MS Excel and VBA for Chemical Engineers

TSEC - Online Certificate Course

PROJECT 1

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1 Shallow water equations

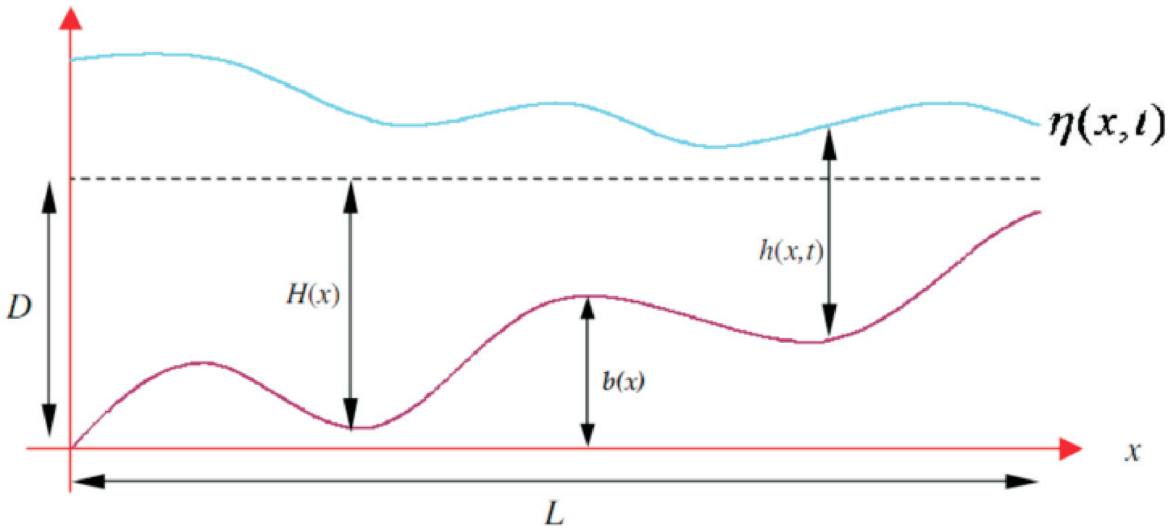

Figure 1: Domain sketch of the 1D shallow water wave equation [ref. 3]

Here D is the average water level; η denotes the surface of free water waves above the average water level; b denotes the bottom topography; h is the height from the free surface to the bottom topography. These equations are given by the following set of partial differential equations.

$$\eta_t + (u(\eta + D - b))_x = 0 \tag{1}$$

$$u_t + \left(\frac{1}{2}u^2 + g\eta\right)_x = 0 \tag{2}$$

Here, u is the velocity of the wave; g is the gravitational constant; and the subscript x denotes the spatial derivative. In its simplified form, we get

$$\frac{\partial \eta}{\partial t} + (\eta + D - b)\frac{\partial u}{\partial x} + u\frac{\partial \eta}{\partial x} - u\frac{\partial b}{\partial x} = 0 \tag{3}$$

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + g\frac{\partial \eta}{\partial x} = 0 \tag{4}$$

To develop the difference equations, the Forward in time, Central in space (FTCS) scheme has been used with an implicit formulation. We substitute the following formula into Equations 3 and 4.

$$\frac{\partial \eta}{\partial t} = \frac{\eta_i^{j+1} - \eta_i^j}{\Delta t}; \qquad \frac{\partial \phi}{\partial x} = \frac{\phi_{i+1}^{j+1} - \phi_{i-1}^{j+1}}{2\Delta x} \tag{5}$$

Where $\phi = \eta/u/b$. The superscripts denote the value at the present time step (j) and the future time step $(j+1)$. The subscripts denote the spatial node location. The variables that have been multiplied as a prefactor have to be evaluated at present time ($u \rightarrow u_i^j$, $\eta \rightarrow \eta_i^j$). Rearranging our equations into the matrix form, we have

$$\begin{aligned} -\Delta t u_i^j \eta_{i-1}^{j+1} + 2\Delta x \eta_i^{j+1} + \Delta t u_i^j \eta_{i+1}^{j+1} - \Delta t(\eta_i^j + D - b_i)u_{i-1}^{j+1} + \Delta t(\eta_i^j + D - b_i)\eta_{i+1}^{j+1} \\ = 2\Delta x \eta_i^j + \Delta t u_i^j (b_{i+1} - b_{i-1}) \end{aligned} \tag{6}$$

and

$$\Delta t g \eta_{i-1}^{j+1} + \Delta t g \eta_{i+1}^{j+1} - \Delta t u_i^j u_{i-1}^{j+1} + 2\Delta x u_i^{j+1} + \Delta t u_i^j u_{i+1}^{j+1} = 2\Delta x u_i^j \tag{7}$$

We solve the implicit equations by bringing all the $j+1$ superscripts to X in the form $AX = B$. Equations on the Right hand side above will remain in the B matrix. This linear system of equations has to be solved for every time step. The given values for the problem are:

1. Domain $= [0, 1]$
2. Time range $= [0, 50]$
3. $dt = 0.1$ sec
4. $dx = 0.01$ km
5. Wave Amplitude $A = 0.45$ km
6. Wave Location $x_A = 0.4$ km

The initial conditions of these equations are

$$\text{For the wave} : \eta(x,0) = A\,\mathrm{sech}\left(\sqrt{\frac{3000}{D^2}}(x - x_A)\right) \tag{8}$$

$$\text{For the velocity} : u(x,0) = 0 \tag{9}$$

And the boundary conditions are Neumann for wave ($\frac{\partial \eta}{\partial x} = 0$) and Dirichlet for velocity ($u = 0$) at both ends.

