

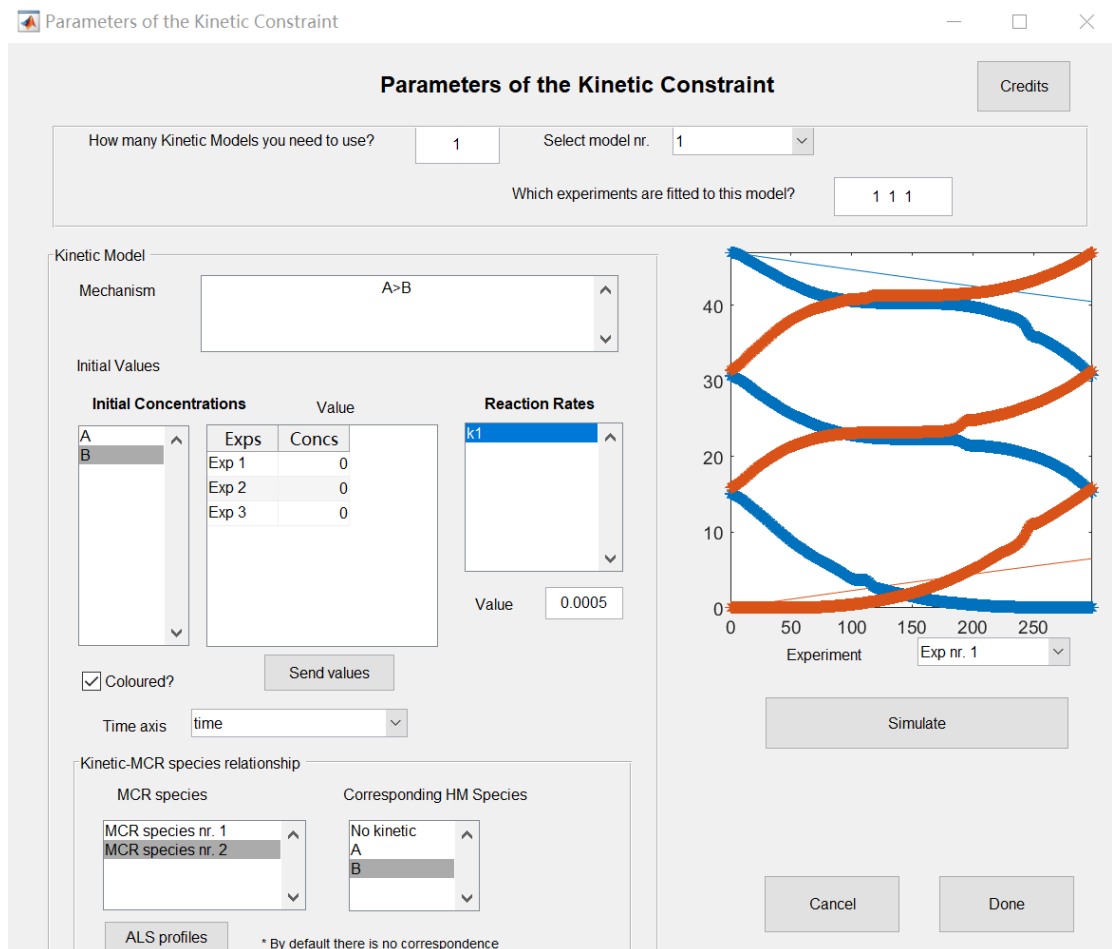
# 动力学作业

## Brief Workflow:

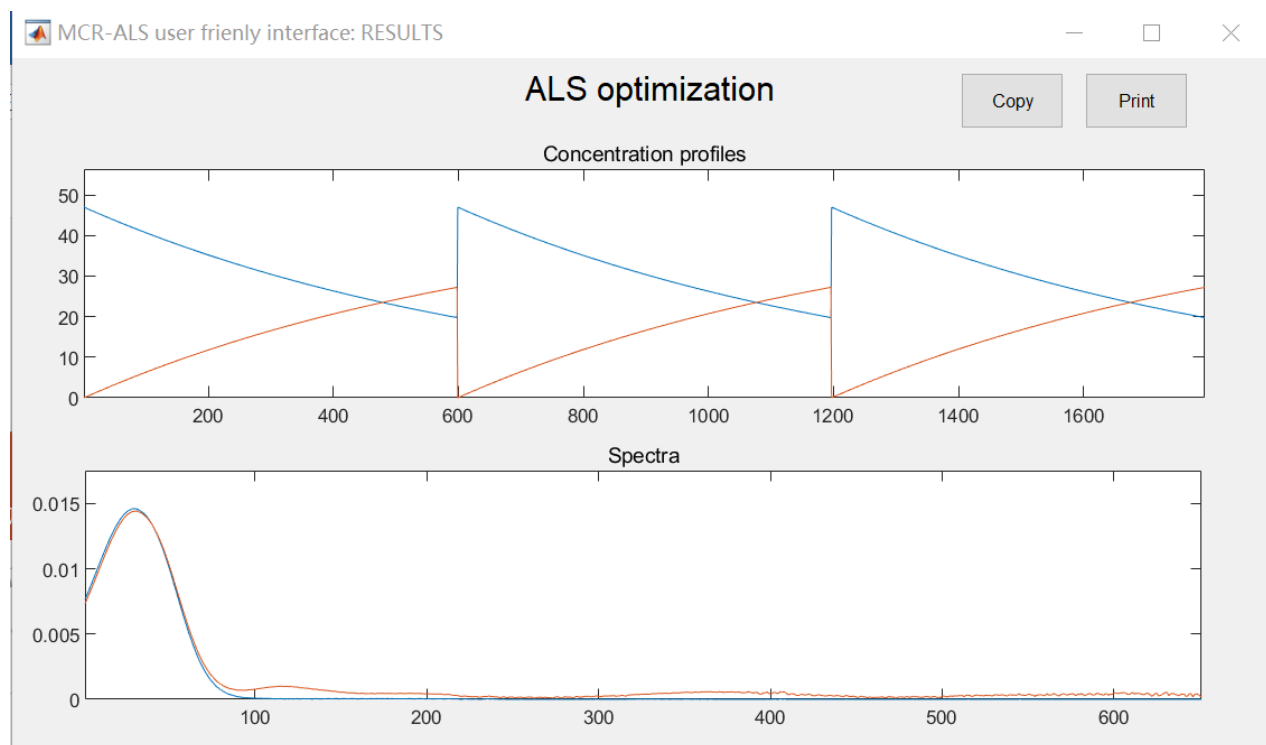
- ✓ Data load
- ✓ Determination of the number of components (SVD)
- ✓ Initial estimation (EFA analysis)
- ✓ Row constraints (Non-negativity + Kinetic Models)
