Computational Design of Intercooled Packing for CO_2 Absorbers

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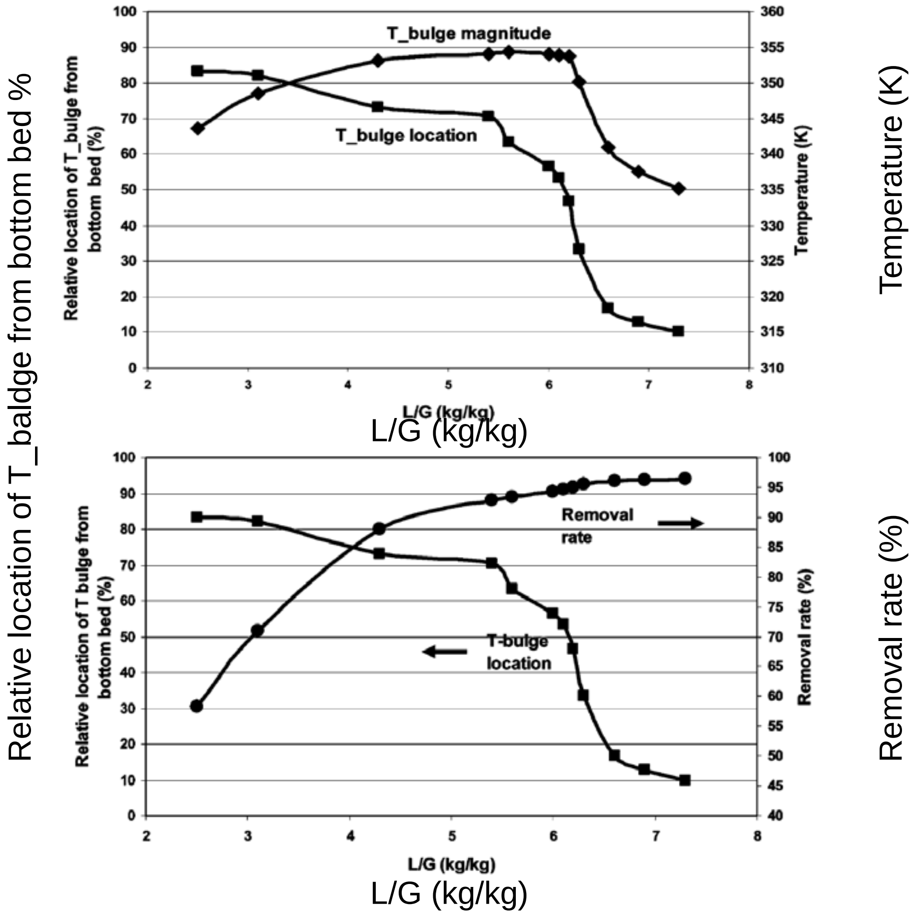
Additively Manufactured Intensified Device for Enhanced Carbon Capture by Monoethanolamine

Background: Temperature Bulge of Liquid

- Occurs as a result of the exothermic reaction of 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)

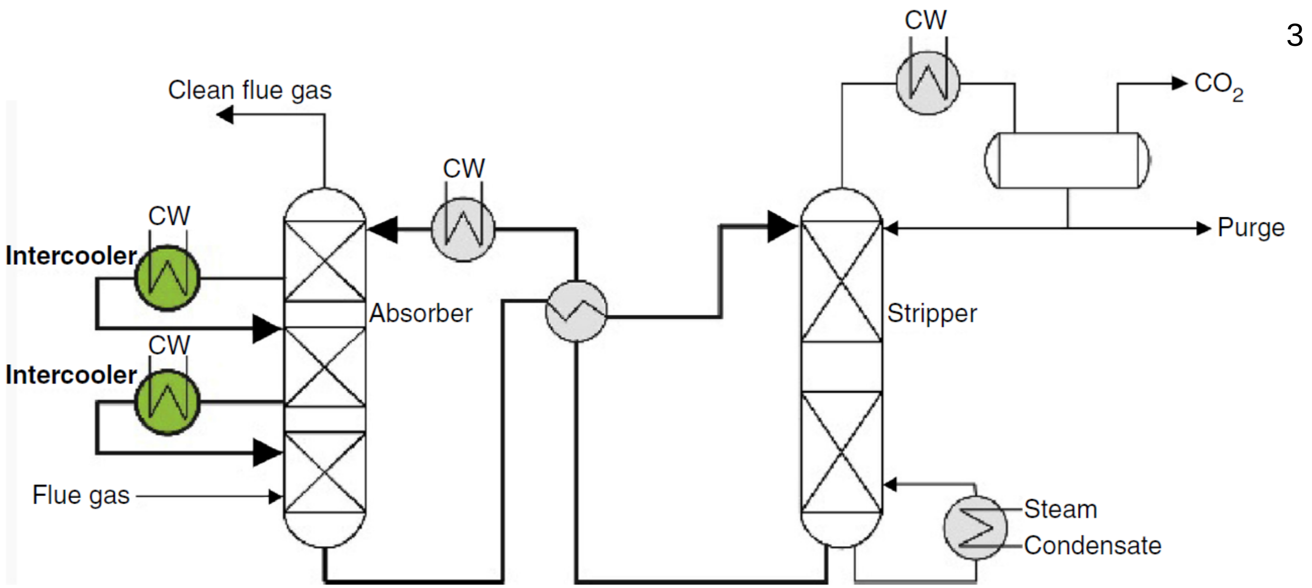
Motivation-New Subtask

- **Hypothesis**
  - Optimization of heat removal could promote more CO_2 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 (3years)**
  - Provide computational and theoretical tools to assist the development, prototyping and validation of enhanced CO_2 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

Process Modeling

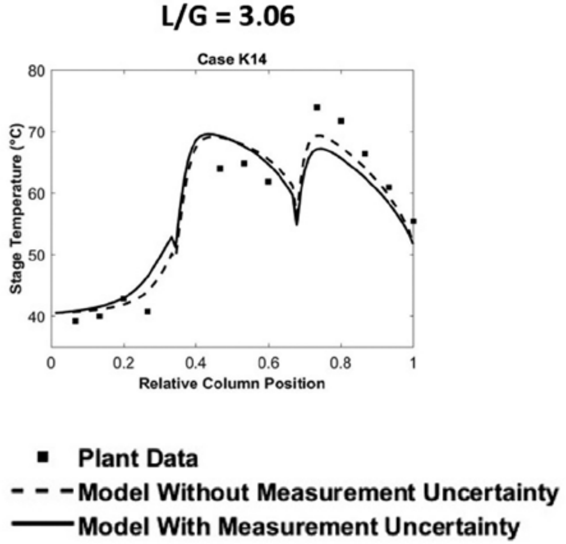
Absorber Model

- Carbon Capture model developed by the CCSI team[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_2O-CO_2 system

