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MATHEMATICAL DESCRIPTION OF THE OPERATION OF A HYBRID BARBOTAGE REACTORS

Barbotage reactors such as airlift reactors (ALR) and bubble column reactors (BCR) due to their two-phase flow are the subject of many studies. Their basic version is used for lifting, mixing, and aeration of liquids, while their hybrid version, supplemented with additional elements, can serve as a rector for transport, lifting, and aeration of liquids. The subject of the research were two design variants of a hybrid barbotage reactor differing in the position of the nozzle for circulation and aeration, both filled with a moving bed. Based on the previously obtained measurement results, a simple mathematical equation was proposed to describe the impact of the type of construction and filling the hybrid reactor with a moving bed on the oxygen concentration and mixing conditions as well as on the transport of liquids. It was found that the greatest impact on the transport of liquid in the hybrid barbotage reactor (HBR) had the location of the H-nozzle, and filling the reactor with a moving bed had the greatest impact on the oxygen conditions and mixing of the liquid in the case of the HBR reactor.

1. INTRODUCTION

Barbotage refers to the flow of multiple gas bubbles through a liquid layer. There are two main types of barbotage reactors: bubble column reactors (BCRs) and airlift reactors (ALRs) [1]. Barbotage reactors that utilize liquid and gas flow have become commonplace in industrial and bioengineering applications. Their simple and reliable design makes it easy to adjust them to the requirements of a given process. Those advantages are exploited in such processes as water and wastewater treatment.

Many researchers have assessed the use of ALR reactors in wastewater treatment as an alternative to conventional systems – stirred tank reactors (STRs) and bubble column

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reactors (BCRs) [2–5]. The use of such reactors for wastewater treatment has been assessed as an alternative to conventional systems [6, 7]. According to the conducted research, higher removal efficiency of different types of contaminants was demonstrated by ALR reactors compared to STR reactors, also, comparable or better results were noticed for ALR reactors than BCRs.

The operation of the barbotage reactors was also assessed based on mathematical models [8–11]. Dluhý et al. [8] analyzed the possibility of using an airlift fluidised bioreactor and a fluidized bed bioreactor for wastewater treatment. Based on the results of mathematical modeling, the conditions for effective decomposition were analyzed and the orthogonal collocation method with the stiff integration procedure was used for the calculations. The simulation calculations showed that the fractional conversion of phenol over 99% was achieved in the airlift reactor with the riser tube height of 2 m and recirculation ratio of 100 with both types of kinetics. The fluidized bed 5 m high enabled a high conversion of phenol but the device 3 m high was not able to perform the process with a desirable effect. Báles et al. [9] analyzed the possibility of eliminating phenol from wastewater by biodegradation. In the study, the kinetics of bacterial degradation of phenol was described (*Alcaligenes xylosoxidans* ssp. *denitrificans* and *Xanthomonas maltophilia*). It was found that taking into account experimental kinetic data, Haldane kinetics was a better option than the Monod equation. Then, a mathematical model of airlift bioreactors was described. A reactor 2 m high was used to calculate phenol degradation and a degradation effect of over 99% was obtained. Tabiś et al. [10] proposed a mathematical model of a two-phase fluidized bioreactor with liquid recirculation and an external aerator. Stationary nonlinear analysis of such a bioreactor for the oxygen process with two-substrate kinetics was performed. The impact of the volume fraction of solid carriers in the liquid phase, the transfer rate of active biomass from the biofilm to the liquid, the concentration of organic substrate, the average liquid holdup time, and the efficiency of the external aerator on the characteristics of bioreactor were analyzed. A method for determining the minimum recirculation coefficient related to oxygen demand and the conditions of a fluidized bed was presented. Based on the obtained results, it is possible to choose reasonable operating conditions for such plants and to determine constraints, while considering acceptable concentrations of a toxic substrate being degraded. Domański et al. [11] conducted numerical studies on the ALR reactor. The hydrodynamics of the reactor was developed and the liquid and gas input for the reactor with external fluid circulation was determined, demonstrating compliance with the results of experimental studies.

