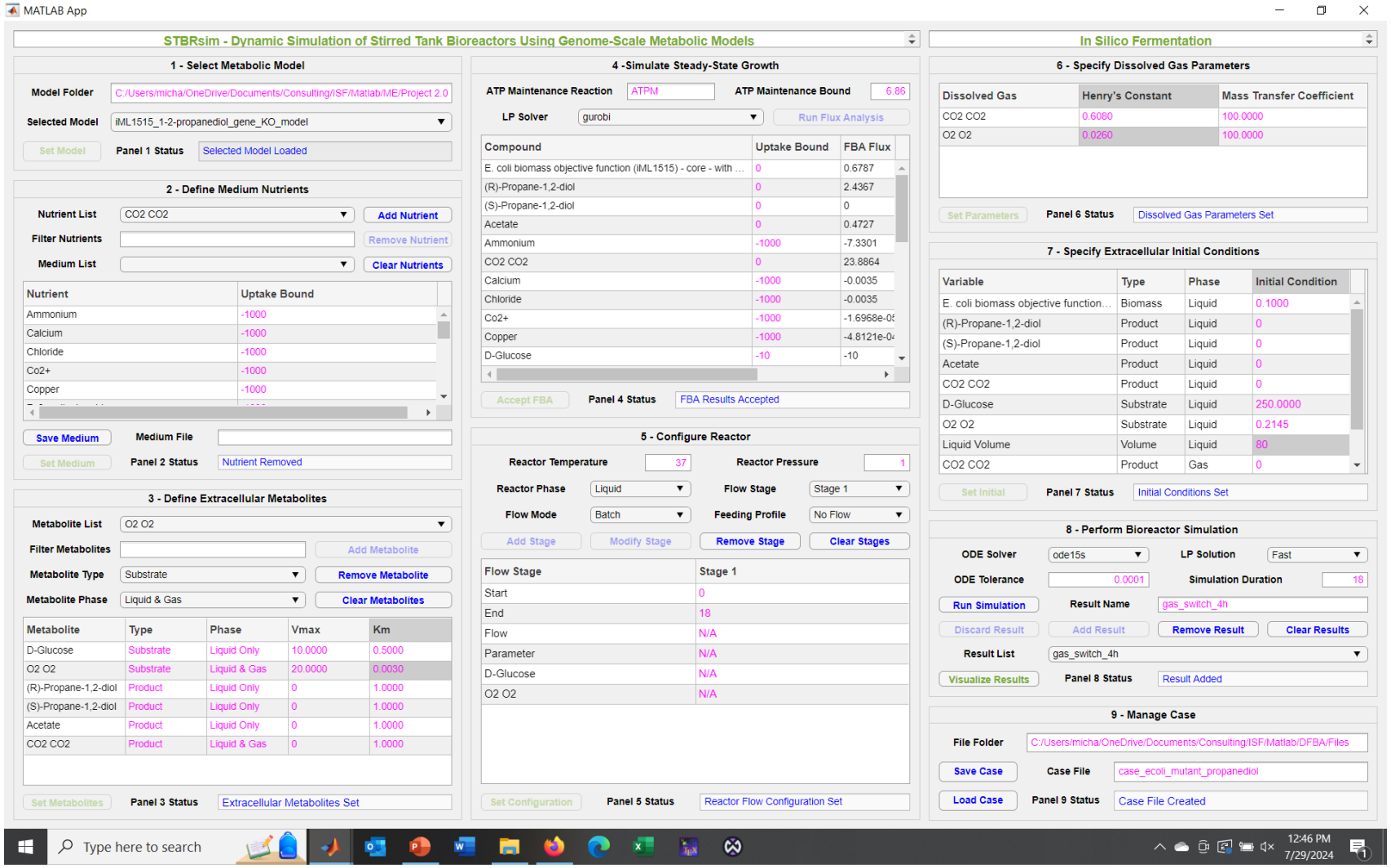
STBRsim – A MATLAB Application for Stirred Tank Bioreactor Simulation

