. Accurate and rapid measurement of fluid thermal conductivity. *Nat Commun.* 2025;16(1):10531. doi:10.1038/s41467-025-65553-x