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Multiphase CFD Modelling of Mixing in a Cubic Single-Use-Technology Bioreactor

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Introduction

Single-use-technologies (SUT) are a class of disposable processing equipment that has become increasingly popular in the bioprocessing industry [1]. Stirred SUT bioreactors use a pre-sterilised polymeric bag which is replaced after use, eliminating the need for cleaning and sterilization in place. Despite the increased levels of plastic waste produced, the overall environmental impact of SUT processes is significantly reduced, largely due to the high energy demands of traditional steam sterilisation [2].

In this work, CFD modeling has been performed using the commercial software ANSYS CFX to investigate multiphase gas-liquid mixing in an industrial cubic SUT bioreactor. This shape is preferred due to the reduced complexity over existing cylindrical SUT designs, the application of which is currently almost exclusively applied to high-value pharmaceutical productions [3]. A magnetically driven, floor-mounted impeller is used so that unused bags can be stacked and no impeller shaft is penetrating the bag.

Mass Transfer Coefficient Models

Five models to describe the mass transfer coefficient k_L are compared in Table 1. All of the chosen models can be calculated from the outputs of the CFD model.

Table 1. Mass coefficient models used to calculate k_La values. D_L = diffusivity, ε = eddy dissipation rate, ν = kinematic viscosity, d_b = bubble diameter, v_b = slip velocity, V_G = superficial gas velocity, g = gravitational acceleration

Model Description	Equation
Penetration model [4] • Based on Higbie's penetration theory of interface transfer • Mass transfer occurs largely due to the small eddies • The Kolmogorov Length Scale is used to describe the contact time	$k_L = \frac{2}{\sqrt{\pi}}\sqrt{D_L\sqrt{\frac{\varepsilon}{\nu}}}$
Eddy cell model [5] • Similar form to the penetration theory but based on the surface renewal model. • It is assumed that the surface renewal rate is calculated using the Kolmogorov Scale model due to the influence of small eddies	$k_L = 0.4\sqrt{D_L\sqrt{\frac{\varepsilon}{\nu}}}$
Slip velocity model [6] • Surface renewal theory is used as a starting point • The renewal of fluid at the surface is assumed to be due to the relative motion of the bulk gas and liquid phases	$k_L = \frac{2}{\sqrt{\pi}}\sqrt{\frac{D_L v_b}{d_b}}$
Rigid model [7] • If a bubble is sufficiently rigid (ie. small bubbles), k_L can be described using the Frossling equation for laminar boundary layers	$k_L = 0.6\left(\frac{v_b}{d_b}\right)^{1/2} D_L^{3/2}\nu^{-1/6}$
Surface renewal stretch model [8] • Combines the continuity equation with aspects of surface renewal theory and the penetration theory for surface stretch	$k_L = \frac{2}{\sqrt{\pi}}\sqrt{D_L\sqrt{\frac{V_G g}{\nu}}}$

Model Development

- 1 m^3 fluid body is modelled with a constant bubble size of 1 mm
- Half of the physical geometry is modelled due to the rotational symmetry in the arrangement of the air spargers (Fig. 1)
- Turbulence is modelled using the k-ε model
- Impeller motion is modelled using the moving reference frame method