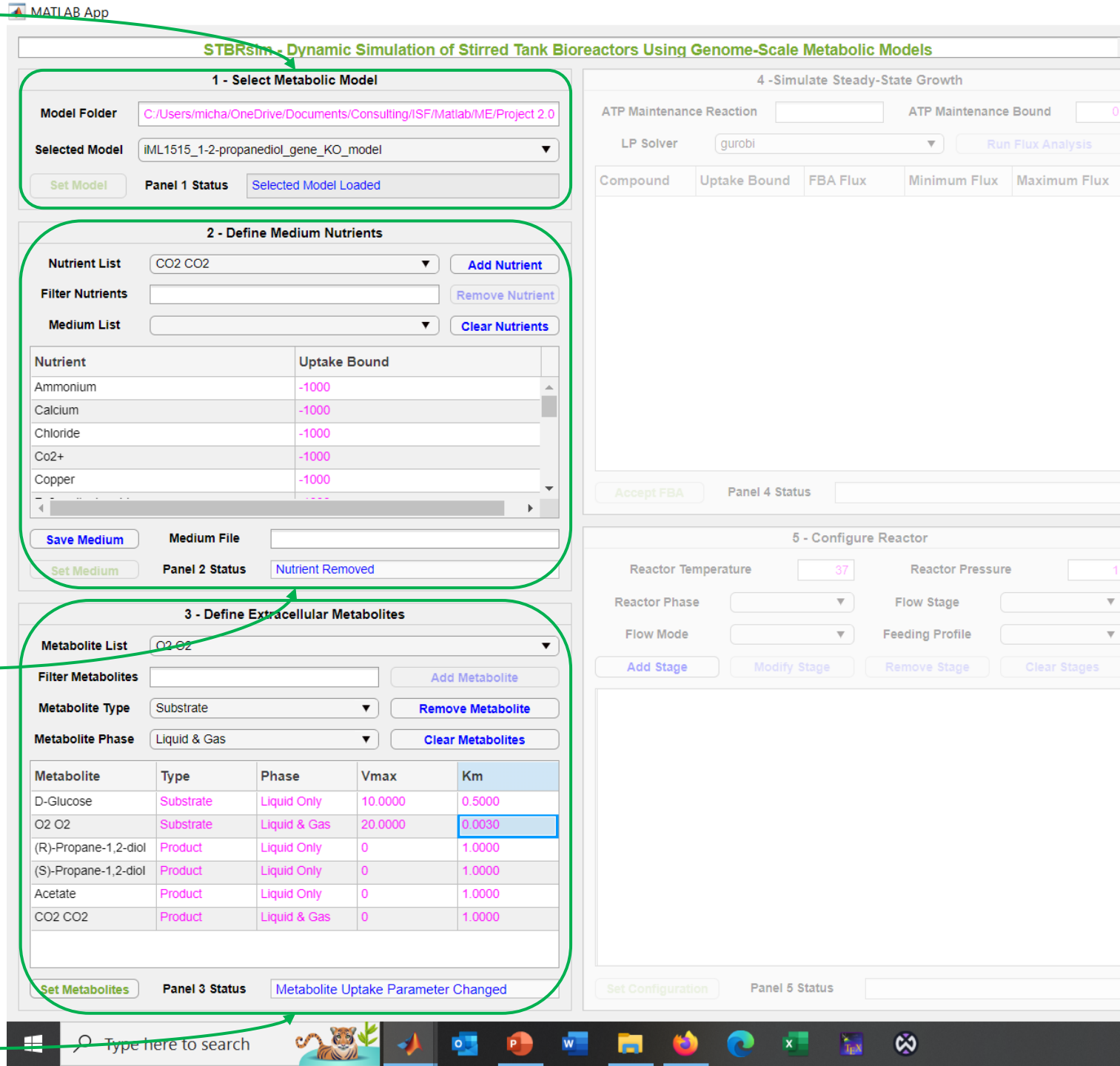


Example – Determine the optimal time for aerobic-to-anaerobic switch to maximize the production of R-1,2-propanediol production in engineered *Escherichia coli*

1. Select the metabolic model for the strain to be simulated. Here we select an *E. coli* strain designed for 1,2-propanediol synthesis.

