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A dimensionless approach to model granule size variation in UASB reactor: Model development and its validation

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Abstract- **Granule size and its variation plays an important role in satisfactory performance of upflow anaerobic sludge blanket (UASB) reactor especially in treatment of industrial and low strength domestic wastewaters. The present study is aimed to model the granule size variation based on fourteen quantifiable variables influencing the granulation and granular size development in UASB reactor. They include organic loading rate, inflow rate, gas production rate, volatile suspended solids, total suspended solids, specific methenogenic activity, sludge volume index, operation time, time for which constant organic loading rate was maintained during the reactor operation, effluent COD concentration, polymer dosing, liquid upflow velocity, granules settling velocity and reactor diameter. Dimensionless mathematical functions are developed for granule size variation using these variables. The non-linear multiplier function with each dimensionless terms as power function is subjected to non-linear regression and the function so developed has been then validated using the experimental results from literature. The results show that the developed non-linear function is capable of predicting the granule size variation in UASB reactor satisfactorily with maximum error in prediction being less than 5.5%. The results of sensitivity analysis show that the liquid inflow rate is the most sensitive parameter among the fourteen variables considered in simulation of granule diameter.**

Key words: **Dimensionless variables, Granulation, Granule size variation, non-linear multiplier function, Polymer dose, UASB reactor**

I. INTRODUCTION

The upflow anaerobic sludge blanket (UASB) reactor is now a days becoming more popular for the treatment of variety of industrial as well as domestic wastewaters. Good efficiency of treatment in UASB reactor is achieved mainly due to the development of granular sludge consisting granules of different sizes ranging between 0.5–5 mm that exhibit good settling characteristics and resist frequent washout of microorganisms from the reactor even at higher. hydraulic and organic loads [1] – [3]. Granules show excellent settling properties due to the higher buoyant densities and their large sizes [4].

Different investigators have tried to enhance the granulation and granule size development in UASB reactors treating variety of wastewaters. But, there are only few studies devoted towards the mathematical modelling of granulation and granule size variations in UASB reactor [5] – [7]. Effect of organic loading rate (OLR) on granulation and granule size development was studied by [5] under different operating conditions. Influence of extracellular polymer (ECP) content and OLR are mentioned as the governing factors in enhancement of granule sizes in UASB reactor [7].

This paper is devoted mainly to develop parameters based mathematical model for assessment of granule size variation with passage of time using dimensionless approach by considering fourteen quantifiable variables influencing the granulation and granule size development in UASB reactor. Different variables such as organic loading rate, liquid upflow velocity, granules settling velocity, sludge volume index, gas production rate, liquid inflow rate, specific methenogenic activity, VSS/SS ratio, polymer loading rate and effluent COD concentration are well documented in literature [1], [2], [8-19]. But, the experimental results of only few investigators for all the fourteen variables are available in the literature.

Mathematical functions are developed using dimensionless approach for granule size variation. The developed non-linear multiplier functions containing powers raised to each dimensionless terms were subjected to non-linear regression analysis using the experimental results of [1] for reactor R4. The resulting parameter based non-linear multiplier function was then validated using the experimental results of [2] for reactor R2 where UASB reactors were operated under more or less similar conditions. Sensitivity analysis was carried out to identify the most sensitive parameters influencing the model predictions.

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II. MODEL DEVELOPMENT

In development of mathematical model for granule size variation, different variables such as organic loading rate (OLR), liquid upflow velocity (V_{up}), granules settling velocity (SV), sludge volume index (SVI), gas production rate (Q_g), liquid inflow rate (Q), specific methenogenic activity (SMA), volatile suspended solids (VSS) concentration, suspended solids (SS) concentration, effluent COD concentration (S_e), polymer loading (P_o), operation time (T), time for which constant organic loading rate was maintained (T_o) during reactor operation and the reactor diameter (D_r) were taken into consideration.

