Computational Design of Intercooled Packing for CO₂ Absorbers

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Additively Manufactured Intensified Device for Enhanced Carbon Capture by Monoethanolamine

**Background: Temperature Bulge of Liquid**

- Occurs as a result of the exothermic reaction of $\text{CO}_2$ with MEA
- The location of the temperature bulge depends on the solvent-to-gas ratio
- The T bulge as well as L/G can significantly affect the removal rate
- The location of where to provide the cooling is not obvious

(Kvaamsdal & Rochelle, 2008)
Motivation-New Subtask

• Hypothesis
  – Optimization of heat removal could promote more CO₂ absorption but tradeoff between capital and operating cost must be taken into consideration

• Background
  – Current capture equipment design: Decoupled unit operations with mass transfer and heat transfer
  – Decoupled stages with external cooling

• Objective (3 years)
  – Provide computational and theoretical tools to assist the development, prototyping and validation of enhanced CO₂ capture with intercooled/intensified devices
  – Develop new computational framework to
    • Understand the effect of operating conditions and material properties on system performance
    • Parameterize geometry and programmatically update CFD model
  – Investigate the effect of geometry through detailed CFD modeling
  – Develop Framework to link CFD, process modeling and performance optimization
Absorber Model

• Carbon Capture model developed by the CCSI team\textsuperscript{1,2} for monoethanolamine (MEA).
• Model tested to be accurate at the NCCC and TCM
• Model includes mass transfer, heat transfer, vapor-liquid equilibrium, and chemistry of the MEA-H\textsubscript{2}O-CO\textsubscript{2} system

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Implementation of Embedded Cooling

- Adaptable to multiple active/inactive cooling sections
- Co-current or counter-current flow

Preliminary Modeling Work II

• Investigating the trade-off between increase in absorption performance and the increase in equipment size
• Geometry of shell and tube type heat exchanger used to relate heat transfer area to increase in absorber size
Investigating the trade-off between increase in absorption performance and the increase in equipment size.

Geometry of shell and tube type heat exchanger used to relate heat transfer area to increase in absorber size.

**Preliminary Modeling Work II**

![Graph showing the relationship between specific cooling area and capture increase](image)

- **Capture Increase**
- **Absorber Size Increase**

*Geometry Matters!*
How do you solve physics problems?
How do you solve physics problems?

Model

Solver

Solution

Fridolin Okkels and Henrik Bruus, Scaling behavior of optimally structured catalytic microfluidic reactors, Physical Review E 75, 016301 2007
How do you solve physics problems?

Governing Eq. + Constitutive Laws + Setup + BC

Model

COMSOL

u, v, p, c

Solver

Solution

Fridolin Okkels and Henrik Bruus, Scaling behavior of optimally structured catalytic microfluidic reactors, Physical Review E 75, 016301 2007

How do you solve physics problems?

Governing Eq. + Constitutive Laws + Setup + BC

Model

? e.g. NS + CDR + BC + Goal

COMSOL

Solver

? TOPOPT

Solution

? Best design

Fridolin Okkels and Henrik Bruus, Scaling behavior of optimally structured catalytic microfluidic reactors, Physical Review E 75, 016301 2007

How do you solve physics problems?

Model

\[ ? \]

e.g. NS + CDR + BC + Goal

Solver

\[ ? \]

TOPOPT

Solution

\[ ? \]

\[ u,v,p,c \]

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Fundamentals of Topology Optimization

\[ \gamma = 0, \text{ Solid} \]
\[ \gamma = 1, \text{ Void} \]

“…Airbus researches use of topology optimization on aircraft wing ribs. It is stated that usage of topology optimization results in around 1000 kg of weight savings per aircraft…”

https://topologyoptimization.wordpress.com/2011/03/11/airbus/

Fundamentals of Optimization Problems

- Optimization Problem = Inverse Problem

Tune the design-variables ($\gamma$) of a problem, such that an objective function ($\Phi$) is minimized, under given constrains.

- Design variables: $\gamma(r), u[\gamma]$
- Objective function: $\min_{\gamma} \Phi(u[\gamma], \gamma)$
- Constrains: $g(u[\gamma], \gamma) \leq 0$
  $0 \leq \gamma(r) \leq 1$
Mathematical Formulation of the PDE problem

We can use the software package COMSOL to solve the reacting flow problem. Requires Partial Differential Equations to be expressed in divergence form.

