processes

Supplementary Materials

Governing equations

In OF v7, `multiphaseEulerFoam` is an incompressible and isothermal solver that can handle dispersed and segregated flows simultaneously by combining the volume of fluid (VOF) approach with the classical Eulerian approach [45]. The governing equations for the Euler multifluid approach are applied for each phase k with its mass (Equation S1) and momentum (Equation S2) equations that account for interfacial forces (Equation S4).

$$\frac{\partial \alpha_k}{\partial t} + \nabla \cdot (\alpha_k u_{R,k}) = 0 \tag{S1}$$

$$\frac{\partial}{\partial t}(\alpha_k \rho_k u_{R,k}) + \nabla \cdot (\alpha_k \rho_k u_{R,k} u_{R,k}) = -\alpha_k \nabla P + \nabla \cdot (\alpha_k (\mu_k + \mu_{t,k}) \nabla u_{R,k}) + \alpha_k \rho_k g + \sum_i F_{i,k} \tag{S2}$$

Where α_k is the (cell) volume fraction of the k^{th} phase ($\sum_i \alpha_i = 1$), ρ is the fluid density, P is absolute pressure, μ is the molecular viscosity, μ_t is the turbulent viscosity computed from the turbulence model, g is the gravitational acceleration, and $\sum_i F_{i,k}$ contains all the additional forces.

Since the multiple reference frame (MRF) approach is used for impeller modelling, u_R is defined by being the relative velocity in the relative rotating frame as:

$$u_R = u - \Omega \times r \tag{S3}$$

with u being the velocity vector in the stationary frame, Ω is the angular velocity vector, and r is the distance vector from the axis of rotation.

In the rotating frame, additional inertial forces are specified (Coriolis and centrifugal), and forces related to the physical system are specified throughout the domain. For this system, it was decided to only include the drag force and surface tension force using OF's default implementation (Equation S4).

$$F_{D,k} = \frac{3}{4} \alpha_c \alpha_d \rho_k C_D \frac{|u_d - u_c|(u_d - u_c)}{d_d}; \qquad F_{S,k} = \sigma \kappa \nabla \alpha_k \tag{S4}$$

where the subscripts c and d denote the continuous and dispersed phases, respectively, d_d is the assumed bubble diameter for the dispersed phase, σ is the surface tension force between phases, and $\kappa = -\nabla \cdot \left(\frac{\nabla \alpha}{\nabla |\alpha|}\right)$ is the local surface curvature. The drag coefficient (C_D) was calculated from the classical Schiller and Naumann correlation [46].

$$C_D = \begin{cases} \dfrac{24(1 + 0.15 {Re_d}^{0.687})}{Re_d}, Re_d \leq 1000 \\ 0.44, Re_d > 1000 \end{cases} \tag{S5}$$

where the Reynolds number is defined with the dispersed phase:

$$Re_d = \frac{\rho_c |u_d - u_c| d_d}{\mu_c} \tag{S6}$$

In regions where both phases are present, the VOF method is used to resolve the interface using the interface compression method of Weller ([45], [47]) as:

$$\frac{\partial \alpha_k}{\partial t} + \nabla \cdot (\alpha_k u_k) + \nabla \cdot \left(\alpha_k u_c (1 - \alpha_k)\right) = 0 \tag{S7}$$

where u_c is the artificial compression velocity, which acts normally upon the phases' interface:

$$u_c = C_\alpha |u| \frac{\nabla \alpha_k}{\nabla |\alpha_k|} \tag{S8}$$

where C_α is a sharpening binary coefficient that is specified for a selected pair of phases. By setting C_α=1, interface capturing takes place, enabling the VOF method in regions with large phase gradients.

CFD model setup of simple Rushton Turbine

A cylindrical vessel, the shaft, and the Rushton turbine were drawn using Siemens NX 12 and exported to STL files, as seen in Figure 1. The mesh is generated using blockMesh and snappyHexMesh OF utilities. Blockmesh generates a hexahedral background mesh (which specifies the cell size of the bulk cells) for the cylinder. In a second stage, snappyHexMesh iteratively adjusts the internal cylinder cells to accommodate internal elements (e.g., shaft and impeller) with the possibility of specifying different refinement regions. The process is fully automated and continues until certain mesh quality constraints are satisfied. A cross-section view of the resulting meshes can be seen in Figure S1. Refinements were focused on properly resolving the fluid's interface and the region close to the impeller blades (where turbulent energy dissipation is expected to be maximal). Additionally, attention was paid to keep nonorthogonality (<70°) and skewness (<4) to a minimum whenever possible based on CFD best practices [48]. Below, a summary is presented in Table S1 of some mesh quality metrics for the three meshes obtained from the OF mesh utility checkMesh.

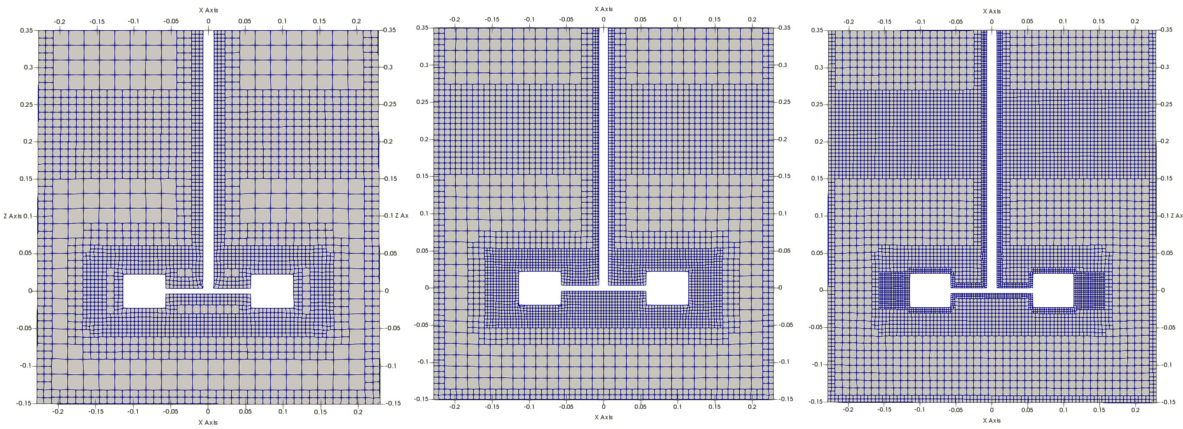

Figure S1: Cross-section view of the mesh for the different refinements (R1: left, R2: centre, R3: right).

Table S1: Mesh quality metrics from checkMesh utility.

	R1	R2	R3
Number of cells	126334	277520	594391
Refinement factor	-	~2.2	~2.1
Hexahedral cells	96766	233526	496999
Max non-orthogonality	65.09	65.85	65.55
Avg. non-orthogonality	10.25	8.06	7.67
Max. skewness	2.84	3.99	4.51

CFD model setup of full-scale reactor

Table S2: Mesh quality metrics from checkMesh utility.

	R1	R2	R3	R4
Number of cells	492659	720165	1160631	1846257
Refinement factor	-	~1.5	~1.6	~1.6
Hexahedral cells	474633	696912	1117262	1715401
Max non-ortho.	65.91	65.21	64.81	66.09
Avg. non-ortho.	5.28	4.88	5.42	5.12
Max. skewness	3.71	4.95	4.66	4.92