A. Dimensionless approach to model the granule diameter

The granule diameter 'Dg' can be regarded as function of the following 14 independent variables and is expressed as:

$$D_g = f\ (VSS, SS, SMA, SVI, OLR, Q, Q_g, T, T_o, S_e, P_o, V_{up}, SV \text{ and } D_r) \quad (1)$$

Using Buckingham π- theorem, various dimensionless groups are formed are-

$$\left(\frac{D_g}{D_r}\right), \left(\frac{V_{up}}{SV}\right), \left(\frac{VSS}{SS}\right), \left(\frac{SMA}{SVI \times OLR}\right), \left(\frac{Q}{Q_g}\right), \left(1+\frac{T}{T_o}\right) and \left(1+\frac{P_o}{S_e}\right) \quad (2)$$

A non-linear multiplier function for dimensionless variable (D_g/D_r) can be written by raising the powers of remaining dimensionless terms of (2) and is expressed as:

$$\left(\frac{D_g}{D_r}\right) = \left[\left(\frac{V_{up}}{SV}\right)^a \cdot \left(\frac{VSS}{SS}\right)^b \cdot \left(\frac{SMA}{SVI \times OLR}\right)^c \cdot \left(\frac{Q}{Q_g}\right)^d \cdot \left(1+\frac{T}{T_o}\right)^e \cdot \left(1+\frac{P_o}{S_e}\right)^f\right] \quad (3)$$

Where, the function D_g/D_r is a non-linear power multiplier function containing each dimensionless terms on R.H.S. as power function. Indices a, b, c, d, e and f are the powers raised to each dimensionless term on R.H.S of (3).

III. MATERIALS AND METHODS

The experimental results/data on granule size variation in UASB reactor were taken from the experimental study of [1] for reactor R4 as referred in [1] for testing of model and the experimental results of [2] for reactor R2 (referred in [2]) for validation of model with more or less similar operating conditions maintained in both the reactors. Experimental results of [1] and [2] are shown in Tables 1 and 2 respectively.

Table 1. Experimental results as per Wang et al. (2004)

Reactor	T	T_o	OLR	SVI	Q_g	SMA	Q	S_e	SV	V_{up}	VSS/SS	D_g
R4	55	15	4.8	0.0299	2.5	1.73	5.28	0.38	40.9	0.0280	0.6501	0.62
	67	16	6.4	0.0301	10.4	1.96	7.04	0.203	48.7	0.0373	0.5942	1.53
	80	14	9.6	0.0227	15.8	2.37	10.56	0.246	51.7	0.0560	0.7272	1.89
	92	11	12.8	0.0141	30.1	1.93	14.08	0.279	64.2	0.0747	0.6756	2.62
	97	7	16	0.0228	30.7	2.13	17.6	0.44	45.9	0.0934	0.7804	1.86
	103	5	19.2	0.0303	34.5	2.12	21.12	0.439	49.4	0.1121	0.7861	1.20

Table 2. Experimental results as per Show et al. (2004)

Reactor	T	T_o	OLR	SVI	Q_g	SMA	Q	S_e	SV	V_{up}	VSS/SS	D_g
R2	26	26	2	-	-	-	1.76	0.62	-	0.009	0.563	0.215
	35	8	4	-	-	-	3.52	0.39	-	0.018	0.549	0.287
	67	31	8	0.028	10.2	2	7.04	0.21	48.7	0.037	0.685	1.269
	80	12	12	0.023	20.9	2.4	10.56	0.38	51.7	0.056	0.695	1.992
	92	11	16	0.019	32.6	2.3	14.08	0.43	58.2	0.074	0.673	2.335
	103	10	24	0.029	37.4	2.1	21.12	0.62	49.4	0.112	0.792	1.185

