

## **Friendly analysis, visualisation and modelling with ChemApp and Python**

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The global metallurgical industry has had a tough time of late. This has pushed companies to question conventional wisdom and innovate. Many existing pyrometallurgical processes are being re-evaluated and new concepts are being developed and tested. Computational thermochemistry is probably the most valuable tool to study high temperature processes and materials in cases where data is available. It provides precious insight and understanding during development, testing and operation. FactSage has served us well for a long time in doing these investigations. Its limitations become apparent, however, when doing large numbers of calculations, when having to do custom result visualisation, and when having to model entire processes beyond single equilibrium calculations. ChemApp gives us complete freedom to do all these things, but it is difficult to be productive in C/C++ and Fortran. ChemAppPy, the friendly Python interface to ChemApp, combines the power of ChemApp and FactSage with the vast Python ecosystem. It enables us to run large volumes of calculations (even in parallel), store results in databases like mongodb, query and manipulate the stored results, and visualise data with the power of matplotlib. It is also now possible to write higher-level software quickly, as demonstrated by a new flowsheet-based mass and energy balance framework that enables us to effectively and productively model and study the steady-state behaviour of processes.