Dept. of Chemical Engineering, NIT Andhra Pradesh

A simulation study of surface temperature influence on localized atmospheric flows and dispersion using shallow water equations

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Motivation

- Atmospheric models are used in
  - Simulation of earth's atmosphere
  - Weather forecast
  - Climate modelling *(Vallis, 2017)*
  - Global Models: GFS, ICON; Regional Models: ETA, COAMPS etc.

- Conventional Models:
  - Governing Equations: Navier-Stokes and Energy Balance Equations
  - Complex and Computationally Expensive.

- Shallow Water Model: Simple to solve and can be used in problems with smaller domains.
  - Can be applicable in Industrial Planning (Identifying Threat Zones and Accident Propagation)
  - Localized Atmospheric Modelling

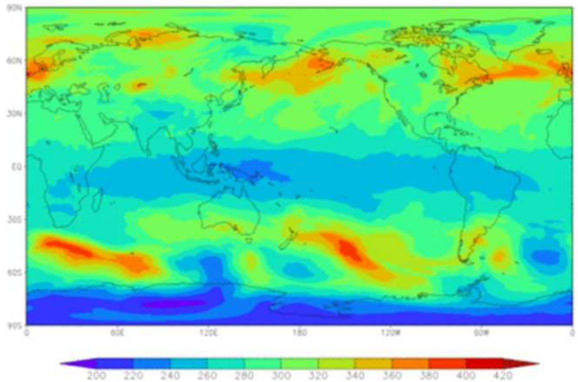

Fig: GFS Temperature contours (atmospheric)

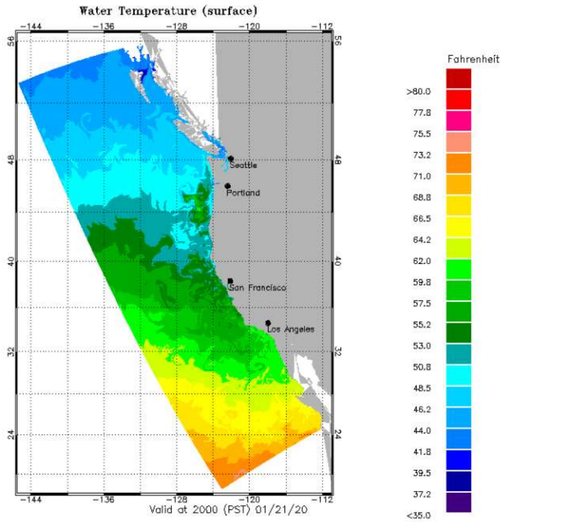

Fig: COAMPS Sea Surface Temperature Contours

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Introduction

- SWEs are hyperbolic/parabolic PDEs derived from the Euler's Equation:

$$\rho\left(\frac{\partial \vec{v}}{\partial t} + \vec{v}.\nabla\vec{v}\right) = -\nabla P$$

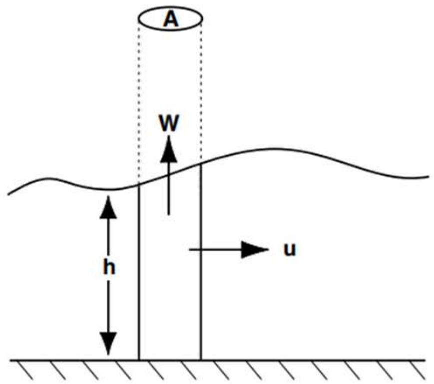
- For 1-D flow(s) the SWEs are written as (*Vallis, 2017*):

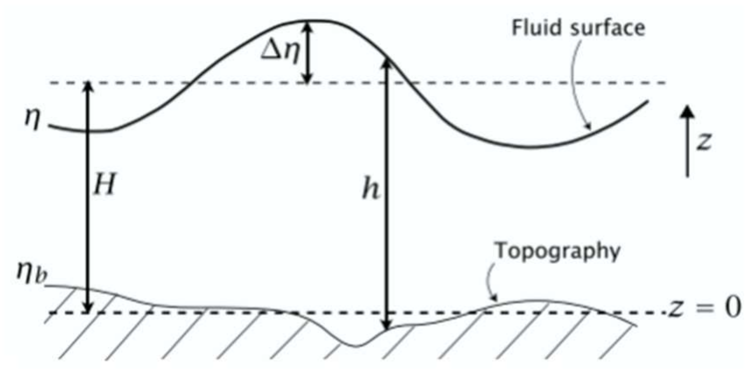
Continuity:

$$\frac{\partial h}{\partial t} + \frac{\partial (uh)}{\partial x} = 0$$

Momentum:

$$\frac{\partial (uh)}{\partial t} + \frac{\partial\left(u^2 h + \frac{1}{2} g h^2\right)}{\partial x} = 0$$





