Development of a thermal deactivation and pretreatment process, using numerical simulation

Enhancing battery recycling through thermal deactivation

The growing use of lithium-ion batteries (LIBs) in electronics, electric vehicles, and energy storage is driving a surge in spent batteries. In pursuit of sustainability and efficient use of finite resources as well as decreasing the global depency on critical raw materials, the European Union has introduced in the Regulation 2023/1542 of 12th July 2023, stricter recycling regulations, including higher collection targets and lithium recovery rates, rising from 50% in 2027 to 80% by 2031. In the conventional state-of-the-art pretreatment process, the batteries are fully discharged, shredded and thermally treated. The idea behind the new method is to deactivate and thermal pretreat the batteries in one process step, followed by mechanical separation.

Battery Pre-Treatment

During battery recycling, the cathode material is the most valuable component, making up to 40% of the cost. However, its firm adhesion to the organic binder and aluminum foil makes recovery challenging. Pre-treatment is essential to separate these materials efficiently, making it a critical first step for a more efficient recycling process.

Among the available solutions for cathode separation, thermal deactivation emerges as a promising alternative enhancing recycling efficiency. In this process, battery cells are exposed to a controlled temperature environment of around 200 °C in a furnace, initiating a controlled thermal runaway. As the battery releases electrolyte gases, the separator collapses, bringing the anode and cathode into direct contact and causing a rapid discharge of stored energy. This triggers a sharp temperature rise to 440 °C, leading to the explosive release of anode and cathode materials while decomposing the organic binder. The resulting products (Figure 1, right) include aluminum and copper foils, the steel case, and cathode and anode materials.

The challenge of this process is to create a furnace that can reliably treat mixtures of different batteries, ensuring that the material characteristics are preserved for further recycling. To achieve this goal a coupled Computational Fluid Dynamics (CFD), Discrete Element Method (DEM) was developed.

Characterization of the thermal deactivation

To investigate the thermal deactivation behavior of different LIBs, an experimental setup was designed, featuring a controlled chamber flushed with inert gas, where a battery is placed at the center (Figure 1, left). The chamber is heated following a defined temperature profile, while temperatures at various locations and the composition of the off-gas are continuously monitored.

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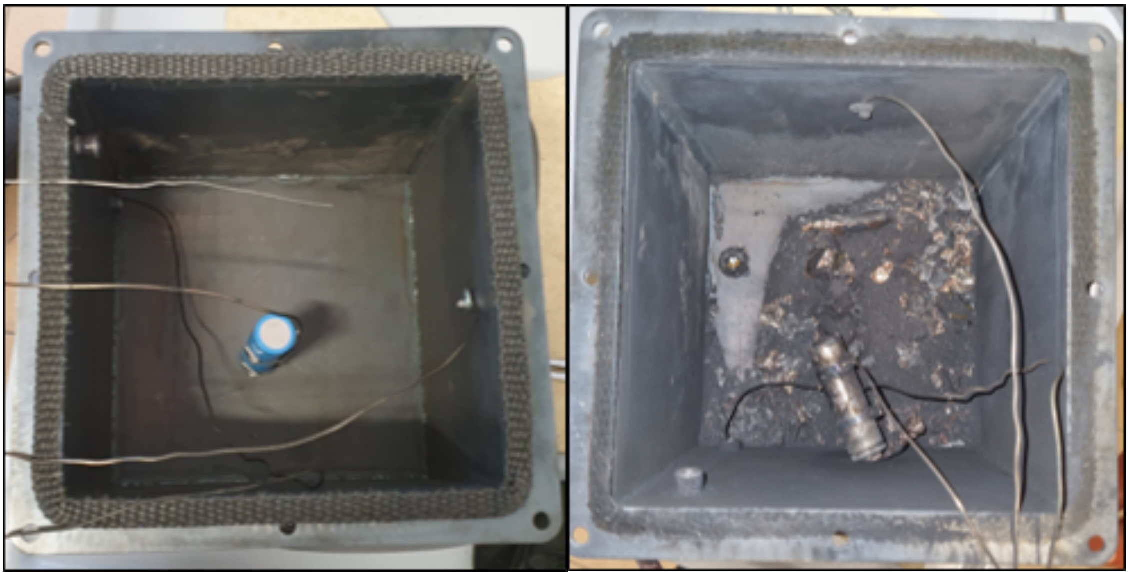

Figure 1: Left: The battery in the measurement enclosure, before thermal deactivation. Right: Remains of the battery after thermal deactivation. These consist of aluminum and copper foils, steel case and cathode and anode materials.

Numerical simulation applied to recycling of LIBs

Based on the data collected from the experiments, mathematical models were developed and added to a DEM particle, representing the battery. This is coupled with a gas phase computed by CFD. This setup allows to analyze the transport phenomena, chemical composition, and temperatures. It provides insights into both small- and large-scale process dynamics that would otherwise require extensive experimental setups and resources, enabling the prediction of thermal deactivation in industrial-size processes for process development and optimization.

