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Short Communication

Test for the Presence of Autocorrelation in the Buchanan-three-phase Model used in the Growth of *Paracoccus* sp. SKG on Acetonitrile

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ABSTRACT

Millions of tonnes of organonitriles are produced annually for use in industry. They are carcinogenic and mutagenic. Bioremediation of acetonitrile, an organonitrile, has been touted as a more economical and feasible method compared to physical and chemical approaches. In this work, we model the growth of growth of *Paracoccus* sp. SKG on acetonitrile from published literature to obtain vital growth constants. We discovered that the Buchanan-three-phase model via nonlinear regression utilizing the least square method was the very best model to explain the growth curve. Nonlinear regression utilizing the least square method typically utilizes the idea that data points usually do not depend upon each other or the value of a data point is not determined by the value of previous or proceeding data points or usually do not display autocorrelation. In this work, the Durbin-Watson statistic to check for the presence of autocorrelation in the growth model was carried out.

INTRODUCTION

Millions of tonnes of organonitriles are produced annually for use in industry. Organonitriles have been demonstrated to be carcinogenic and mutagenic. They're commonly used in industry for example the synthesis of plastics, rubber, herbicides, pharmaceuticals, drug intermediates and pesticides. Furthermore, acetonitrile, an organonitrile, is substantially employed in labs as a solvent and extractant for HPLC (High Performance Liquid chromatography). Organonitriles are classified as priority pollutants. The worldwide industrial consumption of acetonitrile on it's own is more than 4×10^4 tonne in 2001 [1,2]. Consequently, wastewaters from the various usages of organonitriles often contain high contents of organonitrile compounds. Bioremediation of acetonitrile has been touted as a more economical and feasible method compared to physical and chemical approaches. Santoshkumar et al [3] has isolated a bacterial strain that could grow on acetonitrile. The growth profile of the strain showed inhibition of growth at elevated concentrations of acetonitrile. Modelling of the growth curves can yield important parameters that could be used for further secondary modelling exercise such as the inhibitory effect of substrate on growth.

Previously, an acetonitrile-degrading *Paracoccus* sp. SKG has been reported [3]. We have utilized several growth models to model the growth of *Paracoccus* sp. SKG on acetonitrile. We discovered that the Buchanan-three-phase model via nonlinear regression utilizing the least square method was the best model to describe the growth curve (manuscript in preparation). Nonlinear regression utilizing the least square method typically uses the assumption that data points usually do not depend upon each other or the value of a data point is not dependent on the value of previous or proceeding data points. Autocorrelation between data sometimes happens because of events for example temperature drift during time measurements or an overused tungsten lamp in a spectrophotometer. If one would count the quantity of animals each year in a given area the data will be extremely autocorrelated and nonindependence as the quantity of animals within an existing year will be highly influenced by the quantity of animals in the last year [4]. This is very similar to growth of microorganisms where the increase in cellular number in a given time frame can be exponentially fast and any event in time that effect the current or past number of cells would be seen in an amplified manner in future times.

In this work, the Durbin–Watson statistic for the presence of autocorrelation in the growth of *Paracoccus* sp. SKG on acetonitrile as modelled using the Buchanan-three-phase model would be used. The method calculates the level of significance according to the method outlined by Draper and Smith [5].

METHODS

Acquisition of Data

In order to process the data, the graphs were scanned and electronically processed using WebPlotDigitizer 2.5 [6] which helps to digitize scanned plots into table of data with good enough precision [7]. Data were acquired from the works of Santoshkuma et al. [3] from Figure 4 and then replotted, and then assessed using several growth models where the Buchanan-three-phase model was found to be the best (**Fig. 1,** with permission) (Shukor, M.S., Masdor, N.A., Shamaan, N.A., Ahmad, S.A., Roslan, M.A.H. and Shukor, M.Y. 2015. The growth of *Paracoccus* sp. SKG on acetonitrile is best Modelled using the Buchanan Three Phase Model. Manuscript in preparation).

