FINAL RESULTS

Time, (s)

Coefficient of Variation, (\cdot)

Injection

90% mixing

99% mixing
What is syngas fermentation?
Converting syngas (H\textsubscript{2}, CO, CO\textsubscript{2}) into fuels using microorganisms augmented with electrical field to improve selectivity of target products and increase carbon efficiency.

Modeling approach

Macro-scale
- Tool: ANSYS Fluent
- Target: Mass transfer coefficient

Micro-scale
- Tool: OpenFOAM
- Target: Sub-grid model to resolve the mass boundary layer
MACRO-SCALE

\( k_{La} \) → Flow field → Mixing time → Representation of mixing
MACRO-SCALE

Mixing representations

30 probes

5 probes

\[
CoV = \frac{\sigma}{C_{\text{mean}}}
\]

\[
U_{\text{max/min}} = \frac{C_{\text{max}}(t) - C_{\text{min}}(t)}{C_{\text{mean}}}
\]

\[
U(t) = 1 - \frac{\Delta_{\text{max}}(t)}{\Delta_{\text{max}}(0)}
\]

\[
\gamma_a = 1 - \frac{\Sigma(C_i - \bar{C}_i)A_i}{2|C_i|\Sigma A_i}
\]

\[
\Delta_{\text{max}} = \max(C_{\text{max}} - C_{\text{mean}}, C_{\text{mean}} - C_{\text{min}})
\]
## MACRO-SCALE

### Mixing time:

<table>
<thead>
<tr>
<th>rpm</th>
<th>Experiments</th>
<th>CFD</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\bar{t}_m$</td>
<td>$std$</td>
</tr>
<tr>
<td>300</td>
<td>3.1</td>
<td>0.804</td>
</tr>
<tr>
<td>500</td>
<td>1.9</td>
<td>0.141</td>
</tr>
<tr>
<td>800</td>
<td>1.2</td>
<td>0.271</td>
</tr>
</tbody>
</table>
MICRO-SCALE

Problem formulation:

Extremely thin mass boundary layer that should be resolved:

1. Fine mesh
2. Sub-grid scale model
MICRO-SCALE

2D, Half a bubble with axis of symmetry

Sc = 1

Sc = 10

Radial distance, [m]
**MICRO-SCALE**

Scaling boundary layer thickness

\[ \delta \propto \frac{1}{\sqrt{Sc}} \]

**Graph:**
- **Numerical predictions**
- **Sc:0.3**

**Equation:**
\[ \delta = \alpha Sc^\beta, \quad (\alpha = 63.152, \beta = 0.489) \]
MICRO-SCALE

Idea of sub-grid model
MICRO-SCALE

$Sc = 1, \ x = 0.1 \ mm$

$Sc = 10, \ x = 0.1 \ mm$

$Sc = 50, \ x = 0.1 \ mm$
CONCLUDING REMARKS

• Modeling mass transfer for syngas fermentation bioreactor
  
o  Macro-scale:
    ▪ Flow characteristics by mixing time
    ▪ Volumetric mass transfer coefficient (ongoing)
  
o  Micro-scale
    ▪ Resolving the mass boundary layer utilizing fine mesh
    ▪ Developing sub-grid scale models (ongoing)