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Determining an appropriate unstructured kinetic model for batch ethanol fermentation data using a direct search method

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ABSTRACT
In this paper, we study an extracellular process of a biochemical system such as batch ethanol fermentation system by considering an unstructured kinetic model with four different well-known models for the specific growth rate of the yeast cells. Then, we fit the unstructured models to the experimental data for determining the appropriate model that can capture the dynamic behaviour of the batch ethanol fermentation experimental data. The fitting procedure is proceeded by minimising a least-squared error between the model solutions and the experimental data using a direct search method. Our simulations show that the unstructured model with Aiba-type structured model for the specific growth rate of the yeast cell has the best approximating ability to describe the dynamic of the batch ethanol fermentation data.

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KEYWORDS
Batch fermentation data; unstructured model; parameter estimation; direct search method

Introduction
Renewable energy has become an increasingly interesting research topic in recent years. It plays an important role in providing alternative energy sources with a guarantee of sustainability. Bioethanol is one of the highly recommended energy sources, as it is a renewable and environmentally friendly alternative \cite{1,2,3,4}. As one of the renewable and sustainable energy sources, bioethanol has become a potential candidate for replacing fossil fuels, which have greatly contributed to generating high levels of pollution. Along with the development of bioethanol production, optimal production processes and economic feasibility of the ethanol industry are needed. Therefore, optimisation studies through operating the variable design are a common practice in the bioethanol industry, which has an unfeasible complexity.

In studying the optimal production of ethanol, several aspects are investigated, including the fermentation process of the sugars to ethanol performed by yeast. This is a key process in the bioethanol industry where generating a fermentation process with stable performance becomes the biggest challenge for all researchers due to the dependency of the system on the operating variables. Besides that, producing rapid fermentation also becomes the main concern in the ethanol industry.

Several mathematical models have been proposed to investigate the optimal growth of the yeast cells \cite{5,6,7,8,9,10,11,12,13,14,15}. Among the models, the unstructured model is the simple model proposed to describe the growth of yeast cells. A suitable design for the operating parameters of the system can be identified when appropriate models are applied to study the biochemical system. The suitable models are quantified whether they correctly reproduce the dynamic behaviour of the biochemical system. More deeply, the model should fit the experimental data generated from an experimental process. In this research, several models were investigated to find the best model that can capture the behaviour of the experimental data. Four well-known unstructured models were considered to study our batch ethanol fermentation data. We assumed that the yeast cells are entities in solution which interact with the environment in a way that the biomass is described only by its concentration. The four studied models are Monod \cite{15}, Tiessier, Aiba \cite{16} and Tyagi \cite{17} model type for the growth of the yeast cells. Our goal was to carry out a comprehensive analysis of the four mathematical expressions for modelling our batch ethanol fermentation data. This study also aims to understand the impact of some modelling assumptions underlying the system and to provide...