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UNSTEADY STATE PROCESS COMPUTATIONS ON SPREADSHEETS

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ABSTRACT

Spreadsheets are becoming increasingly popular, as a useful tool, for making process engineering calculations. This paper shows the use of spreadsheets for computations of an unsteady state process described by ordinary differential equations. The model equations are numerically solved using the fourth order Runge-Kutta method implemented on a spreadsheet. The spreadsheet implementation of this method demonstrates the possibility and usefulness of spreadsheets for their application in the simulation of dynamic processes.

NOMENCLATURE

A	cross sectional area, (m^2)
$C_{A(t)}$	settleable solids concentration, as a function of time, (mg lit^{-1})
$C_{B(t)}$	non-settleable solids concentration, as a function of time (mg lit^{-1})
$C_{T(t)}$	total solids concentration (mg lit^{-1})
N	total number of tanks
$Q_{(t)}$	wastewater flowrate as a function of time, (m^3 hr^{-1})
S	settleable solids fraction
S_p	scouring parameter
t	time (hr.)
U	settling velocity (m hr^{-1})
V	tank volume, (m^3)
Δt	step size (hr.)

INTRODUCTION

Spreadsheets have until recent years been most often used for business applications such as cost estimation, financial analysis and planning, accounting and budgeting. During the last few years, however, a number of authors have demonstrated the application of spreadsheets in solving a variety of engineering problems (1-15). The advantages of using spreadsheets over the usual computational methods involving programming languages are that spreadsheets are easy to use, are easily available and accessible. They are capable of showing the details of calculations and of displaying the results graphically as a part of the calculations. These features along with their capability of iterative calculations make the spreadsheets more attractive for process engineering applications.

The objective of this paper is to show the suitability of spreadsheets for computations undertaken for the purpose of simulating the behavior of unsteady state processes. The procedure is demonstrated using an example process concerned with the removal of suspended solids from wastewater by settling in continuous flow tanks. The process is employed in sewage treatment plants for the purification of wastewater. In typical industrial settling tanks, the inflowing stream flowrate and the suspended solids concentration vary with time depending on the quantity and the characteristics of the waste water coming to the plant. As a result of these random changes in the influent flowrate and the solids concentration, the process operates under unsteady state condition and steady state operation is never reached. For the purpose of simulation, this unsteady state nature of the settling process can be described by a mathematical model comprising a set of differential equations resulting from the mass balance on the tanks. In this work the model differential equations are solved on a spreadsheet using the fourth order Runge-Kutta method. By doing so this work primarily demonstrates the usefulness of spreadsheets in the process computations requiring the numerical solution of differential equations. It is thought that this work may be of practical interest and usefulness to process engineers interested in the simulation of unsteady state processes.

PROCESS

Figure 1 shows a schematic diagram of a settling tank used in wastewater treatment plants for the removal of suspended solids. The wastewater entering the tank contains settleable and non-settleable solids. In the tank, the settleable

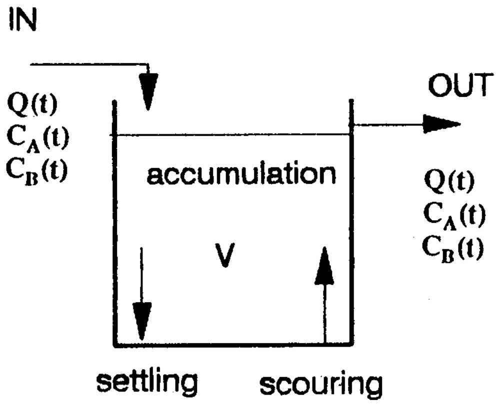

Figure 1: **Schematic diagram of settling process for the removal of solids from wastewater**

solids in the influent wastewater settle by gravity. The effluent stream from the tank consists of solids that have not been settled and the non-settleable fraction. The influent wastewater flowrate and the suspended solids concentration vary randomly with time. The influent wastewater flowrate , Q(t), and the concentrations of both the settleable and non-settleable components, $C_A(t)$ and $C_B(t)$ are therefore taken as functions of time.

The settling solids are accumulated at the bottom of the tank and removed periodically. The tank is provided with a mechanical scraper at the bottom to help removal of the solids from the tank. This scraping of the solids may cause some of the settled solids to be carried with the effluent stream from the tank, the phenomenon known as scouring.

MATHEMATICAL MODEL

The process of solids settling (Figure 1) can be described by the following unsteady state mass balance equations written for the settleable and non-settleable components, respectively.