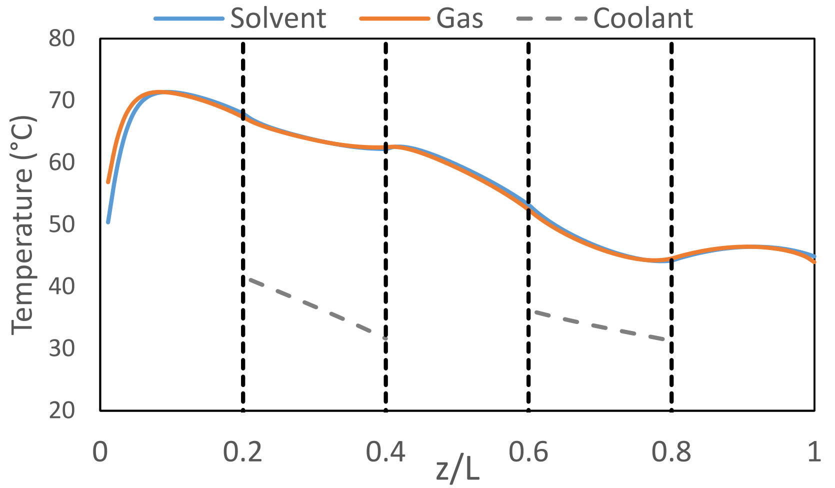


[1] A. Soares Chinen, J. C. Morgan, B. Omell, D. Bhattacharyya, C. Tong, and D. C. Miller, "Development of a Rigorous Modeling Framework for Solvent-Based CO2 Capture. 1. Hydraulic and Mass Transfer Models and Their Uncertainty Quantification," *Ind. Eng. Chem. Res.*, vol. 57, no. 31, pp. 10448–10463, Aug. 2018.
[2] J. C. Morgan *et al.*, "Development of a Rigorous Modeling Framework for Solvent-Based CO2 Capture. Part 2: Steady-State Validation and Uncertainty Quantification with Pilot Plant Data," *Ind. Eng. Chem. Res.*, vol. 57, no. 31, pp. 10464–10481, Aug. 2018.
[3] Debangsu Bhattacharyya1 and David C Miller , Post-combustion CO2 capture technologies — a review of processes for solvent-based and sorbent-based CO2 capture, Chemical Engineering 2017, 17:78–92

Implementation of Embedded Cooling

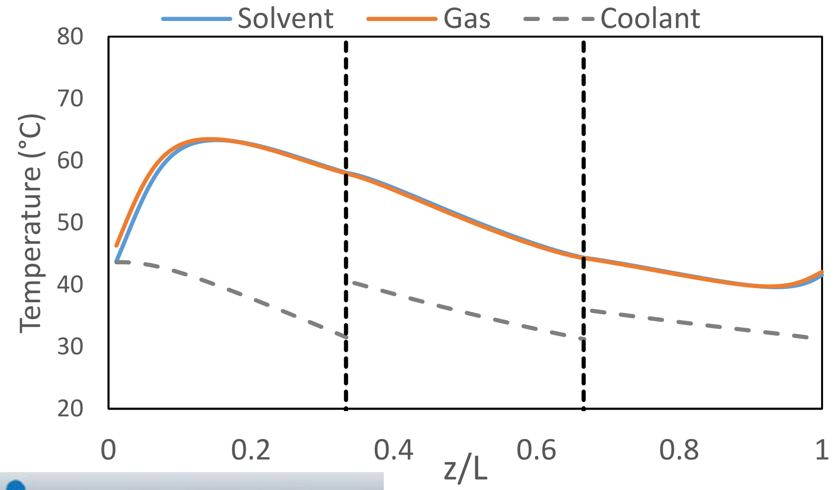


2 Active Sections

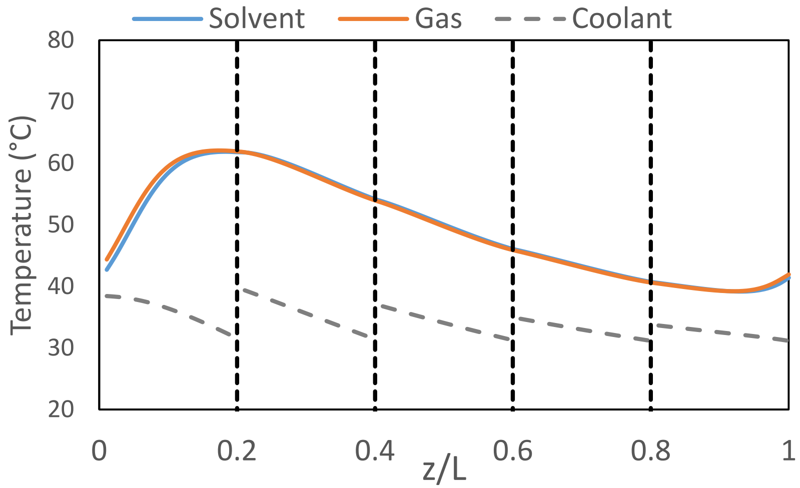


- Adaptable to multiple active/inactive cooling sections
- Co-current or counter-current flow

3 Active Sections



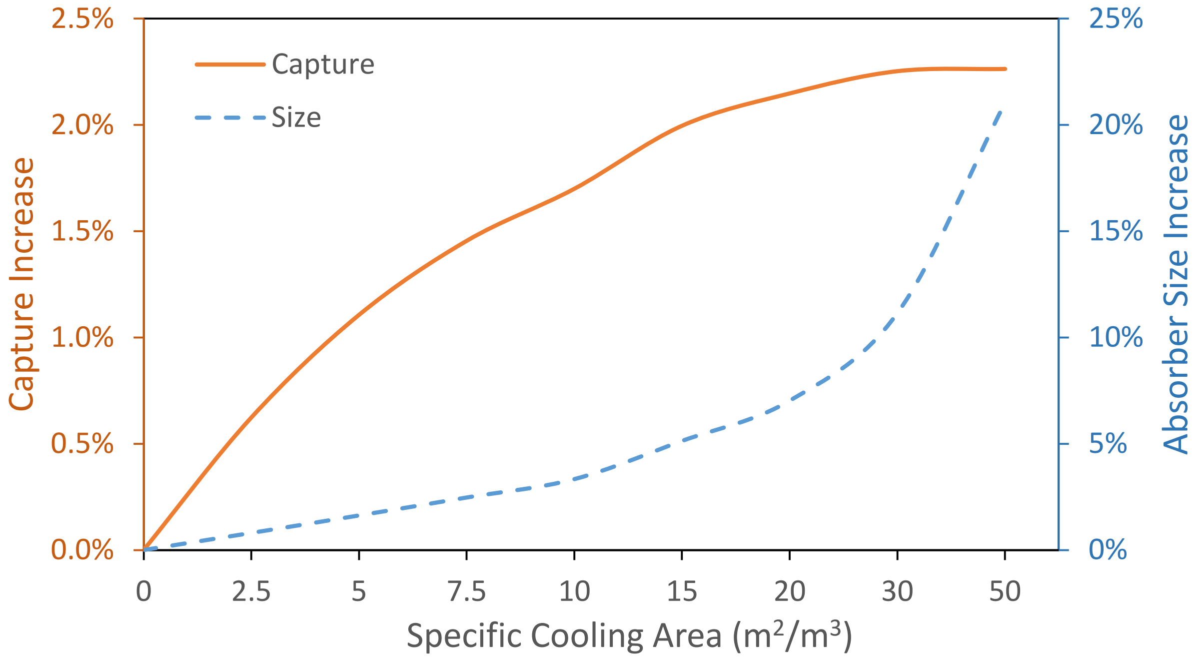
5 Active Sections



J.C. Morgan et al., Development of a Rigorous Modeling Framework for Solvent-Based CO2 Capture. Part 2: Steady-State Validation and Uncertainty Quantification with Pilot Plant Data, Ind. Eng. Chem. Res. 2018, 57, 10464–10481