The non-linear multiplier function represented by (3) was subjected to non-linear regression analysis for the simulation of (D_g/D_r) for reactor R4 using NLINFIT tool of MATLAB 2010a and the indices a, b, c, d, e, and f were determined for best simulation of experimental (D_g/D_r) ratio. The non-linear power function so developed was then validated for experimental granule diameter (D_g/D_r) using the experimental results of [2] for reactor R2. The statistical error estimates viz, sum of residual (SR), sum of square error (SSE), standard deviation (SD) and root mean square error (RMSE) between experimental (D_g/D_r) and predicted (D_g/D_r) were computed using Microsoft Excel software. Sensitivity analysis was carried out to explore the sensitivity of all the variables considered in simulation of granule sizes in UASB reactor using Microsoft Excel software. As per [20] and [21], the sensitivity of the model subjected to variations in the variables can be estimated using the following expression:

$$S_R = \frac{(Y_i - Y_b)}{Y_b} \Big/ \frac{(X_i - X_b)}{X_b}$$

(4)

Where S_R represents the sensitivity of the variables, Y_i is value of function at different parameter values (X_i), Y_b the basic function value at a particular day of reactor operation. X_b is the base parameter value of the variables taken on a particular day of reactor operation and X_i is the parameter values obtained by varying the base parameter values within ±10%. The denominator term was plotted on X-axis against

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the numerator term on Y-axis of (4) and the sensitivity of each parameter was calculated using (4).

IV. RESULTS AND DISCUSSION

A. Testing of model

A non-linear power multiplier function is developed by simulating the experimental granule diameter term i. e. L.H.S term of (3) using NLINFIT tool of MATLAB 2010a using the experimental results of [1] for reactor R4 for reactor operation period of 55-103 days as shown in Table 1.

The resulting non-linear best simulated function is expressed as:

$$\left(\frac{D_g}{D_r}\right)=\left(\frac{V_{up}}{SV}\right)^{0.9595}\cdot\left(\frac{VSS}{SS}\right)^{-0.8275}\cdot\left(\frac{SMA}{SVI\times OLR}\right)^{0.9312}\cdot\left(\frac{Q}{Q_g}\right)^{-0.7666}\cdot\left(1+\frac{T}{T_o}\right)^{-0.1176}\cdot\left(1+\frac{P_o}{S_e}\right)^{6.85E-06} \quad (5)$$

From (5), it can be seen that the indices of each dimensionless terms are obtained based on the parameters values reported in [1] for best simulation of experimental granule diameter (D_g/D_r). These indices may vary to some extent under different operating conditions other than those maintained in reactor R4 of [1]. However, the predicted granule diameters from R.H.S terms of (5) are capable to simulate well the experimental granule sizes in this study. Predicted D_g/D_r values from (5) and the percentage error between the experimental and predicted D_g/D_r values are shown in Table 3.

Table 3. Experimental and predicted granule diameter (D_g) and dimensionless diameter (D_g/D_r)

Models	Experimental D_g/D_r	D_g	Predicted D_g/D_r	D_g	Error (%)
Model testing[a]	0.0062	0.62	0.0063	0.63	0.16
	0.0153	1.53	0.0152	1.52	0.42
	0.0189	1.89	0.0187	1.87	0.78
	0.0262	2.62	0.0264	2.64	1.13
	0.0186	1.86	0.0185	1.85	0.14
	0.0120	1.20	0.0121	1.21	0.23
Model Validation[b]	0.0126	1.26	0.0121	1.21	4.00
	0.0199	1.99	0.0188	1.88	5.40
	0.0233	2.33	0.0224	2.24	3.75
	0.0118	1.18	0.0112	1.12	5.28

[a]Reactor R4 of [1], [b]Reactor R2 of [2]

A comparision between experimental and predicted values of D_g/D_r is shown in fig. 1, where the maximum error lie within ±1.15% error band which is reasonable and well within the acceptable limit in such simulations.

