A Combined Algorithm for Optimization: An Application for Optimization of Gas-Liquid Transition in Stirred Tank Bioreactors

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Abstract. *A combined algorithm for static optimization is developed. The algorithm includes a method for random search of optimal an initial point and a method based on fuzzy sets theory, combined in order to be found for the best solution of the optimization problem. The application of the combined algorithm eliminates the main disadvantage of the used fuzzy optimization method, namely decreases the number of discrete values of control variables. In this way, the algorithm allows problems with larger scale to be solved. The combined algorithm is used for optimization of gas-liquid transition in dependence on some constructive and regime parameters of a laboratory scale stirred tank bioreactor. After the application of developed optimization algorithm significant increase of mass-transfer effectiveness, aeration and mixing processes in the bioreactor are observed.*

Keywords: *Combined algorithm, Optimization, Gas-liquid transition, Fuzzy sets theory, Method of random search with back steps, Fuzzy optimization*

Introduction

The mass-transfer processes in the bioreactor have an immediate and material effect on the growth of the cell population. They influence on the rates of alimentary and energy transfer to cells. Necessary oxygen in an aerobic cultivation is used as energy and substrate source. Its role is dominant. In many cases, the aeration and mass-transfer conditions are determinative for the indexes of the biotechnological processes. The effectiveness of the mass-transfer, aeration, and mixing processes are usually expressed by a criterion characterized gas-liquid transition [7].

Fuzzy sets theory (FST) has a great application in modeling, optimization and optimal control of biotechnological processes [3, 10, 11, 12]. In this paper a method based on FST is used. The general advantage of the method is that the obtained solution is determined directly, so the common weaknesses of the numerical solutions are avoided. A disadvantage of the method is the presentation of variables in a discrete form that makes the method less successful for problems with larger scale [1].

The methods of random search (MRS), do not require a calculated of gradients, they are simple for programming; allow organizing of adaptive algorithms and algorithms for searching of global extremum. MRS are more effective when there are many control variables (more than four), because the study space is always divided in two areas–*felicitous* and *infelicitous*, and the probability for falling in the one or the other does not depend on the number of variables [9].

The methods of random search with back step (RSBS) are used for optimization of the volumetric oxygen mass-transfer coefficient (K_La) for a stirred tank bioreactor in dependence on four factors [6]. Fuzzy optimization is also used to solve the same problems [2]. The comparative analysis between the se methods shows that fuzzy optimization gives better results. Fuzzy optimization is also used for optimization of gas-liquid transition [8]. A combination of both algorithms will allow the disadvantage of the method based of FST, connected with larger scale, to be overcome.

The aim of this paper is a development of a combined algorithm for static optimization and an application for optimization of gas-liquid transition in dependence on some constructive and regime parameters of laboratory stirred tank bioreactors.

A Combined Algorithm for Optimization

Random search with back step (RSBS) algorithm

RSBS algorithm is well known from the literature [9]. Its rate of congruence which is also valid for other algorithms depends on the choice of a beginning point. For augmentation of the congruence rate a preliminary choice of a random set is used on the following scheme:

A beginning point in the admissible space is generated in an accidental method [9]:

$$\mathbf{u}_{0,i} = \mathbf{u}_{min,i} + \xi_i \left(\mathbf{u}_{max,i} - \mathbf{u}_{min,i}\right), \quad i = 1,2,\dots,M; \; M = \begin{cases} 2^m + 4 & at \quad m \le 3 \\ 2m + 4 & at \quad m > 3 \end{cases},$$

where: $\mathbf{u}_{min}$ *and* $\mathbf{u}_{max}$-possible limits for vector of control variable, m-number of the control variables; ξ_i-uniformly distributed random numbers, $\xi_i=URAND(IY)$; $URAND(IY)$ is a random generator of random numbers [0÷1], IY-integer constant, the algorithm of $URAND$ is shown in [5]; M-number of the generated point's.