The purpose of the study was, based on previously obtained measurement results [12], to use a simple mathematical equation to describe the impact of the design and placing the moving bed in the reactor on the conditions of mixing, oxygen, and fluid transport. Testing the aeration efficiency of the HBR and calculations of the technological parameters describing the aeration ability and efficiency was performed according to ASCE standards [13], and German ATV standards [14]. In 2020, the Polish Patent Office granted Patent No. 236340 for the analyzed solution [15]. The reactor variant under assessment was a hybrid with features of an ALR and a BCR [1].

2. EXPERIMENTAL

Research workstation. Hydraulic and technological tests with the use of a physical model were performed using a laboratory installation in the Water Laboratory of the Department of Hydraulic and Sanitary Engineering of the Poznań University of Life Sciences. A 1:1 scale liquid lifting and transport device is shown in Fig. 1 and its conceptual diagram is presented in Figs. 2 and 3.

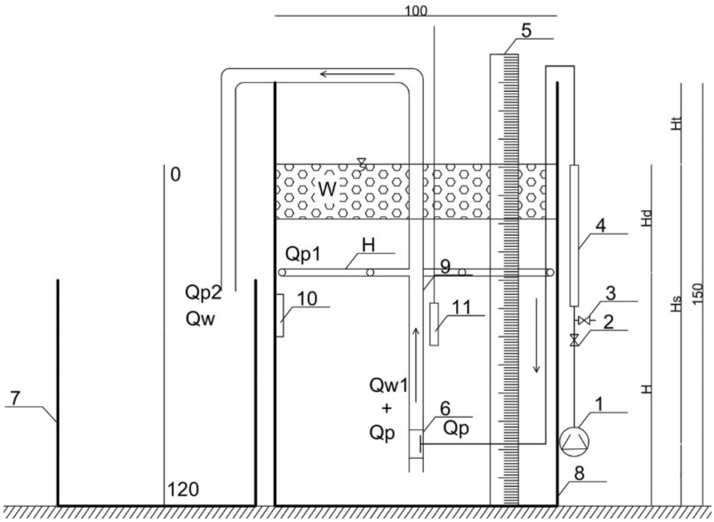


Fig. 1. Diagram of the installation: 1 – air blower, 2 – control valve, 3 – blow off valve, 4 – rotameter, 5 – scale, 6 – diffuser, 7 – recirculation tank, 8 – main tank, 9 – airlift pump with nozzle, 10 – hydrostatic liquid level sensor, 11 – liquid dissolved oxygen sensor (LDO), Qp – supply airflow rate, Qp1 – flow rate of air from nozzle H, Qp2 – flow rate of the exhaust airlift pump, Qw1 – flow rate of water in the section 6-H, H – nozzle, Hs – immersion height, cm, Ht – lifting height, cm

Two variants of tests were performed (S_1 and S_2) and the difference was the position of the aeration and circulation nozzle. In each of the versions, the reactor operated with the filling of 0, 20, 40%, respectively, made of polypropylene fittings.

The objective of this work was to develop a hybrid barbotage reactor in various structural design variants. The structure consisted of a barbotage column of 50 mm in diameter, used to transport a water-air mixture outside the reactor (so-called external loop).