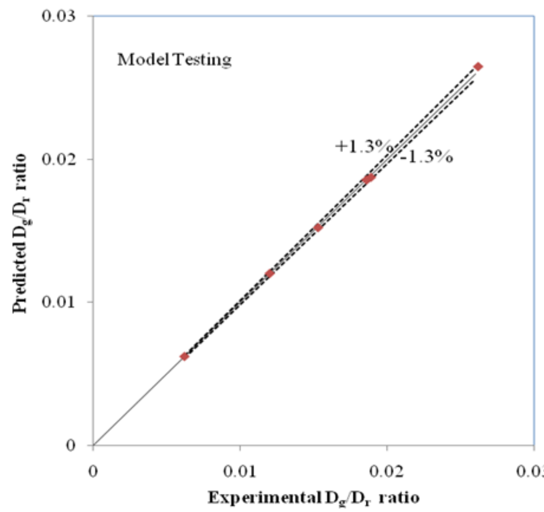

Fig. 1. Comparision between experimental and predicted D_g/D_r for reactors R4 using the experimental results of [1].

Thus, it is inferred that model (5) is a suitable model for simulation of granule diameter within the range of operating variables maintained in reactor R4 of [1].

Statistical error estimates (SR, SSE, SD and RMSE) between experimental and predicted (D_g/D_r) values for reactor R4 are shown in Table 4. From the table, it is evident that SR between experimental and predicted (D_g/D_r) values is of the order of 10^{-4} which shows a small variance between experimental and predicted D_g/D_r values. Smaller values of SSE of the order of 10^{-7} show less error and closeness between experimental and predicted (D_g/D_r) for reactor R4. Standard deviation of the order of 10^{-3} indicates that predicted D_g/D_r tend to vary close to the mean values. Smaller RMSE values indicate that predicted D_g/D_r values are more or less coincident with the experimental D_g/D_r values. Based on the above results, it can be inferred that granules sizes are simulated fairly well by the model (5) in present case.

Validation of model

The non-linear power multiplier function represented by (5) is validated using the experimental results of [2] for reactor R2 for reactor operation period of 26-103 days as shown in Table 2. Model (5) was developed using the experimental results of [1] for reactor R4 fed with polymer dose of 0.02 g/L. Experimental conditions maintained in reactor R4 of [1] were quite similar to those maintained in reactor R2 of [2] with similar dosing of polymer (0.02 g/L). The variations in experimental and predicted D_g/D_r values using the experimental results of [2] for reactor R2 are shown in fig. 2.

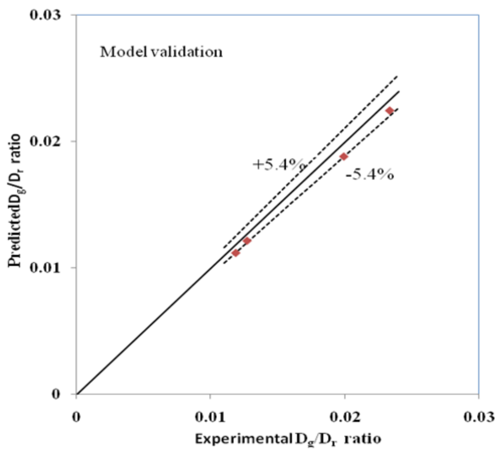

Fig. 2. Comparision between experimental and predicted D_g/D_r for reactor 2 using the experimental results of [2].

From this figure, it is evident that the predicted values of D_g/D_r are close to the experimental D_g/D_r values and the maximum error lie within an error band of ±5.4%. Predicted and experimental granule diameters as well as the percentage error are shown in Table 3 for reactor R2 of [2]. From Table 3, it can be seen that the percentage error in prediction of granule diameter lies between 3.75% to a maximum of 5.40%, which are reasonable and well within the acceptable limits in such simulations. Thus, it can be inferred that the developed model (5) accounting fourteen quantifiable variables influencing the granule size variations can be used satisfactorily to predict the granule diameter in UASB reactor under similar operating and experimental conditions as maintained in the studies of [1] and [2]. Statistical error estimates (SR, SSE, SD and RMSE) between the experimental and predicted (D_g/D_r) values for reactor R2 of [2] are also shown in Table 4.