The point with the best result concerning some criterion J($\mathbf{u}$), is chosen as a beginning point. After that RSBS algorithm is applied.

Fuzzy algorithm

FTS allows a possibility to be developed a "*flexible*" model [1, 2], that reflects in more details all possible values of the criterion and control variables under the developed model. The developed model is examined as the most acceptable. As admissible, but with a less degree of acceptability are examined some diversions from the developed model. The is a presented by a fuzzy set a membership function with a type:

$$\mu_i(\mathbf{u}) = \frac{1}{1+\varepsilon_i^2(\mathbf{u})}, \quad i = 1,\dots,Q, \tag{1}$$

where: $\mathbf{u}$-vector of control variables, ε_i-deviation of the basic model; Q-number of equations in the main model.

Fuzzy criterion is formulated as follows: "*The optimum criterion* J($\mathbf{u}$) *to be possibly higher*" and it is presented by the following membership function:

$$\mu_0(\mathbf{u}) = \begin{cases} 0; & \mathbf{J}(\mathbf{u}) < \alpha_1 \\ \dfrac{\mathbf{J}(\mathbf{u}) - \alpha_1}{\alpha_2 - \alpha_1}; & \alpha_1 \le \mathbf{J}(\mathbf{u}) \le \alpha_2 \\ 1; & \mathbf{J}(\mathbf{u}) > \alpha_2 \end{cases}, \tag{2}$$

where α_1 and α_2 are fuzzy set parameters.

The following optimization problem in the class of fuzzy mathematical programming problems can be formulated:

$$J(\mathbf{u}) \cong \underset{\mathbf{u}=\mathbf{u}[u_1,u_2,\ldots,u_m]}{\widetilde{\max}}\left[J(\mathbf{u})\right], \tag{3}$$

where "$\widetilde{max}$" means *"in possibility maximum"*; "≅" means *"is come into view approximately in following relation"*.

For determination of this problem, an approach generalizing the Bellman-Zadeh's method [1,2] is used. The fuzzy set of the solution is presented with a membership function $\mu_D(\mathbf{u})$, whish is conjunction of the membership functions of the fuzzy set of the criterion $\mu_0(\mathbf{u})$ and the model $\mu_i(\mathbf{u})$:

$$\mu_D(\mathbf{u}) = (1-\gamma)\prod_{i=0}^{Q}\mu_i^{\theta_i}(\mathbf{u}) + \gamma\left\{1 - \prod_{i=0}^{Q}\left[1-\mu_i(\mathbf{u})\right]^{\theta_i}\right\}, \tag{4}$$

where: γ-parameter characterized the compensation degree; θ_i-parameters, those give weights of $\mu_i(\mathbf{u})$, $(i=0,1,\ldots,Q)$.

The solution is received using common *defuzzification* method BADD [4]:

$$\mathbf{u}_0 = \sum_{i=1}^{q}\lambda_i\mathbf{u}_i, \quad \lambda_i = \mu_{D_i}^{\theta_i}(\mathbf{u}) \Big/ \sum_{j=1}^{p}\mu_{D_j}^{\theta_i}(\mathbf{u}), \quad i = 1,\ldots,q; \quad j = 1,2,\ldots,p; \; p = q^m, \tag{5}$$

where: q-number of discrete values of the vector $\mathbf{u}$.

The scheme of combined algorithm (CA) is shown in Fig. 1.

Initial information necessary for RSBS algorithm (Choice 1), is:

1. Number of control variables m.
2. Integer constant IY.
3. Possible area for each control variables $u_{min,i}$ and $u_{max,i}$, $(i=1,2,\ldots,m)$.
4. Steps for each control variable h_i.
5. Beginning point $u_{0,i}$, $(i=1,2,\ldots,m)$.

The corresponding subroutine is called as: **CALL RSBS(m, IY, $\mathbf{u}_{\mathbf{min}}$, $\mathbf{u}_{\mathbf{max}}$, h, $\mathbf{u}_{\mathbf{0}}$, J)**. The **RSBS** returns optimal values of control variables $\mathbf{u}_{\mathbf{0}}$ and criterion J($\mathbf{u}$).

