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PERFORMANCE EVALUATION OF MODIFIED ADVECTION-DISPERSION EQUATION FOR MODELLING RIVER CONTAMINANT TRANSPORT

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Abstract: Modified 2-dimensional advection-dispersion equation has been used in this study to assess pollutant transport in streams. The Advection-Dispersion equation was modified to incorporate temperature. The dispersion term was expressed as a function of stream and air temperature and solved using Laplace transforms. It resulted in a concentration prediction models with temperature term. The model was evaluated using tracer data from experiment conducted to mimic the transport of contaminant in the New-Calabar River, Rivers State, Nigeria. During the evaluation, comparing the experimental data with the predicted concentration, the model predicts well the experimental concentration with a co-efficient of correlation of 0.920 and an average error of 0.01721. Test of significance (T-test) with 5% level of significance results showed that there is no significance difference between the measured value and the predicted values. Inclusion of temperature into the model reduced significantly the discrepancy between the observed and the predicted values and improved the predictive capacity of the model. Keywords: advection-dispersion, temperature, transport, Laplace transform, tracer-experiment

1. INTRODUCTION

In recent years, there has been growing interest in modeling of pollutant transport in streams and rivers because of the increased interest in preserving the quality of the environment, especially for water quality management. Most surface waters around the world are always at risk of constant pollutant discharge especially, those located around industrial areas and cities where there are heavy accumulation of municipal wastes. The Niger Delta region of Nigeria where the New-Calabar River is situated is not exempted from these pollutants discharge because of increase in industrial activities.

The issue of water quality management in Nigeria especially in regards to pollutant's status is not yet taken very seriously due to poor implementation policies on the control and regulation of water quality management. Most of Nigerian citizens and in particular, the Niger Delta region resort to underground water for domestic use without adequate information on the portability of the water being used. Researches geared toward pollutant transport prediction are a viable tool for water quality management. The models for pollutant transport are useful for the simulation of accidental pollutant release in Rivers and streams. The Advection-Dispersion equation has been the generally used approach to description of pollutant transport on surface water (Wallis and Mason, 2004; Socolofsky and Jika, 2005). The advection-dispersion equation has also been widely used to build model on pollutant transport. Although, many reported application of Advection-Dispersion equation was based on the interests the researcher has on the factors that influenced the transport of pollutants on surface water.

The effect of prevailing ambient air and stream temperature on contaminant transport in river, using New Calabar River as a case study was investigated in this work. The ratio of air to river temperature was factored into the dispersion equation. Although, previous studies showed that temperature affects contaminant dispersion in rivers but the effect was greatly investigated with respect to time and direction of lows (UNESCO, 2005). In this work the effect of temperature on contaminant migration was researched for a period of eight months (May to December). However, the months of May and December are only presented in this paper. The air and river temperature were monitored throughout the period of the experiment. The Rhodamine tracer dye was used to mimic the inherent river contaminant. The measured tracer concentrations from the experiment were modeled using the Advection-Dispersion equation. The dispersion coefficient along the longitudinal direction was modified to incorporate temperature parameter, which was expressed as a function of tracer as a function of temperature amongst other terms.

2. MATERIALS AND METHOD

— Case study site

The study area used to conduct the tracer experiment is a section of the new-Calabar river located at Aluu in Rivers state Nigeria. The new Calabar River is one of the most prominent rivers in the state; others include Bonny River, Andoni River, Nun River and Orashi River. New Calabar River is an acidic fresh and non-tidal river which took its rise from Elele-Alimini and empties into some creeks and lagoon bordering the Atlantic Ocean. The

section of the river where sampling and the research was done is located at a geographical co- ordinate between latitude N4^o 55.353'- N4^o 55.365' and longitude E006 ^o 53.785'- E006^o 53.793', at an elevation of 6m above the mean sea level. The new-Calabar river serves as a receiving water body for discharge of point and non-point wastes

from companies that have their operations along the banks of the rivers, which has led to the pollution of the rivers over the years. New Calabar River is situated in the tropical rain forest whose climate is characterized by two seasons which are the raining season which commences from April to November and the dry season which commences from November to March. The people around the New-Calabar River are predominantly fisher men and they engage in a lot of dredging activities to earn their living. The New-Calabar River is sometimes used for recreation, domestic and agricultural purposes. The slope of the study area is generally a gentle sloping terrain as shown in Figure 1.



