

Introduction to Mathematical Modelling Part-3

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Derivation of Mathematical Equations for Understanding Systems Behaviour:

Depending upon the nature of biological process, it is essential to understand different modeling approach as numbers of methods have been used for different biological systems. Functionally, most of the cellular processes are dynamic that change with environmental change such that the signaling or regulation for specific genes when cell is exposed to an extraordinary medium. In order to describe such time-dependent phenomena it is necessary to choose mathematical equations that can capture these dynamic effects. In other biological systems where cellular products/molecules don't change over time i.e., concentration remains same, it is not necessary to describe details of underlying dynamics. For modeling the systems behavior, suitable methods have been developed. Among them are two methods, commonly used in modeling of metabolic process, modeling of signaling and regulatory pathways.

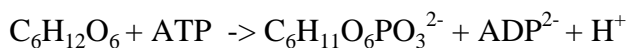
1. Modeling Metabolic Process

Metabolism is an essential process in all living being that provide energy and building blocks for survivability, synthesis of larger molecules and degradation of unnecessary/toxic substance in a cell. Understanding metabolic mechanism have been a part of major research interest for decades but complete interplay of underlying mechanisms has yet not been understood.

One of the key parameter in any metabolic study is the metabolic flux, that is, utilization (conversion) of metabolites along metabolic pathways. Thus, it is important to understand and predict the metabolic flux for all patterns of metabolism that inculcate which biochemical routes are being utilized. Here curve of modeling is fitted into concepts of hypothetical framework or into even known biochemical route so as to identify any particular step in the production/degradation of a desirable molecule (metabolic bottlenecks) by cultured cell/bacteria that in fact limit the overall rate with which the process occur. And result of the study will direct researcher on how to genetically modify the cell or bacteria to optimize the yield of the

particular end product. In overall process, metabolic flux are not concerned much as they are not when biochemical process are operated in steady-state and entry of unnecessary molecule is totally blocked, leaving process to be quasi-stationary without external perturbation to take place.

For such metabolic (quasi-stationary) process, we may consider the conversion of sugar to sugar phosphate. In this process, an enzyme hexokinase adds a phosphate group to the glucose, ($C_6H_{12}O_6$) yielding a compound, glucose-6-phosphate. This reaction should be balanced in terms of atoms and electrical charges. In a chemical notation, the balanced reaction is written as



In the above reaction, both sides of the equation are in a stoichiometric balance. Over investigating more complex metabolic network, each individual chemical reaction is bound with stoichiometric balance constraints such as mass, number of molecules, concentration and charges on reactants that can be used to formulate *mathematical equation*. For such reaction constraints, one should mind that they are not independent from each other and should be solved in parallel to develop a reliable mathematical model. The validity of the models can be tested through wet lab techniques using detectable or radioactively labeled substances. Labeled atoms can be traced across a number of key metabolites, indicating the cellular influx distribution help validate or disapprove metabolic network model.

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