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Doing It Better This Time: Predictive Geochemical Modeling for Responsible Resource Extraction, Waste Minimization, and Risk Reduction

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How can we do it differently and better this time? As highlighted in the session description, “mining, smelting, fossil fuel combustion, and waste disposal release metals, metalloids, and organic contaminants that alter natural geochemical cycles, mobilize toxic species, and degrade water and soil quality.” Historically, geochemical modeling has been applied most extensively in the remediation of soil and water contamination, and it has also served as a predictive tool for evaluating the long-term chemical evolution relevant to safe disposal of high-level nuclear wastes. Yet the rapid transition from fossil fuels to renewable energy systems is creating an unprecedented demand for critical minerals, alongside new contaminant regimes and new opportunities to reduce environmental footprints by design rather than by cleanup.

Going forward, we should harness the predictive power of geochemical modeling proactively. Modeling can help (i) design extraction and processing pathways that generate less waste, (ii) forecast what gets released, how much, and when (for example, the geochemical evolution of pit lakes, tailings, and waste repositories), and (iii) quantify chemical speciation and reaction pathways that govern contaminant mobility and long-term fate in the environment. I will give examples where modeling supports process design with dual environmental and economic benefits, including approaches that couple CO_2 sequestration with nickel and cobalt recovery through peridotite carbonation.

I will also highlight what it takes to elevate geochemical modeling from a computational tool to a shared quantitative framework: a trained workforce that can define chemical systems, understand model inputs and databases, and interpret model outputs; robust, open-source computational codes; and reliable, community thermodynamic and kinetic databases with transparent curation and versioning so that predictions are reproducible and comparable.