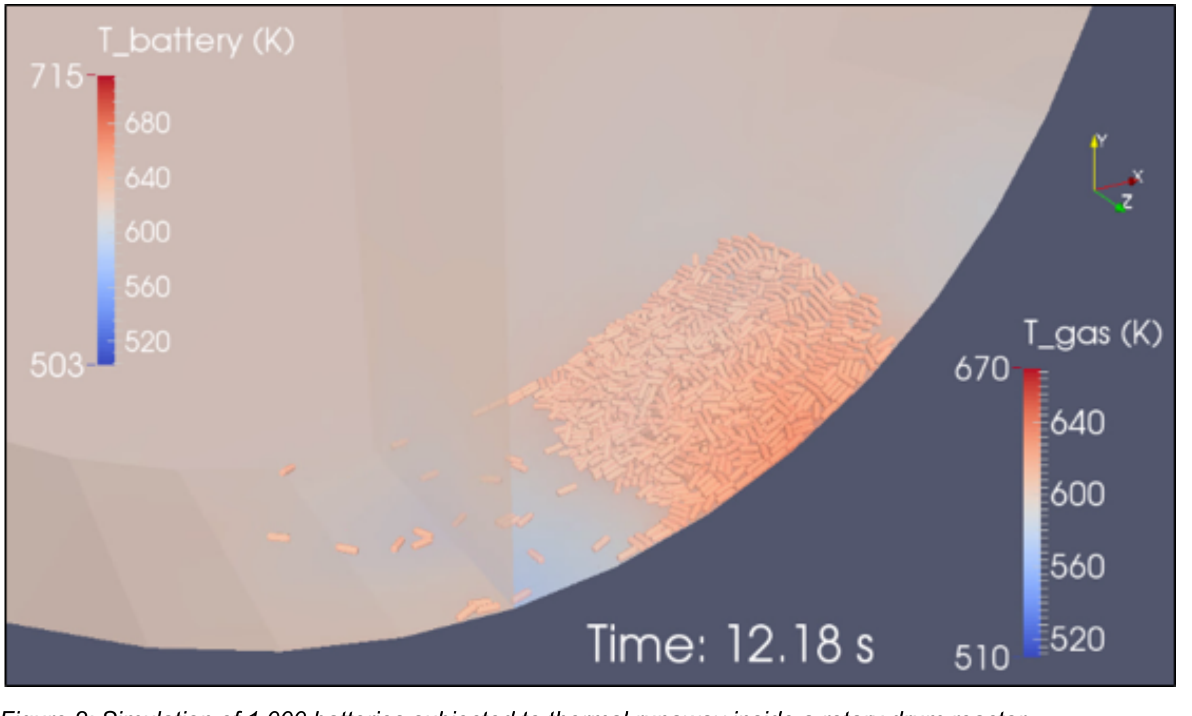

Figure 2: Simulation of 1,000 batteries subjected to thermal runaway inside a rotary drum reactor.

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The second workshop of the COMET-module FuLIBatteR was held on the 20th February 2025 at the BOKU University in Tulln in a hybrid format. There was a lively discussion with external stakeholders about research activities on the sustainable recycling of lithium-ion batteries to enhance an efficient and sustainable recovery of critical raw materials from LIBs.

Figure 3: 2nd FuLIBatteR workshop, BOKU University, Tulln.

Further selected dissemination activities in the FuLIBatteR module in the first quarter of 2025 were:

- Sieber, A., Spiess, S., Rassy, W. Y, Schild, D., Rieß, T., Singh, S., Jain, R., Schönberger, N., Lederer, F., Kremser, K., Guebitz, G. M., Fundamentals of bio-based technologies for selective metal recovery from bio-leachates and liquid waste streams, Frontiers in Bioengineering and Biotechnology 12, 1528992
- „Verwertungs- und Entsorgungsstrategien für Li-Antriebsbatterien – aktuelle Trends und Entwicklungen“, 18th March 2025, Vienna (Austria), Presentation by J. Rieger „Rückgewinnung kritischer Rohstoffe aus verschiedenen LIB-Anwendungen“ (Contribution from Project 1, 2 and 3)

The Module FuLIBatteR is supported by COMET (Competence Center for Excellent Technologies), the Austrian programme for competence centres. COMET is funded by the Federal Ministry of Innovation, Mobility and Infrastructure, the Federal Ministry of Economy, Energy and Tourism, the Federal States of Upper Austria and Styria as well as the Styrian Business Promotion Agency (SFG). Furthermore, Upper Austrian Research GmbH continuously supports the Module. The consortium includes (listed alphabetically) acib GmbH, Audi AG, BOKU University of Natural Resources and Life Sciences Vienna, BRAIN Biotech AG, Coventry University, Ebner Industrieofenbau GmbH, Montanuniversitaet Leoben, RHI Magnesita GmbH, Saubermacher Dienstleistungs AG, TUEV SUED Landesgesellschaft Oesterreich GmbH, UVR-FIA GmbH, voestalpine High Performance Metals GmbH and VTU Engineering GmbH. The project consortium is coordinated by K1-MET GmbH as consortium leader.

For more information about the FuLIBatteR project and its progress, please visit LinkedIn and the K1-MET-Website.

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