Data in Brief

Dataset on modeling and optimization analysis of biodegradation of paracetamol

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Abstract

This article contains the experimental and statistical data related to degradation of acetaminophen (paracetamol, APAP) by bacterial strains. The strains used in this study were isolated from wastewater by enrichment culture method. The optimization was important to identify the physical conditions at which the strain degraded the APAP effectively. Therefore, the Box-Behnken design (BBD) was used to know the influence of physical parameters (viz. pH, temperature, agitation speed, and concentration) on the degradation of APAP. The effects of the physical factor on the degradation process were investigated by a mathematical model, and this had indicated that all physical factors having some effect on the biodegradation of the APAP. Analysis of variance (ANOVA) showed that the strains DPP1, DPP3, DKP1, and DKP2 had the F-value of 12.89, 6.45, 4.58, and 5.31, respectively. This indicated, the model was significant with regression coefficient (R) value of 0.01%, 0.06%, 0.37%, and 0.18%, respectively. The experimental values, predicted data, and ANOVA analysis has suggested that the model was satisfactory.

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Specifications table

| Subject area | Environmental science |
|--------------|-----------------------|
| More specific subject area | Biodegradation |
| Type of data | Table and Figures |
| How data was acquired | The bacterial strains viz. Staphylococcus sciuri DPP1 (MN744326), Bacillus subtilis DPP3 (MN744327), Bacillus paralicheniformis DKP1 (MN744324) and Enterococcus faecium DKP2 (MN744325) were isolated from sewage water, has the potential to degrade APAP in shake flask. Further, to know the effect of physical factors (viz. pH, temperature, agitation speed, and concentration of APAP) on degradation Box-Behnken design was used for the optimization of experimental conditions. |
| Data format | Raw (Table 1) and analyzed (Table 2) |
| Parameters for data collection | Physical factors used for degradation of APAP were, pH (3–11), temperature (10–70 °C), agitation speed (50–250 rpm), and concentration of APAP (20–1200 mg/L). Statistical analysis of biodegradation of APAP, using Box-Behnken design (BBD). The 3D- plots indicated the effect of physical factors on biodegradation. |
| Data source location | Deenbandhu Chhotu Ram University of Science and Technology, Murthal-131039, Sonepat, Haryana, India. |
| Data accessibility | Data information is available in this article only. |
| Related research articles | Chopra S, Kumar D (2020) Characterization, optimization and kinetics study of acetaminophen degradation by Bacillus drentensis strain S1 and waste water degradation analysis. Bioresour Bioprocess 7: |

Value of the data

This data analysis was focused on the optimization of physical parameters viz. pH, temperature, agitation speed, and concentration of APAP, employed for the degradation of APAP. The degradation efficiency of strains can be increased by performing degradation at optimal physical conditions. This is not only eco-friendly but also a cost-effective technique for the removal of such compounds with better efficiency. The statistical data will be useful for the optimization of the degradation of APAP from wastewater. The data will be further used for improving the degradation of APAP using co-degradation, and the effect of various nutrients on the degradation of strains at the optimal physical conditions. BBD of Design Expert® software was successfully used to design the experiments. After that, the predicted value for the biodegradation of APAP, was predicted by it. Further, this helps in the optimization of parameters which reduces the number of runs required to perform the experiment.

Data description

The data represented the use of Box-Benkin Design (BBD) for the optimization of physical condition for the degradation of paracetamol (APAP) also known as acetaminophen by four bacterial strains. These strains were isolated from sewage sources using enrichment culture methods [1]. The physical factors pH, temperature, agitation speed, and concentration of APAP were used to understand the degradation (Table 1). The model suggested 29 experiments with varied physical factors predicted through BBD of Design Expert® software (Design-Expert® Version 12.0.3.0; State-ease, Inc.) (Table 2). Further, the analysis of variance (ANOVA) was predicted for each strain. This model suggested that the F-value of 12.89 indicated that the model is significant for DPP1 and 0.01% chance in the F-value due to noise ratio. P-values less than 0.0500 indicated that the model was significant and B, A², C², D² were the significant model terms. The lack of fit F-value of 0.41 indicated the lack of fit was not significant relative to pure error (Table 3).
Table 1
Physical factors and experimental ranges for experiments.

| Factor code | Factor             | Units | Box-Behnken Design | Mean | Std. Dev. |
|-------------|--------------------|-------|--------------------|------|-----------|
| A           | pH                 |       | Low (-1)           |      |           |
|             |                    |       | High (+1)          |      |           |
| B           | Temp               | °C    |                    |      |           |
| C           | Agitation Speed    | rpm   |                    |      |           |
| D           | APAP Concentration | mg/l  |                    |      |           |

Fig. 1. The contour plots and 3D-plots between physical parameter, A: temperature, B: pH, C: Agitation speed and D: concentration of APAP. a) The 3D-plots showing APAP degradation by DPP1 between D and A, b) The contour plots showing APAP degradation by DPP1 between D and A, c) The 3D-plots showing APAP degradation by DPP3 between D and A, d) The contour plots showing APAP degradation by DPP3 between D and A.