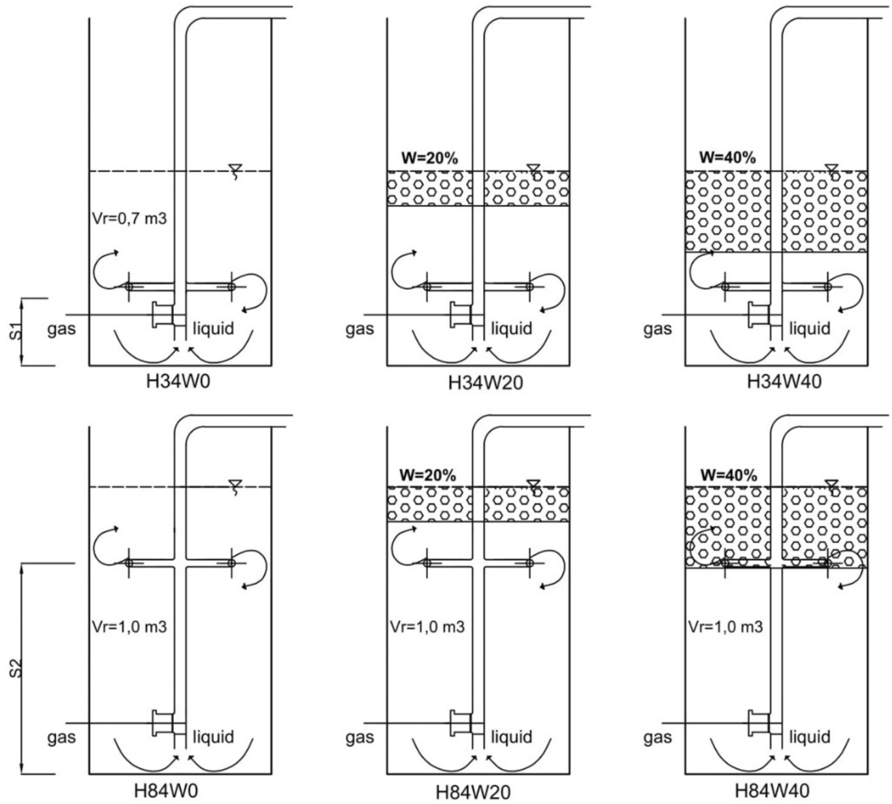


Fig. 2. Structural design variants of a hybrid barbotage reactor

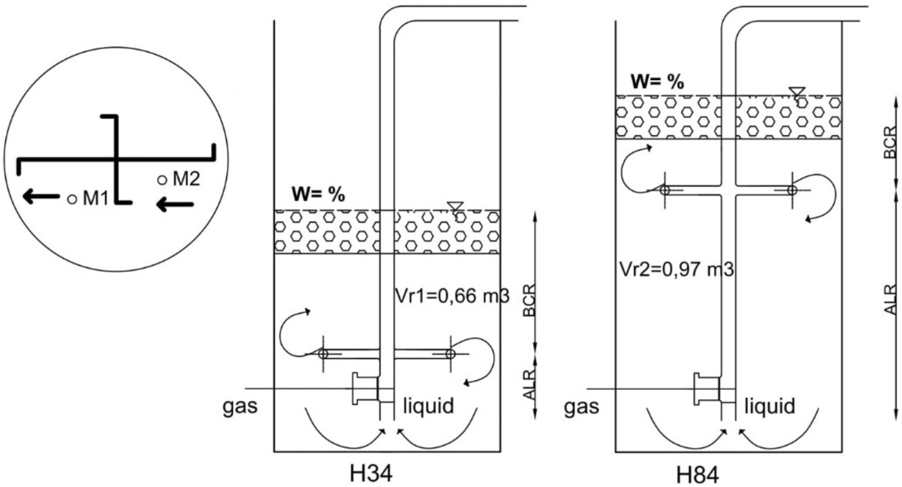


Fig. 3. Diagram of hydraulic and technological tests: M1, M2 – liquid velocity measuring profiles, ALR – airlift reactor zone, BCR – bubble column reactor zone

The installation was additionally equipped with a nozzle to improve mixture aeration and circulation efficiency. The nozzle was mounted at various heights of the column pump segment (S_1 and S_2). Additionally, the reactor was equipped with a moving bed in two variants of the reactor capacity W (20 and 40%) to determine its effect on the mixture aeration and circulation conditions. Based on the measurement results, aeration curves were constructed for various design and column packing variants of the reactor. Properties of the two-phase mixture were determined for both parts – ALR and BCR. Technological and energy parameters of the aeration process were calculated, and the circulation velocity for the measuring profiles M1 and M2. A detailed description of the methodology of technological and hydraulic laboratory tests can be found in the study by Kujawiak et al. [12].

Mathematical description of the HBR reactor. Based on detailed results of hydraulic tests [12] (reactor efficiency, mixing intensity) and technological tests (aeration), the equations describing the impact of geometric altitude (X_1) and filling with moving bed (X_2) on hydraulic conditions (y_1), aeration (y_2) and mixing (y_3) were created. A two--criteria optimization was applied for the position of the nozzle, 34 cm (H34) and 84 cm (H84) above the bottom of the tank, and, and the filling of the reactor of 20 and 40% (W20 and W40). The general form of the equation $y = f(X_1, X_2)$ for the four directional factors a, b, c, d is

$$y = a + bX_1 + cX_2 + dX_1X_2 \tag{1}$$

where a is a free factor, b, c, d – factors depending on the position H of the nozzle (b), filling with moving bed W (c), and interactions X_1 and X_2 (d), X_1 – the ratio of the immersion depth of the nozzle H_d to the immersion depth of the airlift pump H_s, $X_1 = H_d/H_s$, X_2 – the level of filling the reactor with moving bed W (from 0.2 to 0.4). The values of X_1 were calculated following the values assumed in the conducted laboratory tests [12]. The values of X_2 taken 0.2 or 0.4.

