动力学作业

Brief Workflow:

- ✓ Data load
- ✓ Determination of the number of components (SVD)
- ✓ Initial estimation (EFA analysis)

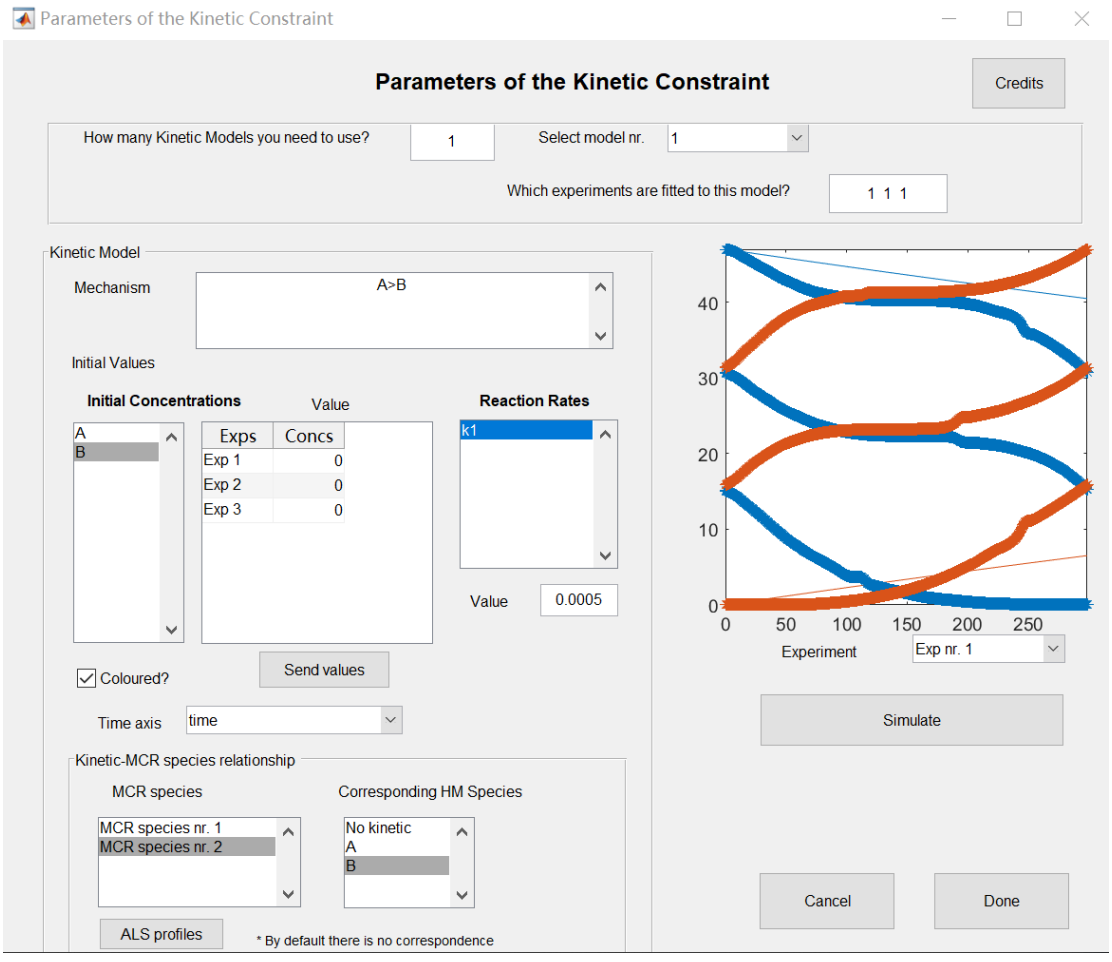
- ✓ Row constraints (Non-negativity + Kinetic Models)
- ✓ Column constraints (Non-negativity)

- ✓ ALS optimization (Iteration:200, convergence criterion:0.1)