- ✓ Column constraints (Non-negativity)
- ✓ ALS optimization (Iteration:200, convergence criterion:0.1)
- ✓ Output (分解矩阵 concentrations + spectra; 残差矩阵)

## Outcomes: (Graphs)

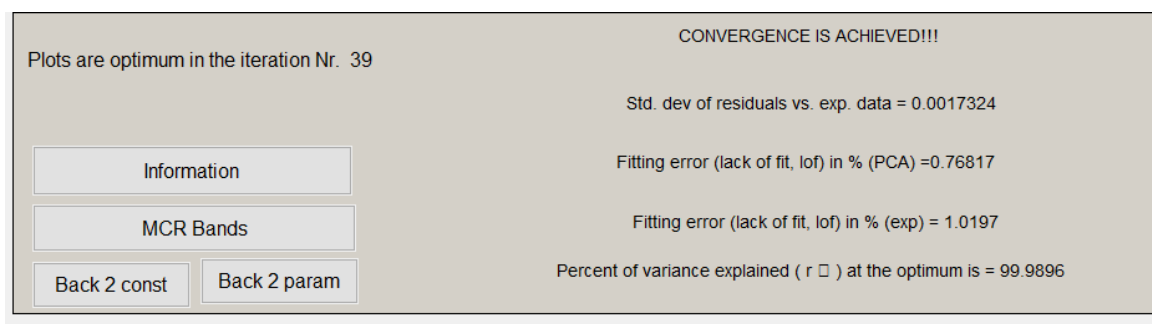
### 漆酶+底物体系 (LAC\_SUB)



