

Accelerated Fluid Discovery for Data Center Immersion Cooling

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ABSTRACT

Rapid expansion of data centers to support high-performance computing has amplified the demand for efficient thermal management solutions. Immersion cooling offers a promising approach, but it introduces new challenges in identifying a suitable coolant compatible with this technology. Along with optimized thermophysical properties, electrical properties and material compatibility are also critical considerations. This study focuses on developing a self-driving lab to accelerate the discovery of optimal coolants. An automated high-throughput AI-powered screening platform has been developed to analyze key properties, including viscosity, density, heat capacity, thermal conductivity, dielectric constant, and additive compatibility. The system analyzes up to five samples per hour, achieving a 100x higher throughput than conventional methods. A machine learning platform is first benchmarked using >1,000 data from ten liquids and their binary and ternary mixtures. The pure liquids include esters, alcohols, ketones, ethers, and aldehydes. These data points were gathered at 40 °C to ensure the liquids meet real-world operating conditions. The developed platform will be used to discover the optimum mixture from a large chemical space, guiding the next experiment in the fluid discovery loop. This integrated approach significantly reduces the number of required tests, leading to substantial time and material savings. This work advances the development and adoption of next-generation cooling technologies, addressing the increasing thermal management demand posed by high-performance computing in data centers.