$h = h(x, t)$: thickness of liquid column
H : mean height
η : height of free surface
$h = \eta - \eta_b$: height of floor of the container
u = velocity of stream

Contd..

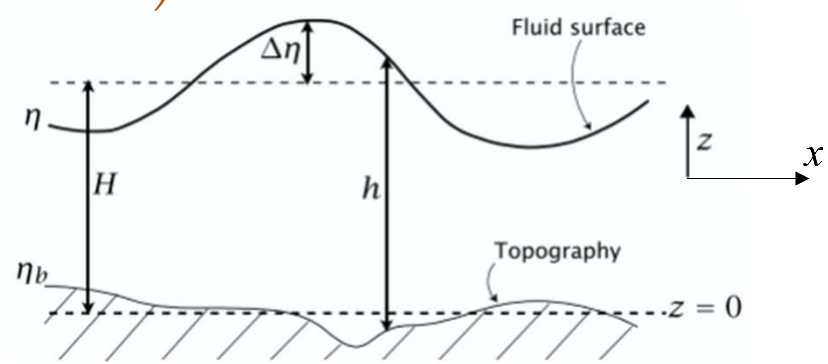
Introduction

Euler's Equation:

$$\rho\left(\frac{\partial\vec{v}}{\partial t}+\vec{v}.\nabla\vec{v}\right)=-\nabla P$$

Continuity: $$\frac{\partial h}{\partial t}+\frac{\partial(uh)}{\partial x}=0$$

Momentum: $$\frac{\partial(uh)}{\partial t}+\frac{\partial\left(u^2h+\frac{1}{2}gh^2\right)}{\partial x}=0$$



- Basic assumptions for the current set of equations (*Vallis, 2017)*:
  - 1-D flow
  - Inviscid (Assumed due to high Re: Atmospheric flows)
  - Incompressible flow.
  - Negligible Coriolis (Body) forces.
  - Horizontal length scale is very large as compared to the height of the stream. (h<<<L)

h = h(x, t): thickness of liquid column
H : mean height
η : height of free surface
$h=\eta-\eta_b$: height of floor of the container
u = velocity of stream

Contd..

Literature Review

- **Pritchard, D. and Hogg, A. (2002)**
- **Cao et al. (2004)**

- 1-D and 2-D Hydrodynamic Models built on SWEs to simulate sediment transport under dam break, using finite volume solvers.
- Regular Terrains

- **Shuangcai et al. (2012):**
  - Discussed about modelling of coupled system of PDEs (Dispersion and Shallow Water) and their outcomes over the un-coupled models.
  - A 2-D Shallow Water Model coupled with Dispersion equation was developed.
  - Simulated for Advection of Pollutant in Square Cavity and with an Asymmetric Dam Break using Finite Volume Solver.

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Literature Review & Gap

- **Chistyakov et al.(2020):**
  - 3D Hydrodynamic Model for Salt dispersion and Heat Transfer.
  - 3D Navier-Stokes + Heat & Mass Transport.
- **Kissami Imad., et al. (2021):**
  - Pollutant dispersion using SWE and Dispersion
- **Staples et al. (2023):**
  - The model uses publicly available meteorological data and is applicable to shallow waterbodies less than 1 meter deep.
  - Empirical model that is highly reliant on the publicly available data.

Gap

No heat transfer + SWE coupled Models

Objective

To develop an SWE+HT Model to be used in problems with smaller domains.

