Indian Journal of Science and Technology Vol. 4 No. 5 (May 2011) ISSN: 0974- 6846

Role of constraints on process parameters in artificial neural network based simulation of composting of agricultural waste

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Abstract

This paper focuses on the effect of process constraints on success of the artificial neural network (ANN) program in predicting the compost process. Agricultural waste (sugarcane bagasse, soya husk, and wood straw) was composted aerobically and data on experimentally determined carbon dioxide evolved was used for simulation of composting process. A computer program was developed using ANN technique for simulation purpose. The ANN based model was tested for fitting a combination of exponential functions on experimental data, for two different rates of reaction, corresponding to easily and moderately hydrolysable waste. Initial trials failed to give satisfactory fit, but introduction of certain constraints like relative magnitude of the two reaction rates and constraint on total carbon helped in convergence of the solution. This study reveals the important role of constraints on process parameters in modeling of aerobic composting of agricultural waste. ANN program required initial estimates of process parameters to start the convergence process. Effect of these estimates is also discussed here.

Keywords: Agricultural waste, compost, artificial neural network, carbon.

Introduction

Composting of agro-wastes has been an area of active research during the last two decades (Marugg *et al*., 1993; Martinez-Inigo & Almendros, 1994; Paredes *et al*., 2001; Paredes *et al.,* 2002; Komilis & Ham, 2003). During aerobic decomposition, agricultural solid waste is first hydrolyzed due to which solid carbon forms enters the aqueous media (Komilis, 2006). The hydrolysis rates of different components vary due to difference in binding of cellulose by hemicelluloses and lignin. The products of decomposition of cellulose and hemicelluloses are water soluble. The aqueous media also contains other components such as different sugar types, alcohols, organic acids and amino acids. A part of carbon in aqueous media gets converted into carbon dioxide, while residual carbon is retained by the humic substance as the final stabilized produce of bio-degradation of organic agro-waste. Production of carbon dioxide during composting can be used as a measure of hydrolysis rate of different carbon fractions in agro-waste substrate (Komilis & Ham, 2000; Komilis, 2006). Artificial neural networks (ANN) have been used in earlier works for modeling of bacterial growth (Najjar *et al*., 1997; Geeraerd *et al*., 1998; Jeyamkondan *et al*., 2001; Hajmeer & Basheer, 2002).

Experimental data was obtained through aerobic composting of a mixture of sugarcane bagasse, soya husk, wood straw, mixed with food waste (to support growth of microbes, particularly during the initial phase). The hydrolysis reaction rate constants were obtained for easily hydrolysable, moderately and difficult hydrolysable carbon fractions. Data on experimentally determined carbon dioxide evolved was used for simulation of composting process. The ANN based model was tested for fitting a combination of exponential functions on experimental data, for two different rates of reaction, corresponding to easily and moderately hydrolysable waste. Initial trials failed to give satisfactory fit, but introduction of certain constraints like relative magnitude of the two reaction rates and constraint on total carbon helped in convergence of the solution. Research with ANN has shown that this technique may have some limitations in predicting the results under certain circumstances (Tu, 2000). The present work attempts to highlight similar conditions for prediction of composting of agro-wastes. ANN program required initial estimates of process parameters to start the convergence process. Effect of these estimates is also discussed here.

In this work, effect of initial estimates of carbon fraction in aqueous media of a composting system is studied using ANN for prediction of other process parameters. Experimental data was obtained from a composting system comprising an aerobic digester for composting of a mixture of agricultural and food waste, operating in near-optimal conditions with regards to adequacy of oxygen and temperature in the system. The ANN model was assigned the task of fitting a combination of exponential functions, for two different rates of reaction, corresponding to easily and moderately hydrolysable waste. Comparison of experimental observations with results predicted by the ANN model indicate that effectiveness of ANN in predicting evolution of carbon dioxide is affected by use of constraints on process parameters, as well as the initial value of process parameters in the system. These observations emphasize the importance and necessity of using constraints on process parameters when ANN based models are to be employed for simulation and modeling of aerobic composting.