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



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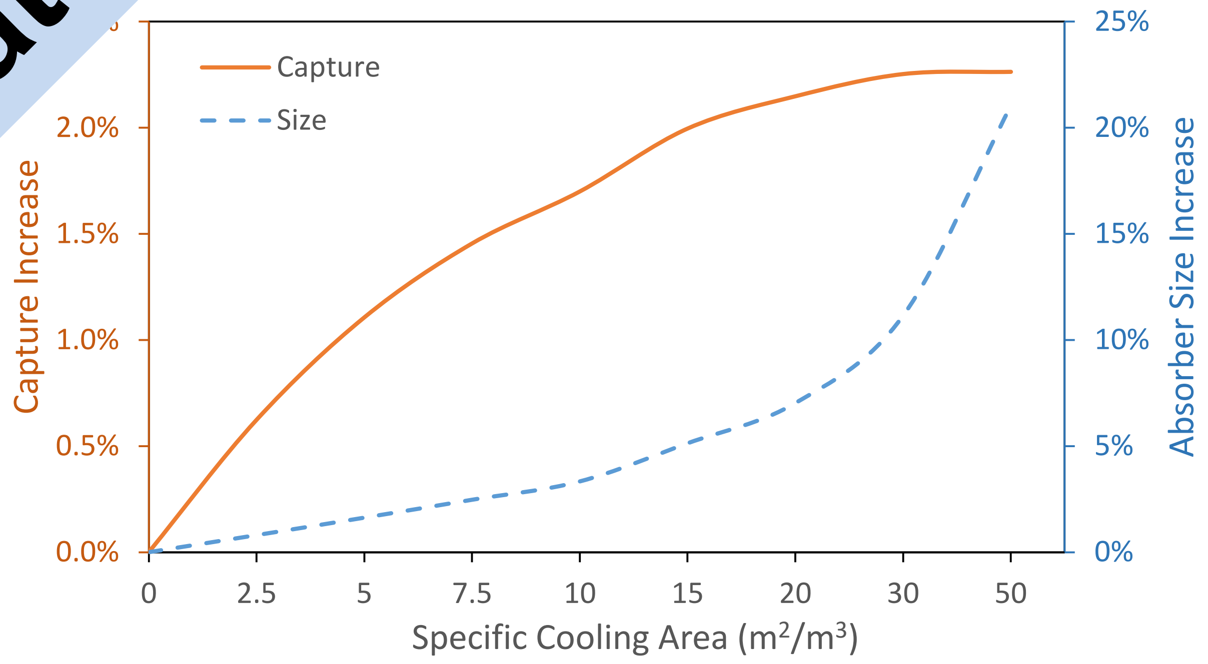
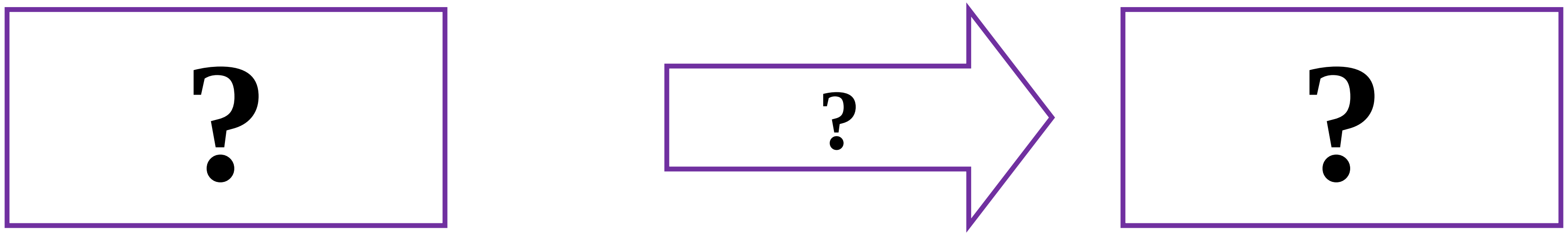
Geometry Matters!!



How do you solve physics problems?



Fridolin Okkels and Henrik Bruus, Scaling behavior of optimally structured catalytic microfluidic reactors, Physical Review E 75, 016301 2007
L.H. Olesen et al. A high-level programming-language implementation of topology optimization applied to steady-state Navier–Stokes flow, Int. J. Numer. Meth. Engng 2006; 65:975–1001

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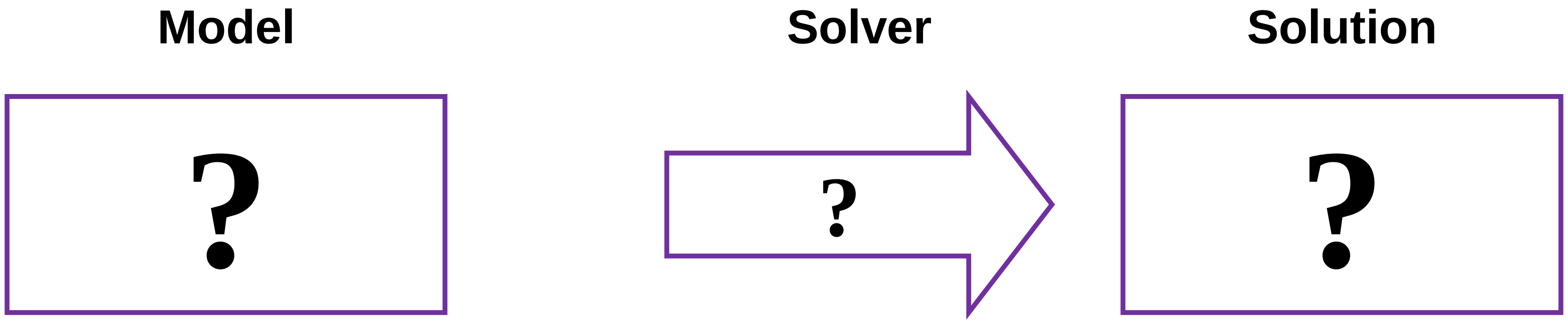