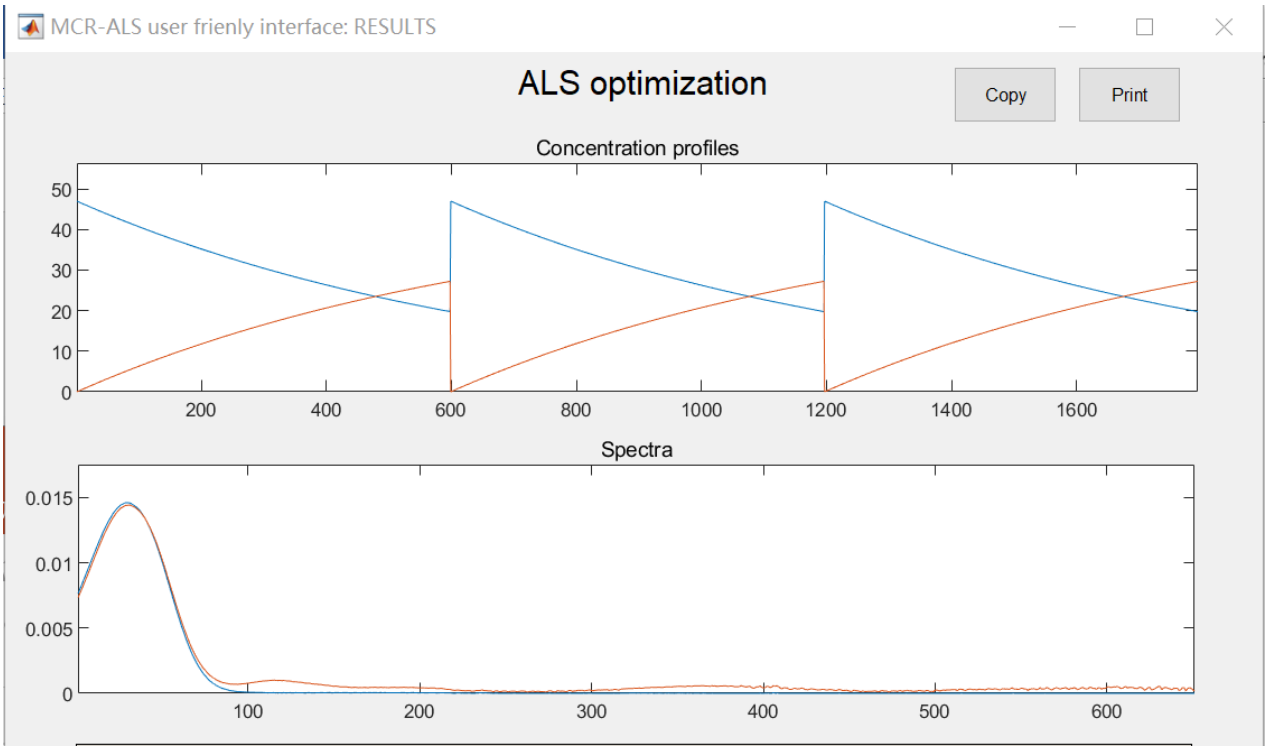
- ✓ Output (分解矩阵 concentrations + spectra; 残差矩阵)