Figure 1: Area Map of Cross-Section of New-Calabar River

— Experimental procedure

A tracer experiments was carried out to mimic the transport of contaminant in the stream. Soluble tracer can be used to simulate the transport and dispersion of solute in surface water because they have virtually the same phenomenon (Shaw, 1977). The use of soluble tracer to quantify the transport and dispersion in streams and rivers has been used by various authors. Dispersion number is however usually determined by tracer studies (Polpaset et al., 1983; Marecos-domonte and Mara, 1987). The tracer dispersion study was conducted for a period of eight months to cater for period of low and high temperature in the stream. Table 1 summarizes the data obtained for eight months and the computed dispersion-coefficient along the longitudinal flow.

— Development of the river transport model

The governing equation for the transport of contaminant in 2-dimensional flow case is given by

$$\frac{\partial C}{\partial t} + V_x \frac{\partial C}{\partial x} + V_y \frac{\partial C}{\partial y} = D_L \frac{\partial^2 C}{\partial x^2} + D_T \frac{\partial^2 C}{\partial y^2}$$
(1)

In this work, we have applied the Buckingham π -theorem from the following variables, shear velocity, river velocity, depth, river temperature, ambient air temperature to obtain the dispersion coefficient in the longitudinal direction as follows.

Let the no. of variables be represented by Φ , and the no. of fundamental units be represented by Γ . Then, the no. of pie group is

$$\Pi = \Phi - \Gamma \tag{2}$$

$$7 - 3 = 4$$

Hence, for Π_1, Π_2, Π_3 and Π_4 were obtained as

$$\Pi_{1} = f_{1}(\Pi_{2}, \Pi_{3}, \Pi_{4})$$
(3)

$$\Pi_1 = UBT_S D_L \tag{4}$$

$$\Pi_2 = UBT_S H \tag{5}$$

$$\Pi_3 = UBT_S V \tag{6}$$

$$\Pi_4 = UBT_S T_a \tag{7}$$

Analyzing dimensional homogeneity

$$\Pi_1 = \frac{D_L}{U_*} B \tag{8}$$

$$\Pi_2 = \frac{H}{B} \tag{9}$$

$$\Pi_3 = \frac{V}{U_*} \tag{10}$$

$$\Pi_4 = \frac{T_a}{T_S} \tag{11}$$

Hence, after substitution and simplification, the dispersion coefficient was obtained as

$$D_{L} = a * (UB)^{b} * \left(\frac{H}{B}\right)^{c} * \left(\frac{V}{U_{*}}\right)^{d} * \left(\frac{T_{a}}{T_{s}}\right)^{c}$$
(12)

In this paper the governing equation is modified to incorporate the dispersion coefficient term along the longitudinal direction, D_L as a function of dimensionless temperature. The dimensionless temperature is expressed as the ratio of ambient air temperature to the stream temperature. Again, to reduce the complexity of the model, we simplified equation (12) as follows.

$$D_{L} = \alpha \left(\frac{T_{s}}{T_{a}}\right)^{e}$$
(13)

where:

$$\alpha = a * (UB)^{b} * \left(\frac{H}{B}\right)^{c} * \left(\frac{V}{U_{*}}\right)^{d}$$
(14)

Substituting equation (13) into (1), the modified equation becomes

$$\frac{\partial C}{\partial t} + V_x \frac{\partial C}{\partial x} + V_y \frac{\partial C}{\partial y} = \alpha \left(\frac{T_s}{T_a}\right)^e \frac{\partial^2 C}{\partial x^2} + D_T \frac{\partial^2 C}{\partial y^2}$$
(15)

The above modified 2-Dimensional Advection-Dispersion model is solved analytically using the Laplace transform to obtain a concentration model which predicts the concentration profile of the discharged contaminant. The following assumptions were made in solving the equation:

- (1) The pollutants are conservative and non-decaying
- (2) Instantaneous discharge from a point source
- (3) Flow is uniform, steady and incompressible
- (4) Neglect wind shear on velocity

