Passive Scalar Transport Equation

Core Components and Initialization

The `PassiveScalarTransportEq` class, implemented in C#, models the transport of a passive scalar (e.g., a tracer or pollutant) in an estuary. The domain spans a length L, discretized into n grid points with spatial step $\Delta x = L/n$. Key parameters include:

- Estuary length: L
- Grid points: n
- Spatial step: $\Delta x = L/n$
- River boundary concentration: C_{river}
- Ocean boundary concentration: C_{ocean}
- Salt wedge position: x_s

The class initializes arrays for the passive scalar concentration (C) and relies on external inputs for velocity (u) and eddy diffusivity (κ).

Functioning Logic

The `SolvePassiveScalarTransport` method advances the passive scalar concentration over a time step Δt, performing:

1. Advection-diffusion computation using a finite difference scheme.
2. Application of boundary conditions at the river ($x = 0$) and ocean ($x = L$).
3. Mixing adjustment near the salt wedge position using a Gaussian weighting function.

Transport Computation

The method solves the advection-diffusion equation for the passive scalar concentration:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = \frac{\partial}{\partial x}\left(\kappa\frac{\partial C}{\partial x}\right) \tag{1}$$

using an explicit finite difference scheme:

- **Advection term**: Central difference approximation:

$$u\frac{\partial C}{\partial x} \approx u_i\frac{C_{i+1} - C_{i-1}}{2\Delta x} \tag{2}$$

- **Diffusion term**: Second-order finite difference:

$$\frac{\partial}{\partial x}\left(\kappa\frac{\partial C}{\partial x}\right) \approx \frac{\kappa_{i+1}(C_{i+1} - C_i)/\Delta x - \kappa_i(C_i - C_{i-1})/\Delta x}{\Delta x} \tag{3}$$

- **Time update**: Explicit Euler step:

$$C_i^{n+1} = C_i^n + \Delta t \left(-u_i \frac{C_{i+1} - C_{i-1}}{2\Delta x} + \frac{\kappa_{i+1}(C_{i+1} - C_i) - \kappa_i(C_i - C_{i-1})}{\Delta x^2} \right) \tag{4}$$

Boundary conditions are:

- River ($x = 0$): $C_0 = C_{\text{river}}$
- Ocean ($x = L$): $C_{n-1} = C_{\text{ocean}}$

Mixing Near Salt Wedge

A Gaussian mixing factor is applied near the salt wedge position x_s:

$$m_i = \exp\left(-\frac{(i\Delta x - x_s)^2}{0.1L^2} \right) \tag{5}$$

The concentration is adjusted as:

$$C_i^{n+1} = (1 - m_i)C_i^{n+1} + m_i C_i^n \tag{6}$$

This smooths the concentration field near x_s, simulating enhanced mixing at the salt wedge interface.

Physical and Mathematical Models

The `PassiveScalarTransportEq` class simulates the transport of a passive scalar using the following models:

- **Advection-Diffusion Equation**:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = \frac{\partial}{\partial x}\left(\kappa \frac{\partial C}{\partial x}\right) \tag{7}$$

  where C is the scalar concentration, u is the velocity, and κ is the eddy diffusivity.

- **Finite Difference Discretization**:
  - Advection: $u_i \frac{C_{i+1}-C_{i-1}}{2\Delta x}$
  - Diffusion: $\frac{\kappa_{i+1}(C_{i+1}-C_i)-\kappa_i(C_i-C_{i-1})}{\Delta x^2}$
  - Time stepping: $C_i^{n+1} = C_i^n + \Delta t\,(-\text{advection} + \text{diffusion})$
- **Boundary Conditions**:

$$C_0 = C_{\text{river}} \tag{8}$$
$$C_{n-1} = C_{\text{ocean}} \tag{9}$$

- **Salt Wedge Mixing**:

$$m_i = \exp\left(-\frac{(i\Delta x - x_s)^2}{0.1L^2}\right) \tag{10}$$

$$C_i^{n+1} = (1 - m_i)C_i^{n+1} + m_i C_i^n \tag{11}$$

These models capture the transport and mixing of a passive scalar in an estuarine environment, with numerical stability ensured by explicit time stepping and boundary constraints.