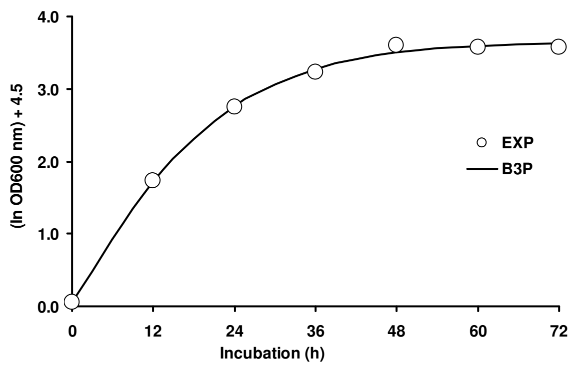

Fig. 1. Growth curves of *Paracoccus* sp. SKG on acetonitrile fitted by the Buchanan-three-phase model.

Durbin-Watson test

The Durbin–Watson statistic calculates the level of significance according to the method outlined by Draper and Smith [5].

$$d=\frac{\sum_{t=2}^{T}\left(\hat{e}_t-\hat{e}_{t-1}\right)^2}{\sum_{t=1}^{T}\hat{e}_t^2} \quad \textbf{(1)}$$

The hypothesis H_0: ρ= 0 versus the alternative $H1$: $\rho > 0$ is tested. The statistic is about equal to 2(1− p). The Durbin-Watson test statistic equals 2 when the ρ value is zero while a ρ value of one equals a Durbin-Watson test statistic of 0. Non-autocorrelation is specified by a d value near 2 while a value towards 0 indicates positive autocorrelation. Negative autocorrelation is indicated by d values nearing 4 (**Eqn**. 1).

The null hypothesis should be rejected for a low value of the Durbin-Watson test statistic indicating significant autocorrelation. Unlike the t- or z-statistics, the distribution of the Durbin-Watson test statistic is not available for ρ-value associated with d and tables must be used in the hypothesis testing.

The decision rule for the Durbin-Watson bounds test is
• if d > upper bound, fail to reject the null hypothesis of no serial correlation,
• if d < lower bound, reject the null hypothesis and conclude that positive autocorrelation is
present,
• if lower bound < d < upper bound, the test is inconclusive.

RESULTS AND DISCUSSION

The runs test has additionally been utilized as a method to test for autocorrelation in time-series regression models. Nonetheless, simulation studies employing Monte Carlo have demostrated that the runs test generates noticeably asymmetrical error rates in the two tails [8]. The investigation is carried out to analyse the empirical properties of the runs test utilizing (a) sample sizes of between 12 and 100 (b) using non-intervention and intervention regression models, (c) utilizing directional and nondirectional tests (d) with three levels of α, and (e) with 19 levels of autocorrelation among the errors. In addition, both directional and nondirectional tests produce no satisfactory results with respect to Type I error. The increase of the ratio of degrees of freedom to sample size to as high as .98 could also not remedy the situation. Hence, the Durbin-Watson method would be the method of choice to assess autocorrelation.

The Durbin–Watson statistic (DW) can calculate for the presence of serial correlation of residuals. Autocorrelation, also known as serial correlation, is the cross-correlation of a signal with itself. The DW is used to test whether a model has been successful in describing the underlying trend. Informally, it is the similarity between observations as a function of the time lag between them. It is a mathematical tool for finding repeating patterns, such as the presence of a periodic signal obscured by noise [4,5,9].

The value of the Durbin-Watson statistics was d = 0.346/0.131 = 2.634. As usual the hypothesis H_0: ρ= 0 versus the alternative $H1$: ρ > 0 is tested. The statistic is approximately equal to 2(1− p). The Durbin-Watson test statistic equals 2 when the ρ value is zero while a ρ value of one equals a Durbin-Watson test statistic of 0. Non-autocorrelation is indicated by a d value near 2 while a value towards 0 indicates positive autocorrelation. Negative autocorrelation is indicated by d values nearing 4. The null hypothesis should be rejected for a low value of the Durbin-Watson test statistic indicating significant autocorrelation. Unlike the t- or z-statistics, the distribution of the Durbin-Watson test statistic is not available for ρ-value associated with d and tables must be used in the hypothesis testing. For a three-parameter model like Buchanan-three-phase model, the upper critical valued_U was 2.102 while the lower critical value d_L was 0.229. Since d was higher than the upper critical value then the null hypothesis that no positive autocorrelation exist is not rejected i.e. there appears to be no evidence of positive autocorrelation and the Buchanan-three-phase model used for fitting the growth curve was adequate. Autocorrelation occurs when covariances of errors are not zero, a problem often seen in time series data such as microbial growth curves. A consequent of the presence of autocorrelation is that estimators for the models used even though are still considered linear and unbiased, but they there not efficient and not the best.

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