Combining the power of computational thermochemistry with the convenience of Python programming:

My experience with ChemAppPy

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1. My background

- I am metallurgical engineer specialised in modeling, control and optimization of metallurgical furnaces (steelmaking, non-ferrous metallurgy)

- 10 years of experience using thermochemical application
  - FactSage™ regularly
  - SimuSage for dynamic process modeling, in a close cooperation with GTT (oxygen converter, lead smelting in the TSL process)

- Limited experience with coding:
  - Applications developed mainly by co-workers (programmers)
  - Moderate experience using the software Matlab:
    - University days
    - Mathematical process modeling + solving numerical problems (with assistance)
2. Why ChemAppPy?
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- FactSage
  - a powerful tool that I use on a daily basis for evaluating the thermodynamic equilibrium state relevant to our processes
  - there has always been a need to use FactSage calculation options as an integrated module into a programming environment so that we can
    - automate thermochemical calculation tasks
      - inputs for the calculations
      - the post-processing of the results
    - integrate computational thermochemistry into existing digital platforms in SMS group
  
  those possibilities are provided by: ChemApp + ChemAppPy
2. Why ChemAppPy?

Digital TWINNING resource systems of SMS: Integrating our expertise, in-depth understanding of technology, and theoretical knowledge into digital platforms
2. Why ChemAppPy?

- **ChemApp** provides the flexibility that we are seeking
  - is an API (application programmer’s interface)
  - However, there was a *language* issue!
    - It has an interface to C and Fortran
    - For someone with a little programming experience, learning those coding languages is challenging
    - this was the case for me during learning DELPHI and C#
      - made me question the *effort-benefit* since I will use those programs only „occasionally“
  - Python was recommended to me as a much easier to learn coding language
2. Why ChemAppPy?

- **ChemAppPy**: became commercially available in 2019
  - made ChemApp available in a Python environment
  → we considered this as a chance to achieve our goals
  - The original functions in ChemApp are now grouped into few classes, which are easier to remember and work with:
    - Info, Units, ThermochemicalSystem, EquilibriumCalculation, StreamCalculation, PhaseMapCalculation

- Further additional functions are included in order to
  - make the calculations easier and quicker to do
  - post-processing and visualizing the calculation results.
3. What I gained so far
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- Programming with Python:
  - using thermochemistry in Python made me part of a large online community from which there is a lot to learn and exchange!
  - The effort to learn Python was considerably less than for other coding languages:
    - Python-Training is one part of ChemAppPy-Training: The fundamental concepts + the basic functions needed for ChemAppPy are introduced.
    - It took me about 2 weeks with an effort of 2-4 h/day to get the basics of Python and be able to work with it by myself
    - once getting over the „hurdle“ of learning how to code
      - I can now use many powerful python packages such as Pandas (data preparation and analysis) and Matplotlib (visualization)
3. What I gained so far

- Enjoying not only the power but also the **friendliness** of ChemAppPy
  - The calculation functions are grouped into few **Classes**
  - when the class is called, a list of the corresponding functions appears:

- The indexing adopted is consistent throughout the program (**A** for amount, **ph** for phase, **pc** for phase const,.....)

  focus more on **what** I want to do rather on **how** to do it

  less learning effort Vs. more **comfort** and **fun** working with the program!
Conclusion

- The need to flexibly use thermochemistry in SMS has been there for a while.
- The development and availability of ChemAppPy brought us closer to achieving our goals.
  - We were now able to automate the thermochemical calculations and thus work more efficiently.
  - We are heading into our goal of integrating ChemAppPy into our digital platforms in the scope of a close cooperation between:
    - SMS group: R&D + Non-Ferrous Process and Technology
    - SMS digital
    - GTT and Ex Mente
Thank you for your attention!

Questions? please contact me under:

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