\[ \mathbf{\Gamma}_1 \equiv \begin{bmatrix} \sigma_{11} \\ \sigma_{21} \end{bmatrix}, \quad \mathbf{\Gamma}_2 \equiv \begin{bmatrix} \sigma_{12} \\ \sigma_{22} \end{bmatrix}, \quad \mathbf{\Gamma}_3 \equiv \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \quad \mathbf{\Gamma}_4 \equiv \begin{bmatrix} -J_1 \\ -J_2 \end{bmatrix} \]

\[ F_1 \equiv \rho(\mathbf{v} \cdot \nabla)v_1 + \alpha v_1, \quad F_2 \equiv \rho(\mathbf{v} \cdot \nabla)v_2 + \alpha v_2, \quad F_3 \equiv \nabla \cdot \mathbf{v} \quad F_4 \equiv \mathbf{v} \cdot \nabla c + R \]

Then the reacting flow problem can be written as:

\[ \nabla \cdot \mathbf{\Gamma}_i = F_i \quad \text{in } \Omega, \]

\[ R_i = 0 \quad \text{on } \partial \Omega, \quad \text{Dirichlet b.c.} \]

\[ -n \cdot \mathbf{\Gamma}_i = G_i + \sum_{j=1}^{3} \frac{\partial R_i}{\partial u_i} \mu_j \quad \text{on } \partial \Omega, \quad \text{Neumann b.c.} \]
The Finite Element Method (FEM)

- Expand both $u$ and $\gamma$ on a finite basis set
  
  $$u_i(r) = \sum_n u_{i,n} \varphi_{i,n}(r)$$  
  $$\gamma(r) = \sum_n \gamma_{4,n}(r)$$

- Use P1 basis for $p(r)$, $c(r)$ and $\gamma(r)$

- Use P2 basis for $u(r)$

Finite element mesh; basis function $\varphi_j$ has small support
Constrained optimization problem

- Minimize objective function $\Phi(u)$ subject to constraints

$$\begin{align*}
\min_{\gamma} & \quad \Phi(u, \gamma) \\
\text{subject to} & \quad \int_{\Omega} \gamma(r) \, dr - \beta |\Omega| \leq 0, \\
& \quad 0 \leq \gamma(r) \leq 1, \\
& \quad \nabla \cdot \Gamma_i = F_i, \quad \text{Volume constraint} \\
& \quad R_i = 0, \quad \text{Design variable bounds} \\
& \quad -\mathbf{n} \cdot \Gamma_i = G_i + \sum_{i=1}^{3} \frac{\partial R_j}{\partial u_i} \mu_j, \quad \text{Governing equations} \\
& \quad \text{Dirichlet b.c.} \\
& \quad \text{Neumann b.c.}
\end{align*}$$
Setup and procedure for micro-reactor
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Modeling

COMSOL GUI
Setup and procedure for micro-reactor

Modeling

- COMSOL GUI
- MMA.m (MATLAB)

Method

- COMSOL Script
  - TOPOPT.m
  - Adj-Pr.m

Setup and procedure for micro-reactor

Modeling
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Visualization/Analysis
- COMSOL Script
- COMSOL/MATLAB
- General export

Topology Optimized Micro-Reactors

- Characteristic Examples

\[ \text{Iter} = 188 \]

\[ \text{Iter} = 227 \]

\[ Da = 10^{-5}, D = 1 \cdot 10^{-8} \frac{m^2}{s}, dp = 0.1 \text{ Pa}, k_a = 1 \]

\[ Da = 10^{-5}, D = 1 \cdot 10^{-8} \frac{m^2}{s}, dp = 0.5 \text{ Pa}, k_a = 1 \]
Characteristic Examples

\[
\begin{align*}
\text{Iter} &= 121 \\
\text{Iter} &= 227
\end{align*}
\]

\[
\begin{align*}
\text{Da} &= 10^{-5},
D &= 1 \cdot 10^{-8} \frac{m^2}{s}, 
\text{dp} &= 0.5 \text{ Pa}, 
k_a &= 0.25 \\
\text{Da} &= 10^{-5},
D &= 1 \cdot 10^{-8} \frac{m^2}{s}, 
\text{dp} &= 0.5 \text{ Pa}, 
k_a &= 1
\end{align*}
\]
Partnership with ORNL and WVU

- Models and numerical campaign to inform experimental work
- Experimental campaign to collect data to improve models

NETL
Local Information- High fidelity CFD

ORNL
Experimentation, manufacturing and testing

WVU
Process modeling
Moving Forward

- **Improve process model in terms of Coolant model and improved discrete or continuous design of cooling locations**
- **Link CFD with Process Modeling**
- **Study Process economics**
- **Calibrate model and validate computational and theoretical work against actual 3D printed structured packing**

- **Develop CFD framework to simulate**
  - Multiphase flow
  - Chemical reactions
  - Thermal coupling between chemistry and fluid flow on limiting mechanisms
  - Packing
  - Fluid properties
  - Operating conditions

- **MEA+Mellapak equivalent, to match literature performance**
- **MEA+Intensified reactor Goal: improve packing with in situ continuous cooling (absorber) and heating (stripper)**

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**CCSI**

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For more information
https://www.acceleratecarboncapture.org/

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