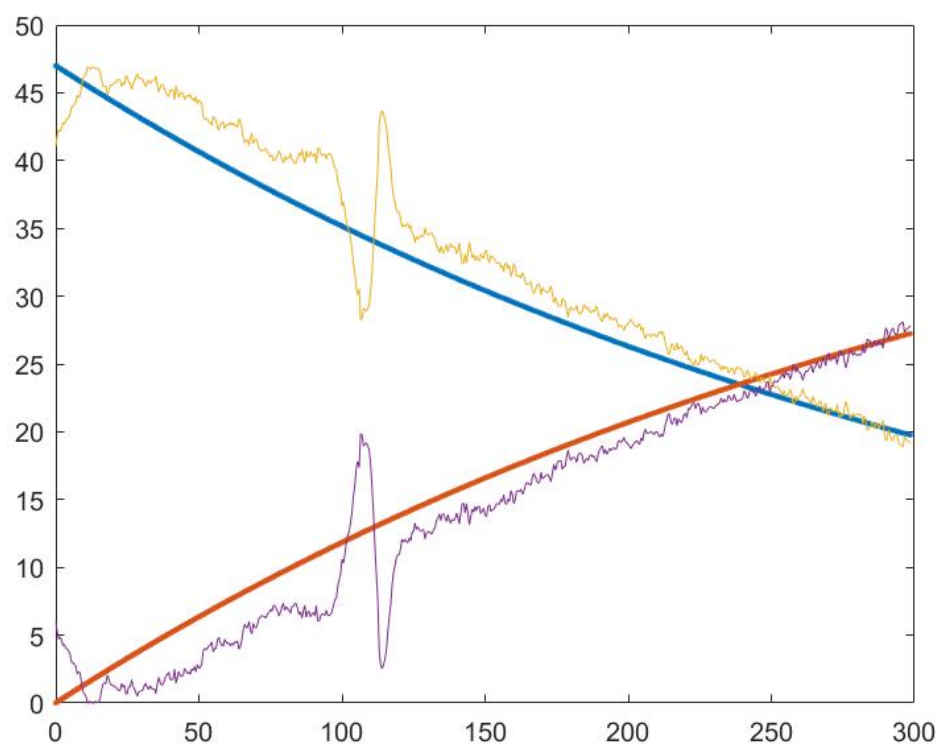
动力学模型限制步骤 (模拟+ALS)