Experimentation, modeling and simulation

A mixture of agricultural waste comprising sugarcane bagasse, soya husk, and wood straw, mixed with food

Indian Journal of Science and Technology Vol. 4 No. 5 (May 2011) ISSN: 0974- 6846

Fig1. Experimental setup

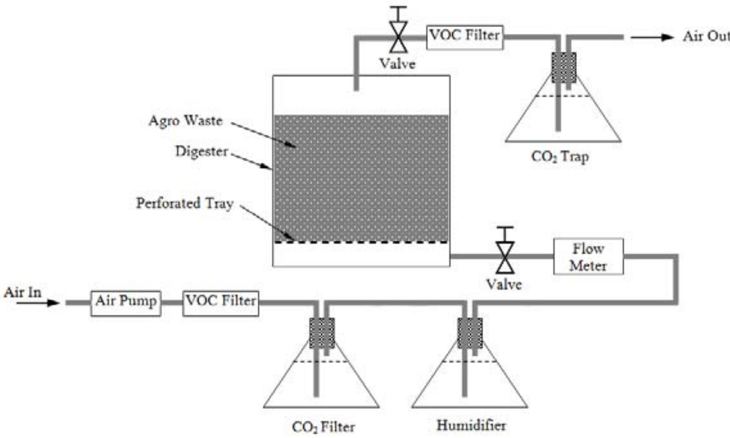


Fig.2. Compost model

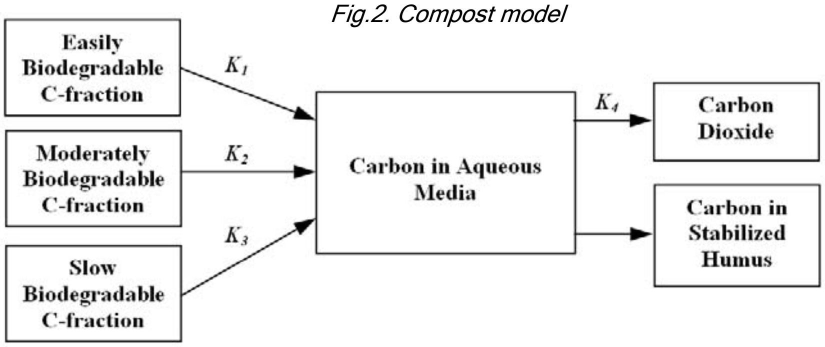


Fig.3. Sum of squared errors after data fitting

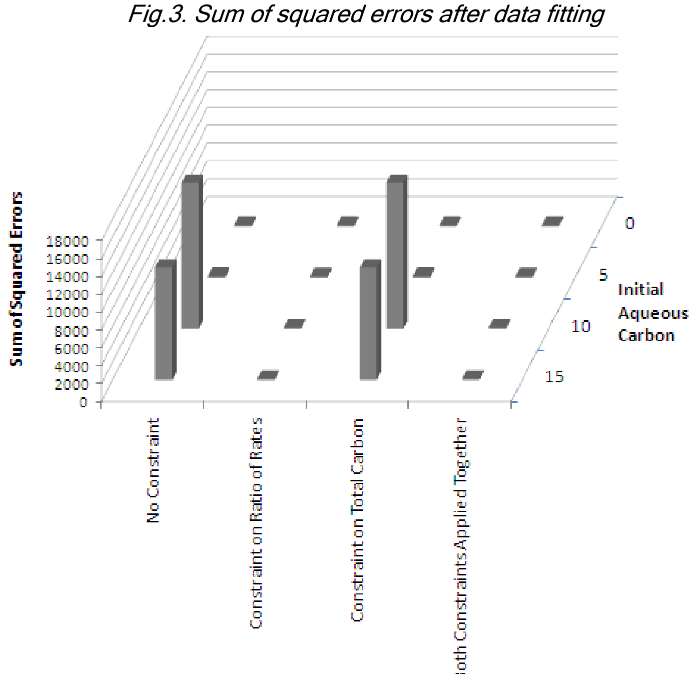


Fig.4. Predicted initial aqueous carbon

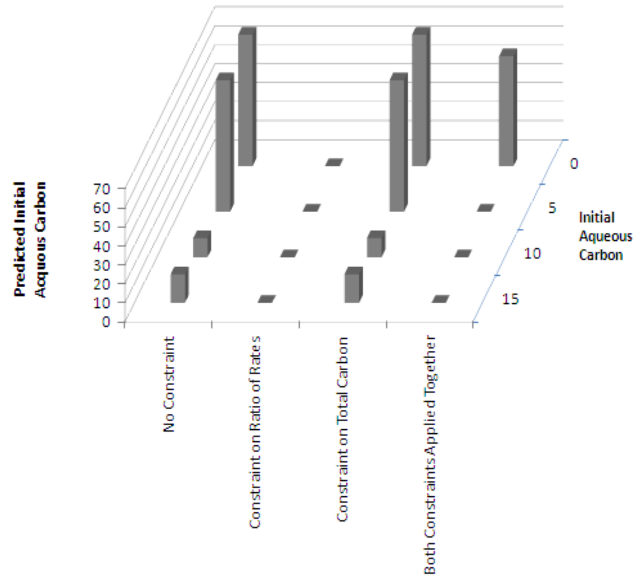
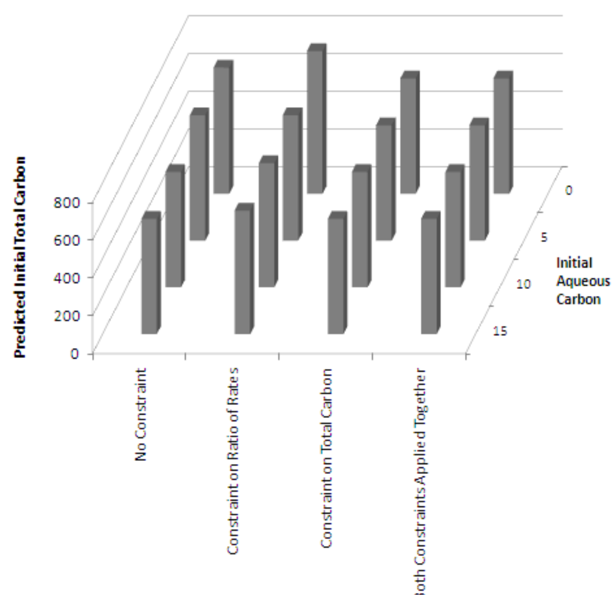


Fig. 5. Predicted total carbon



waste was composted aerobically. The setup used for this is shown schematically in Fig.1.

In aerobic decomposition of agricultural solid waste, hydrolysis is the first stage as followed by entering of various carbon components of solid waste into aqueous media. The hydrolysis rate of a particular component depends upon its micro structure defined by binding of cellulose by compounds like hemicelluloses and lignin. Part of carbon in aqueous media is converted into carbon dioxide and remaining carbon is retained by the humus. Fig.2 shows the schematic presentation of this phenomenon.