Outcomes:（Graphs）

漆酶+底物体系（LAC_SUB）

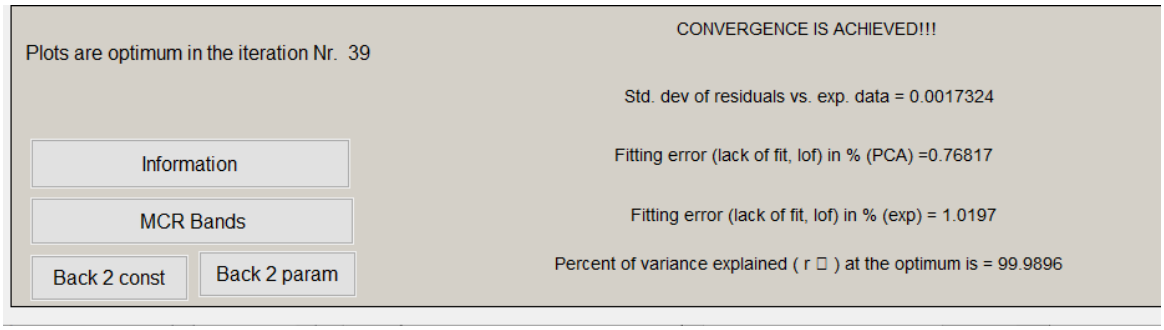


动力学模型限制步骤（模拟+ALS）



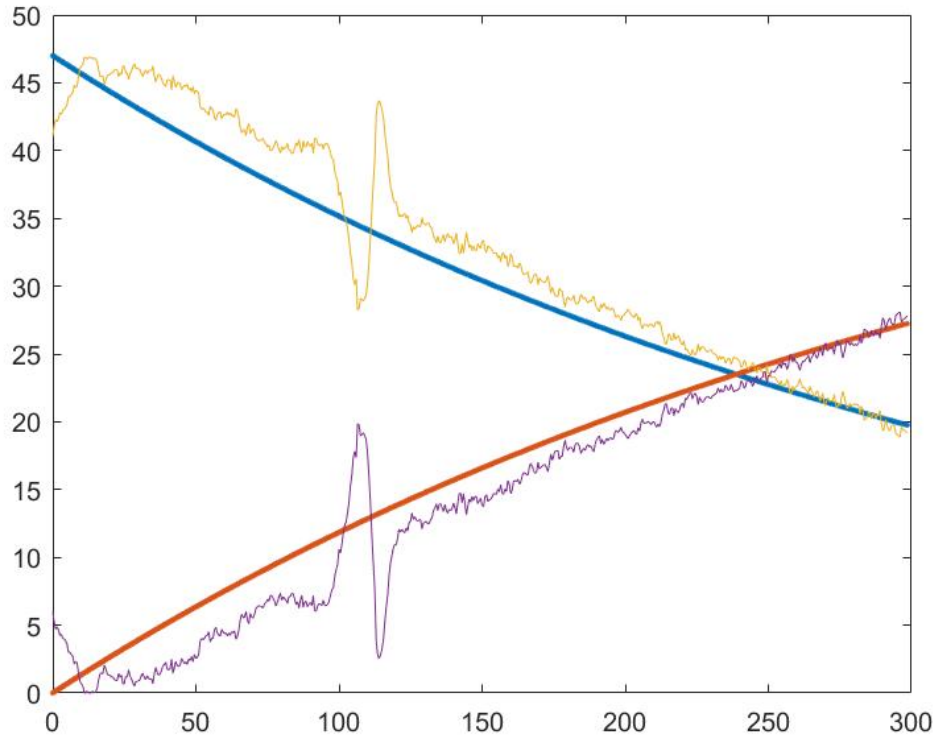
ALS 优化结果