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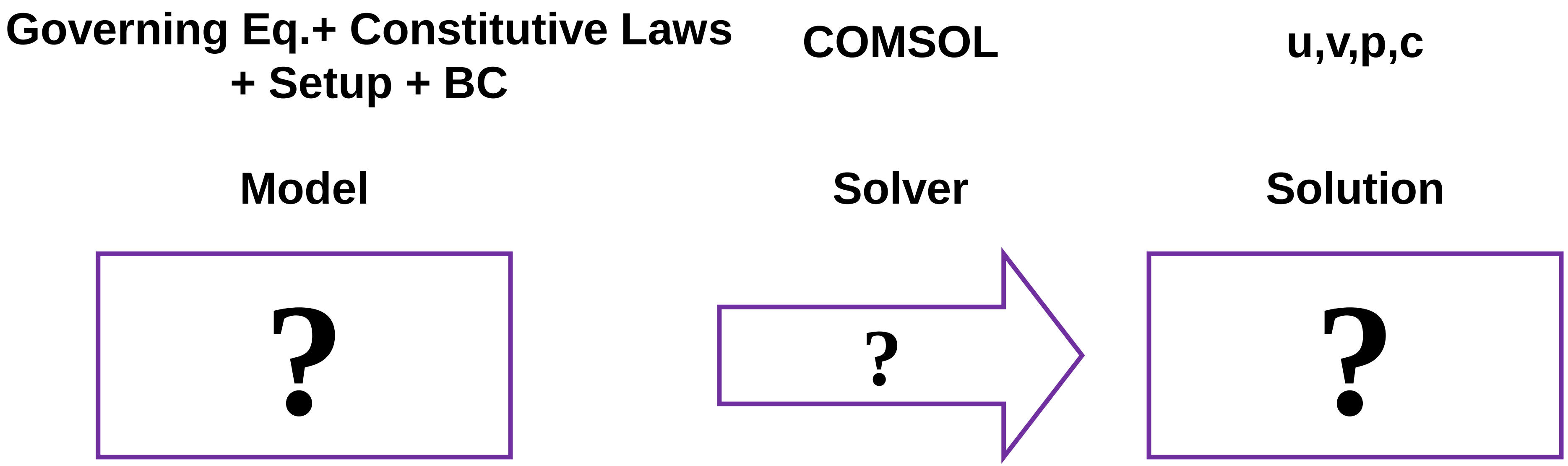

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How do you solve physics problems?

Governing Eq.+ Constitutive Laws + Setup + BC	COMSOL	u,v,p,c
Model	**Solver**	**Solution**
?	? →	?
e.g. NS + CDR+ BC + <u>Goal</u>	TOPOPT	<u>Best</u> design

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How do you solve physics problems?

normally

Model	Solver	Solution
Governing Eq.+ Constitutive Laws + Setup + BC	COMSOL	u,v,p,c
?	?	?
e.g. NS + CDR+ BC + <u>Goal</u>	TOPOPT	<u>Best</u> design

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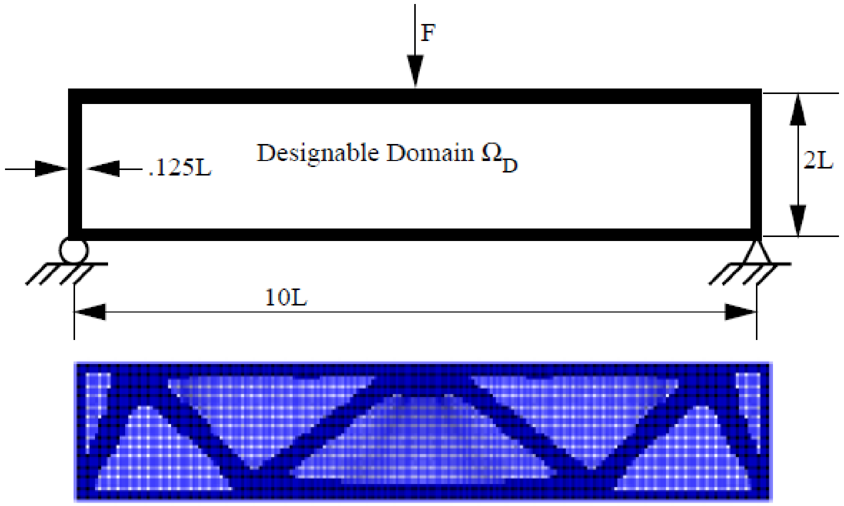
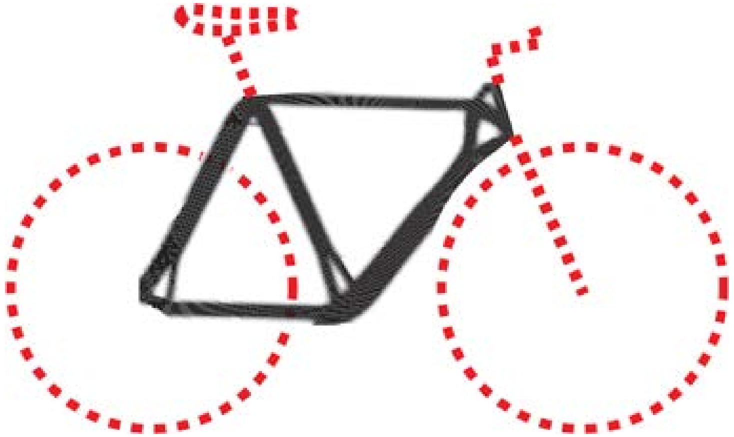
Fundamentals of Topology Optimization





$\gamma = 0$, Solid
$\gamma = 1$, Void

M.P.Bendsøe and O. Sigmund, *Topology Optimization - Theory, Methods and Applications*, Springer (2003)

Topology Optimization in Aircraft Design

"…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/

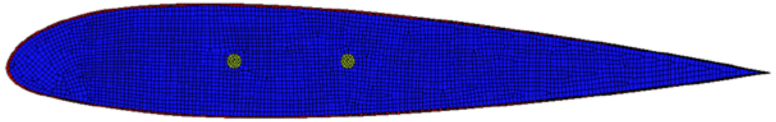


Figure 5.a. Topology optimization design space for 2D airfoil test case.

Figure 5.b Topology optimization results for simple 2D airfoil test case.

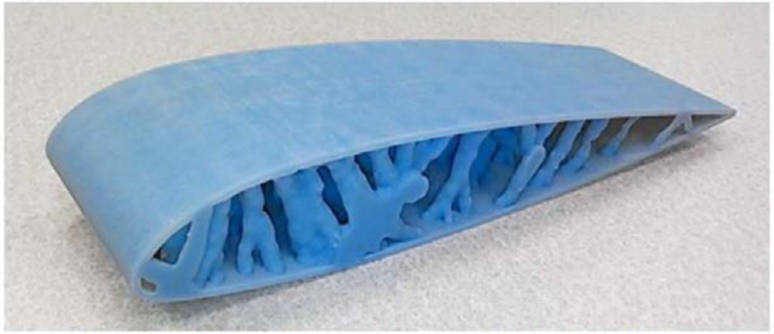


Figure 7. 3D printed wing section for a NACA 23015 airfoil.