To determine the factors the a, b, c, d, equation (1) was converted:

$$y = y_1 = \frac{H_t}{H_s} \tag{2}$$

where H_t is the lifting height of the airlift pump, m, H_s – the immersion depth of the airlift pump, m.

Calculations were performed for four design variants (H34W20, H34W40, H84W20, H84W40), which allowed the assessment of the influence of a geometrical factor (position of the nozzle), and a technological factor (the level of filling the reactor with a moving bed) on the hydraulic conditions resulting in the reactor performance.

The value of the y_2 function was calculated with the use of the equation:

$$y = y_2 = \frac{c_{30}}{c_s} \tag{3}$$

where c_{30} is the average concentration of oxygen in the reactor after 30 min of aeration, mg/dm^3, c_s – temperature-dependent saturation concentration, mg/dm^3.

Calculations were performed for four design variants (H34W20, H34W40, H84W20, H84W40) to assess the impact of the same factors on the oxygen conditions, the effect of which is the degree of removal of contamination in the hybrid reactor. y_2 is the ratio of oxygen concentration in the reactor after 30 min of aeration to the maximum obtainable value (saturation concentration). A period of 30 min was sufficient to obtain the oxygen concentration of 2–3 mg/dm^3, which was sufficient for wastewater treatment.

Based on the zonal measurement results of the fluid circulation velocity in the hybrid reactor, the y_3 value was calculated for the two measurement profiles – M1 and M2 (Fig. 3):

$$y = y_{3\mathrm{M1}} = \frac{V_{\mathrm{BCR_{M1}}}}{V_{\mathrm{ALR_{M1}}}} \tag{4}$$

$$y = y_{3\mathrm{M2}} = \frac{V_{\mathrm{BCR_{M2}}}}{V_{\mathrm{ALR_{M2}}}} \tag{5}$$

where V_{BCR} is the average circulation velocity in the BCR zone, cm/s, V_{ALR} – average circulation velocity in the ALR zone, cm/s.

Aeration capacity. Based on the results of tests on the aeration capacity of the reactor and the values of the increase in oxygen concentration over time, a mathematical model was created to show the aeration process in the barbotage reactor, depending on the position of the circulation and aeration nozzle H and filling with moving bed W.

A mathematical growth model with third-degree exponential association equations was used to describe the oxygenation capacity over time (OC, g/(m^3·h)), for five design variants: H34W0, H34W20, H34W40, H84W0, H84W20

$$OC = \alpha\left(\beta - \mathrm{e}^{-\gamma t}\right) \tag{6}$$

where t is the time interval, min, α, β, γ – directional factors of the model.

For the H84W40 variant, it was not possible to use the growth model due to the unusual course of the aeration process caused by a large amount of bedding and the aeration nozzle placed too high.

Oxygen concentration. To describe the oxygen concentration (S_{O_2}, mg/m^3) during aeration of the barbotage reactor overtime, the mathematical growth model with second-degree exponential association equations was used for six design variants: H34W0, H34W20, H34W40, H84W0, H84W20, H84W40

$$S_{O_2} = A\left(1 - e^{-Bt}\right) \tag{7}$$

where t is the time interval, min, A, B – directional factors of the model.

3. RESULTS

3.1. IMPACT OF GEOMETRY OF A REACTOR ON ITS OPERATING CONDITIONS. A TWO-CRITERIA ANALYSIS

The values of X_1 and X_2 used in equation (1) were calculated following the values assumed in the conducted laboratory tests [12]. The results of the calculations are presented in Table 1.

Table 1

The values of parameters X_1 and X_2 for position H and filling W

X_1	H34	H84
	0.83	0.42
X_2	W20	W40
	0.2	0.4

Using equations (2)–(5), by applying corresponding values, the values of functions $y_1, y_2, y_{3M1}, y_{3M2}$ were obtained as shown in Table 2.