The boundary condition applied or solving 2-d advection-dispersion model are

$$t = 0 \qquad 0 < x < \infty ; C = 0$$
 (16)

$$t > 0 \qquad x = \infty; \quad C = 0 \tag{17}$$

$$t > 0$$
 $x = 0$; $C = C_0$ (18)

After all necessary manipulations and simplifications, the solution to equation (15) was solved analytically as

$$C(\mathbf{x},\mathbf{y},\mathbf{t}) = \frac{C_{o}}{2} \left\{ \operatorname{erfc} \left[\frac{\mathbf{x} + \mathbf{y}\sqrt{D_{T}}}{2\sqrt{D_{L}}\left[1 + \left(\frac{D_{T}}{D_{L}}\right)^{2}\right]\mathbf{t}} \right] + \operatorname{erfc} \left[\frac{\mathbf{x} + \mathbf{y}\sqrt{D_{T}}}{2\sqrt{D_{L}}\left[1 + \left(\frac{D_{T}}{D_{L}}\right)^{2}\right]\mathbf{t}} \right] \right] \times \exp \left[\frac{V_{x}\left[2\left(\mathbf{x} + \mathbf{y}\sqrt{D_{T}}\right) - V_{x}\mathbf{t}\right]}{4D_{L}\left[1 + \left(\frac{D_{T}}{D_{L}}\right)^{2}\right]} \right] \right]$$
(19)

However, the measured velocity and dispersion coefficient in the transverse direction were insignificant. Thus, the transport of the river contaminants was dominant along the longitudinal direction. Therefore equation (19) is only accounted for dispersion along the longitudinal direction, and hence, reduces to equation (20).

$$C(\mathbf{x},\mathbf{t}) = \frac{C_{o}}{2} \left\{ \operatorname{erfc} \left[\frac{\mathbf{x} - \mathbf{V}_{\mathbf{x}} \mathbf{t}}{2\sqrt{\alpha(T)^{e} \mathbf{t}}} \right] + \operatorname{erfc} \left[\frac{\mathbf{x} + \mathbf{V}_{\mathbf{x}} \mathbf{t}}{2\sqrt{\alpha(T)^{e} \mathbf{t}}} \right] \right\} \times \exp \left(\frac{\mathbf{V}_{\mathbf{x}} [2\mathbf{x} - \mathbf{V}_{\mathbf{x}} \mathbf{t}]}{4\alpha(T)^{e}} \right)$$
(20)

- Previously Development Transport Models used for Comparison

In order to ascertain the reliability of the developed model, we further compare results obtained with those of Kumar and co-workers and van-Genuchten and co-workers. The model developed by Kumar et al. (2010) is given in equation (21), while that developed by van-Genuchten et al. (2013) is given in equation (22).

$$C(\mathbf{x},\mathbf{t}) = \frac{C_{o}}{2} \left[\operatorname{erfc}\left(\frac{\frac{x}{f(\mathbf{mt})} - V_{x}\mathbf{t}}{2\sqrt{D_{x}\mathbf{t}}}\right) + \exp\left(\frac{Vx}{D_{x}f(\mathbf{mt})}\right) \operatorname{erfc}\left(\frac{\frac{x}{f(\mathbf{mt})} + V_{x}\mathbf{t}}{2\sqrt{D_{x}\mathbf{t}}}\right) \right]$$
(21)

where f(mt) = 1 for m=0

$$C(\mathbf{x},\mathbf{t}) = \frac{C_{o}}{2} \left\{ \operatorname{erfc}\left[\frac{\mathbf{x} - \mathbf{V}_{\mathbf{x}}\mathbf{t}}{\sqrt{4D_{\mathbf{x}}\mathbf{t}}}\right] + \sqrt{\frac{\mathbf{V}^{2}\mathbf{t}}{\pi D_{\mathbf{x}}}} \exp\left[-\frac{(\mathbf{x} - \mathbf{V}\mathbf{t})^{2}}{4D_{\mathbf{x}}\mathbf{t}}\right] - \frac{1}{2} \left(1 + \frac{\mathbf{V}\mathbf{x}}{D_{\mathbf{x}}} + \frac{\mathbf{V}^{2}\mathbf{t}}{D_{\mathbf{x}}}\right) \exp\left(\frac{\mathbf{V}_{\mathbf{x}}\mathbf{x}}{D_{\mathbf{x}}}\right) \operatorname{erfc}\left[\frac{\mathbf{x} + \mathbf{V}_{\mathbf{x}}\mathbf{t}}{\sqrt{4D_{\mathbf{x}}\mathbf{t}}}\right] \right\}$$
(22)

The models above were simulated and implemented in MATLAB to facilitate the computation. The data obtained from the MATLAB simulation were analyzed using Excel math tools.