Similarly, through ANOVA, it was concluded that for the bacterial isolates DPP3 (Table 4), DKP1 (Table 5), and DKP2 (Table 6). The F-values of 6.45, 4.58, and 5.31, respectively. The significance with DPP3 (0.06%), DKP1(0.37%), and DKP2(0.18%) (Tables 4, 5, 6). Further, the contour plots and 3-D plots showing the APAP degradation between physical factors, viz. A: temperature, B: pH, C: Agitation speed and D: concentration of APAP were constructed between various parameters like The 3D-plots showing APAP degradation: by DPP1 between D and A, (Fig 1a), by DPP3 between D and A (Fig 1c), by DKP1 between B and A (Fig 2b), by DKP2 between B and A (Fig 2d), etc. Similarly, the contour plots showing APAP degradation by DPP1 between D and A (Fig 1b), by DPP3 between D and A (Fig 1d), by DKP1 between D and C (Fig 2a), by DKP2 between B and A (Fig 2c), etc. The P-values less than 0.0500 for each strain indicates that the model was significant with B, A^2, C^2, D^2 are significant model terms for DPP3; A is a significant model term for DKP1 and A^2, D^2 are significant model terms for DKP2. The lack of fit F-value for DPP3, DKP1, and DKP2 of 0.56, 1.48, and 0.64, respectively. This has suggested that the lack of fit was not significant relative to the pure error. Finally, the solution table was generated by the BBD-quadratic model. This table suggested that the strains DPP1, DPP3, DKP1, and DKP2 have the optimal pH at
Table 2
Experimental design and individual factor study using box-behnken design, and corresponding response for APAP biodegradation.