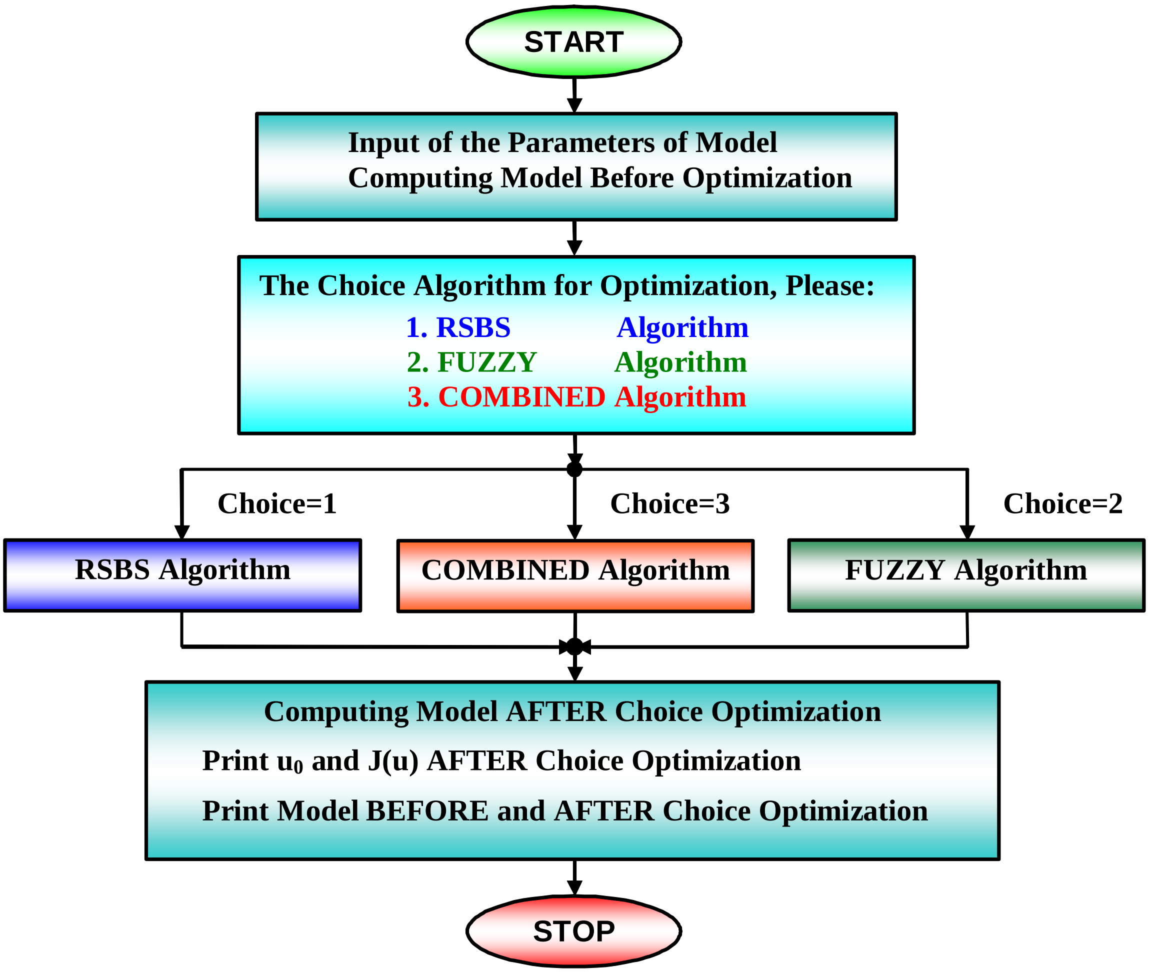

Fig. 1 Block scheme of combined algorithm

Initial information necessary for FUZZY Algorithm (Choice 2), is:

1. Number of control variables m.
2. Possible area for each control variables $u_{min,i}$ and $u_{max,i}$, $(i=1,2,\ldots,m)$.
3. Steps for each control variable h_i.
4. Initial values for fuzzy sets parameters α_1^0 and α_2^0.
5. Fuzzy sets parameters γ and θ_i, $(i=1,2,\ldots,Q)$.