- Localized Atmospheric Modelling

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Numerical Analysis

System of Governing Equations

Continuity: $$\frac{\partial h}{\partial t} + \frac{\partial (uh)}{\partial x} = 0$$

Momentum: $$\frac{\partial (uh)}{\partial t} + \frac{\partial \left(u^2 h + \frac{1}{2} g h^2\right)}{\partial x} = 0$$

$$h = h(x,t);\ u = u(x,t)$$

Finite difference method

"pdepe" solver subroutine:

sol = pdepe(m, pdefun, icfun, bcfun, xmesh, tspan, options)

Code equation: $c\left(x,t,u,\frac{\partial u}{\partial x}\right)\left(\frac{\partial u}{\partial t}\right) = x^{-m}\frac{\partial}{\partial x}\left(x^m f\left(x,t,u,\frac{\partial u}{\partial x}\right)\right) + s\left(x,t,u,\frac{\partial u}{\partial x}\right)$

m = 1

$c = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ *(diagonal values only)*

$$f = \begin{bmatrix} -uh \\ -(u^2 h + \frac{1}{2} g h^2) \end{bmatrix}$$

$$s = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

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1D Dispersion Model

$$\frac{\partial h}{\partial t} + \frac{\partial (uh)}{\partial x} = 0 \qquad -(1)$$

$$\frac{\partial (uh)}{\partial t} + \frac{\partial \left(u^2 h + \frac{1}{2} g h^2\right)}{\partial x} = 0 \qquad -(2)$$

SWE

$$\frac{\partial (\psi h)}{\partial t} + \frac{\partial (\psi u h)}{\partial x} = \frac{\partial \left(\mu \frac{\partial c}{\partial x}\right)}{\partial x} \qquad -(3)$$

Dispersion Equation

- ψ = depth averaged volumetric concentration
- c = local concentration

Heat Dispersion Equation (After Non dimensionalisation)

$$\frac{\partial (\psi_h h)}{\partial t} + \frac{\partial (\psi_h u h)}{\partial x} = \frac{\partial \left(h_t \frac{\partial T}{\partial x}\right)}{\partial x}$$

T: Temperature

h_t: Overal Heat Transfer Coefficient

Ref: Shuangcai et al. (2012)

CURRENT WORK..

Solution Methods

- Some common numerical schemes:
  - Finite Difference Approach
    - First Order Upwind Scheme
    - Lax-Wendroff Scheme
  - Finite Element Approach
  - Finite Volume Approach
- FDM: Approximates the derivatives using finite difference approximations, depending on the scheme, it may be forward difference, backward difference or central difference.

- FEM: Approximations using Piecewise continuous functions, (linear or polynomial) on a spatially discretized domain.

Ref: Jain & Iyengar

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Solution Methods

- FOU Scheme:
  - First Order Scheme
  - Ensures solution stability (Further discussed in CFL Criteria)
  - It approximates the derivatives using one-sided differences

- Lax- Wendroff Scheme:
  - Second Order Finite Difference Scheme
  - Used for Hyperbolic PDEs, especially for conservation laws.
  - Uses a second order central difference at current time level → For time derivative
  - Uses a second order central difference at current node → For spatial derivative

Ref: Jain & Iyengar

Lax-Wendroff Scheme

- Approximates the solution twice: Once at the half time step, and again at the full time step, as a predictor-corrector approach.

- General scheme of estimation of solution:
  - At half time-step:

$$y_m = y_0 + \frac{1}{2}\Delta T \,.\, f(y_0)$$

  - At full time step

$$y_{m+1} = y_0 + \Delta T \,.\, f(y_m)$$

Governing Equations

$$U = \begin{bmatrix} h \\ uh \\ \psi h \end{bmatrix}; \mathrm{E} = \begin{bmatrix} uh \\ u^2 h + \frac{1}{2} g h^2 \\ \psi u h \end{bmatrix}; \mathrm{S} = \begin{bmatrix} 0 \\ 0 \\ \mu\left(\frac{\partial c}{\partial x}\right) \end{bmatrix}$$

$$\frac{\partial U}{\partial t} + \frac{\partial E}{\partial x} = S$$

Ref.: C. B. Moler.

CFL criteria for numerical analysis

- CFL : Courant-Friedrichs-Lewy condition

- To ensure the number of time-steps and the number of nodes are complying with the following inequality to prevent the loss of convergence at the boundaries.

$$dt \leq \frac{dx}{|u| + \sqrt{gh}}$$

- If we reduce *dx*, we may have to reduce *dt* as well, if we are near the CFL limit.