| Std | Run | A: pH | B: Temp | C: Agitation Speed | D: APAP Concentration | Response 1 | Response 2 | Response 3 | Response 4 |
|-----|-----|-------|---------|-------------------|-----------------------|------------|------------|------------|------------|
|     |     | rpm   | mg/L    | % Observed | Predicted | % Observed | Predicted | % Observed | Predicted | % Observed | Predicted |
| 26  | 1   | 40    | 150     | 610      | 89        | 80.60      | 74        | 75.00      | 47        | 51.00      | 82        | 70.80      |
| 29  | 26  | 40    | 150     | 610      | 88        | 43.04      | 90        | 50.67      | 43        | 24.96      | 76        | 35.54      |
| 25  | 22  | 40    | 150     | 610      | 85        | 11.17      | 67        | 17.13      | 54        | 67.58      | 76        | 14.33      |
| 28  | 24  | 40    | 150     | 610      | 84        | 12.17      | 92        | 17.29      | 62        | 35.25      | 78        | 20.00      |
| 15  | 28  | 10    | 250     | 610      | 79        | 10.04      | 76        | 13.33      | 48        | 27.79      | 68        | 16.54      |
| 16  | 25  | 70    | 250     | 610      | 74        | 62.79      | 82        | 60.71      | 57        | 58.13      | 80        | 56.96      |
| 21  | 6   | 70    | 150     | 20       | 67        | 41.17      | 24        | 31.13      | 38        | 47.75      | 42        | 38.50      |
| 13  | 9   | 10    | 50      | 610      | 67        | 66.79      | 63        | 68.04      | 57        | 56.13      | 68        | 65.63      |
| 23  | 8   | 10    | 150     | 1200     | 65        | 74.67      | 62        | 70.96      | 58        | 66.42      | 72        | 74.00      |
| 27  | 15  | 40    | 150     | 610      | 57        | 9.67       | 52        | 3.46       | 49        | 59.58      | 42        | 8.00       |
| 8   | 21  | 40    | 250     | 1200     | 57        | 41.29      | 52        | 13.21      | 49        | 49.96      | 45        | 45.13      |
| 5   | 27  | 40    | 50      | 20       | 56        | 16.29      | 38        | 10.21      | 62        | 39.79      | 39        | 19.13      |
| 22  | 18  | 70    | 150     | 20       | 47        | 13.29      | 52        | 8.38       | 49        | 63.13      | 42        | 10.63      |
| 1   | 2   | 3     | 10      | 150      | 45        | 13.67      | 56        | 9.96       | 34        | 26.25      | 29        | 7.33       |
| 7   | 29  | 40    | 50      | 1200     | 43        | 80.60      | 27        | 75.00      | 65        | 51.00      | 39        | 70.80      |
| 6   | 23  | 70    | 250     | 20       | 36        | 27.54      | 23        | 31.33      | 57        | 69.29      | 26        | 29.04      |
| 14  | 7   | 70    | 50      | 610      | 35        | 20.54      | 32        | 26.00      | 46        | 49.13      | 39        | 18.04      |
| 24  | 11  | 70    | 150     | 1200     | 34        | 48.29      | 26        | 49.87      | 45        | 46.96      | 36        | 47.46      |
| 2   | 16  | 11    | 10      | 150      | 21        | 23.79      | 24        | 25.54      | 63        | 25.96      | 15        | 17.46      |
| 20  | 20  | 11    | 40      | 250      | 610      | 19         | 21.79      | 16        | 20.71      | 69        | 68.29      | 14        | 20.96      |
| 4   | 17  | 11    | 70      | 150      | 18        | 60.04      | 14        | 56.17      | 42        | 56.63      | 13        | 57.54      |
| 18  | 13  | 11    | 40      | 50       | 610      | 17         | 80.60      | 15        | 75.00      | 67        | 51.00      | 18        | 70.80      |
| 19  | 19  | 3     | 40      | 250      | 610      | 17         | 44.54      | 15        | 36.83      | 26        | 57.63      | 11        | 38.88      |
| 3   | 5   | 3     | 70      | 150      | 610      | 16         | 80.60      | 14        | 75.00      | 36        | 51.00      | 19        | 70.80      |
| 17  | 12  | 3     | 40      | 50       | 610      | 16         | 62.67      | 11        | 63.46      | 43        | 53.42      | 27        | 63.33      |
| 10  | 3   | 11    | 40      | 150      | 20       | 15         | 80.60      | 27        | 75.00      | 69        | 51.00      | 28        | 70.80      |
| 12  | 10  | 11    | 40      | 150      | 1200     | 14         | 53.54      | 11        | 45.50      | 67        | 60.46      | 13        | 50.04      |
| 9   | 14  | 3     | 40      | 150      | 20       | 13         | 69.17      | 23        | 66.29      | 19        | 52.08      | 13        | 57.83      |
| 11  | 4   | 3     | 40      | 150      | 1200     | 12         | 35.04      | 18        | 19.83      | 28        | 62.46      | 17        | 37.71      |
Table 3
Analysis of variance (ANOVA) for the APAP Degradation by DPP1.

| Source                      | Sum of Squares | df  | Mean Square | F-value | p-value |
|-----------------------------|----------------|-----|-------------|---------|---------|
| Model                       | 18,729.77      | 14  | 1337.84     | 12.89   | < 0.0001 significant |
| A-pH                        | 18.75          | 1   | 18.75       | 0.1807  | 0.6772  |
| B-Temp                     | 1200.00        | 1   | 1200.00     | 11.56   | 0.0043  |
| C-Agitation Speed           | 192.00         | 1   | 192.00      | 1.85    | 0.1953  |
| D-APAP Concentration       | 6.75           | 1   | 6.75        | 0.0650  | 0.8024  |
| AB                          | 169.00         | 1   | 169.00      | 1.63    | 0.2227  |
| AC                          | 0.2500         | 1   | 0.2500      | 0.0024  | 0.9615  |
| AD                          | 0.0000         | 1   | 0.0000      | 0.0000  | 1.0000  |
| BC                          | 182.25         | 1   | 182.25      | 1.76    | 0.2063  |
| BD                          | 30.25          | 1   | 30.25       | 0.2915  | 0.5977  |
| CD                          | 289.00         | 1   | 289.00      | 2.78    | 0.1174  |
| A²                          | 15,712.09      | 1   | 15,712.09   | 151.41  | < 0.0001 |
| B²                          | 240.70         | 1   | 240.70      | 2.32    | 0.1500  |
| C²                          | 1028.43        | 1   | 1028.43     | 9.91    | 0.0071  |
| D²                          | 2521.60        | 1   | 2521.60     | 24.30   | 0.0002  |
| Residual                   | 1452.78        | 14  | 103.77      |         |         |
| Lack of Fit                | 739.58         | 10  | 73.96       | 0.4148  | 0.8819  not significant |
| Pure Error                 | 713.20         | 4   | 178.30      |         |         |
| Cor Total                  | 20,182.55      | 28  |             |         |         |