D. Walker et al. *Topology Optimization of an Aircraft Wing,* 56th AIAA/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference

Fundamentals of Optimization Problems

- Optimization Problem = Inverse Problem

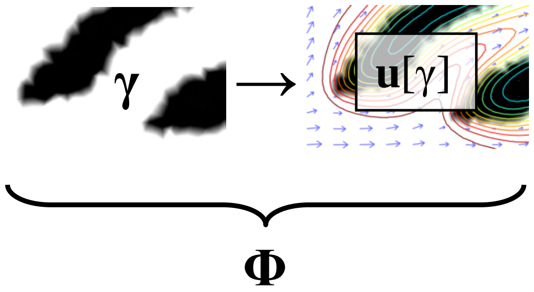
Tune the design-variables (γ) of a problem, such that an objective function (Φ) is minimized, under given constrains.

- Design variables: $\gamma(\vec{\mathbf{r}}) \qquad \mathbf{u}[\gamma]$

- Objective function: $\min\limits_{\gamma} \; \Phi\big(\mathbf{u}[\gamma], \gamma\big)$

- Constrains: $g\big(\mathbf{u}[\gamma], \gamma\big) \leq 0$

$$0 \leq \gamma(\mathbf{r}) \leq 1$$



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

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

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

Then the reacting flow problem can be written as:

$$\mathbf{\nabla} \cdot \mathbf{\Gamma}_i = F_i \qquad \text{in } \Omega,$$

$$R_i = 0 \qquad \text{on } \partial\Omega, \qquad \textit{Dirichlet b.c.}$$

$$-\mathbf{n} \cdot \mathbf{\Gamma}_i = G_i + \sum_{j=1}^{3} \frac{\partial R_j}{\partial u_i} \mu_j \qquad \text{on } \partial\Omega, \qquad \textit{Neumann b.c.}$$

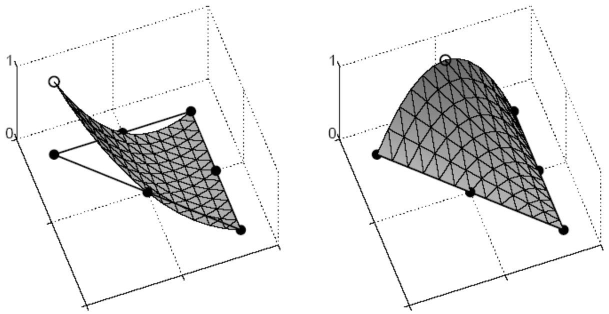
The Finite Element Method (FEM)

- Expand both u and γ on a finite basis set

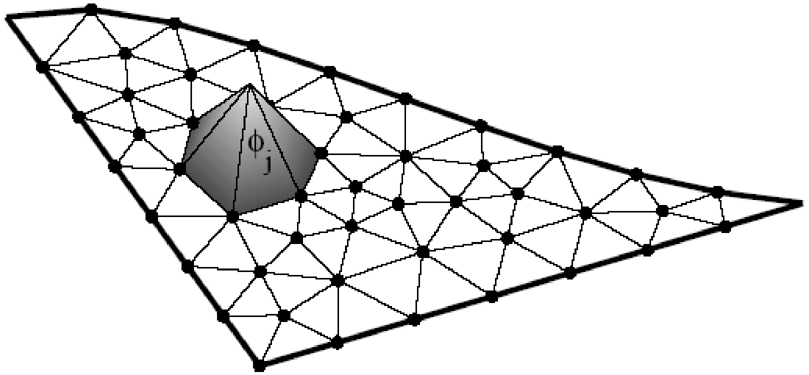
$$u_i(\mathbf{r}) = \sum_n u_{i,n}\, \varphi_{i,n}(\mathbf{r}) \qquad\qquad \gamma(\mathbf{r}) = \sum_n \gamma_n\, \varphi_{4,n}(\mathbf{r})$$

- Use *P*1 basis for *p*(r), c(r) and γ(r)

- Use *P*2 basis for u(r)