- Here $\sqrt{gh}$ measures motion due to gravity waves.

Ref.: S. C. Chapra and R. P. Canale.

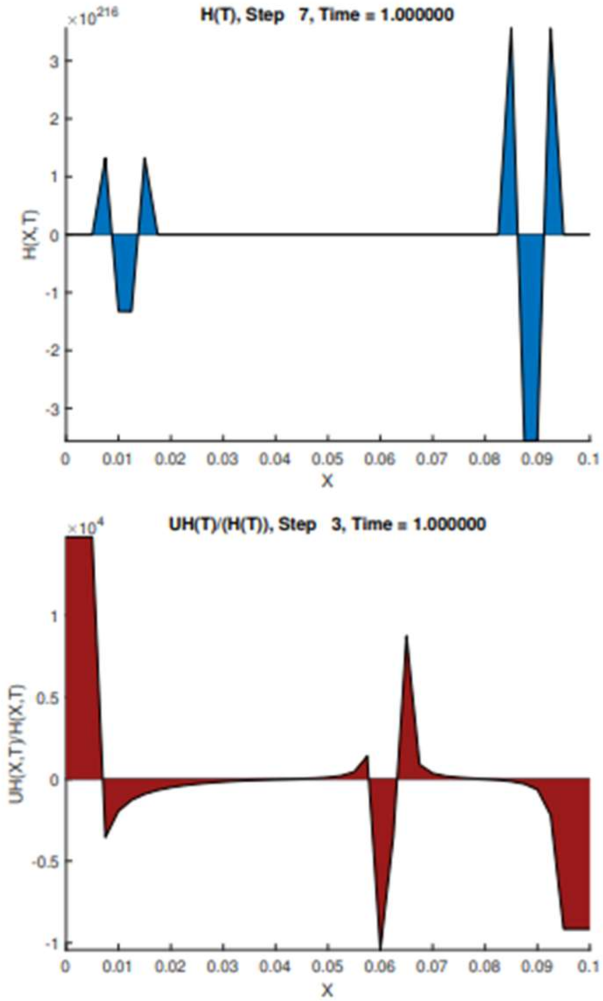

Figure: Output plots for a condition where dx and dt do not satisfy the CFL Criteria

Model Validation

Governing Equations

$$U = \begin{bmatrix} h \\ uh \\ \psi h \end{bmatrix}; \mathrm{E} = \begin{bmatrix} uh \\ u^2 h + \frac{1}{2} g h^2 \\ \psi uh \end{bmatrix}; \mathrm{S} = \begin{bmatrix} 0 \\ 0 \\ hK\left(\frac{\partial c}{\partial x}\right) \end{bmatrix}$$

$$\frac{\partial U}{\partial t} + \frac{\partial E}{\partial x} = S$$

Scarcity of relevant data for the SWE+HT modeling. Consequently compared the Lax-Wendroff and ANSYS-Fluent CFD solutions.

Estimation of each variable using discretized equations, for each node at each time step.

For Instance, at Half time-step, estimation of *h* becomes:

$$hm(i) = \frac{h(i) + h(i+1)}{2} - \frac{\Delta t}{2} \frac{uh(i+1) - uh(i)}{\Delta x}$$

At full time-step:

$$hm(i) = h(i) + \left(h(i+1)\right) - \Delta t \frac{\left(uh(i+1) - uh(i)\right)}{\Delta \mathrm{x}}$$

The estimation of the other variables in the system can be estimated similarly

Contd..

