

Computing and Graphing Fluxes to Facilitate QSP/PhysioPD™ Model Development and Calibration

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Typical QSP models / PhysioPD Platforms include interacting species that regulate each other. A species may have multiple influx and efflux reactions, each of which could in turn contain non-linear functions of other species in the Platform. In this context, it can become quite challenging to discern which reaction rates are the biggest drivers of the change in species value at different points in time, for different parameterizations, and under different simulated experimental conditions.

To address this challenge, Rosa & Co. has developed the RateCalculator, a MATLAB script that calculates a set of reaction rates from an existing SimBiology model and plots the resulting values in an organized and informative way. This script allows for quantitative assessment of the fluxes that determine the rate of change for a given species. Model object and simulation outputs provided by the user in the MATLAB workspace are parsed and the necessary species, parameters, and rules for reaction rate calculations are extracted. The user specifies the species of interest, and the script automatically computes all influx and efflux reactions, which are then organized into a single, intuitive plot. Requirements for successful script execution include: 1) Species have unique names even across compartments; 2) Rules are active if used in reaction rates; 3) All reactions for a chosen species contain the species name in its reaction definition. The resulting plot is formatted using Rosa's proprietary style, but can be customized by the user. In the future, this tool can be readily expanded with additional features such as computing multiple species at a time and/or computing the same species for different simulated experimental conditions.

We will demonstrate the use of this script in the context of a PhysioPD Platform to highlight both the mechanics of using it, and its utility in developing QSP/PhysioPD models.