Finite element mesh;
basis function φ_j has small support

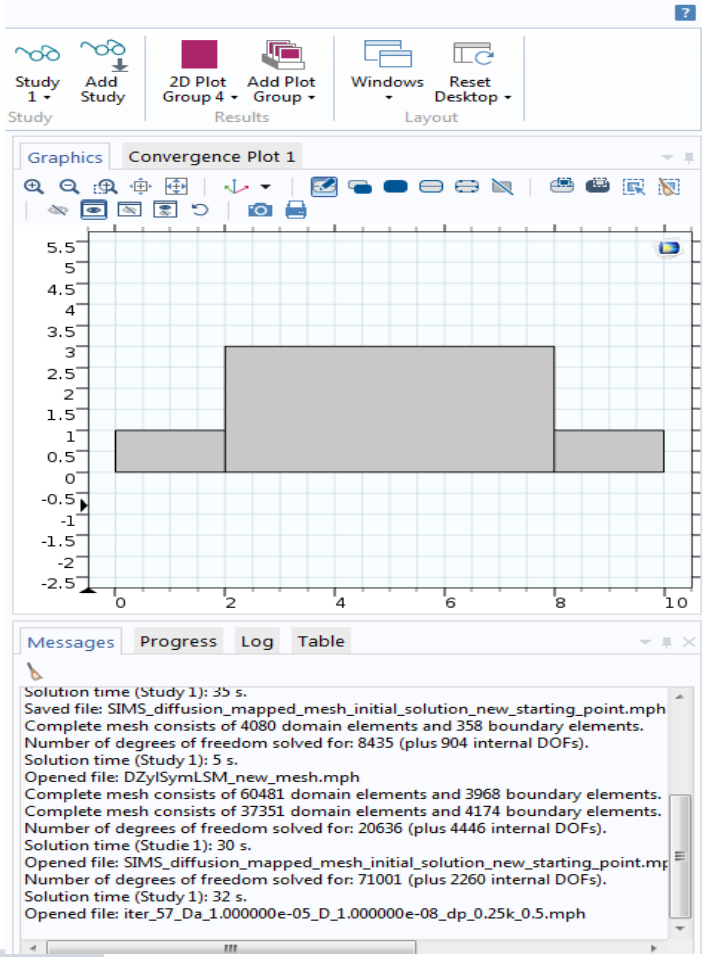


Constrained optimization problem

- Minimize objective function Φ(u) subject to constraints

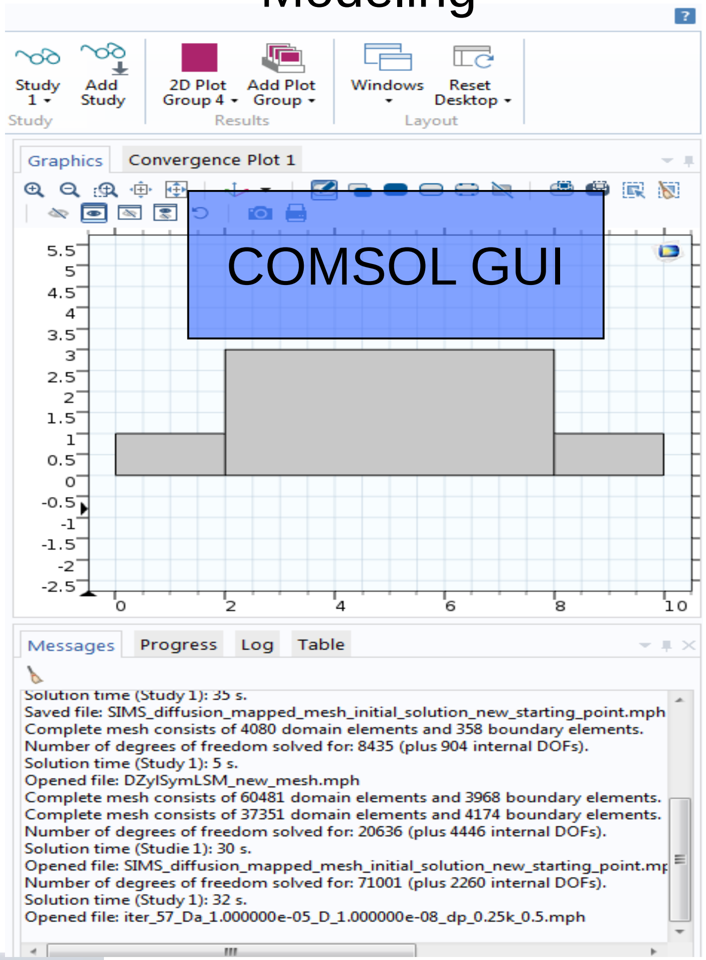
$$
\begin{aligned}
&\min_{\gamma}\ \Phi(\mathbf{u},\gamma) && \\
&\text{subject to}\quad \int_{\Omega}\gamma(\mathbf{r})\,\mathrm{d}\mathbf{r}-\beta\,|\Omega|\le 0, && \textit{Volume constraint}\\
&\qquad 0\le\gamma(\mathbf{r})\le 1, && \textit{Design variable bounds}\\
&\qquad \boldsymbol{\nabla}\cdot\boldsymbol{\Gamma}_i = F_i, && \textit{Governing equations}\\
&\qquad R_i = 0, && \textit{Dirichlet b.c.}\\
&\qquad -\mathbf{n}\cdot\boldsymbol{\Gamma}_i = G_i+\sum_{j=1}^{3}\frac{\partial R_j}{\partial u_i}\mu_j, && \textit{Neumann b.c.}
\end{aligned}
$$