Table 4. Statistical error estimates in simulated dimensionless diameter (D_g/D_r)

Statistical parameters	SR	SSE	S.D	RMSE
Model testing[a]	1.04E-04	1.16E-07	6.9E-03	1.50E-04
Model validation[b]	3.08E-03	2.58E-06	5.4E-03	1.92E-04

[a]Reactor R4 of [1], [b]Reactor R2 of [2]

From Table 4, it is evident that the error estimates show better closeness of predicted (D_g/D_r) values with experimental D_g/D_r values and hence good accuracy in prediction of D_g/D_r values by the model (5).

From the above results, it has been inferred that the granules size variations as per model (5) are validated reasonably well using experimental results of [2]. Due to lack of experimental results of other investigators for all the fourteen variables under more or less similar operating conditions within reactor, further validation of model (5) could not be performed in the present work. However, further validation of (5) can be attempted in future studies with experimental results of other investigetors with UASB reactors operated under more or less similar operating conditions.

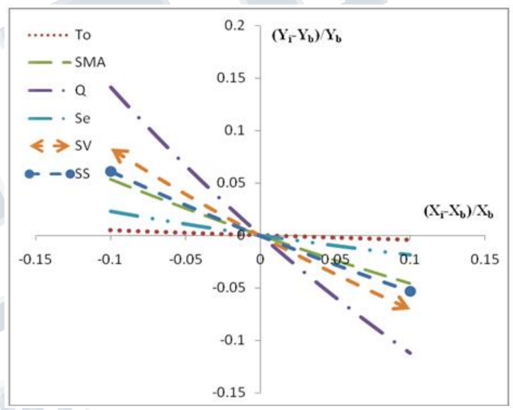

Fig. 3. Sensitivity analysis of parameters under Group-Iusing the experimental results of [1]

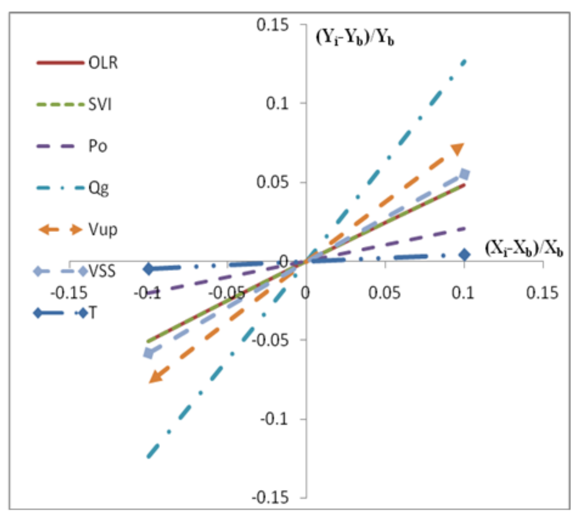

Fig. 4. Sensitivity analysis of parameters under Group-II using the experimental results of [1].

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Sensitivity analysis

Sensitivity analysis was carried out to assess the sensitivity of variables considered in the model (5) for prediction of (D_g/D_r) values for reactor R4 of [1].

Sensitivity of 13 variables (except D_r) namely, OLR, Q, Q_g, VSS, SS, SMA, SVI, T, T_o, S_e, P_o, V_{up} and SV influencing the granule diameter was determined using (4). Variables were grouped in two broad categories: T_o, SMA, Q, S_e, SV and SS in group-I and OLR, SVI, P_o, Q_g, V_{up}, T and VSS in group II depending upon the nature of sensitivity variations examined.

The sensitivity of all the thirteen variables are plotted in figs. 3 and 4 respectively for group-I and group-II variables for reactor R4 of [1]. From Fig. 3, it is obseved that the parameters T_o, SMA, Q, S_e, SV and SS do have little influence on prediction of granule diameter. Among the six variables of group- I, liquid inflow rate (Q) is observed to be the most sensitive parameter and therefore needs proper attention during reactor operation to avoid any shortcircuiting and possible washout of viable microorganisms. Settling velocity (SV) of granule is the next most sensitive parameter which governs the setteability and retention capability of granules within the reactor. The concentration of suspended solids (SS), specific methenogenic activity (SMA), effluent COD concentration (S_e) and operation time (T_o) are relatively less sensitive parameters in decreasing order of their sensitivity as seen from Fig. 3 for group-I parameters. Following is the decreasing order of sensitivity for group- I parameters: Q > SV > SS > SMA > Se > T_o