Table 2

The values of functions y_1, y_2, y_3 for position H and filling W

Design variant	Result for			
	$y_1 = H_t/H_s$	$y_2 = c_{30}/c_s$	y_{3M1} = BCR$_{M1}$/ALR$_{M1}$	y_{3M1} = BCR$_{M2}$/ALR$_{M2}$
H34W20	0.84	0.52	6.11	1.59
H34W40	0.86	0.46	1.93	1.02
H84W20	0.22	0.61	0.98	2.01
H84W40	0.23	0.65	3.44	1.26

Factors a, b, c, d in equation (1) were calculated for the values of the functions given in Table 2, and are shown in Table 3.

Table 3

The value of directional factors for function *y*

Function factor	y_1	y_2	y_{3M1}	y_{3M2}
a	–0.36	0.57	–13.51	3.36
b	1.83	0.01	28.67	–1.43
c	0.1	0.68	46.23	–4.62
d	–0.12	–1.17	–80.87	2.1

Based on the calculations of the factors, it can be seen that factor *b* (position of the nozzle *H* in the reactor) has the greatest impact on the value of function y_1. Factor *c* (filling *W* of the reactor with a moving bed) has a small impact on the hydraulic conditions, derived from the reactor's performance. In turn, factor *b* (position of the nozzle *H* in the reactor), has a small impact on the value of function y_2 and, consequently, on the oxygen conditions in the reactor. Factor *c* (filling *W* the reactor with a moving bed) has an impact on the oxygen conditions, the consequence of which is the efficient removal of pollutants. The impact of circulation was assessed with the use of factors determined for function y_3 (measurement profiles M1 and M2 in the HBR reactor). Based on the data in Table 3, it was found that factor *b* (position of the nozzle *H* in the reactor), has a small impact on the mixing conditions in the reactor for both measurement points. Factor *c* (filling *W* of the reactor with a moving bed) has a significant impact on mixing conditions, the consequence of which is the efficient removal of pollutants and intensity of aeration.

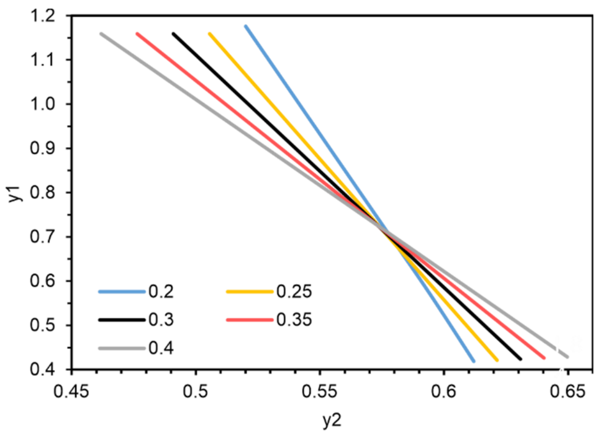


Fig. 4. A two-criteria analysis of the HBR reactor depending on the filling of the reactor with a moving bed *W* with the positions of the nozzle *H* = 34 and 84 cm

Using the factors *a*, *b*, *c*, *d*, the values of the functions y_1 and y_2 (eqs. (2) and (3)) were calculated for the intermediate values of X_1 (for H34, 44, 54, 64, 74 and 84) and X_2 (W20, 25, 30, 35, 40) for each variant of parameter *X* (Tables 4 and 5). The results are presented in Fig. 4 which allows assessing the performance of a barbotage reactor depending on the hydraulic and oxygen conditions. Based on the above graph, it can be concluded that the barbotage reactor with 30% filling with a moving bed is the best one in terms of Pareto optimality. Using the calculated factors for functions y_2 and y_3 (Table 3), the values of the functions described earlier as y_{3M1}, y_{3M2} were calculated for the intermediate values X_1 and X_2 (eqs. (4) and (5)).