3. RESULTS AND DISCUSSION

The profiles of all the results obtained for each of the month are similar, though, different in numerical values, but the months of May and December were chosen for this report. Comparison was also made between modified and convectional models (without temperature). Further, the modified model was compared with Advection-Dispersion models developed by other researchers.

– Coefficient of Transport Model

In order to satisfactorily use the developed models and the dispersion coefficient model in equation (12), the variables shown in Table 1 were measured in-situ, which were used to determine the dispersion coefficient. Table 1: The Summary of the Data Collected for Eight Month Dispersion Studies

Tuble 1. The building of the build boliceted for Eight Month Dispersion beddies							
Month	$T_s(^{\circ}C)$	$T_a(^{\circ}C)$	U∗(m/s)	$Vel_{(x)}(m/s)$	H(m)	B(m)	$D_L(m^{2/s})$
May	17.5	22.1	0.805	0.3439	1.654	10	6.364
June	18.4	23.6	0.745	0.2793	1.787	10	4.863
July	23.8	35.3	0.673	0.4537	1.556	10	9.298
August	24.5	30.1	0.745	0.3400	1.700	10	5.839
September	24.6	30.4	0.681	0.3737	1.644	10	5.572
October	25.1	30.2	0.745	0.4167	1.73	10	8.343
November	25.6	29.3	0.682	0.2991	1.653	10	5.581
December	26.6	35.4	0.687	0.3919	1.6431	10	7.417

where: T_s =River temperature, T_a =ambient air temperature, V=river velocity, U*=shear velocity, H=depth, B=width and D_L =longitudinal dispersion coefficient.

The above results are average values taken once every week per month in order to reduce sources of error due to variability of atmospheric conditions and the river. The average of the river and ambient temperatures for the months of May and June are 5°C greater than the rest of the months, indicating variability in temperature.

— Variation of the tracer concentration

The variation in tracer concentartion along the flow of the River current was modeled and compared as shown in Tables 2 and 3, while the profiles of the tabulated data are presented in Figures 2 and 3 for the months of May and December respectively.

Table 2. Concentration of tracer for modified and convectional models for way				
Distance (m)	Experiment (mg/l)	Model with temperature (mg/l)	Model without temperature (mg/l)	
0	500	500	500	
3	352.52	397.82	404.70	
6	242.51	302.21	314.74	
9	160.46	218.52	234.61	
12	102.02	149.98	167.23	
15	62.82	97.48	113.78	
18	38.52	59.88	73.76	
21	24.75	34.70	45.50	
24	17.16	18.94	26.67	
27	11.38	9.72	14.84	
30	3.07	4.69	7.83	

Table 2: Concentration of tracer for modified and convectional models for May



Figure 2: Comparison of experimental, temperature dependent and non-temperature dependent model for the month of May

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Longitudinal Distance (m)	Experiment	Model With Temperature	Model Without	
0 (/	Ŧ	Ľ	Temperature	
0	500	500	500	
3	381.25	405.24	413.95	
6	274.35	315.73	331.85	
9	196.52	235.87	257.11	
12	139.72	168.59	192.20	
15	90.18	115.05	138.41	
18	62.46	74.84	95.91	
21	35.4	46.33	63.86	
24	21.22	27.26	40.82	
27	13.64	15.22	25.03	
30	7.38	8.06	14.71	



Figure 3: Comparison of experimental, temperature dependent and non-temperature dependent model for the month of December

The temperature dependent concentration model obtained from the analytical solution of the Advection-Dispersion equation modified, which included temperature term and the solution to the Advection-Dispersion model without temperature term were simulated and compared. The result shows that the concentration model with temperature predicted the actual measured concentration from the field than the model independent of temperature. As can be seen in the Figures 2 and 3, the profile of concentration for the modified model (temperature dependent model) was closer to that of the experiment than the convectional model (temperature independent model). However, due to metrological condition, the performance of the model with respect to the monthly analysis was observed to have varied.

