

Pseudo-CFD Model for Impeller Mixed Stirred Tank Bioreactor for Energy Dissipation Rate (EDR)

1. Purpose of the Model

The goal is to estimate local shear rate ($\dot{\gamma}$) and energy dissipation rate (ϵ) distribution inside a mixing tank without running CFD. This helps predict zones of high and low mixing intensity, average vs. maximum EDR, and scale-up comparability between reactors.

2. Core Assumptions

Concept	Simplified Assumption in Model
Fluid Type	Newtonian (viscosity constant, water-like: $\mu = 0.001 \text{ Pa}\cdot\text{s}$)
Density (ρ)	Constant throughout volume
Impeller Power	Estimated by classic correlation $P = N_p \rho N^3 D^5$
Flow Pattern	Approximated by a Gaussian intensity field (no CFD mesh solving)
Shear Rate	Estimated locally from power density $\dot{\gamma} \approx \sqrt{(\epsilon/\nu)}$
Energy Dissipation	Derived from $\epsilon = \mu \dot{\gamma}^2$
Boundary & Baffles	Ignored (axisymmetric assumption)

3. Step-by-Step Logic

Step 1: Input & Geometry

- The user provides tank diameter (T), liquid volume (V), and impeller data (diameter, speed, clearance, power number).
- Tank height H is computed from the volume:

$$H = \frac{V}{\pi(R)^2}$$

where $R = T/2$.

Step 2: Impeller Power Calculation

Each impeller contributes mechanical power:

$$P_i = N_{p,i} \rho N^3 D_i^5$$

All impellers' power adds up to total:

$$P_{total} = \sum P_i$$

Then, the global power density (P/V) is:

$$\frac{P_{total}}{V}$$

This represents an *average* EDR in the entire tank.

Step 3: Define Spatial Grid (Pseudo-CFD Field)

- The tank is divided into a 2D grid ($r \times z = 50 \times 50$ cells).
- Each cell represents a small annular volume $dV = 2\pi r dr dz$.
- Arrays `intensity[j][i]` hold local “power density proxy” values.

Step 4: Local Power Distribution Around Impellers

Each impeller produces a *Gaussian decay* of power with distance from its center (r, z):

$$\varepsilon(r, z) = \varepsilon_0 \exp \left[-\left(\frac{r}{0.75D} \right)^2 - \left(\frac{z - z_i}{0.6D} \right)^2 \right]$$

where

- $\varepsilon_0 = P_i/V$ = average contribution from that impeller
- z_i = clearance height
- D = impeller diameter

This defines an energy “cloud” centered around each impeller.

Step 5: Compute Shear and Local EDR

Once local ϵ (power density) is estimated for every grid cell:

- Shear rate is approximated from local ϵ and kinematic viscosity (ν):

$$\dot{\gamma} = \sqrt{\frac{\epsilon}{\nu}}$$

- EDR (Energy Dissipation Rate) is then:

$$\epsilon_{local} = \mu \dot{\gamma}^2$$

Thus, each grid point gives:

- Local shear rate (1/s)
- Local EDR (W/m³)

Step 6: Compute Averages

Two averages are calculated:

1. Simple arithmetic mean

$$\bar{\epsilon}_{simple} = \frac{1}{N} \sum \epsilon_{local}$$

2. Volume-weighted mean

$$\bar{\epsilon}_{vol} = \frac{\sum \epsilon_{local} V_{cell}}{\sum V_{cell}}$$

This is directly comparable to P/V from power balance.

The maximum EDR (ϵ_{max}) is also tracked to capture the most energetic (or shear-intensive) zone in the tank.

7. Physical Interpretation

Parameter	Meaning	Significance
avgEDR_W_m3_volumeWeighted	Volume-weighted mean EDR	Comparable to mechanical P/V, good for scale-up
maxEDR_W_m3	Maximum EDR in domain	Indicates shear “hot spots” that may damage cells or proteins
avgShearRate_1_per_s	Mean flow-averaged shear rate	Related to overall mixing intensity
maxShearRate_1_per_s	Peak shear rate	Predicts cell damage potential

8. Strengths and Limitations

Strengths: Fast, physics-based, CFD-like, suitable for comparative and scaling studies.

Limitations: Axisymmetric, no turbulence model, assumes Newtonian fluid, ignores baffles and free-surface effects.

9. Practical Use

The model helps compare impeller designs, estimate energy uniformity, assess scale-up consistency, and visualize pseudo-CFD contour plots in Retool dashboards or process reports.