Model Validation

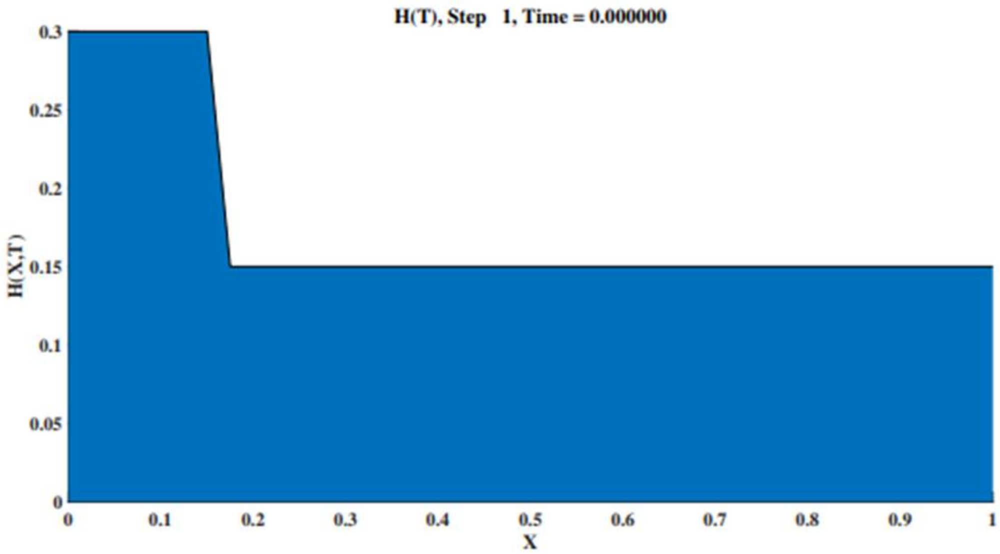

Figure: Initial time-steps after dam-break (Lax-Wendroff)

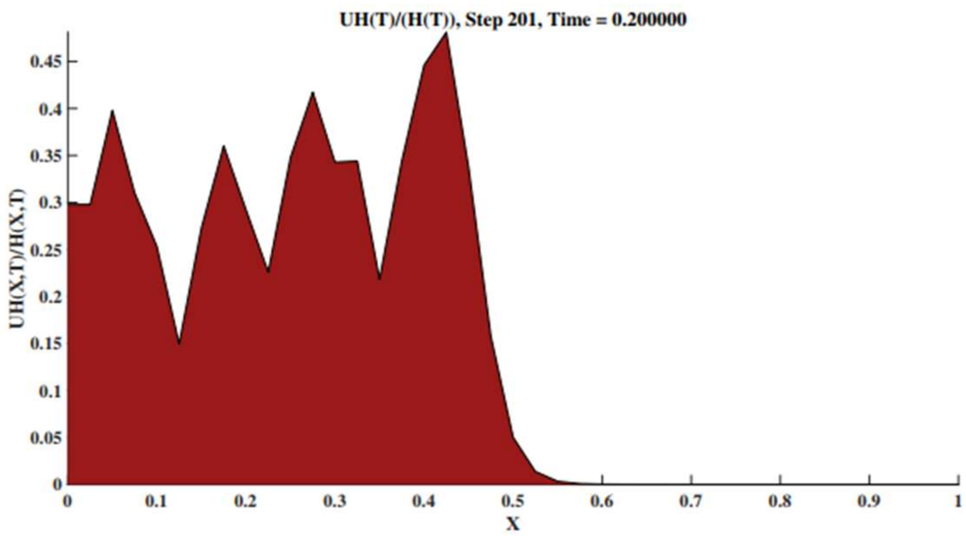

Figure: Velocity plot at the final time-step (Lax-Wendroff)

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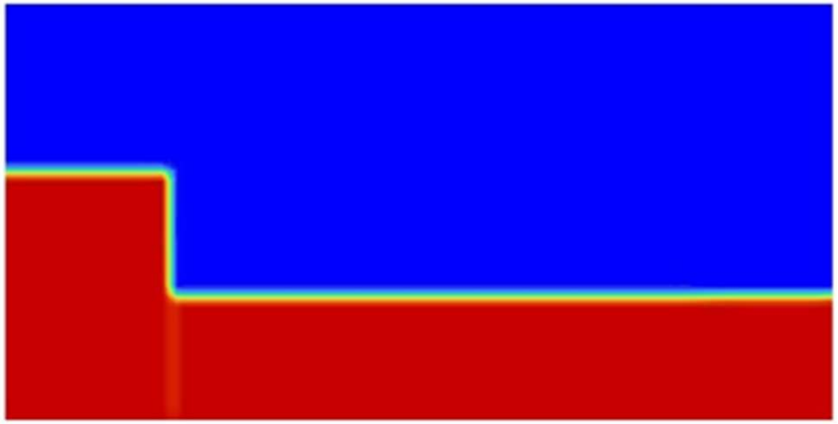