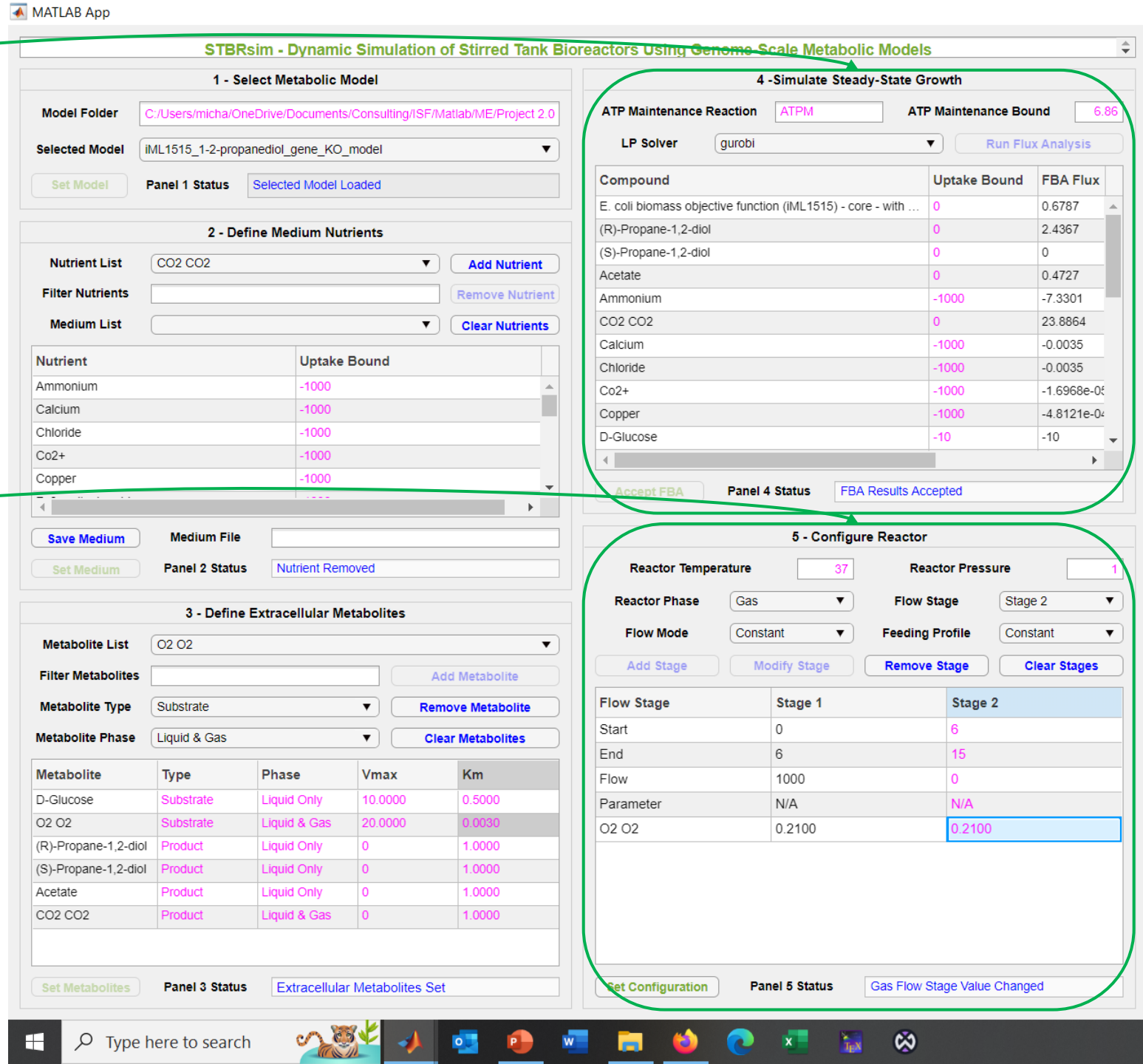
2. Define the culture medium in terms of unlimited nutrients and their maximum uptake rates. The nutrients can be extracted from the model, specified manually, or loaded from a saved file.