The generalized FUZZY Algorithm scheme is:
BEGIN

1. Computing criterion before optimization $J_0(\mathbf{u})$.
2. Computing fuzzy sets parameters α_1 and α_2: $\alpha_1 = \alpha_1^0 J_0(\mathbf{u}), \alpha_2 = \alpha_2^0 J_0(\mathbf{u})$.
3. Computing number of discrete values of vector $\mathbf{u}$: $q = INT\left[1+\left(\mathbf{u}_{max}-\mathbf{u}_{min}\right)/\,\mathbf{h}\right]$.
4. Computing discrete values of each control variable: $\mathbf{u}_i = \left[\mathbf{u}_{min} + k\left(\mathbf{u}_{max}-\mathbf{u}_{min}\right)\right]/\left(q-1\right)$, $(k=0,1,\ldots,q)$, $(i=1,2\ldots,q)$.
5. Computing of deviations ε_i from the basic model;
6. Computing of membership function of the criterion $\mu_0(\mathbf{u})$ from (2).
7. Computing of membership functions of the model $\mu_i(\mathbf{u})$, $(i=1,2\ldots,Q)$ from (1).

8. Computing of optimization criterion J(**u**) from (3).
9. Computing of membership function of the decision μ_D(**u**) from (4).
10. Obtaining of solution $\mathbf{u_0}$ using *defuzzification* operator from (5)
11. Returns optimal values of control variables $\mathbf{u_0}$ and criterion J(**u**).

END

The corresponding subroutine is called as:

CALL FUZZY(m, $\mathbf{u_{min}}$, $\mathbf{u_{max}}$, h, α_1^0, α_2^0, Gamma, Theta, $\mathbf{u_0}$, J).

Initial information necessary for CA (Choice=3), is:

1. Number of control variables *m*.
2. Integer constant *IY*.
3. Steps for each control variable h_i.
4. Fuzzy sets parameters γ and θ_i, ($i=1,2,\ldots,Q$).

The generalized COMBINED Algorithm scheme is:

BEGIN

1. **CALL RSBS(m, IY, $\mathbf{u_{min}}$, $\mathbf{u_{max}}$, h, $\mathbf{u_0}$, J).**
2. Optimal value of the criterion J(**u**), received from **RSBS**.
3. Fuzzy sets parameters are determined based on relation: $\alpha_1 = 1.1J(\mathbf{u}), \alpha_2 = 1.5J(\mathbf{u})$.
4. Beginning point $\mathbf{u}_0$ is accepted equal to the one received from **RSBS**.
5. Possible area for each control variables $\mathbf{U}_{min}$ and $\mathbf{U}_{max}$, are determined in the vicinity of $\pm 10\%$ the received with RSBS point: $\mathbf{U}_{min} = 0.9\mathbf{u}_0$ and $\mathbf{U}_{max} = 1.1\mathbf{u}_0$.
   If the lower or upper bound exceeds the admissible values $\mathbf{u}_{\text{min}}$ or $\mathbf{u}_{\text{max}}$, then the bounds they are accepted equal to them.
6. Computing number of discrete values of vector **u**: $q = INT\left[1 + \left(\mathbf{U}_{max} - \mathbf{U}_{min}\right) / \mathbf{h}\right]$.
7. Computing discrete values of each control variable: $\mathbf{u}_i = \left[\mathbf{U}_{min} + k\left(\mathbf{U}_{max} - \mathbf{U}_{min}\right)\right] / \left(q - 1\right)$.
8. **CALL FUZZY(m, $\mathbf{U_{min}}$, $\mathbf{U_{max}}$, h, α_1, α_2, Gamma, Theta, $\mathbf{u_0}$, J).**
9. Returns optimal values of control variables $\mathbf{u_0}$ and criterion J(**u**).