Figure: Dam Break Initialization using VOF in Ansys

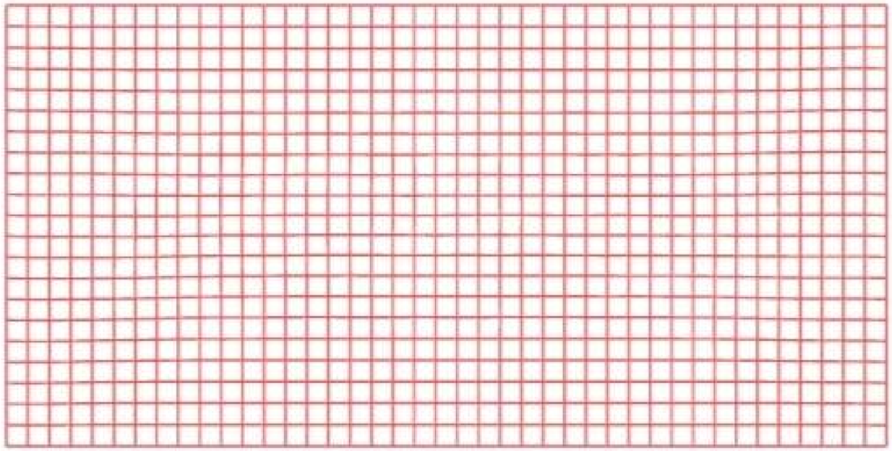


Figure: Fluent Meshing

Model Validation

- The mesh is generated in such a way that there are 41 nodes in the X-Direction, as discretized in the Lax-Wendroff Solver discussed in the previous section.
- 200 timesteps each of a size 0.1 seconds
- "SIMPLEC Pressure Velocity Coupling scheme" along with a First order Implicit method for the Transient formulation.
- Inviscid Volume of Fluids approach.

Contd..