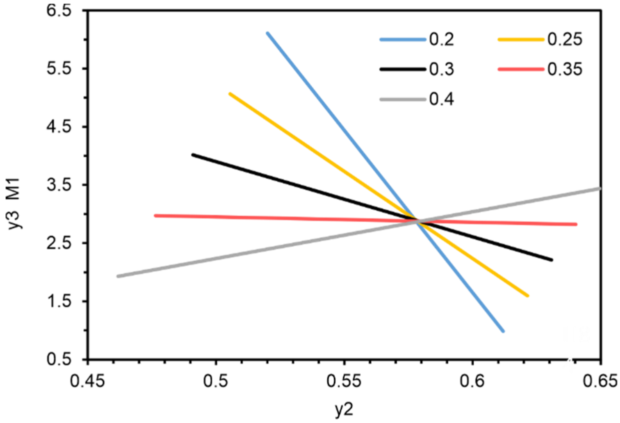


Fig. 5. The dependence of circulation in the HBR reactor on the oxygen conditions at different levels of filling and the positions of the nozzles (measurement profile M1)

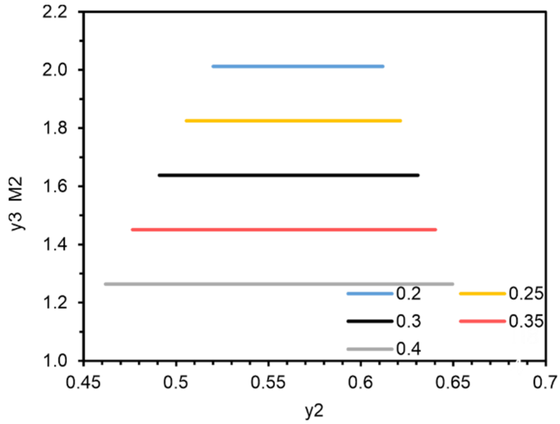
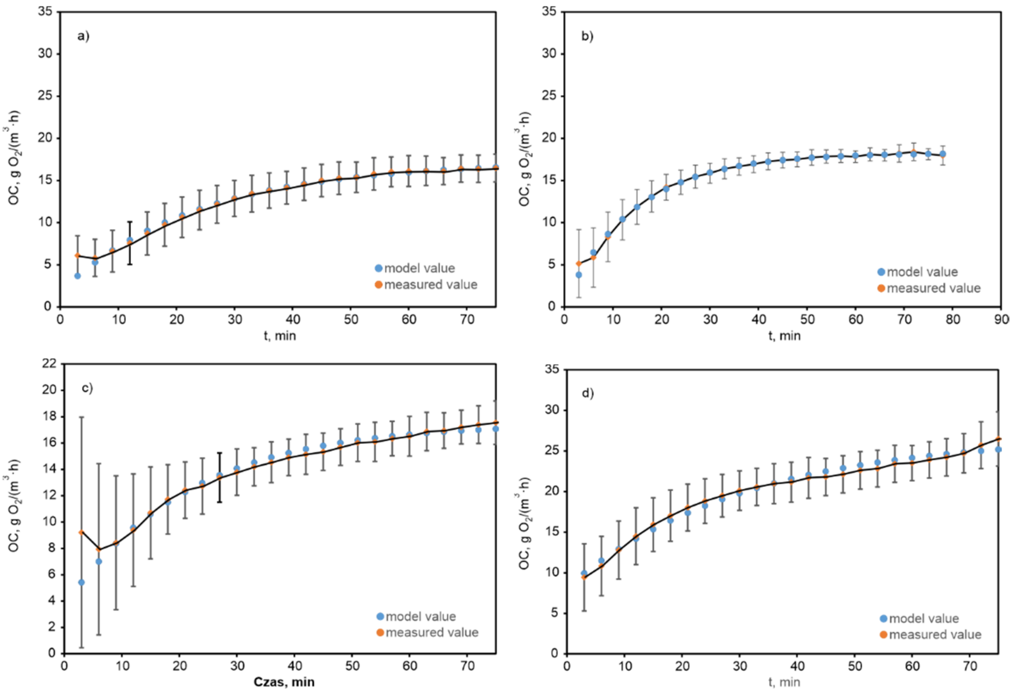


Fig. 6. The dependence of circulation in the HBR reactor on the oxygen conditions and on the filling with moving bed W with the positions of nozzles H = 34 and 84 cm (measurement profile M2)

The results of the calculations are presented in Figs. 5 and 6. Based on the above graphs, it was found that the lower the amount of filling of the hybrid reactor with a moving bed, the higher intensity of circulation in the BCR zone.

