

Exercises 2 - PASB 2025

Hands-on session on Thermodynamic Flux Analysis (TFA) in a reduced metabolic model of *E. coli*

Part 1. Simulating Growth

You are given a reduced metabolic model of *E. coli* (small_ecoli.mat) on MOODLE. Compare the growth yield among alternative carbon sources in aerobic and anaerobic conditions for FBA and for TFA. Assume a maximal uptake rate of 10 mmol/hr/gDW for each respective carbon source, while setting the others to zero.

Do you observe any differences in the growth rates?

To create the TFA model you first need to load the thermodynamic data (thermo_data.mat) that you can find on MOODLE. Then to build the TFA model structure you should use in the following order the matTFA functions: 1) prepModelForTFA, 2) convToTFA, and 3) addNetFluxVariables. To help you understand the usage of the previous functions and the structure of the TFA model we provide on MOODLE a TFA CheatSheet.

Substrates	Max. yield AEROBIC		Max. yield ANAEROBIC	
	FBA	TFA	FBA	TFA
D-Glucose				
D-Lactate				
Acetate				
Ethanol				

Part 2. Integrating concentration data

You are given a set of metabolomics (metaboloimics_data.csv) on MOODLE. Find the metabolites that are represented in your model and integrate their concentration ranges (one standard deviation - if none is given, assume a relative error of 0.5) into the TFA model. Assume a maximal uptake rate of 10 mmol/hr/gDW for each of respective carbon source, while setting the others to zero. Round your results to the third digit.

Do you observe any differences in the growth rates? Provide a list with the metabolites that are part of your model and the ones that are not.

Substrates	Max. yield AEROBIC		Max. yield ANAEROBIC	
	FBA	TFA	FBA	TFA
D-Glucose				
D-Lactate				
Acetate				
Ethanol				