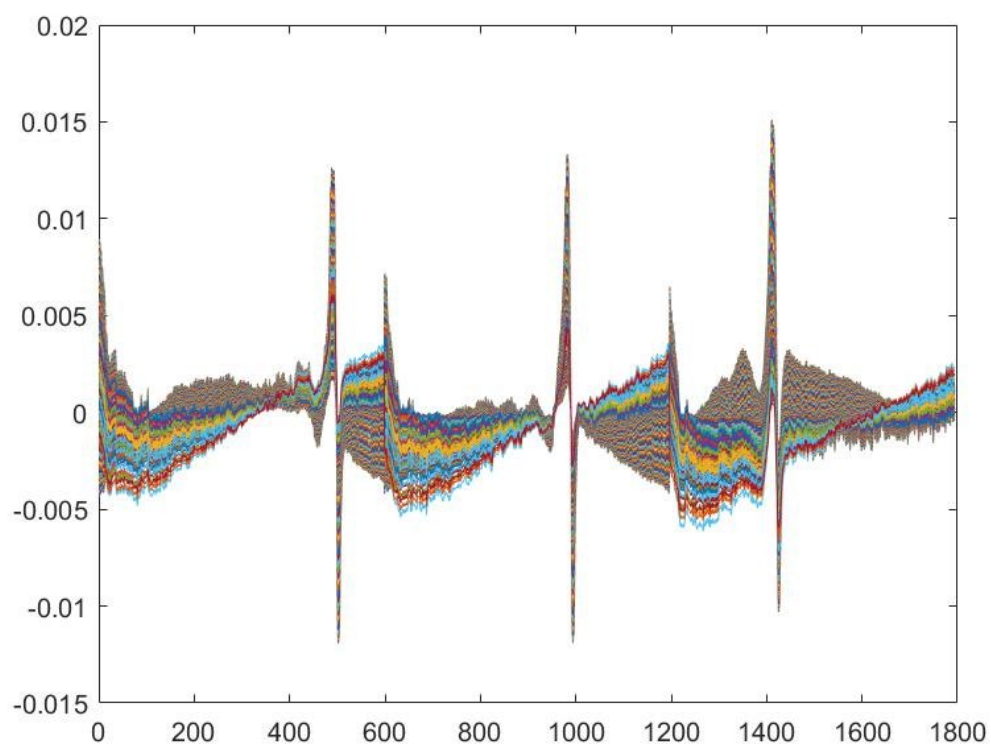
ALS 优化结果  
分解得到两个矩阵（上：浓度矩阵，下：光谱矩阵）



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)

Parameters of the Kinetic Constraint

How many Kinetic Models you need to use?  Select model nr.

Which experiments are fitted to this model?

Kinetic Model

Mechanism

Initial Values

Initial Concentrations

	Exps	Concs
A	Exp 1	0
B	Exp 2	0
	Exp 3	0

Reaction Rates

Value

☒ Coloured?

