Estimation of K-centric parameters from temperature programmed GC

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* Similar idea like in several previous papers, like Hou2018, McGinitie and others
* Here estimation for the K-centric parameters, of which one (Tchar) can roughly be estimated from elution temperature (Blumberg2017, Brehmer2022)
* Simulation of GC is the backbone of this paper (Leppert2022)
* Simulation is differentiable (AutoDiff) in the Julia code
* Investigate different optimization algorithms (Optimization.jl), e.g. Nelder-Mead (McGinitie), Newton-method (Hou2018) and others
* Compare results with parameters estimated using isothermal measurements
* Test results by simulate new GC separations and compare them to measurements