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## ACCEPTED MANUSCRIPT

**Biotechnology and Bioengineering** 

### Novel Kinetic Model for the Simulation Analysis of the Butanol Productivity of *Clostridium acetobutylicum* ATCC 824 under Different Reactor Configurations

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**Abstract.** Acetone-Butanol-Ethanol (ABE) fermentation process can be exploited for the generation of butanol as biofuel, however it does need to overcome its low volumetric solvent productivity before it can commercially compete with fossil fuels technologies. In this regard, mathematical modelling and simulation analysis are tools that can serve as the base for process engineering development of biological systems. In this work, a novel phenomenological kinetic model of *Clostridium acetobutylicum* ATCC 824 was considered as a benchmark system to evaluate the behaviour of an ABE fermentation under different process configurations using both free and immobilized cells: single stage batch operation, fed-batch, single stage Continuous Stirred Tank Reactor (CSTR) and multistage CSTRs with and without biomass recirculation.

The proposed model achieved a linear correlation index  $r^2 = 0.9952$  and  $r^2 = 0.9710$  over experimental data for free and immobilized cells respectively. The predicted maximum butanol concentration and productivity obtained were 13.08 g·L<sup>-1</sup> and 1.9620 g·L<sup>-1</sup>·h<sup>-1</sup> respectively, which represents an increase of 1.01 % and 990 % versus the currently developed industrial scale process reported currently into the literature. These results provide a reliable platform for the design and optimization of the ABE fermentation system and showcase the adequate predictive nature of the proposed model.

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