Unsteady state Component Mass Balance Equations :

a) Settleable Component (A) :

(Rate of inflow) - (Rate of outflow) - (Rate of settling) + (Rate of scouring) = (Rate of accumulation)

$$[\,Q(t)\,.\,C_A(t)\,]_{in} - [\,Q(t)\,.\,C_A(t)\,]_{out} - [\,U.\,A.\,C_A(t)\,] + [\,S_p.\,U.\,A.\,C_A(t)\,] = V\,d[\,C_A(t)\,]\,/\,dt \qquad (1)$$

b) Non-settleable Component (B) :

(Rate of inflow) - (Rate of outflow) = (Rate of accumulation)

$$[\,Q(t)\,.\,C_B(t)\,]_{in} - [\,Q(t)\,.\,C_B(t)\,]_{out} = V\,d[\,C_B(t)\,]\,/dt \qquad (2)$$

The concentrations of components (A) and (B) are related to the total inlet solids concentration, $C_T(t)$ by

$$C_A(t) = S.\,C_T(t) \text{ and } C_B(t) = (1-S).\,C_T(t) \qquad (3)$$

In equation 1 the term scouring represents the rate of solids coming in the effluent stream as a result of the mechanical scraping of the accumulated solids at the bottom of the tank. The rate of scouring is considered as a fraction of the settling rate. This fraction is defined as the scouring parameter.

An underlying assumption in the above equations is that the tank contents are completely mixed so that the components concentrations in the effluent stream can be considered as representative of the concentrations inside the tank. This assumption of complete mixing, however, is not practically fulfilled in actual tanks. To account for this deviation the process in an actual tank is theoretically represented (16, 17) by a mathematical model which considers N perfectly mixed tanks operated in series (Figure 2). The number of tanks, N, is the model parameter determined so that to give the same performance as that of a tank with imperfect mixing.

In the N tanks model the well mixed tanks are assumed of equal volumes operated in series under constant volume conditions ($V_1 = V_2 = ... = V_{n-1} = V_n = V$ and $Q_1(t) = Q_2(t) = ... = Q_{n-1}(t) = Q_n(t) = Q(t)$). The inlet flow rate of the wastewater and the total inlet concentration of the suspended solids to each tank are considered to be functions of time. The component mass balance equations 1 and 2 are written for each tank in the model giving a total of 2N equations for the process. Equations 1 and 2 written for any tank , n, become:

$$[\ Q(t)\ .\ C_A(t)_{n-1}\ ]_{in} - [\ Q(t)\ .\ C_A(t)_n\ ]_{out} - [\ U.\ A.\ C_A(t)_n\ ] + [\ S_p.\ U.\ A.\ C_A(t)_n\ ] = V\ .\ d[\ C_A(t)_n\ ]\ /\ dt \qquad (1.a)$$

$$[\ Q(t)\ .\ C_B(t)_{n-1}\ ]_{in} - [\ Q(t)\ .\ C_B(t)_n\ ]_{out} = V\ .\ d[\ C_B(t)_n\ ]\ /\ dt \qquad (2.\ a)$$

where $C_A(t)_{n-1}$ and $C_B(t)_{n-1}$ are given by

$$C_A(t)_{n-1} = S.C_T(t)_{n-1} \text{ and } C_B(t)_{n-1} = (1-S).\ C_T(t)_{n-1} \qquad (3.\ a)$$

SPREADSHEET TEMPLATE

A spreadsheet template was developed using Quattro Pro (version 4) to solve equations 1.a and 2.a numerically with the fourth order Runge-Kutta method. The spreadsheet consisting of 219 rows and four column (A-D) was arranged in blocks as described below.

1. Data Input

The block for data input is shown in Figure 3. In the beginning of this block, instructions are given to help the user enter the required data. Column A lists the names used for the various data items. The user is required to enter the data in the adjacent cells in columns B, C and D as shown in the figure. There are two types of data required in the solution of the model. The operating data related to the settling process and the data on the model parameters such as the number of tanks, initial concentrations of suspended solids in tanks 1-5 and the step size for integration of the differential equations. The operating data consist of tank volume and cross sectional area, settleable fraction of the inlet stream, scouring parameter, settling velocity and the inlet stream flowrate and suspended solids total concentration as functions of time.