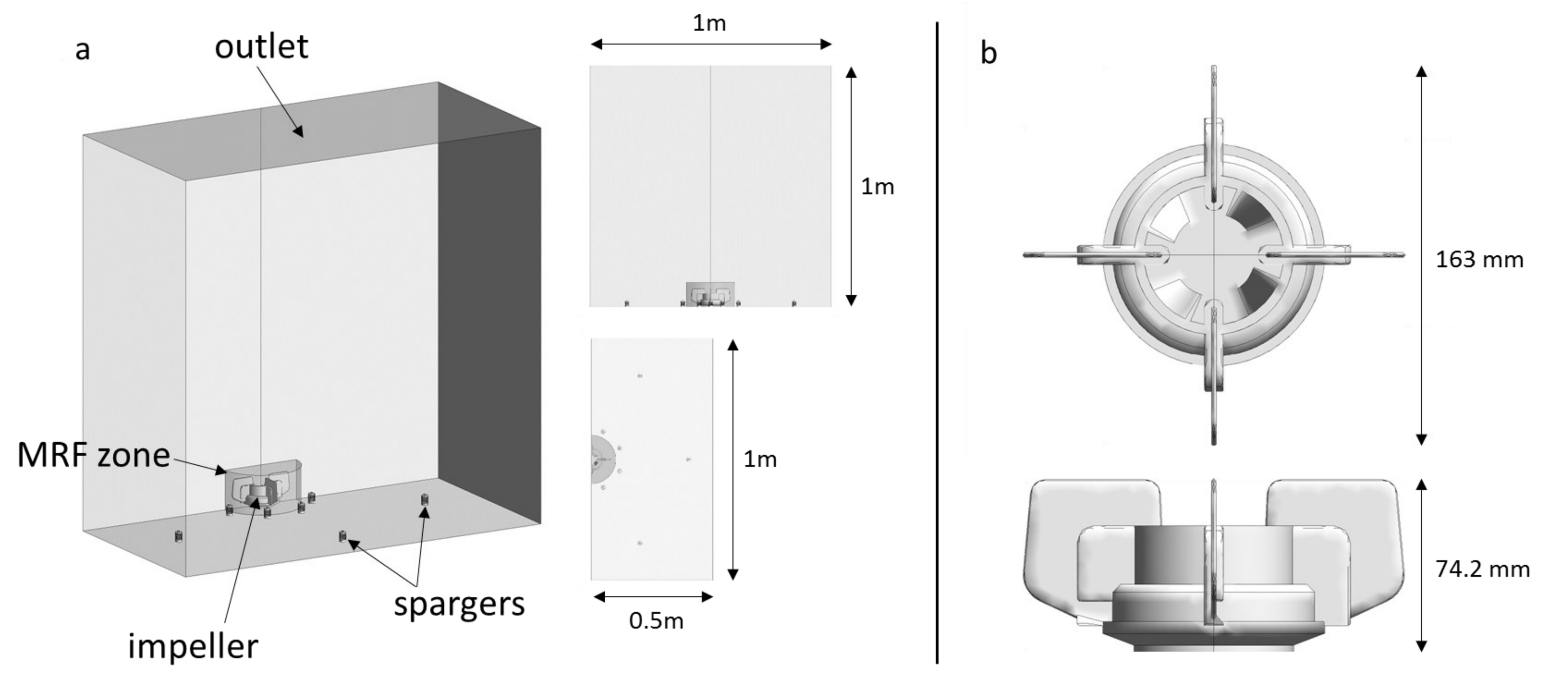

Figure 1. 3D modelled geometry a) modelled fluid domain b) magnetically driven impeller

Results & Discussions

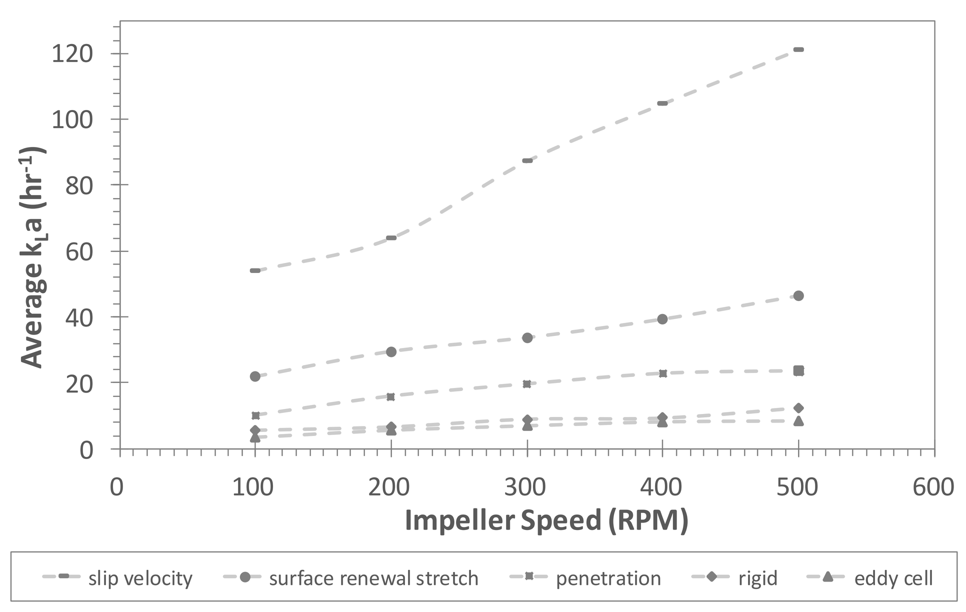

Figure 2. Comparison of volume-averaged k_La values for different mass transfer models