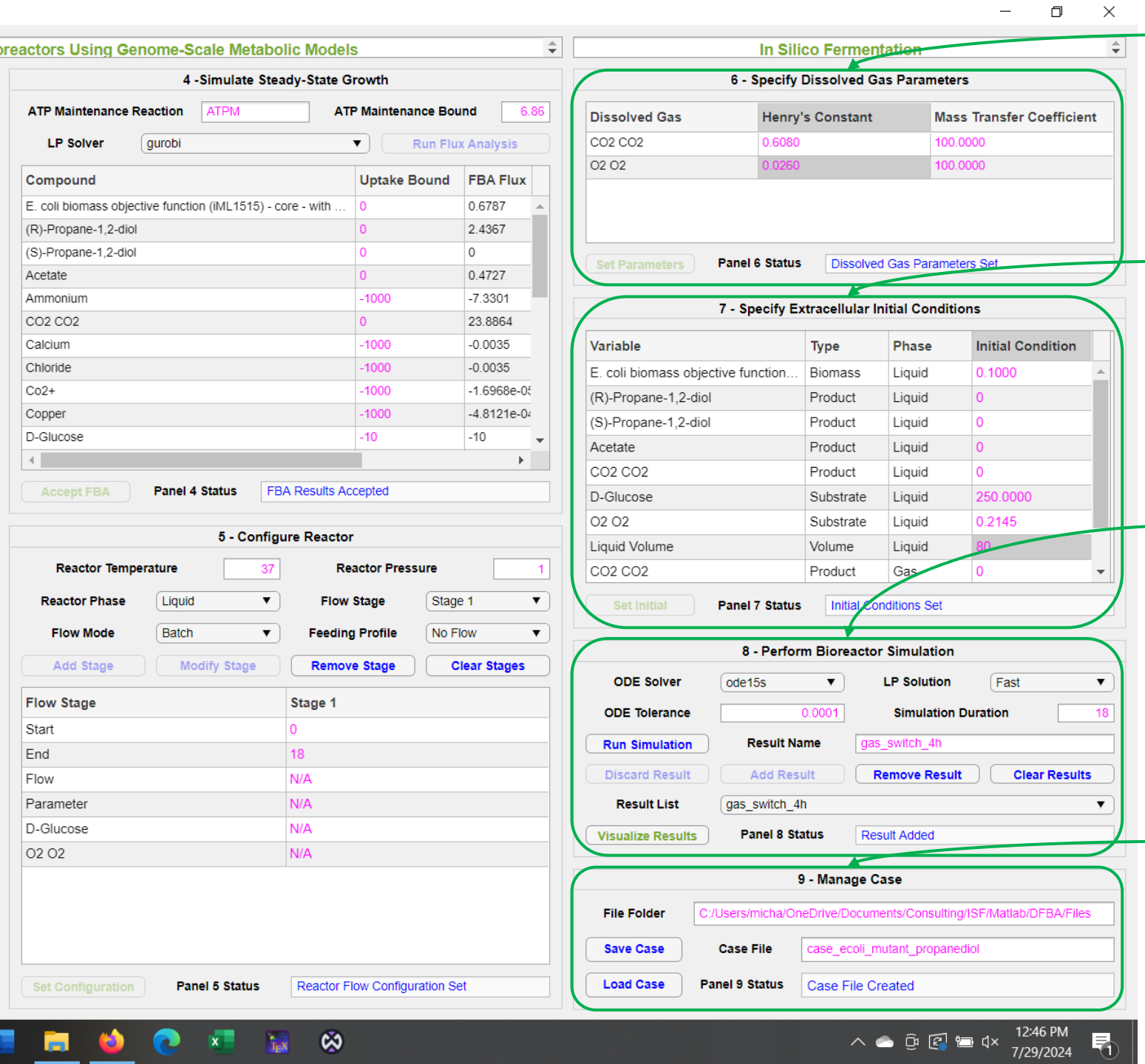
3. Define balanced extracellular metabolites, including growth-limiting substrates and secreted products. Each metabolite is characterized by its phases(s) and uptake kinetic parameters.



4. Perform flux balance analysis to analyze steady-state growth. Maximum uptake rates can be changed to determine their effects on cellular growth, substrate uptake and product secretion rates.

5. Configure liquid and gas flow stages to implement time-based feeding strategies. The flow mode (e.g., fed-batch), feeding profile (e.g., ramp), start/end times, flow rate parameters, and feed substrate values can be specified for each stage.





