Equation of State

Core Components and Initialization

The `EqOfState` class, implemented in C#, calculates seawater density based on salinity, temperature, and pressure, using a polynomial approximation suitable for estuarine circulation modeling. This static class provides a single method, `ComputeDensity`, which is integrated into the `AsymmTidalMix` framework to determine density-driven dynamics in estuarine environments.

Functioning Logic

The `ComputeDensity` method computes seawater density (ρ) in kg/m³, taking:

- Salinity (S): Practical Salinity Units (PSU)
- Temperature (T): Degrees Celsius (°C)
- Pressure (P): Decibars (dbar, where 1 dbar = 10^4 Pa)

Input parameters are constrained to physical ranges to ensure numerical stability:

- $S \in [0, 40]$ PSU
- $T \in [-2, 40]$ °C
- $P \geq 0$ dbar

Density Computation

The method uses a polynomial equation of state to compute density, incorporating contributions from pure water, salinity, temperature-salinity interactions, and pressure effects via compressibility. The computation proceeds in steps:

1. **Pure Water Density** (ρ_0) at zero pressure:

$$\rho_0 = a_0 + a_1 T + a_2 T^2 + a_3 T^3 + a_4 T^4 + a_5 T^5 \tag{1}$$

   where coefficients are:

   - $a_0 = 999.842594$
   - $a_1 = 6.793952 \times 10^{-2}$
   - $a_2 = -9.095290 \times 10^{-3}$
   - $a_3 = 1.001685 \times 10^{-4}$
   - $a_4 = -1.120083 \times 10^{-6}$
   - $a_5 = 6.536332 \times 10^{-9}$

2. **Salinity Contribution**:

$$S_{\text{term}} = b_0 + b_1 T + b_2 T^2 + b_3 T^3 + b_4 T^4 \tag{2}$$

where coefficients are:

- $b_0 = 8.24493 \times 10^{-1}$
- $b_1 = -4.0899 \times 10^{-3}$
- $b_2 = 7.6438 \times 10^{-5}$
- $b_3 = -8.2467 \times 10^{-7}$
- $b_4 = 5.3875 \times 10^{-9}$

3. **Temperature-Salinity Interaction**:

$$I_{\text{term}} = c_0 + c_1 T + c_2 T^2 \tag{3}$$

where coefficients are:

- $c_0 = -5.72466 \times 10^{-3}$
- $c_1 = 1.0227 \times 10^{-4}$
- $c_2 = -1.6546 \times 10^{-6}$

4. **Salinity $S^{1.5}$ Term**:

$$S_{\text{sqrt}} = d_0 S^{3/2}, \quad d_0 = 4.8314 \times 10^{-4} \tag{4}$$

5. **Density at Atmospheric Pressure**:

$$\rho = \rho_0 + S \cdot S_{\text{term}} + S \cdot I_{\text{term}} + S^{3/2} \cdot d_0 \tag{5}$$

6. **Compressibility (Secant Bulk Modulus)**:

$$K_0 = e_0 + e_1 T + e_2 T^2 + e_3 T^3 + e_4 T^4 \tag{6}$$
$$K_1 = f_0 + f_1 T + f_2 T^2 + f_3 T^3 \tag{7}$$
$$K_2 = g_0 + g_1 T + g_2 T^2 \tag{8}$$
$$K = K_0 + S \cdot K_1 + S \cdot S^{1/2} \cdot K_2 \tag{9}$$

where coefficients are:

- $e_0 = 19652.21$, $e_1 = 148.4206$, $e_2 = -2.327105$, $e_3 = 1.360477 \times 10^{-2}$, $e_4 = -5.155288 \times 10^{-5}$
- $f_0 = 54.6746$, $f_1 = -0.603459$, $f_2 = 1.09987 \times 10^{-2}$, $f_3 = -6.1670 \times 10^{-5}$
- $g_0 = 7.944 \times 10^{-2}$, $g_1 = 1.6483 \times 10^{-2}$, $g_2 = -5.3009 \times 10^{-4}$

7. **Pressure-Corrected Density**:

$$\rho = \rho \cdot \frac{1 + P/(K - P)}{1} \tag{10}$$

Physical and Mathematical Models

The `EqOfState` class employs the following model for seawater density:

- **Density at Atmospheric Pressure**:

$$\rho = \left(a_0 + \sum_{i=1}^{5} a_i T^i\right) + S \cdot \left(b_0 + \sum_{i=1}^{4} b_i T^i\right) + S \cdot \left(c_0 + c_1 T + c_2 T^2\right) + d_0 S^{3/2} \quad (11)$$

- **Secant Bulk Modulus**:

$$K = \left(e_0 + \sum_{i=1}^{4} e_i T^i\right) + S \cdot \left(f_0 + \sum_{i=1}^{3} f_i T^i\right) + S \cdot S^{1/2} \cdot \left(g_0 + g_1 T + g_2 T^2\right) \quad (12)$$

- **Pressure Correction**:

$$\rho \leftarrow \rho \cdot \left(1 + \frac{P}{K - P}\right) \quad (13)$$

This model provides accurate density calculations for estuarine waters, accounting for salinity, temperature, and pressure effects, with bounds ensuring numerical stability in simulations.