From Fig. 4, for sensitivity of group-II parameters (7 variables), Q_g is observed to be the most sensitive parameter in the prediction of granule diameter. Gas production rate (Q_g) plays a key role in granulation and formation of denser granules in the sludge bed region. Higher gas production rate in the sludge bed leads to the shearing of loose flocs and hence facilitates the formation of denser granules with good settleability. Liquid upflow velocity (V_{up}) is the next most sensitive parameter and has an important role in variation of granule sizes in the sludge bed region [1]. As V_{up} increases, the granules may disintegrate due to shearing and the resulting loose fragments which are liable to wash out from the reactor [22]. The concentration of volatile suspended solids (VSS), organic loading rate (OLR), sludge volume index (SVI), polymer loading (P_o) and operation time (T) are relatively less sensitive parameters in decreasing order of their sensitivity as can be seen from Fig. 4 for group-II parameters. The following is the decreasing order of sensitivity for group-II parameters: Q_g >V_{up} >VSS > OLR > SVI > P_o > T.

Sensitivity of all the thirteen parameters considered in the present study reveals that the sensitivity of parameter Q is followed by Q_g , SV, $V_{up,}$ SS, VSS, SMA, OLR, SVI, S_e, P_o and $T_{o,}$ while T is having minimum sensitivity in prediction of granule diameter among the parameters of both the groups. The decreasing order of sensitivity of all the thirteen parameters can be expressed as follows: Q > Q_g > SV > V_{up} > SS > VSS > SMA > OLR > SVI > S_e >P_o > T_o > T.

CONCLUSIONS

In this study, a mathematical function to model the granule size variation in UASB reactor has been developed using dimensionless approach and incorporating fourteen quantifiable variables for which experimental results were available in the literature. From the analysis of non-linear multiplier function developed using the experimental results of [1], it has been concluded that the parameter based non-linear power multiplier function predicts the granule size variation satisfactorily in UASB reactor. Validation of the developed non-linear multiplier function using the experimental results of other investigator [2] reveals that the developed non-linear power multiplier function simulates the experimentally observed granule sizes satisfactorily in UASB reactor with maximum error in predictions being 5.40%. Sensitivity analysis reveals that the liquid inflow rate (Q) is the most sensitive parameter influencing the predictions of granule size variations while operation time being the least sensitive. The decreasing order of the sensitivity of all the thirteen variables is observed as follows: Q > Q_g > SV > V_{up} > SS > VSS > SMA > OLR > SVI > S_e >P_o > T_o > T

The results of the present study may prove useful in the assessment of granule sizes in UASB reactor with high methanogenic activity and good settling characteristics that are essential for its successful operation and performance in treating industrial as well as domestic wastewaters. However, the model of the present work requires further validation in future investigations.

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ABBREVIATIONS

D_g	Granule diameter, mm
D_r	Reactor diameter, mm
OLR	Organic loading rate, g.COD/L.d
P_o	Polymer dose, g/L
Q	Flow rate, L/d
Q_g	Gas production rate, L/d
R^2	Coefficient of determination
S_o	Influent COD concentration, g COD/L

S_e Effluent COD concentration, g COD/L
SMA Specific methenogenic activity, g CH_4-COD/g VSS.d
S_R Sensitivity of the variable
SV Settling velocity, m/h
SVI Sludge volume index, L/gm
T Operation time, d
T_o Time for which a particular OLR is maintained constant, d
V_{up} Upflow liquid velocity, m/h
X_b Base parameter value of the variables taken on a particular day of reactor operation
X_i Parameter values
Y_b Basic function value at a particular day of reactor operation
Y_i Value of function at different parameter values,

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