END

The corresponding subroutine is called as:

CALL COMBINED(m, IY, $\mathbf{u_{min}}$, $\mathbf{u_{max}}$, h, Gamma, Theta, $\mathbf{u_0}$, J).

All programmed is also written using Compaq Visual FORTRAN Professional Edition 6.6. All computations have been performed on an AMD Athlon 64 2800+ computer using Microsoft Windows XP Pro Edition operating system.

CA will be used for optimization of gas-liquid transition in a laboratory stirred tank bioreactor in dependence on some regime and constructive parameters.

Formulation of the optimization problem

The effectiveness of mass-transfer, aeration and mixing processes is determined by criterion characterized the gas-liquid transition [7]:

$$\max_{\mathbf{u}=u_1,\dots,u_m}\left[J(\mathbf{u})\right]= C_G^0\,\frac{K_L a\ V}{\rho_G\ \ u_7}\,\frac{\left[X^*(t)-Y(t)\right]}{X(\eta,t)}\ , \tag{6}$$

where: C_G^0-oxygen concentration in the air, $C_G^0=0.21$ *kg/m*^{3}; V-volume, $V=0.25\pi D^2 u_8$, m^3; D-bioreactor diameter, $D=0.120$ *m*; ρ_G-gas density, $\rho_G=1.141$ *kg/m*^{3}; u_7-gas flow rate, m^3/s; η-dimensionless coordinate, $0\le\eta\le 1$; t-time, s; $X^*(t)$–dimensionless mean oxygen concentration in the liquid-phase, $Y(t)$-dimensionless oxygen concentration in the liquid-phase; $X(\eta,t)$-dimensionless oxygen concentration in the gas-phase.

Chosen control variables and their admissible values are shown in Table 1.

Table 1. Control variables and their intervals of change

N^0	Control Variables		Symbol	$\mathbf{u}_{min}$	$\mathbf{u}_{max}$
1.	Angle of the blades of the impeller,	α	u_1	45^0	90^0
2.	Eccentricity of impeller,	δ	u_2	*0.0 mm*	*1.5 mm*
3.	Number of impeller,	z_i	u_3	*1*	*3*
4.	Width of the baffle assembly,	b	u_4	*9 mm*	*15 m*
5.	Impeller diameter,	d	u_5	*40 mm*	*60 mm*
6.	Rotation speed,	n	u_6	*200 min*$^{-1}$	*1200 min*$^{-1}$
7.	Gas flow rate,	Q_G	u_7	*50 l/h*	*275 l/h*
8.	Level of liquid in the bioreactor,	L	u_8	*100 mm*	*200 mm*

The $X(\eta,t)$, $X^*(t)$ and $Y(t)$ are calculated by the solution of the combined model of the mass-transfer [8]:

$$X(\eta,t)=A_0\exp(r_1\eta)+B_0\exp(r_2\eta)+C_0$$
$$X^*(t)=A_0\left[\exp(r_1)-1\right]/r_1+B_0\left[\exp(r_1)-1\right]/r_2+C_0$$
$$Y(t)=X^*(t)\left[1-\exp(-a_2 t)\right],$$

where: $r_{1,2}=0.5Pe\pm\sqrt{(0.5Pe)^2+a_1}$; $A_0=a_3B_0$; $C_0=1-a_4B_0$; $B_0=\exp(-a_2t)/a_4$;

$a_1=Pe\,\dfrac{K_L a\,u_8}{\varepsilon_G\,m_L\,W_G}$; $a_2=\dfrac{K_L a}{(1-\varepsilon_G)}$; $a_3=-(r_2/r_1)\exp\left(-2\sqrt{(0.5Pe)^2+a_1}\right)$; $\eta=0.5$ and $t=30$ s;

Pe-Peclet number, $Pe=W_G u_8/D_L$; $a_4=1+a_3-(a_3 r_1+r_2)/Pe$; W_G-gas velocity,

$W_G=4u_7/(\pi D)$, m/s; m_L-Henry's law constant, $m_L=82.86$; $D_L=1.16x10^{-4}$, m^2/s.