Agro-wastes like sugarcane bagasse, soya husk, and wood straw contain such components as easily hydrolysable, moderately hydrolysable, or difficult to hydrolyze in different proportions. The reaction kinetics of the process is defined by the system of simultaneous differential equations (1) to (5)

$$\frac{dx_1}{dt} = -K_1 . x_1 \quad (1)$$

$$\frac{dx_2}{dt} = -K_2 . x_2 \quad (2)$$

$$\frac{dx_3}{dt} = -K_3 . x_3 \quad (3)$$

$$\frac{dx_4}{dt} = -K_1 . x_1 + K_2 . x_2 + K_3 . x_3 - K_4 . x_4 \quad (4)$$

$$\frac{dx_5}{dt} = K_4 . x_5 \quad (5)$$

Where,

x_1 : easily biodegradable carbon fraction in substrate,

x_2 : moderately biodegradable carbon fraction in substrate,

x_3 : difficult biodegradable carbon fraction in substrate,

x_4 : carbon fraction in aqueous media,

x_5 : carbon in the form of $C0_2$ produced from aqueous media,

K_1: reaction rate for hydrolysis of easily biodegradable carbon fraction.

K_2: reaction rate for hydrolysis of moderately biodegradable carbon fraction

K_3: reaction rate for hydrolysis of difficult biodegradable carbon fraction.

K_4: reaction rate for mineralization of aqueous carbon fraction.