- The eddy cell model gives the best fit to an experimental k_La value of 18 hr^{-1} at 400 RPM (Fig. 2)
- There is no benefit seen from increasing the stirrer speed above 400 RPM for the chosen model (Fig. 2)
- Significant radial distribution of gas bubbles occurs at stirrer speeds of 300 RPM and above (Fig. 3)

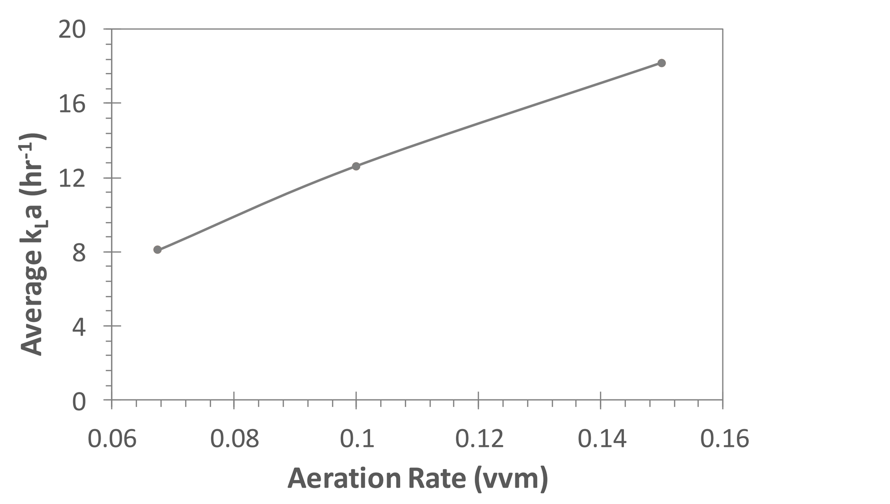

Figure 4. Effect of increasing aeration rate at a stirrer speed of 400 RPM

- Increasing the supply of air to the tank will result in higher k_La values (Fig. 4)
- This will be limited as the sparger region could become flooded if the aeration rate is too high