For use in the sheet, the data on tank volume, tank cross-sectional area and the inlet flowrate and the solids total inlet concentration were taken from Bradley (18). These data were reported for the settling tanks of a wastewater treatment plant in Brazil. Bradley measured the inlet flowrate and the inlet

DATA INPUT

ENTER DATA AS FOLLOWS IN COLUMNS B, C AND D

TANK VOLUME, V, M**3	7832		
X-AREA, A, M**2	1783.4		
SETTLEABLE FRACTION, S	0.63		
SCOURING PARAMETER, SP	0		
SETTLING VELOCITY, U, M/HR	1.88		
NO. OF TANKS, N	5		
TIME, t, HOURS,	t	Q(t)	CT(t)
FLOWRATE, Q(t), M**3/HR	0	3170.57	190.0
AND TOTAL CONC. ,CT(t)	2	2972.40	180.0
	4	2774.25	120.0
	6	2477.00	140.0
	8	2972.40	190.0
	10	3566.89	240.0
	12	3665.96	185.0
	14	4260.45	330.0
	16	4359.53	220.0
	18	4458.60	250.0
	20	4359.53	240.0
	22	3963.20	220.0
	24	3765.04	200.0
	26	2972.40	160.0
	28	2774.25	255.0

STEP SIZE	0.05	
INITIAL CONCENTRATIONS IN TANKS 1-5		
CA1(t)		0.00
CA2(t)		0.00
CA3(t)		0.00
CA4(t)		0.00
CA5(t)		0.00
CB1(t)		0.00
CB2(t)		0.00
CB3(t)		0.00
CB4(t)		0.00
CB5(t)		0.00

Figure 3: Spreadsheet block for data input

solids total concentration at intervals of two hours. The data on the settleable fraction and settling velocity for the same tanks were calculated by Javed and Ahmad (17) and are used in the spreadsheet template. The value of scouring parameter was taken as zero as recommended by Alarie (16). The number of tanks in the model considered in this problem was 5 and the step size of 0.05 was used. The number of tanks more than 5 has only marginal effect on the simulated outlet solids concentration (17). The value of 0.05 for the step size was found to give a stable solution of the model.

2. Calculations and Results Display

After the data have been entered by the user the spreadsheet is ready for making calculations. The procedure adopted for initiating and performing the spreadsheet calculations is shown in Figure 4. The user can start iterative calculations entering either 0 or 1 in cell B57. An entry of 0 sets the initial conditions for the solution of the differential equations and the number of iterations and the time counter to zero. If the entry in cell B57 is 1 the sheet is set in the ready mode. The calculations are made by pressing the F9 key. The sheet can be set to carry out a given number of iterations each time the F9 key is pressed. The maximum allowable iterations in Quattro Pro are 255. In the present case a total of 500 iterations are required with the chosen step size of 0.05 and the total time of 25 hours. These 500 iterations can be handled by choosing 250 iterations per calculation cycle. The user therefore is required to press F9 key twice to complete the solution. This obviously may vary from a problem to problem as the total number of iterations required would depend on the step size and the total time of integration.

In this block the simulated results which are calculated in the later parts of the spreadsheet are graphically displayed as solids concentration Vs time. When the user enters 0 in cell B57, the curves in this display are set to the initial conditions and as the user starts calculations by entering 1 in cell B57, the curves display is updated with iterations. This allows the user to observe the simulated values as a function of time from the initial conditions through successive time intervals as the solution of the model equations proceeds . The curves shown in Figure 4 give the solids concentration in the last tank (i.e. 5th tank) with time for the data shown in Figure 3.

3. Interpolation and Runge-Kutta method

The interpolation of the time dependent inlet flowrate and the solids

CALCULATION AND RESULTS DISPLAY

INSTRUCTIONS FOR USERS :

1) ENTER 0 OR 1 IN CELL B57, PRESS RETURN KEY AND THEN PRESS F9 KEY
(0 SETS THE SPREADSHEET IN INITIAL CONDITION AND 1 STARTS THE ITERATIONS)
2) PRESS F9 KEY ONCE FOR EACH SET OF ITERATIONS
3) STOP ITERATIONS WHEN STOP TIME COUNTER (CELL B59) EQUALS THE TOTAL TIME
4) THE CALCULATED RESULTS ARE SHOWN IN ROWS 190-217
5) GRAPHICAL DISPLAY OF THE SIMULATED CONCENTRATION VS TIME IS GIVEN IN ROWS 61-74