Model Validation

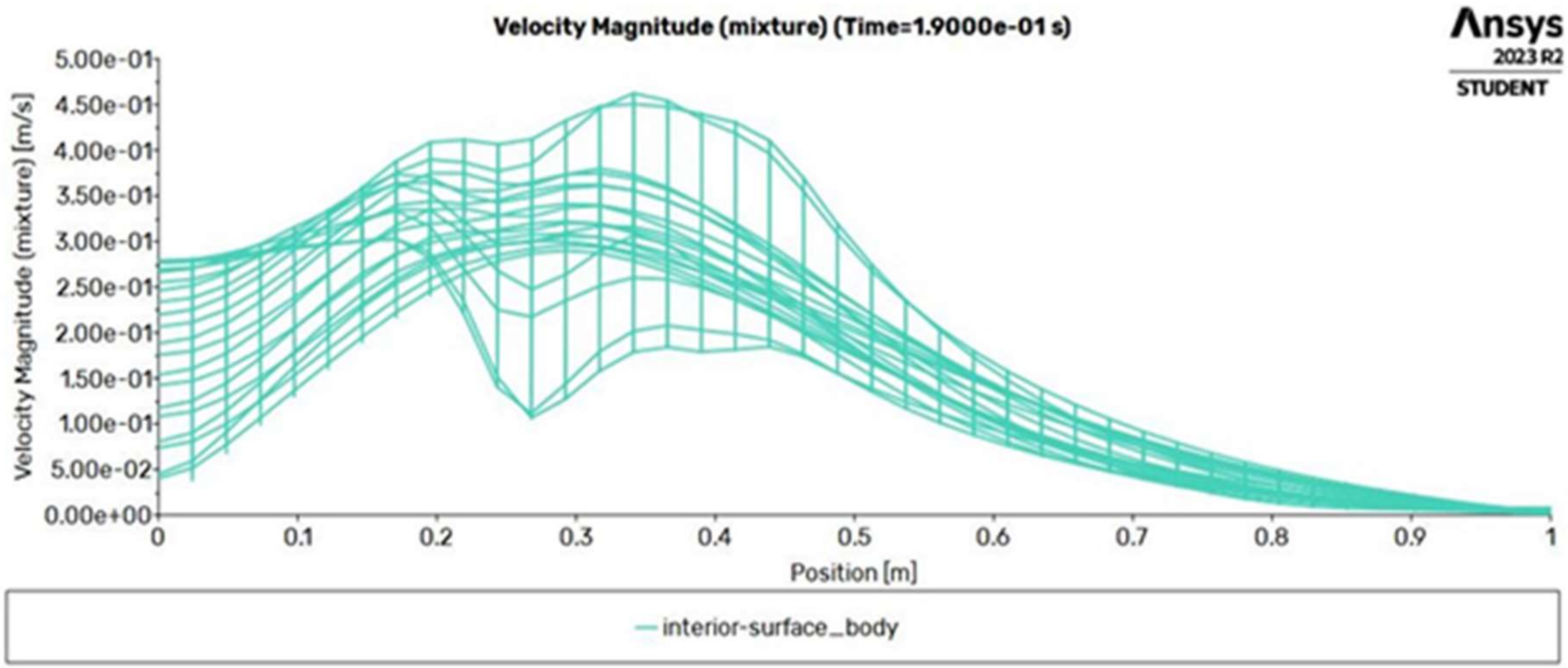
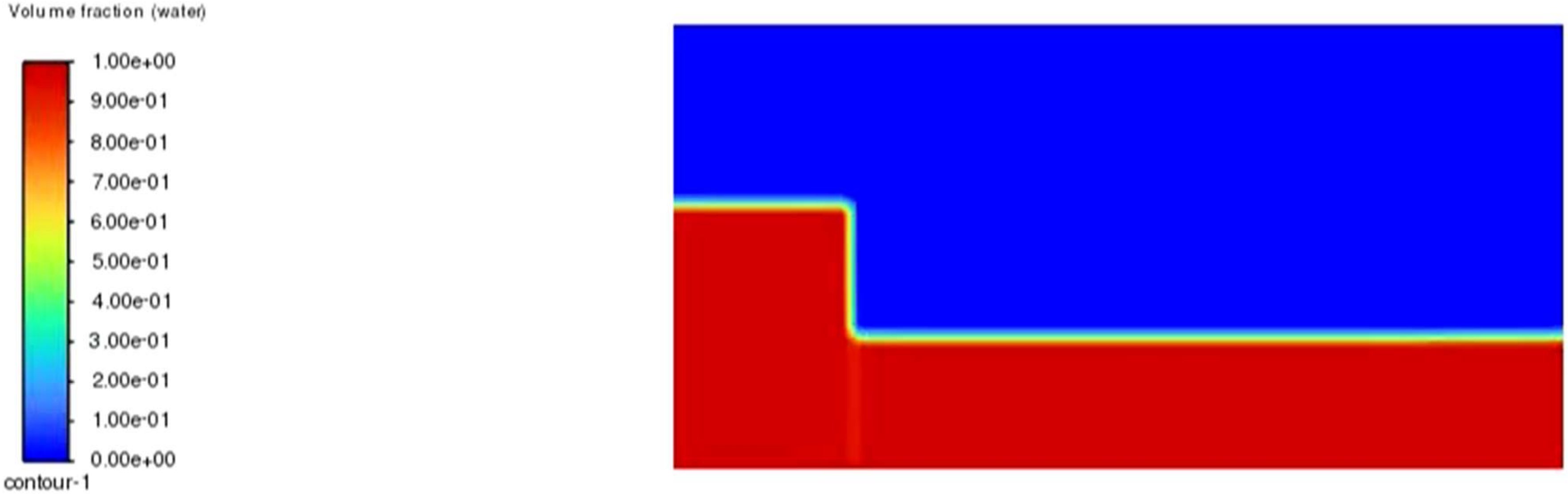


Figure: Velocity Plot for timestep corresponding to the timestep of the Lax-Wendroff Scheme

Contd..


Volume fraction (water)
1.00e+00
9.00e-01
8.00e-01
7.00e-01
6.00e-01
5.00e-01
4.00e-01
3.00e-01
2.00e-01
1.00e-01
0.00e+00
contour-1

Heat Transfer Incorporation

- Flat Plate steady state heat transfer: Analytical Solution.
- Numerical unsteady state problem studied using the current scheme.

