

**Modeling surface gas transfer in agitated vessels using  
Computational Fluid Dynamics**

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**Abstract**

Surface gas transfer into agitated vessels is an important phenomenon in many industries applications. This work focuses on the development of a novel approach to model surface gas transfer using computational fluid dynamics (CFD). The methodology was developed to understand oxygen-water surface transfer in agitated vessels. Experimental data in the form of dissolved oxygen (DO) curves were used to verify the modeling approach. To increase computational efficiency, a species transport model was used as an alternative to more traditional multiphase approaches. DO profiles and  $kLa$ 's obtained from CFD models were comparable to experimental data for a range of tank scales and designs. This approach provides an efficient way to design vessels with specific  $kLa$  requirements using CFD and thus reducing the cost of experimentation.