3.2. ANALYSIS OF AERATION CAPACITY

As previously mentioned, for the H84W40 design variant, due to a different distribution of points, it was not possible to describe the aeration capacity using a growth model. The time course of OC oxygenation/aeration capacity is presented in Fig. 7. A comparison of the curves for the design variants depending on the filling with a moving bed proves that placing the moving bed in the reactor reduces by half the time the reactor reaches maximum OC values.



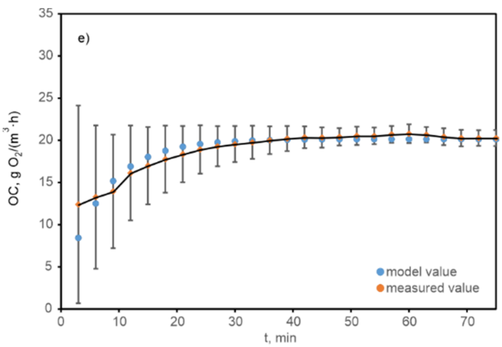


Fig. 7. Verification of the mathematical model describing the oxygenation capacity in a barbotage reactor, design versions: a) H34W0, b) H34W20, c) H34W40, d) H84W0, e) H84W20

Apart from the values calculated with the use of the exponential equations (eq. (6)), the measured values and the error bar (standard deviation of the mean) are presented in

Fig. 7. The model curve in its entire course falls within the error limit of the OC value measurement. The value of the correlation coefficient is very high (from 0.96 to 0.99), which proves a good fit of the model to the actual results of the function (Table 4).

Table 4

Factors for the model of oxygenation capacity overtime: growth model exponential, association 3

H [cm]	*W* [%]	α	β	γ	*S*	*r*
34	0	15.34	1.12	0.04	0.652	0.989
	20	17.72	1.03	0.07	0.342	0.998
	40	13.89	1.26	0.05	1.133	0.963
84	0	18.61	1.44	0.03	0.652	0.991
	20	17.99	1.12	0.14	1.089	0.971

H – position of the nozzle, *W* – filling with moving bed, *S* – standard error, *r* –– correlation coefficient, α, β, γ – coefficients of eq. (6).

3.3. ANALYSIS OF THE OXYGEN CONCENTRATION IN THE REACTOR

Figure 8 shows the oxygen concentration in the reactors under study for all design variants. Measured values with standard deviation and model curves are marked.

Table 5

Table 5. Factors for the model of oxygen concentration during the aeration of the barbotage reactor over time, growth model exponential association 3

H [cm]	*W* [%]	*A*	*B*	*S*	*r*
34	0	16.89	0.01	0.437	0.992
	20	12.70	0.02	0.328	0.996
	40	14.91	0.01	0.313	0.996
84	0	11.18	0.03	0.029	1.000
	20	10.92	0.03	0.209	0.998
	40	10.34	0.04	0.078	1.000

A, *B* – coefficients of eq. (7), other symbols as in Table 4.

It was found that the model curves are within the error limit with a correlation coefficient above 0.99 (Table 5), which proves a good fit for the model.

The oxygen concentration in the reactor at the level of 3 mg/dm^3 was obtained within 10 to 20 min, while increasing the level of filling the reactor with a moving bed shortened the time to obtain the expected oxygen concentration.