The gas hold-up is computed by the following relation [7]:

$\varepsilon_G=0.2\,(P_G/V)^{0.7}\,W_G^{0.2}$,

where: P_G-power input with aeration, W; $P_G=0.8\left[u_7/(u_6u_5^3)\right]^{-0,011}P_L$;

P_L-power input without aeration, W; $P_L=\begin{cases}179.5\rho u_6^3u_5^5Re^{-0.40} & at\ u_2\le 0\\ 60.9\rho u_6^3u_5^5Re^{-0.18}\left(u_2/u_5\right)^{-0.23} & at\ u_2>0\end{cases}$;

Re-Reynolds number; ρ-liquid density, kg/m^3.
K_La is determined using following regression model [6]:

$$K_L a = 137.0 + 8.9u_1 + 13.0u_3 + 7.3u_2u_4 + 6.1u_3u_4 - 7.9u_1^2 - 34.0u_2^2 - 9.3u_3^2 + 23.5u_4^2 .$$

The optimization problem is formulated in the following way: to be founded such values of control variables $\mathbf{u}=\mathbf{u}[u_1, u_2, \ldots, u_m]$ that ensure maximal value of the criterion (6). The formulated optimization problem is solved by the developed CA (Fig. 1) for $m=8$.

Results and Discussion

The total computing time for solving of optimization problem by CA is of the order of *10 s*. Otherwise, both methods are used consecutively, the computing time for solution using RSBS is of the order of *2 s*, and for solution of FA necessary time is of the order of *50 s.* Based on the received results it can be concluded that the combination of both algorithms decreases vastly the computing times vastly – around 5 times. Obtained optimal values of the criterion and control variables are shown in Table 2. The basic indexes characterized mass-transfer, aeration and mixing processes.

Table 2. Optimization results

Method / Control Variables	u_1 *0*	u_2 *mm*	u_3 *Num.*	u_4 *mm*	u_5 *mm*	u_6 *min^{-1}*	u_7 *l/h*	u_8 *mm*	J(**u**) -
Initial point	80	0.83	3	15	57	600	*60*	120	0.130
Beginning point from random set	76	1.15	2	14	30	929	72	117	0.145
RSBS	70	1.13	2	13	32	908	50	134	0.242
FA	71	0.86	2	13	56	595	58	124	0.161
CA	69	1.00	2	12	32	904	50	144	0.282
Merthod / Basic indexes	V *l*	W_G *mm/s*	P_L *W*	P_G *W*	$(P_L - P_G)/V$ *W/l*	ε_G *%*	K_La *h^{-1}*	Pe -	Percent *%*
Initial point	1.36	1.47	7.40	6.23	0.870	15.78	172.78	1.50	11.5
Beginning point from random set	1.32	1.76	0.55	0.46	0.068	2.67	132.44		
RSBS	1.52	1.23	0.66	0.55	0.072	2.55	124.55	1.40	66.9
FA	1.41	1.43	6.58	5.54	0.738	14.08	142.90	1.50	23.8
CA	1.63	1.13	0.70	0.59	0.067	2.51	131.58	1.39	16.5

The change of the gas-liquid transition in the time before and after the optimization is shown in Fig. 2, where superscript '0' denotes before optimization, superscript '1'-after optimization with RSBS and superscript '2'-after optimization with CA.

