TERM PROJECT-I

Title

Implementation of Navier-Stokes Equations in Chemical Engineering: The Working behind Chemical Reactors

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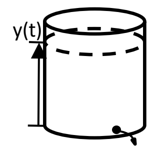
Problem Statement: "Develop a mathematical model based on the Navier-Stokes ordinary differential equations (ODEs) to deduce the level of reactant left in a chemical reactor, provided the reactant follows the incompressibility property, which can be useful in determining the flow rate and time required in emptying the container or adding more to it."

Solution: The Navier-Stokes equations are partial differential equations that describe the motion of fluid substances, including gases and liquids, under the influence of various forces. In the case of incompressible fluids, these equations reduce to ordinary differential equations which can be solved to find the desired output.

Illustration: A tank contains water at an initial depth y_o = 1 m. The tank diameter is D = 250 mm. A hole of diameter d = 2 mm appears at the bottom of the tank. A reasonable model for the water level over time is



$$dy/dt = -(d/D)^2\sqrt{2gy} \qquad y(0) = y_o$$

Using 11-point and 21-point Euler methods, estimate the water depth after t = 100 min, and compute the errors compared to the exact solution

$Y_{exact}(t) = [\sqrt{y_o} - (d/D)^2\sqrt{(gt/2)}]^2$

Approach: To solve the Navier-Stokes Equation for incompressible fluid flow, we assume that the velocity and pressure of the fluid do not change with time. The general form of the equation can be written as:

$$\rho(\partial v/\partial t + v \cdot \nabla v) = -\nabla p + \mu\nabla^2 v + f$$

The equation in the illustration above is based on this special case of Navier-Stokes Equation (Incompressible fluid flow) where specific boundary conditions when applied to the equation makes it solvable as an ODE. This ODE can be solved using Euler's method.

Euler Methods: -

y_i, y_{i+1} = value of y in the i^{th} and $(i+1)^{th}$ iteration respectively

h = step size = $(x_N - x_O)/N$ where x_N, x_O are values of x at first and last boundary points and N is the total number of points when counted from 0

- Explicit Euler method: $y_{i+1} = y_i + hf(x_i, y_i)$
- Implicit Euler Method: $y_{i+1} = y_i + hf(x_{i+1}, y_{i+1})$

The Implicit Euler method is unconditionally stable on proper parameters hence it is better suited.

Applications of the above situation-based Navier-Stokes equation: The Navier-Stokes equations are approximated in reactor analysis. These simplifications include steady state, incompressible flow, or reactor specificities without violating the accuracy of the system.

- The Navier-Stokes equations can be implemented to determine the flow patterns and velocity distribution of fluids inside reactors, which is important in optimizing reactor design and operation.

- The Navier-Stokes equations help in comprehending the mass transfer limitations, calculating the concentration profiles, and analyzing the reaction kinetics.