References

1. Crowhurst, P., & Li, Z. (2013, April). Numerical solutions of one-dimensional shallow water equations. In 2013 UKSim 15th International Conference on Computer Modelling and Simulation (pp. 55-60). IEEE.

2. Riestiana, V. A., Setiyowati, R., & Kurniawan, V. Y. (2021, February). Numerical solution of the one dimentional shallow water wave equations using finite difference method: Lax-Friedrichs scheme. In AIP Conference Proceedings (Vol. 2326, No. 1). AIP Publishing.

3. Setiyowati, R. (2019, August). A simulation of shallow water wave equation using finite volume method: Lax-Friedrichs scheme. In Journal of Physics: Conference Series (Vol. 1306, No. 1, p. 012022). IOP Publishing.

2 Report writing

You need to prepare a report for this topic to include this as a project in your CV. Use the following format to fill up the report. (Preferably use LaTeX to write your report. It is very easy to learn it by your own. Youtube link: LaTeX for Students – A Simple Quickstart Guide)

- Project title
- Mention that you have done it as a part of the Excel Certificate course from TSEC
- Your name, Instructor's name
- Affiliations
- Contents of the report
  1. Introduction: Write in detail about the Project title and explain its physical system.
  2. Derivation: Can start the derivation from the Navier-Stokes Equations.
  3. Methodology: Describe how you have set up the problem. Describe in detail about the discretisation scheme you have used in your problem. Mention how you have used Excel and VBA to generate your results.
  4. Results and Discussion: Take screenshots of the system at different times and describe what is happening in the system. Discuss on other configurations of the system, like different initial conditions, different boundary conditions, different bottom topology, etc. Also identify where this methodology fails. (There is still scope to improve the results from this problem. Researchers are still working on generating more efficient numerical methods for this problem).
  5. Conclusion: Give your final thoughts on this problem.
- References

Appendix: AX = B form

$$\begin{bmatrix} 1 & -1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ -\Delta t u_2^j & 2\Delta x & \Delta t u_2^j & 0 & 0 & \cdots & -\Delta t(\eta_2^j + D - b_2) & 0 & \Delta t(\eta_2^j + D - b_2) & 0 & 0 & \cdots & 0 \\ 0 & -\Delta t u_3^j & 2\Delta x & \Delta t u_3^j & 0 & \cdots & 0 & -\Delta t(\eta_3^j + D - b_3) & 0 & \Delta t(\eta_3^j + D - b_3) & 0 & \cdots & 0 \\ 0 & 0 & -\Delta t u_4^j & 2\Delta x & \Delta t u_4^j & \cdots & 0 & 0 & -\Delta t(\eta_4^j + D - b_4) & 0 & \Delta t(\eta_4^j + D - b_4) & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ -\Delta t g & 0 & \Delta t g & 0 & 0 & \cdots & 2\Delta x & \Delta t u_2 & 0 & 0 & 0 & \cdots & 0 \\ 0 & -\Delta t g & 0 & \Delta t g & 0 & \cdots & -\Delta t u_3 & 2\Delta x & \Delta t u_3 & 0 & 0 & \cdots & 0 \\ 0 & 0 & -\Delta t g & 0 & \Delta t g & \cdots & 0 & -\Delta t u_4 & 2\Delta x & \Delta t u_4 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & -\Delta t g & 0 & \Delta t g & 0 & 0 & 0 & 0 & \cdots & -\Delta t u_{n-1} & 2\Delta x \end{bmatrix} \begin{bmatrix} \eta_1^{j+1} \\ \eta_2^{j+1} \\ \eta_3^{j+1} \\ \eta_4^{j+1} \\ \vdots \\ \eta_n^{j+1} \\ u_2^{j+1} \\ u_3^{j+1} \\ u_4^{j+1} \\ \vdots \\ u_{n-1}^{j+1} \end{bmatrix} = \begin{bmatrix} 0 \\ 2\Delta x \eta_2^j + \Delta t u_2^j (b_3 - b_1) \\ 2\Delta x \eta_3^j + \Delta t u_3^j (b_4 - b_2) \\ 2\Delta x \eta_4^j + \Delta t u_4^j (b_5 - b_3) \\ \vdots \\ 0 \\ 2\Delta x u_2^j \\ 2\Delta x u_3^j \\ 2\Delta x u_4^j \\ \vdots \\ 2\Delta x u_{n-1}^j \end{bmatrix}$$