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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 modelling 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 $k_a$ are compared in Table 1. All of the chosen models can be calculated from the outputs of the CFD model.

<table>
<thead>
<tr>
<th>Model Description</th>
<th>Equation</th>
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<tbody>
<tr>
<td>Penetration model [4]</td>
<td>$k_a = \frac{2}{3} \frac{\varepsilon}{\sqrt{\varepsilon}}$</td>
</tr>
<tr>
<td>Eddy cell model [5]</td>
<td>$k_a = \frac{2}{3} \frac{\varepsilon}{\sqrt{\varepsilon}}$</td>
</tr>
<tr>
<td>Slip velocity model [6]</td>
<td>$k_a = \frac{2}{3} \frac{\varepsilon}{\sqrt{\varepsilon}}$</td>
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<tr>
<td>Rigid model [7]</td>
<td>$k_a = \frac{2}{3} \frac{\varepsilon}{\sqrt{\varepsilon}}$</td>
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<tr>
<td>Surface renewal stretch model [8]</td>
<td>$k_a = \frac{2}{3} \frac{\varepsilon}{\sqrt{\varepsilon}}$</td>
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Model Development

- 1 m³ 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

Results & Discussions

- The eddy cell model gives the best fit to an experimental $k_a$ 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)

230L Geometry Model

- A proposed 230 L design was modelled with the same sparger inlet velocity (0.1 m/s)
- 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

Summary

- The eddy cell model provides the best fit for $k_a$ values
- A stirrer speed of 300 RPM or greater is needed for significant bubble distribution in the 1 m³ 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
- $k_a$ values in the 1 m³ 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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