Table 4
Analysis of variance (ANOVA) for the APAP degradation by DPP3.

| Source                      | Sum of Squares | df  | Mean Square | F-value | p-value |
|-----------------------------|----------------|-----|-------------|---------|---------|
| Model                       | 17,180.20      | 14  | 1227.16     | 6.45    | 0.0006  significant |
| A-pH                        | 33.33          | 1   | 33.33       | 0.1752  | 0.6819  |
| B-Temp                     | 1365.33        | 1   | 1365.33     | 7.18    | 0.0180  |
| C-Agitation Speed           | 574.08         | 1   | 574.08      | 3.02    | 0.1043  |
| D-APAP Concentration       | 30.08          | 1   | 30.08       | 0.1581  | 0.6969  |
| AB                          | 256.00         | 1   | 256.00      | 1.35    | 0.2654  |
| AC                          | 2.25           | 1   | 2.25        | 0.0118  | 0.9149  |
| AD                          | 110.25         | 1   | 110.25      | 0.5796  | 0.4591  |
| BC                          | 342.25         | 1   | 342.25      | 1.80    | 0.2012  |
| BD                          | 110.25         | 1   | 110.25      | 0.5796  | 0.4591  |
| CD                          | 506.25         | 1   | 506.25      | 2.66    | 0.1251  |
| A²                          | 12,110.01      | 1   | 12,110.01   | 63.66   | < 0.0001 |
| B²                          | 13.80          | 1   | 13.80       | 0.0725  | 0.7916  |
| C²                          | 1575.18        | 1   | 1575.18     | 8.28    | 0.0122  |
| D²                          | 2551.53        | 1   | 2551.53     | 13.41   | 0.0026  |
| Residual                   | 2663.25        | 14  | 190.23      |         |         |
| Lack of Fit                | 1555.25        | 10  | 155.53      | 0.5615  | 0.7908  not significant |
| Pure Error                 | 1108.00        | 4   | 277.00      |         |         |
| Cor Total                  | 19,843.45      | 28  |             |         |         |

7.6, 4.1, 6.9, and 6.1 respectively, and the optimal temperature was at 47°C, 37°C, 11°C, and 53°C respectively. Similarly, the model suggested optimal agitation speed was at 140 rpm, 115 rpm, 77 rpm and 161 rpm, respectively and the concentration of APAP in mg/L was at 886, 1171, 558, and 1065, respectively.

Experimental design, materials, and methods

Materials

The acetaminophen (99% pure) was obtained from Sigma Aldrich (USA) and all other highly pure chemicals were purchased from HiMedia (Mumbai, India), to perform degrading experi-
Table 5
Analysis of variance (ANOVA) for the APAP degradation by DKP1.

| Source                  | Sum of Squares | df | Mean Square | F-value | p-value | Significant |
|-------------------------|----------------|----|-------------|---------|---------|-------------|
| Model                   | 4608.88        | 14 | 329.21      | 4.58    | 0.0037  | Significant |
| A-pH                    | 3234.08        | 1  | 3234.08     | 45.00   | < 0.0001|             |
| B-Temp                  | 225.33         | 1  | 225.33      | 3.14    | 0.0984  |             |
| C-Agitation Speed       | 56.33          | 1  | 56.33       | 0.7839  | 0.3909  |             |
| D-APAP Concentration    | 0.7500         | 1  | 0.7500      | 0.0104  | 0.9201  |             |
| AB                      | 132.25         | 1  | 132.25      | 1.84    | 0.1964  |             |
| AC                      | 90.25          | 1  | 90.25       | 1.26    | 0.2813  |             |
| AD                      | 72.25          | 1  | 72.25       | 1.01    | 0.3330  |             |
| BC                      | 100.00         | 1  | 100.00      | 1.39    | 0.2578  |             |
| BD                      | 6.25           | 1  | 6.25        | 0.0870  | 0.7724  |             |
| CD                      | 2.25           | 1  | 2.25        | 0.0313  | 0.8621  |             |
| A²                      | 310.32         | 1  | 310.32      | 4.32    | 0.0566  |             |
| B²                      | 10.82          | 1  | 10.82       | 0.1506  | 0.7038  |             |
| C²                      | 175.96         | 1  | 175.96      | 2.45    | 0.1400  |             |
| D²                      | 61.67          | 1  | 61.67       | 0.8581  | 0.3700  |             |
| Residual                | 1006.08        | 14 | 71.86       |         |         |             |
| Lack of Fit             | 792.08         | 10 | 79.21       | 1.48    | 0.3758  | not significant |
| Pure Error              | 214.00         | 4  | 53.50       |         |         |             |
| Cor Total               | 5614.97        | 28 |             |         |         |             |