Setup and procedure for micro-reactor



Setup and procedure for micro-reactor

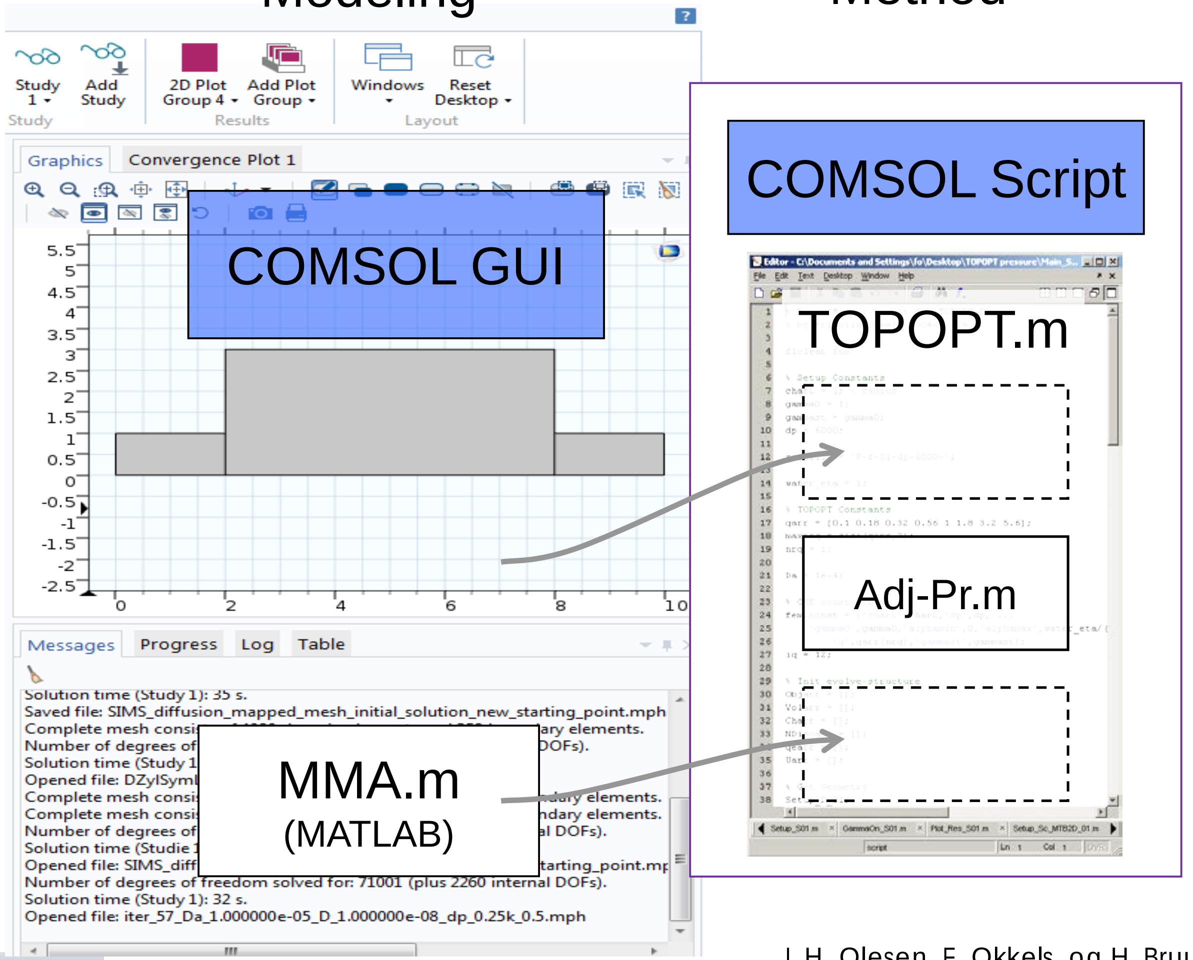
Modeling



Setup and procedure for micro-reactor

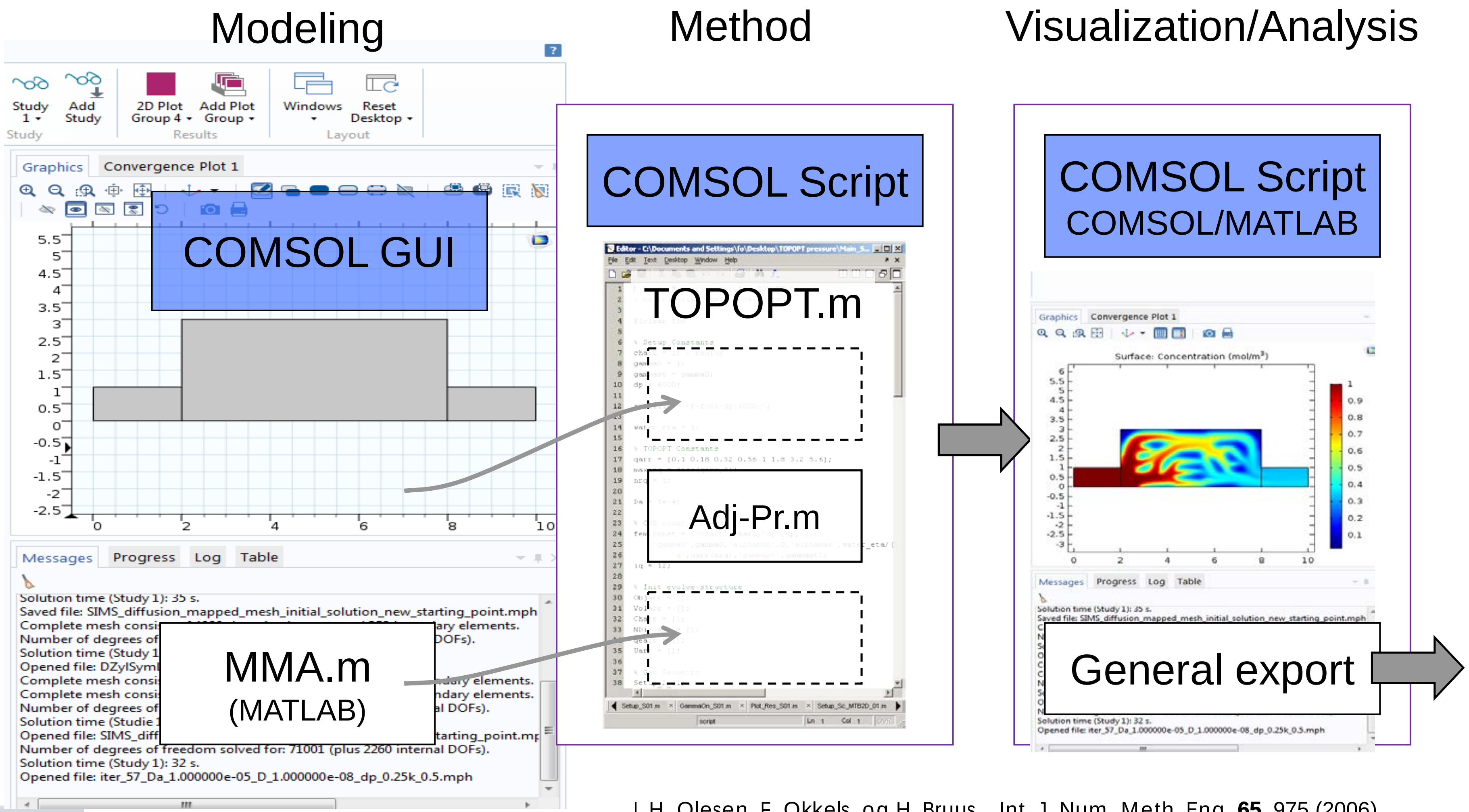
Modeling

Method



L.H. Olesen, F. Okkels, og H. Bruus, Int. J. Num. Meth. Eng. **65**, 975 (2006)

Setup and procedure for micro-reactor



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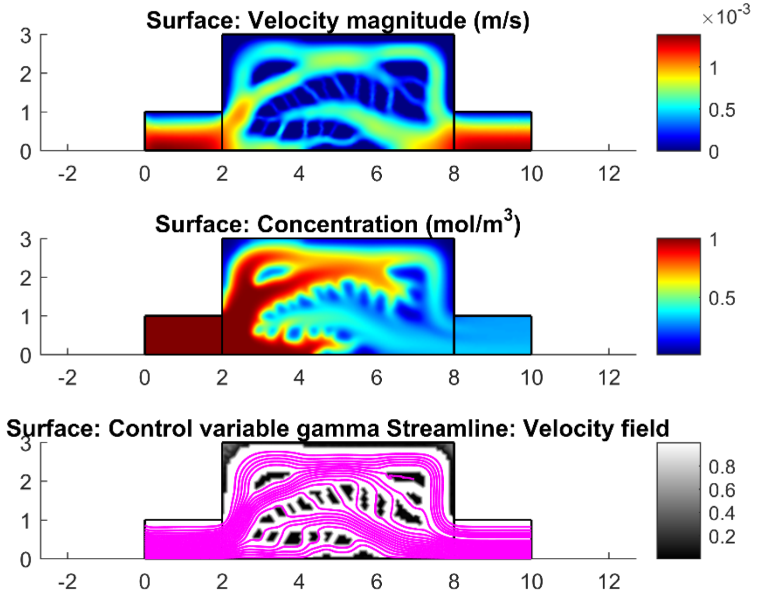
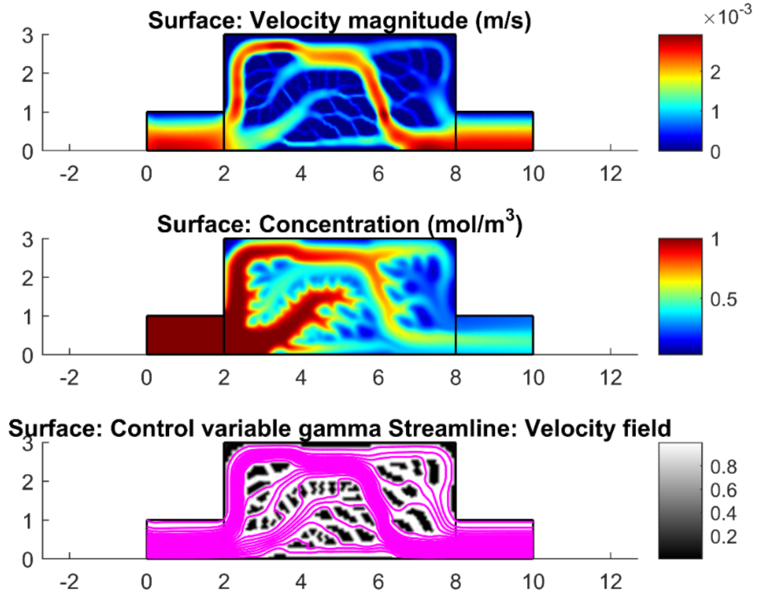
Topology Optimized Micro-Reactors