分解得到两个矩阵（上：浓度矩阵，下：光谱矩阵）

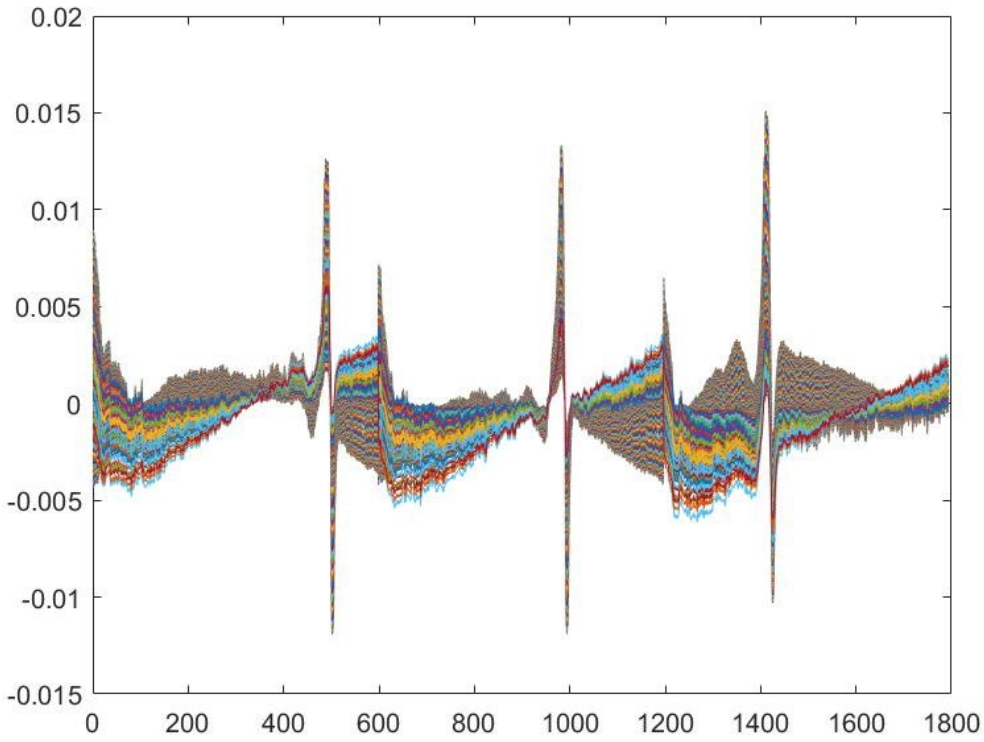


在第 39 次迭代达到最优

优化性能参数如上列出

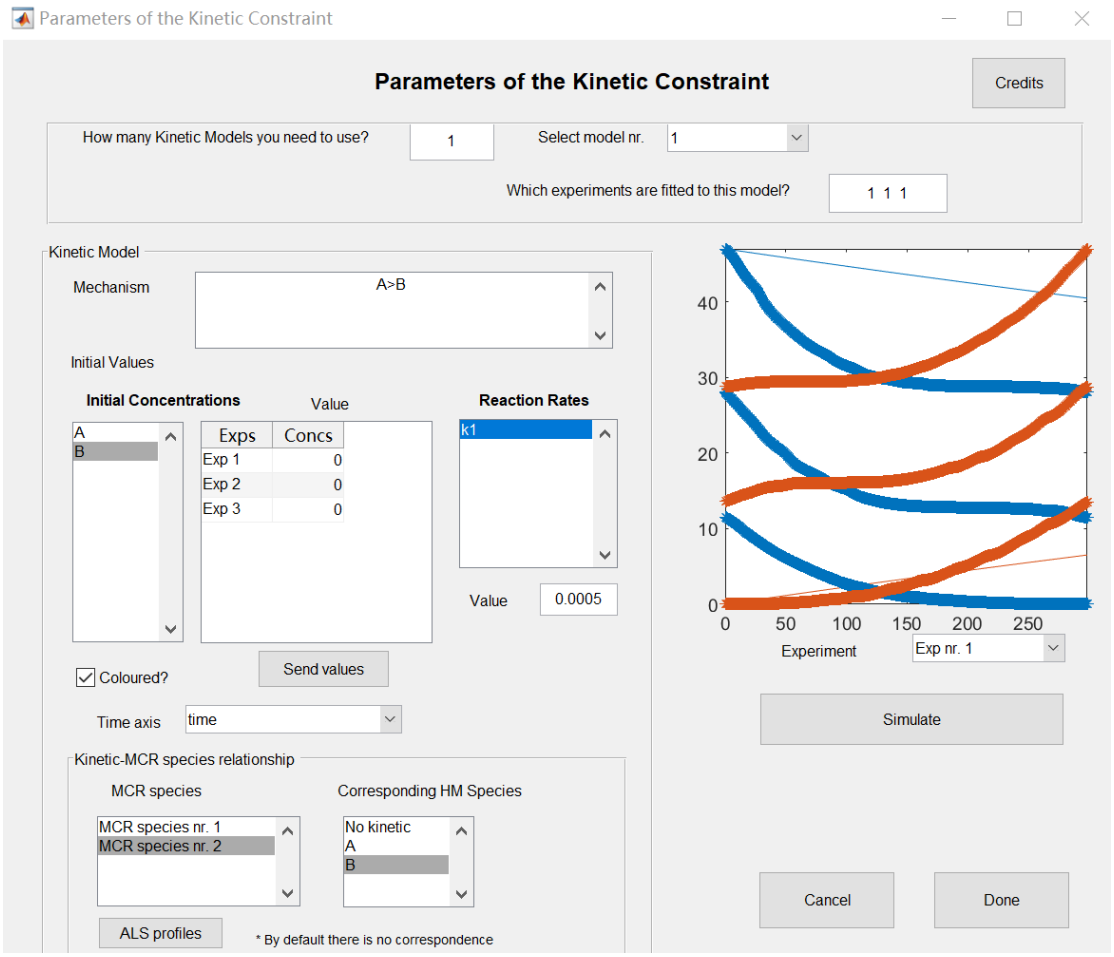


分解矩阵迭代优化过程，逐渐收敛

