SimBiology of Metabolic Pathway of Biobutanol Production by *Clostridium acetobutylicum*

Nooshin Asadi\(^1\), Mohammadhadi Jazini\(^2*\), Keikhosro Karimi\(^3\)

1- MSc Student, Department of Chemical Engineering, Isfahan University of Technology, Isfahan, Iran
2- Assistant Professor, Department of Chemical Engineering, Isfahan University of Technology, Isfahan, Iran
3- Associate Professor, Department of Chemical Engineering, Isfahan University of Technology, Isfahan, Iran

\(^*\)m.h.jazini@cc.iut.ac.ir

**Abstract**

Butanol is known as a fuel blended more readily with gasoline and hydrocarbon products and contains higher heat value in comparison with ethanol. *Clostridium acetobutylicum* is able to produce a considerable amount of butanol. Acetone and ethanol are products of the other metabolic path of this strain. The simple models describing the production of these metabolites like Monod model are restricted to prognosticate intracellular processes. The mathematical expression of intracellular metabolites production, as a method, is applied to optimize the production of the desired compound, especially, in cellular metabolic engineering.

In this study, the structured model of the cellular metabolic pathway of *Clostridium acetobutylicum* was utilized to describe and predict the dynamical variations of intra and extracellular metabolites. Mathematical equations of the model were solved by SimBiology metabolic path stimulator and the obtained results were compared with experimental data, which revealed an appropriate conformity. The effects of butyrate and acetate on the butanol production were investigated and the results demonstrated that the butanol production increased at the presence of those substances in the culture media. The presence of butyrate in the media led to an increase in butanol production and decrease in time required to attain the maximum butanol production. The butanol concentration was 120.48 mM when the initial concentrations of acetate and butyrate are 100 and 0 mM, respectively and one is 138.35 mM with 100 mM of butyrate and 0 mM of acetate initial concentrations. Due to the irreversible production reaction of acetone in the metabolic pathway, butanol production was not influenced by the acetone concentration, but its elimination from the cell pathway increased the butanol production.

**Keywords:** Biobutanol, Modeling, SimBiology, *Clostridium acetobutylicum*, Metabolic pathway.