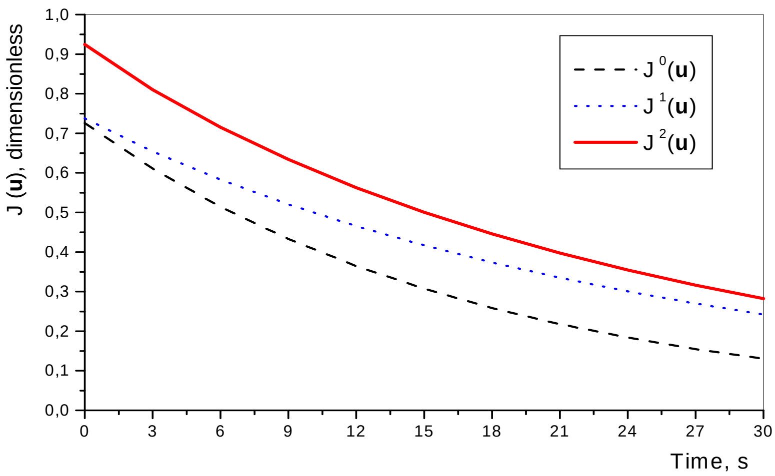

Fig. 2 Gas-liquid transition, before and after the optimization

From the obtained results with different optimization algorithms (Table 2, Fig. 2), the following conclusions can be made:

1. After preliminary chosen from random sets beginning point, the criterion increases its value with more than 11 percents ($J_{Initial}=0.145$ *and* $J_{Begin}=0.13$) in comparison with the initial point.
2. The application of the RSBS algorithm increases the criterion value with more than *66 percents* ($J_{RSBS}=0.242$ *and* $J_{Initial}=0.145$) toward the optimal beginning point.
3. The application of the FA is, on the one hand, the slowest one **(**~*50 s*), and, on another hand it leads to the criterion increase with only *24* percents ($J_{FA}=0.161$ *and* $J_{Begin}=0.13$), in comparison with the initial point. This could be explained with a fact that it has been performed a search in the whole admissible interval of control variables change and the obtained extremum could not be a global.
4. The application of CA leads to the criterion increase with more than *16* percents ($J_{CA}=0.282$ *and* $J_{RSBS}=0.242$) toward its value received with RSBS method.
5. The general improvement of the criterion is more than *90* percents ($J_{CA}=0.282$ *and* $J_{Begin}=0.145$) toward the optimal beginning point and more than *110* percents ($J_{CA}=0.282$ *and* $J_{Initial}=0.13$) toward the initial point.

Obtained results (Table 2) for the indexes of aeration and mixing processes ε_G and $(P_L - P_G)/V$ show vastly decrease of their values. The gas hold-up decrease, more than 6 times ($\varepsilon_G=15.78$ percents-before and $\varepsilon_G=2.51$ percents-after optimization). The relative power input $(P_L - P_G)/V$ decrease, more than 12 times: $(P_L - P_G)/V = 0.87$ -before and $(P_L - P_G)/V = 0.067$ -after optimization.

Basic mass-transfer index K_La decrease, its value (Table 2) with *24%* ($K_La=172.78\ h^{-1}$-before and $K_La=131.56\ h^{-1}$-after optimization). This shows a good effectiveness of the gas-liquid transition. Higher value of K_La does not provide a good gas-liquid transition, so it should be accepted some mean value, but not the maximal one.

The general conclusion after the optimization of constructive bioreactor parameters is that the impeller with fewer diameters should be used (Table 2, parameter u_5). It will reduce the diameter of the impeller shaft. Rest parameters do not force a large change of the construction.

Conclusions

1. Proposed combined algorithm for static optimization, based of random search method with back step and fuzzy sets theory, decreases vastly the time for the solution of the optimization problem. This algorithm get over the main disadvantage of used fuzzy optimization method, namely decreases number of discrete values of the control variables. In this way the algorithm allows problems with larger scale to be solved.
2. Developed combined algorithm can be used for decision of other static optimization problems in the area of bioprocess systems.
3. Developed optimization of gas-liquid transition in dependence on considered constructive and regime bioreactor parameters maximizes the apparatus effectiveness at aerobic cultivation of microorganisms.

4. Based on developed optimization of the constructive parameters it could be concluded that an impeller with fewer diameters should be used. That will reduce the diameter of the impeller shaft.

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