This model was solved using artificial neural network (ANN). The input to ANN was arbitrarily selected trial data given in Table 1. With this trial data carbon dioxide generation during the entire duration of composting process was estimated using the mathematical model defined by Equations (1) to (5) under the four trial conditions. These four trials differ in terms of value of aqueous carbon fraction selected for first input to the ANN. The squared errors were determined for each of the four starting estimates of carbon dioxide evolution. The errors in prediction were calculated using experimental carbon dioxide evolution and those predicted by the model with initial conditions. The output of ANN program was used for back propagation training of the network. Four different constraint sets were considered for the analysis

Results and discussion

Four different constraint sets were used for simulation: (a) no constraints on total carbon or reaction rates, (b) constraint on ratio of reaction rates of easily biodegradable carbon fraction and that of moderately degradable carbon fraction, (c) constraint on total carbon in all fractions, and (d) combined constraint on ratio of reaction rates of easily biodegradable carbon fraction and that of moderately degradable carbon fraction, along with constraint on total carbon in all fractions. For each constraint set four different values of initially assumed aqueous carbon fraction were used for simulation named as trial 1 to 4 for each of the individual constraint sets. Initially assumed values for other carbon fractions were kept the same for all the cases. Tables 1 to 4 present the initially assumed values and the corresponding values

Table 1. No Constraint on total weight or reaction constants

	Trial 1		Trial 2		Trial 3		Trial 4	
	Input	Output	Input	Output	Input	Output	Input	Output
Initial Aqueous Carbon	15	15	10	10	5	69	0	69
Sum of Squared Errors	18716	12600	25022	16371	32328	193	40633	193
Total Carbon	610	610	610	610	610	662	610	667

Table 2. Constraint on reaction constants

	Trial 1		Trial 2		Trial 3		Trial 4	
	Input	Output	Input	Output	Input	Output	Input	Output
Initial Aqueous Carbon	15	0	10	0	5	0	0	0
Sum of Squared Errors	18716	189	25022	189	32328	189	40633	189
Total Carbon	610	653	610	658	610	663	610	754

Table 3. Constraint on total carbon in all fractions

	Trial 1		Trial 2		Trial 3		Trial 4	
	Input	Output	Input	Output	Input	Output	Input	Output
Initial Aqueous Carbon	15	15	10	10	5	69	0	69
Sum of Squared Errors	18716	12600	25022	16371	32328	193	40633	193
Total Carbon	610	610	610	610	610	610	610	610

Table 4. Constraints on reaction constants and total carbon

	Trial 1		Trial 2		Trial 3		Trial 4	
	Input	Output	Input	Output	Input	Output	Input	Output
Initial Aqueous Carbon	15	0	10	0	5	0	0	58
Sum of Squared Errors	18716	189	25022	189	32328	189	40633	192
Total Carbon	610	610	610	610	610	610	610	610

obtained by simulation. Each table corresponds to one constraint set described above.

Table 5. Sum of squared of errors

Initial Aqueous Carbon	15	10	5	0
No Constraint	12600	16371	193	193
Constraint on Ratio of Rates	189	189	189	189
Constraint on Total Carbon	12600	16371	193	193
Both Constraints Applied Together	189	189	189	192

Table 6. Predicted initial aqueous carbon

Initial Aqueous Carbon	15	10	5	0
No Constraint	15	10	69	69
Constraint on Ratio of Rates	0	0	0	0
Constraint on Total Carbon	15	10	69	69
Both Constraints Applied Together	0	0	0	58

Table 5 presents variations of sum of squared errors obtained through simulation for all the sixteen combinations (four constraint sets with four initially assumed aqueous carbon fraction). Table 6 presents variations of predicted initial aqueous carbon fraction obtained through simulation for all the sixteen combinations. Table 7 presents variations of predicted total carbon for all the sixteen combinations.

Table 7. Predicted total carbon

Initial Aqueous Carbon	15	10	5	0
No Constraint	610	610	662	667
Constraint on Ratio of Rates	653	658	663	754
Constraint on Total Carbon	610	610	610	610
Both Constraints Applied Together	610	610	610	610