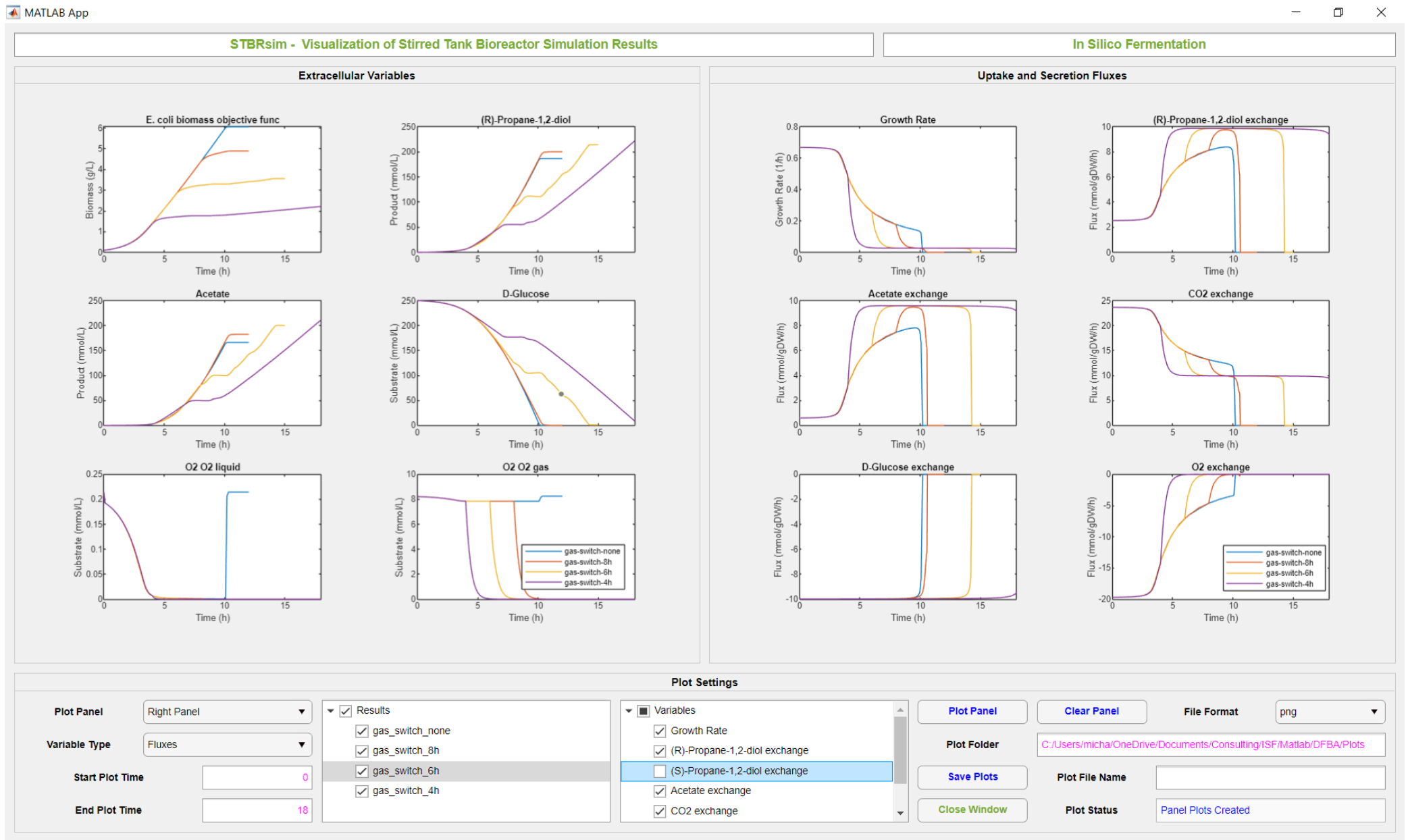
6. Specify dissolution and mass transfer parameters for the dissolved gases.

7. Specify initial conditions for all extracellular variables in the liquid and gas phases.

8. Perform dynamic simulation for the current parameters. Different simulations can be stored to allow comparison through a companion visualization App.

9. Save current case to completely capture the current App state for subsequent loading.

STBRsim – Companion App for Result Visualization and Comparison



Batch Production of R-1,2-propanediol in Engineered *Escherichia coli*

Gas Switch Time (h)	Total Batch Time (h)	Final R-1,2-BD Titer (mmol/L)	Volumetric Productivity (mmol BD/L/h)	Product Yield (g BD/g glucose)
None	10.3	187	18.2	0.32
8	10.8	200	18.5	0.34
6	14.4	214	14.9	0.36
4	17.0	230	13.5	0.39