Table 6
Analysis of variance (ANOVA) for the APAP degradation by DKP2.

| Source                  | Sum of Squares | df | Mean Square | F-value | p-value | Significant |
|-------------------------|----------------|----|-------------|---------|---------|-------------|
| Model                   | 14,630.02      | 14 | 1045.00     | 5.31    | 0.0018  | Significant |
| A-pH                    | 18.75          | 1  | 18.75       | 0.0953  | 0.7620  |             |
| B-Temp                  | 675.00         | 1  | 675.00      | 3.43    | 0.0851  |             |
| C-Agitation Speed       | 56.33          | 1  | 56.33       | 0.2865  | 0.6009  |             |
| D-APAP Concentration    | 30.08          | 1  | 30.08       | 0.1530  | 0.7016  |             |
| AB                      | 16.00          | 1  | 16.00       | 0.0814  | 0.7796  |             |
| AC                      | 36.00          | 1  | 36.00       | 0.1831  | 0.6753  |             |
| AD                      | 90.25          | 1  | 90.25       | 0.4589  | 0.5092  |             |
| BC                      | 420.25         | 1  | 420.25      | 2.14    | 0.1659  |             |
| BD                      | 30.25          | 1  | 30.25       | 0.1538  | 0.7008  |             |
| CD                      | 240.25         | 1  | 240.25      | 1.22    | 0.2877  |             |
| A²                      | 12,382.45      | 1  | 12,382.45   | 62.96   | < 0.0001|             |
| B²                      | 34.81          | 1  | 34.81       | 0.1770  | 0.6803  |             |
| C²                      | 657.33         | 1  | 657.33      | 3.34    | 0.0889  |             |
| D²                      | 1400.08        | 1  | 1400.08     | 7.12    | 0.0184  |             |
| Residual                | 2753.22        | 14 | 196.66      |         |         |             |
| Lack of Fit             | 1692.42        | 10 | 169.24      | 0.6382  | 0.7432  | not significant |
| Pure Error              | 1060.80        | 4  | 265.20      |         |         |             |
| Cor Total               | 17,383.24      | 28 |             |         |         |             |

ments. The strains used in this data analysis were isolated from the wastewater flow in the drains present in Sonipat, Panipat, Karnal, and Yamunanagar (Haryana, India); Delhi, India [1].

Design of experiment

Primarily, the experiments were designed with Box-Behnken design (BBD) Design expert® (Design-Expert® Version 12.0.3.0; State-ease, Inc.). In the model, four variables (physical factors) were used and a total of 29 experiments were designed [2]. The four physical factors used were pH (A), temperature (B), agitation speed (C), and concentration of APAP (D). Further, the response variables, APAP degradation by DPP1, DPP3, DKP1, and DKP2, were determined through experiments conducted in the lab and by system responses. After that, the mathematical model,
Fig. 2. The contour plots and 3D-plots between physical parameter, A: temperature, B: pH, C: agitation speed and D: concentration of APAP. a) The contour plots showing APAP degradation by DKP1 between D and C, b) The 3D- plots showing APAP degradation by DKP1 between Band A, c) The contour plots showing APAP degradation by DKP2 between Band A, d) The 3D- plots showing APAP degradation by DKP2 between Band A.

ANOVA was applied, and finally, the creation of response surface method plots. The main goal to optimize the maximum degradation under physical factors was evaluated through the interactions between these factors, and modeling mathematical data.

The degradation of APAP was monitored with a UV spectrophotometer at OD$_{254}$ using the colorimetric method [1,3,4]. The degradation percentage (R) of APAP was calculated by Eq. (1):

$$R = \left( \frac{C_0 - C_t}{C_0} \right) \times 100$$  \hspace{1cm} (1)

Here, $C_0$ is the absorbance at the initial concentration of APAP and $C_t$ is the absorbance after incubation at time.

**Declaration of Competing Interest**

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.dib.2020.105826.

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