Time axis

Kinetic-MCR species relationship

MCR species

Corresponding HM Species

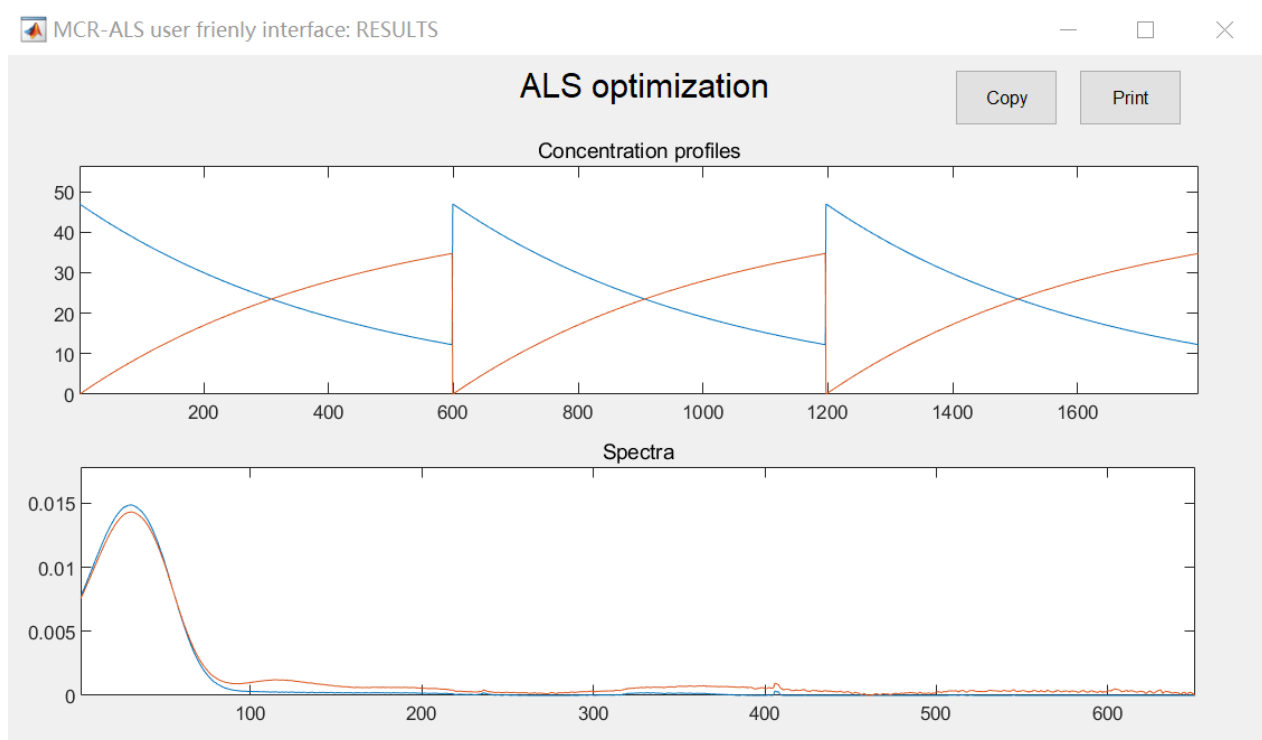
ALS profiles

\* By default there is no correspondence

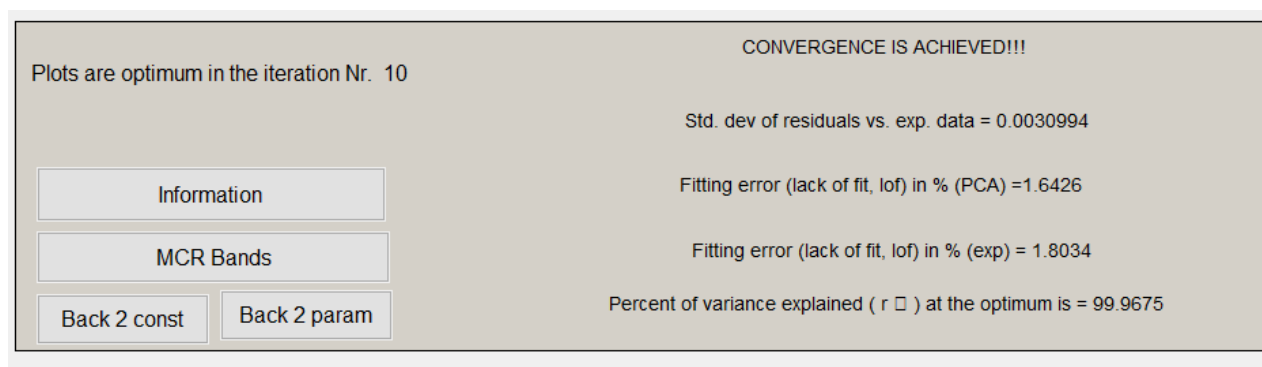