Thus, with the measured River and air temperatures of 17.5° C and 22.1° C respectively, and dimensionless temperature value of 0.792, the concentration of the tracer in the River decreased from an initial value of 500 mg/l to 3.07 mg/l after covering a distance of 30m. With the temperature dependent model, the racer concentration decreased from 500 mg/l to 4.6 mg/l, while the temperature independent model at same initial concentration decreased to 7.8 mg/l after 30m from the point source. The coefficient of determination R² for the temperature dependent model and temperature independent model were obtained to be 89.36% and 81.99% respectively, indicating that the modified model explained the experimental results better.

Like in the month of May, similar trends were observed for the month of December. Thus, the tracer concentration for the experiment, temperature dependent and temperature independent models decreased from the initial 500mg/l to 7.38mg/l, 8.06mg/l and 14.7mg/l respectively after 30m away from the point source. Also, the measured River and air temperatures are 26.6°C and 35.4°C, while the dimensionless temperature was 0.751. The coefficient of determination R^2 of the temperature dependent and temperature independent models for December were obtained as 96.09% and 89.10%. This again, proved that the modified model predicted the experimental results better than the convectional model.

— Comparison of model with established models

The developed temperature dependent model was also compared with other literature reported model. Thus, the Advection-Dispersion models developed by Kumar et al. (2010) and van-Genucheten et al. (2013) were subjected into the experimental results using the model coefficients obtained from the field analysis. Table 4 showed the results obtained from the respective models, while Figure 4 shows their profiles.

rape 4. Experimental and predicted values nom various concentration models					
Distance (m)	This work	van Genuchten et al.	Kumar et al. (2010)	Experimental	
	(IIIg/1)	(2015) (IIIg/1)	(111g/1)	(111g/1)	
0	500	500	500	500	
3	397.82	417.38	428.75	352.52	
6	302.21	335.63	353.65	242.51	
9	218.52	258.63	279.81	160.46	
12	149.98	190.47	211.84	102.02	
15	97.48	133.73	153.16	62.82	
18	59.88	89.35	105.55	38.52	
21	34.70	56.71	69.23	24.75	
24	18.94	34.14	43.16	17.16	
27	9.72	19.47	25.54	11.38	
30	4.69	10.51	14.34	3.07	

Table 4: Experimental and predicted values from various concentration models



Figure 4: Comparison of modified and other Advection-Dispersion models

The comparison of the models for the month of May showed that the concentration of the tracer in the River decreased from initial 500mg/l to 4.69mg/l for temperature dependent model, 500mg/l to 10.51mg/l for van-Genuchten et al. and 500mg/l to 14.34mg/l for Kumar et al. after 30m away from the point source. From Figure 4, it can be observed that the profile of the modified model (Chiedozie 2017) was closer to the experiment than the others.

Also, statistical analysis shows that the developed temperature dependent concentration model gave an R² value of 0.92 and root-mean-square error of 5.2. The model developed by van-Genuchten et al. (2013) gave an R^2 value of 0.85 and root-mean-square error of 2.7, while the model developed by Kumar et al. (2010) gave an R^2 value of 0.77 and root-mean-square of 6.5. Base on this statistical analysis, the developed model is said to be reliable in the evaluation of pollutant transport in Rivers and streams.

4. CONCLUSION

The level of prediction of pollutant distribution along the Rivers by the modified Advection-Dispersion model showed that temperature is really a factor that can influence the transport of River pollutant. Thus, evaluation of pollutant migration in water using Advection-Dispersion equation should not only consider coefficients like seepage velocity dispersion coefficient, but temperature of the studied water body should also be considered. Thus, the developed modified Advection-Dispersion model showed it was effective for the evaluation of pollutant transport in Rivers. This was further confirmed by the statistical results, which showed higher R² than both the convectional model and the selected literature Advection-Dispersion models. Besides, temperature, it should be noted that the correct determination of key component of dispersion and velocity coefficient will determine the robustness of the developed model. Finally, future investigation on River or stream contaminant process should also consider the effect of wind speed variable.

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