Fig.3 shows variation of sum of squared errors after final run of the ANN program for the various combinations of constraint sets and initially assumed aqueous carbon fraction. It is observed that the program could not reduce the sum of squared errors satisfactorily for the following four cases: (a) no constraints, initial aqueous carbon fraction 15 gC/kg substrate, (b) no constraints, initial aqueous carbon fraction 10 gC/kg substrate, (c) constraint set 3 (constraint on total carbon), initial aqueous carbon fraction 15 gC/kg substrate, (d) constraint set 3, initial aqueous carbon fraction 10 gC/kg substrate. However, the constraint set 2 (constraint on ratio of reaction rates of easily degradable carbon fraction and moderately degradable carbon fraction), as well as constraint set 4 (combined constraint on ratio of reaction rates of easily biodegradable carbon fraction and that of moderately degradable carbon fraction, along with constraint on total carbon in all fractions), produced. It is evident that constraint on ratio of reaction rates minimized the sum of squared errors for the four combinations of initial aqueous carbon. Constraint on total carbon alone could not control the sum of squared errors on its own, however, in combination with constraint on ratio of reaction rates, the results could be achieved. It is also observed in Table 5 that constraint of ratio of reaction rates alone reduced the sum of squared errors to 189 for all the four cases of initial aqueous carbon. But under combined constraints (set 4), same value of sum of squared errors could be achieved in only three cases (initial aqueous carbon of 15, 10, and 5 gC/kg substrate). For the value of 0 gC/kg substrate the sum of squared errors could be reduced to 192. This may also be due to cumulative truncation errors during numerical solution of the differential and exponential equations.

Fig.4 shows the variation of predicted initial carbon fraction after data fitting by the ANN program, for the sixteen combinations of constraints and initially assumed aqueous carbon. It is observed that variation in results is most prominent for initial aqueous carbon values of 0 gC/kg and 5gC/kg. For initial aqueous carbon values of 10 gC/kg and 15 gC/kg the variations are small and almost similar. It may be observed that the constraint set 3 (constraint on ratio of reaction rates) resulted in predicted value of initial aqueous carbon of 0 gC/kg for all the four assumed values of this parameter. These results were not obtained for the four cases by other constraints. It is worth noting here that for combined constraints (constraint set 4), predicted aqueous carbon was 58 gC/kg for initial assumed value of 0 gC/kg. Here it may be argued that during the initial stages of biodegradation value of aqueous carbon fraction should be practically zero, because source of aqueous carbon fraction is hydrolysis of different fractions of carbon in the solid waste. Thus, prediction of 0 gC/kg initial aqueous carbon is justified. Therefore it may be concluded that constraint on ratio of reaction rates gives more reliable results when used alone; in combination with constraint on total carbon the results got misleading, even when a realistic value of initial of aqueous carbon fraction was taken as input to the ANN program.

Fig.5 shows variation of predicted total carbon for all the combinations of constraint sets and initially assumed aqueous carbon. It is obvious that for constraint sets 3 and 4, where constraint on total carbon was used, the final value of total carbon remained the same as initially assumed values. Variations were observed with constraint sets 1 and 2; these being more prominent with constraint set 2 (constraint on ratio of reaction rates). This indicates that use of constraint on ratio of reaction rates makes changes in the total estimate of carbon, which might be due to variations in values of individual carbon fractions. This finding needs further investigation, which is being done by the authors.

Conclusion

ANN based model was used for simulation of aerobic composting of mixture of sugarcane bagasse, soya husk, and wood straw. The carbon dioxide produced during this process was measured. An ANN based program was used to determine the process parameters using the experimental data. Initial trials indicated that the ANN program did not produce satisfactory results under certain circumstances. In order to overcome this problem, additional constraints were imposed. Four constraint sets were used: (a) no constraints on total carbon or reaction rates, (b) constraint on ratio of reaction rates of easily biodegradable carbon fraction and that of moderately degradable carbon fraction, (c) constraint on total carbon in all fractions, and (d) combined constraint on ratio of reaction rates of easily biodegradable carbon fraction and that of moderately degradable carbon fraction, along with constraint on total carbon in all fractions. Constraint on ratio of reaction rates turned out to be most important. Constraint on total carbon alone could not control the sum of squared errors on its own; however, in combination with constraint on ratio of reaction rates, the results could be achieved. It was also observed that combination of the above two constraints tends to deteriorate the performance of ANN program under circumstance. Constraint on ratio of reaction rates gives more reliable results when used alone; in combination with constraint on total carbon the results got misleading, even when a realistic value of initial of aqueous carbon fraction was taken as input to the ANN program. Use of constraint on ratio of reaction rates, without imposing constraint on total carbon, makes changes in the total estimate of carbon, which might be due to variations in values of individual carbon fractions. Further research in this line is under progress.

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