Simulate

Cancel Done

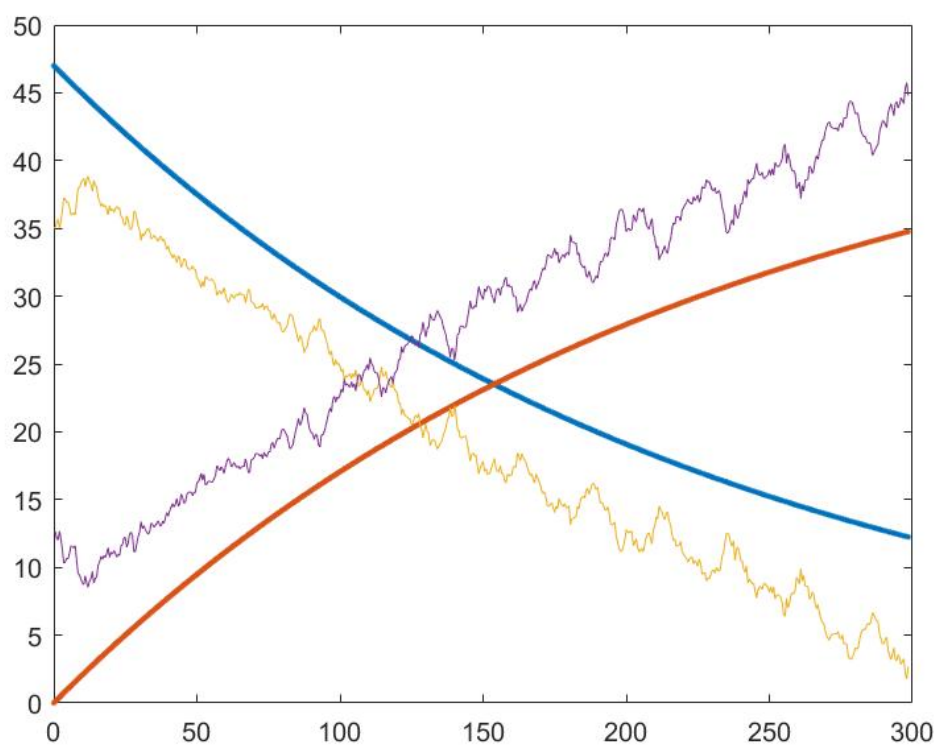
动力学模型限制步骤 (模拟+ALS)



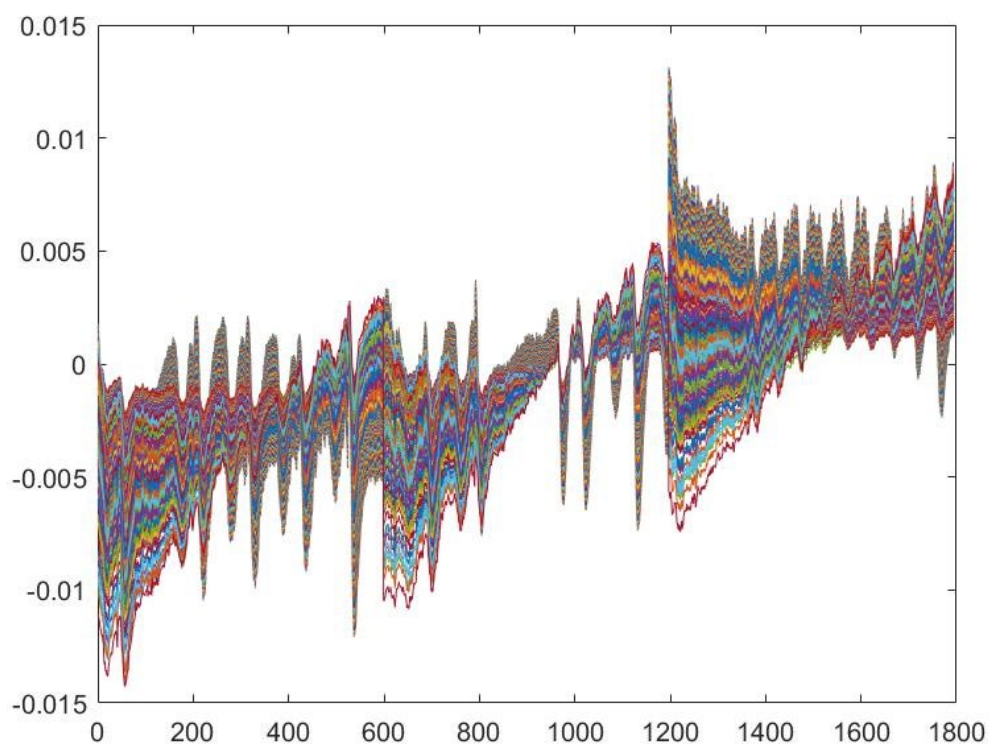
ALS 优化结果  
分解得到两个矩阵（上：浓度矩阵，下：光谱矩阵）



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