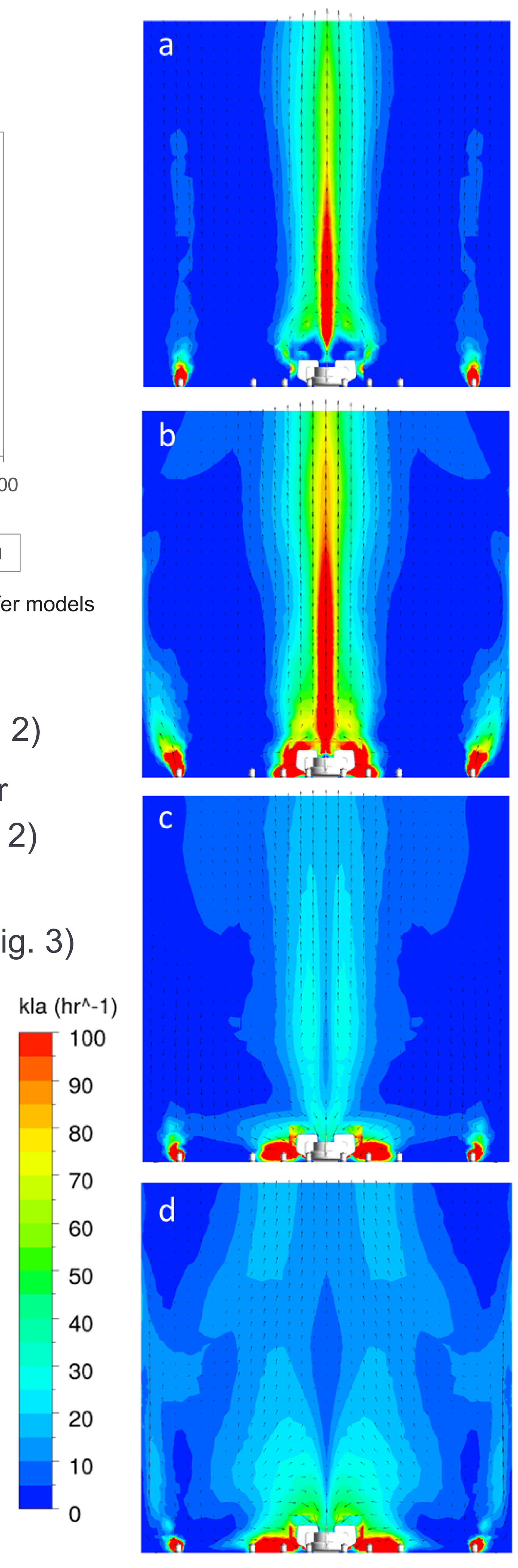

Figure 3. Combined contour and vector plot of k_La and liquid velocity for a) 100 RPM b) 200 RPM c) 300 RPM d) 400 RPM

230L Geometry Model

- A proposed 230 L design was modelled with the same sparger inlet velocity (0.1 ms^{-1})
- Mass transfer is significantly improved at a stirrer speed of 400 RPM due to a higher gas flow rate per unit volume
- Greater recirculation of the liquid phase is seen, however a central region develops with no gas phase recirculation

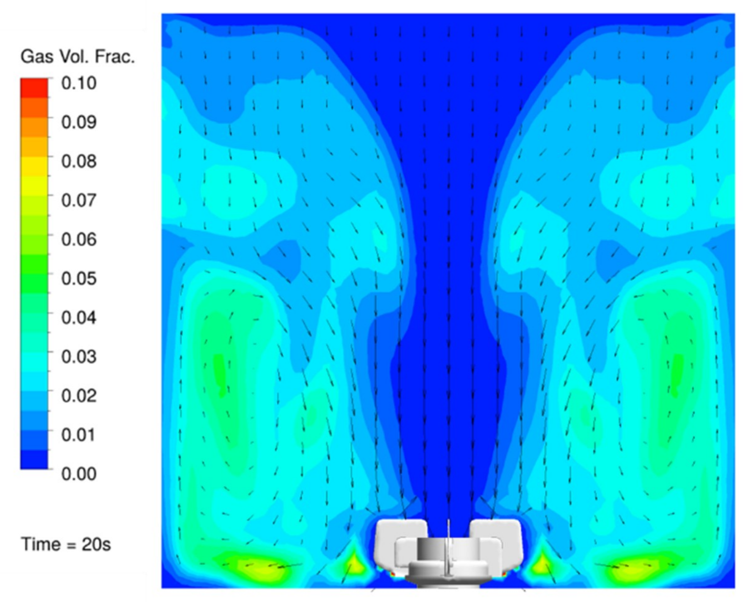

Figure 5. Combined contour and vector plot of gas volume fraction and liquid velocity in the 230L vessel at 400 RPM

Summary

- The eddy cell model provides the best fit for k_La values
- A stirrer speed of 300 RPM or greater is needed for significant bubble distribution in the 1 m^3 bioreactor reactor modelled
- Increasing the stirrer speed form 400 to 500 RPM shows no significant benefit in terms of mass transfer of oxygen
- Increasing the aeration rate increases mass transfer as long as the reactor is not flooded
- Using a smaller tank volume with the same inlet gas velocity will significantly increase mass transfer and promote greater recirculation
- k_La values in the 1 m^3 bioreactor modelled are currently much lower than traditional stainless steel fermenters, limiting the current applicability to low oxygen demand species only
- Ongoing work includes model validation via Laser Doppler Anemometry (LDA) in a lab-scale cubic vessel, the direct modelling of interphase mass transfer for oxygen and the incorporation of a model to predict bubble size distributions

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