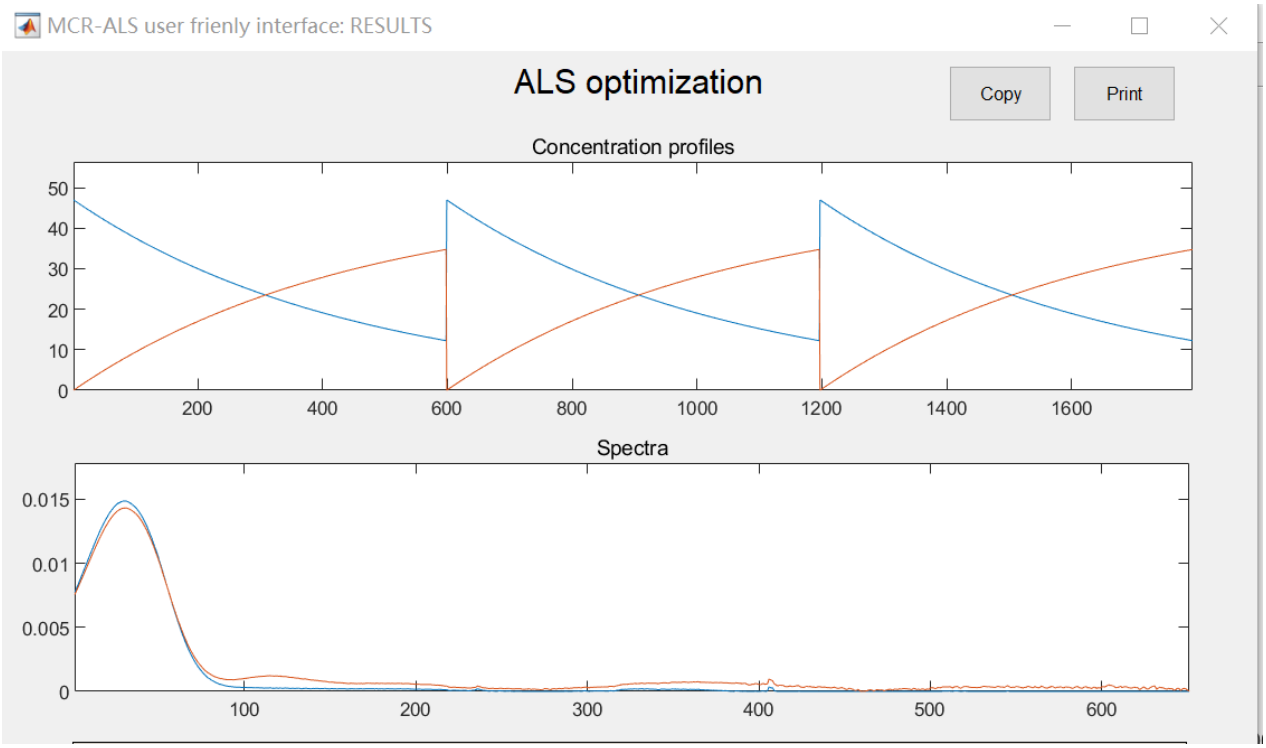


误差矩阵示意图

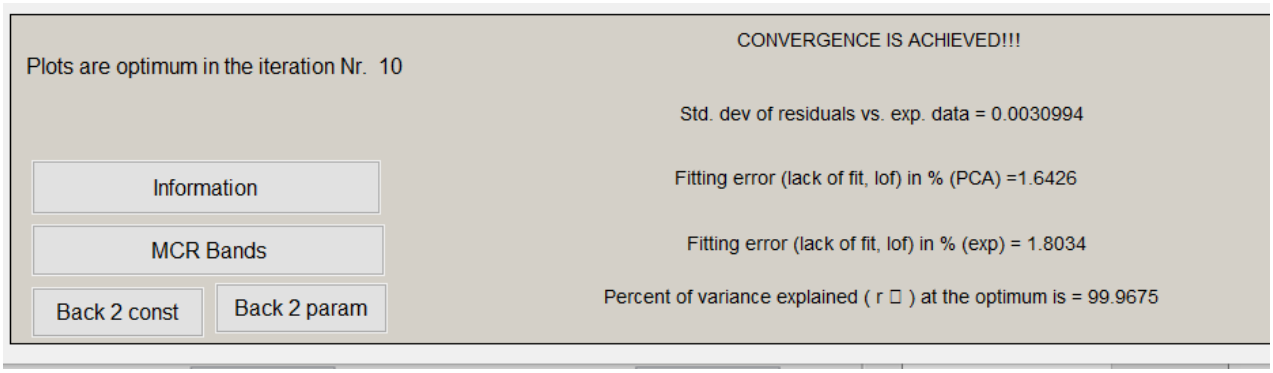
漆酶+介体 TEMPO+底物体系（LAC_TEMPO_SUB）



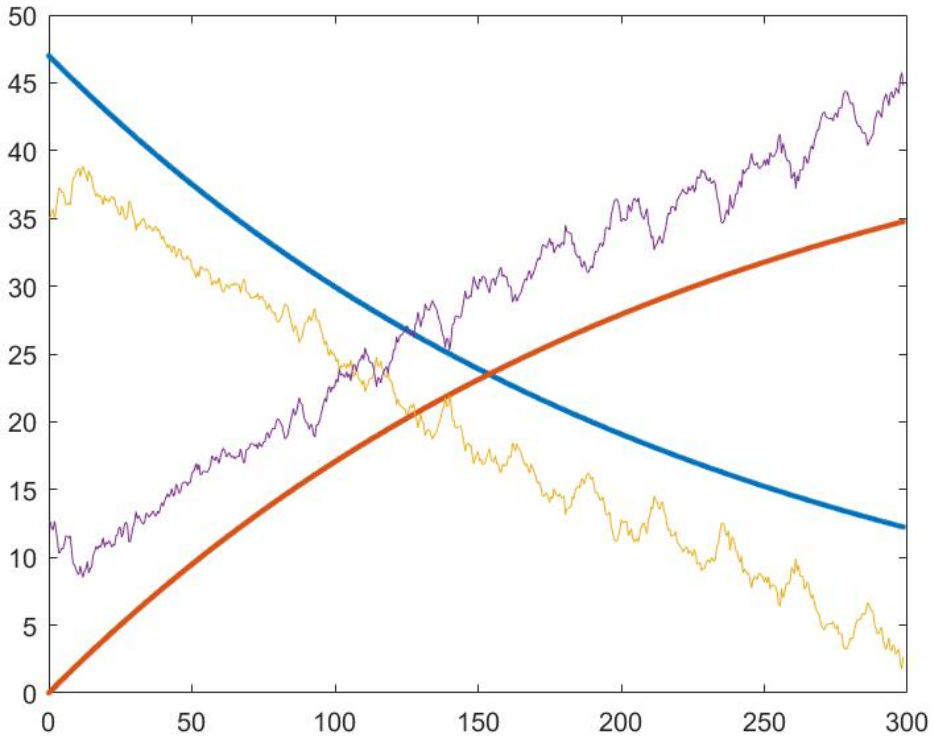