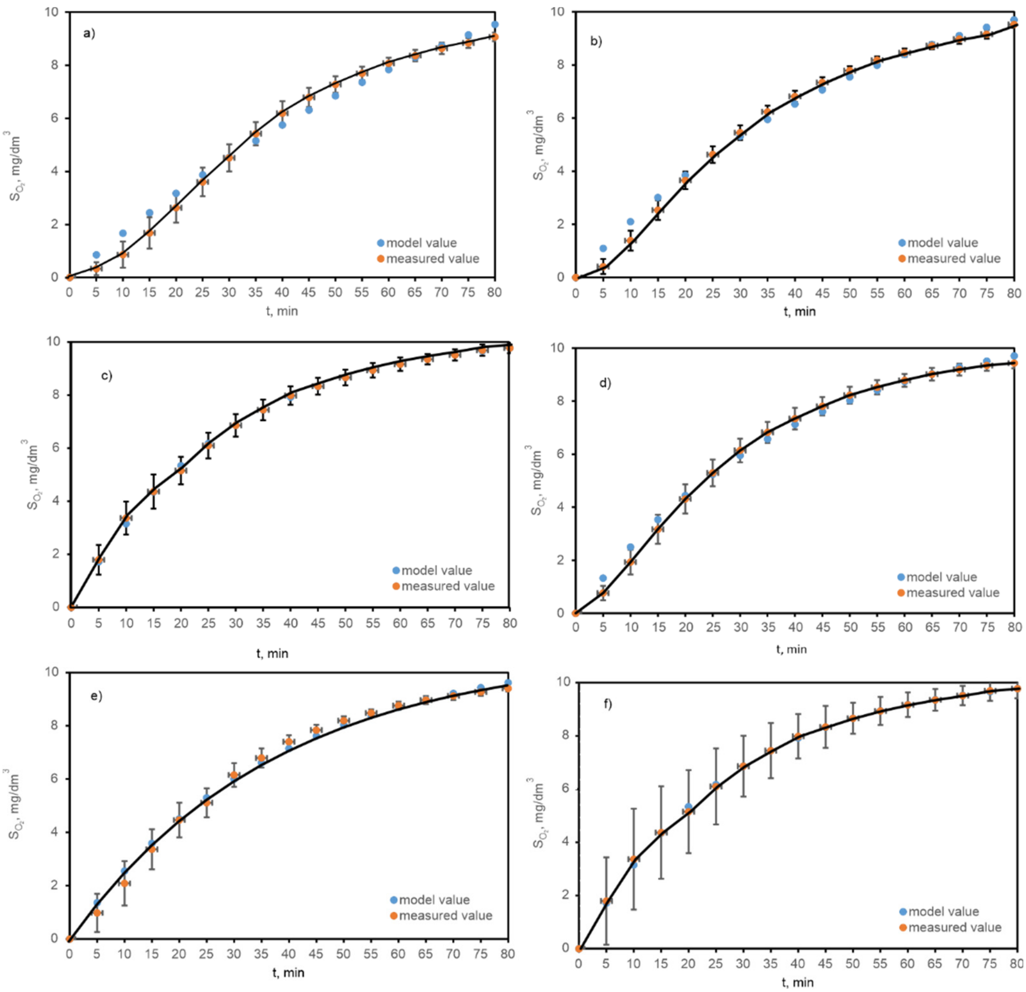


Fig. 8. Verification of a mathematical model used to describe the oxygen concentration in a barbotage reactor, design versions: a) H34W0, b) H34W20, c) H34W40, d) H84W0, e) H84W20

4. DISCUSSION

The study presents an assessment of the impact of the type of design and filling of a barbotage reactor on hydraulic and oxygen conditions.

With the use of a two-criteria analysis and a model equation, the impact of the position of the nozzle *H* and filling *W* of the reactor with a moving bed on hydraulic (reactor's performance, mixing, and circulation) and oxygen conditions is described. Additionally, with the use of the growth model, the aeration capacity and oxygen concentration for different types of design variants of the HBR reactor are described.

The position of the nozzle has the greatest impact on the performance of the reactor. The above is consistent with the previously presented research results [7, 12, 16]. Changing the position of the aeration nozzle causes a change in the amount of hydraulic loss at the outflow of the mixture in the discharge section of the lift mechanism, depending on *H*.

The level of filling the reactor with a moving bed had the greatest impact on the oxygen conditions, circulation, and mixing of liquids in the HBR reactor. The moving bed increases the holdup time of air bubbles in the liquid and significantly reduces the speed of liquid circulation in the reactor, especially in its upper zone, marked as BCR.

The growth model with second and third-degree exponential association equations was used to describe mathematically the aeration capacity and oxygen concentration. The equations proved a very good fit of the model to the experimental data. It can be noticed that filling the hybrid reactor with a moving bed causes flattening of the obtained curves, and the time over which the reactor reaches its maximum values of OC and the expected S_{O_2} is significantly shorter.

5. CONCLUSIONS

Based on the mathematical analysis of the hydraulic and technological tests performed for the hybrid barbotage reactor, it was found that:

- The greatest impact on the performance of the HBR reactor has the position of the aeration nozzle *H*.
- Filling the hybrid reactor with a moving bed has a greater impact on the improvement of oxygen conditions in the reactor than the position of the circulation nozzle, reduces the intensity of mixture circulation, especially in the BCR zone, and significantly reduces the time it takes to reach the maximum and expected values of oxygen capacity (OC) and oxygen concentration (So_2).

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