START ITERATIVE CALCULATIONS	1
ITERATIONS	500
STOPTIME COUNTER	25

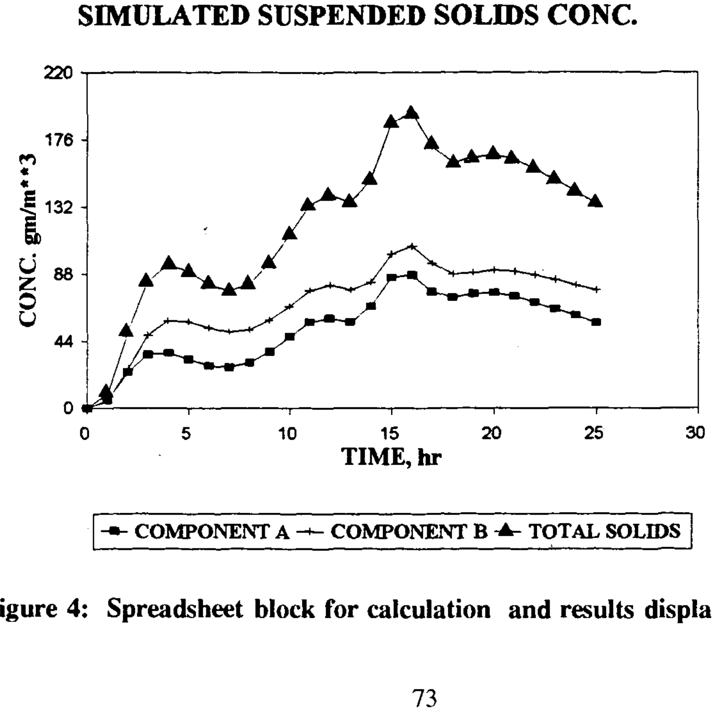

Figure 4: Spreadsheet block for calculation and results display

concentration was required to obtain the instantaneous values of these parameters for use in the Runge-Kutta method. For interpolation the input data values of time, flowrate and total solids concentration are used to generate a table containing the difference between the two consecutive values of these data. For each step size during the integration the values of these parameters were calculated using the linear interpolation formula.

$$y_i = y_{i-1} + (t_i - t_{i-1})(y_{i+1} - y_{i-1})/(t_{i+1} - t_{i-1}) \tag{4}$$

Where y_i is the parameter to be interpolated, at time t_i between the time interval $(t_{i+1} - t_{i-1})$ and i is an integer value.

The fourth order Runge-Kutta method is widely used for solving ordinary differential equations. The method is based on an algorithm which allows the solution of a differential equation say, $dC/dt = f(C, t)$, by calculation of the dependent variable, C, at any time, t_{i+1}, using equation 5.

$$C_{i+1} = C_i + (k_1 + 2k_2 + 2k_3 + k_4)/6 \tag{5}$$

Where, C_i and C_{i+1} are the values of C at time t_i and t_{i+1}, respectively. The values of k_1 to k_4 are calculated from

$$\begin{aligned} k_1 &= \Delta t\, f(C_i, t_i) \\ k_2 &= \Delta t\, f(C_i + k_1/2, t_i + \Delta t/2) \\ k_3 &= \Delta t\, f(C_i + k_2/2, t_i + \Delta t/2) \\ k_4 &= \Delta t\, f(C_i + k_3, t_i + \Delta t) \end{aligned} \tag{6}$$

The solution of ordinary differential equations requires the initial conditions for starting the solution. The values of the dependent variable are calculated at differential time intervals (i.e. step size) and summed up over the total specified time. For a set of differential equations the above algorithm is followed in sequence for each differential equation.

In this work the above procedure was implemented on the spreadsheet to solve equations 1.a and 2.a. Since there were two components and five tanks, in each iteration the concentration of each component and values for k_1 through k_4 had to be calculated for each tank. The calculated values of the concentrations of component (A), component (B) and the total concentration in the 5th tank are written as a function of time at the end of the sheet. These concentrations are also shown graphically in the calculation block explained earlier so that the user has a facility of observing the calculated values during the simulation period.

CONCLUSION

The usefulness of spreadsheets in the simulation of an unsteady state process was demonstrated by solving a mathematical model consisting of a set of ordinary differential equations. The model equations were solved on a spreadsheet using the fourth order Runge-Kutta method. The implementation of this numerical technique for solving differential equations on a spreadsheet, as shown in this work, indicates the suitability of spreadsheets for computations required in the simulation of dynamic processes.

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Note: A copy of the spreadsheet template can be obtained from the first author by sending a blank 5.25 inch diskette.