动力学模型限制步骤（模拟+ALS）



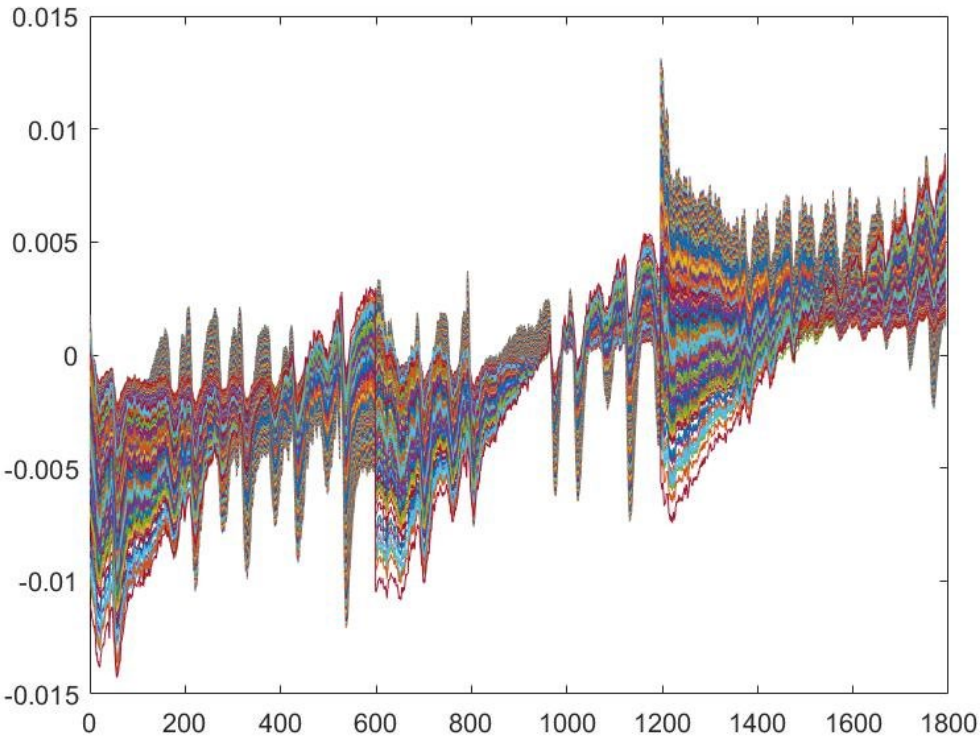
ALS 优化结果
分解得到两个矩阵（上：浓度矩阵，下：光谱矩阵）



在第 10 次迭代达到最优
优化性能参数如上列出



分解矩阵迭代优化过程，逐渐收敛



误差矩阵示意图