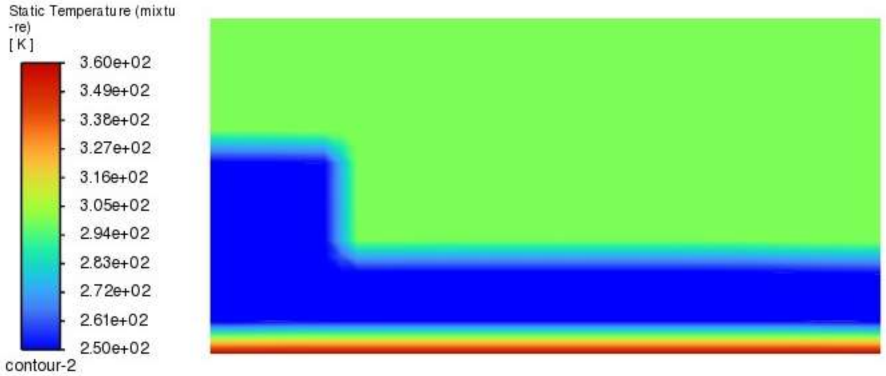


Figure: Initial Condition before Dam Break for Heat Transfer

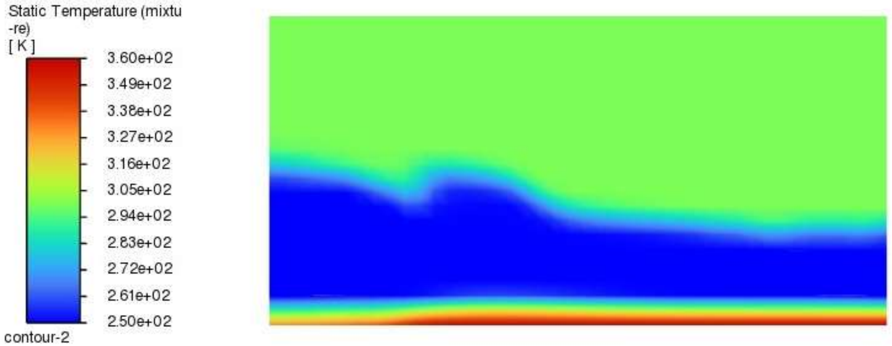


Figure: Final timestep for Dam Break along with Surface Heat Transfer

Poor heat transfer from the surface to the fluid as time proceeds, because of the absence of vertical advection in the model.

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Heat transfer performance by introducing obstacle

- Introducing an obstacle has led to variation in the local velocity magnitude more than for the smooth bottom case. Hence slightly better heat transfer performance is observed.

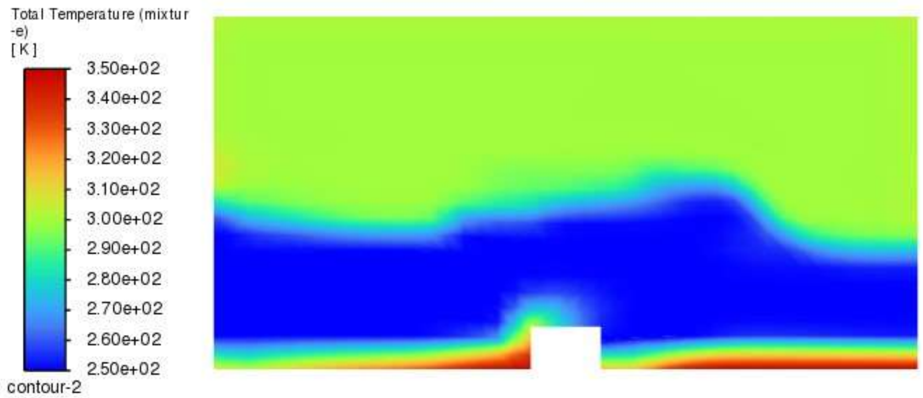

Figure: Evaluation of Heat transfer performance using obstacle

Future Work & Recommendations

- The project should shift from a first-order approach to a second-order one to properly evaluate this model's effectiveness.

- The project focused solely on smooth bottom scenarios. However, results improved with obstacles, indicating a need for broader study incorporating realistic scenarios.

- To enhance heat transfer predictions, a new coupled system derived from thermodynamic Equations of States (EOS) can incorporate vertical advection, crucial for accurate local temperature and pressure estimation.

- Because of insufficient prior research, the model's validation and verification require expansion through experimental evaluations in specific cases.

- While the Dam-Break Problem is well-researched for hydrodynamics, studying it for atmospheric air flow is impractical. Alternative relevant scenarios are necessary.

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