- Characteristic Examples



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

Iter=188

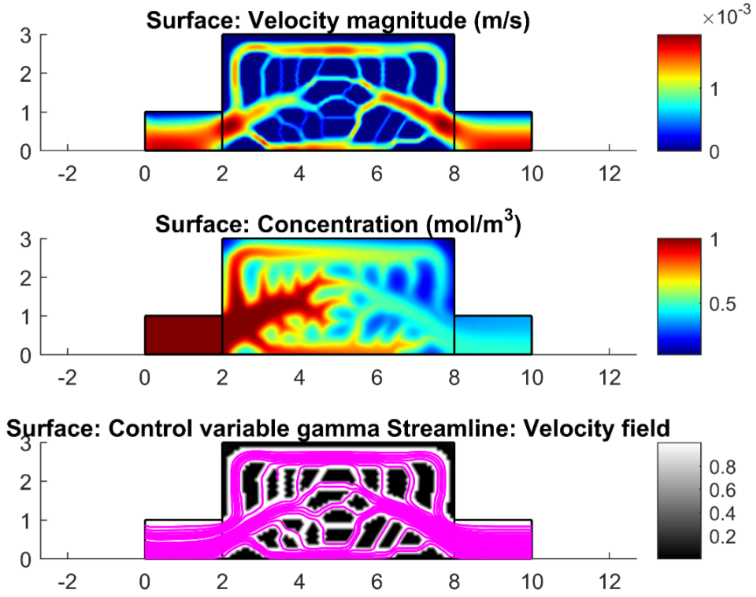


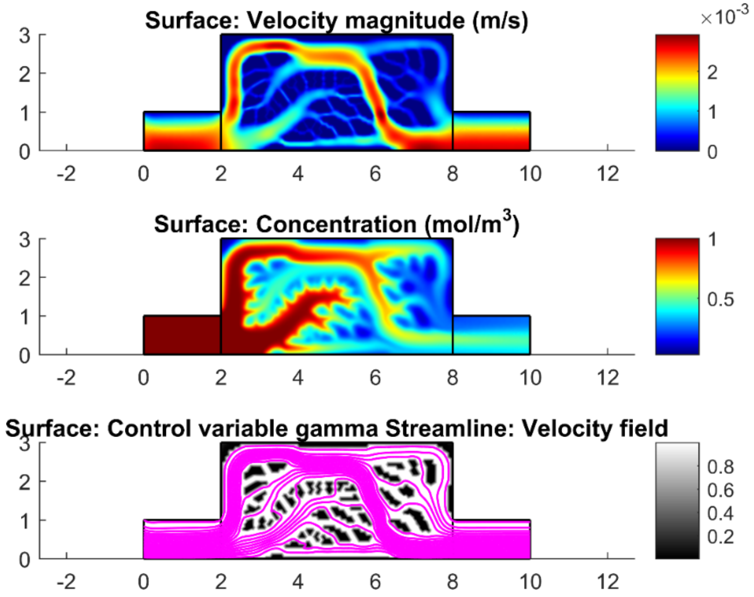
$$\mathrm{Da} = 10^{-5}, \mathrm{D} = 1 \cdot 10^{-8}\,\frac{\mathrm{m}^2}{\mathrm{s}}, \mathrm{dp} = 0.5\ \mathrm{Pa}, \mathrm{k_a} = 1$$

Iter=227

Topology Optimized Micro-Reactors

- Characteristic Examples





$$\mathrm{Da} = 10^{-5}, \mathrm{D} = 1 \cdot 10^{-8}\,\frac{\mathrm{m}^2}{\mathrm{s}}, \mathrm{dp} = 0.5\ \mathrm{Pa}, \mathrm{k_a} = 0.25$$

$$\mathrm{Da} = 10^{-5}, \mathrm{D} = 1 \cdot 10^{-8}\,\frac{\mathrm{m}^2}{\mathrm{s}}, \mathrm{dp} = 0.5\ \mathrm{Pa}, \mathrm{k_a} = 1$$

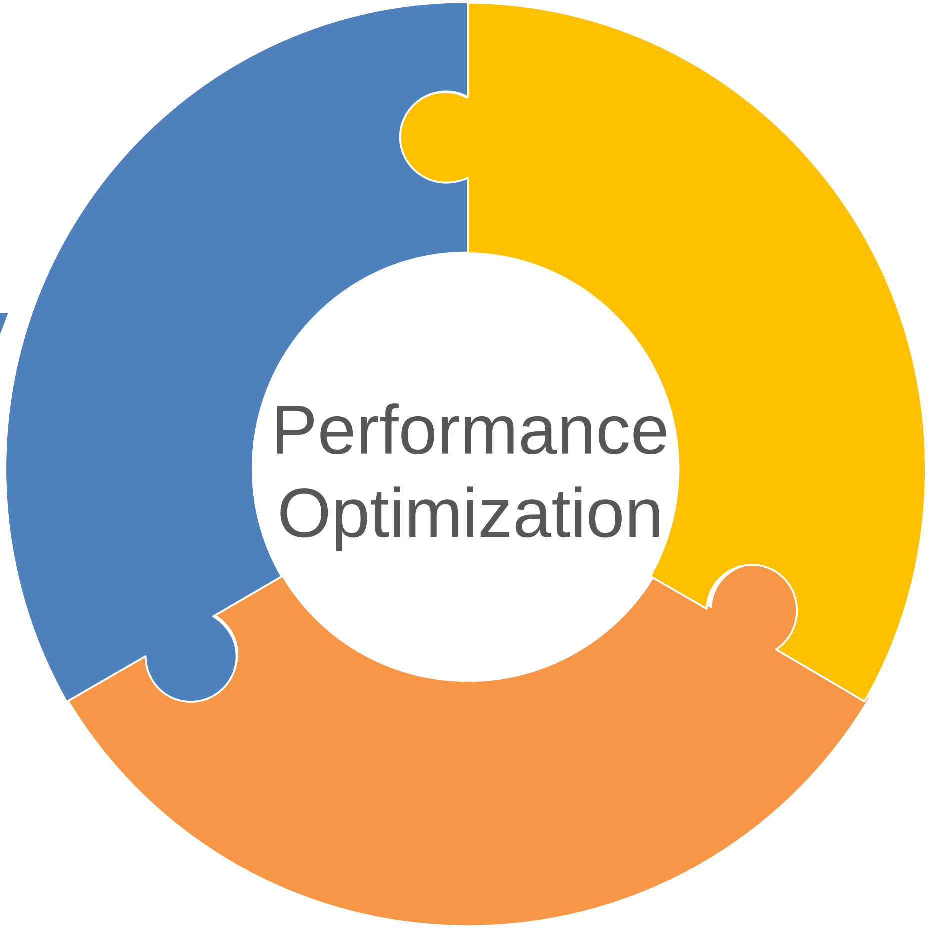
Iter=121

Iter=227

Partnership with ORNL and WVU

NETL
Local Information- High fidelity CFD

WVU
Process modeling



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

ORNL
Experimentation, manufacturing and testing

Moving Forward

MEA+Mellapak equivalent, to match literature performance

MEA+Intensified reactor Goal: improve packing with in situ continuous cooling (absorber) and heating (stripper)

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

- 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

Acknowledgements

Carbon Capture Simulation for Industry Impact (CCSI^2)

ORNL: Xin Sun, Costas Tsouris, Lonie Love, Canhai Lai

NETL: Michael Matuszewski, Benjamin Omell

WVU: Debangsu Bhattacharyya, Ryan Hughes, Goutham Kotamreddy

CCSI²

Carbon Capture Simulation for Industry Impact

For more information

https://www.acceleratecarboncapture.org/

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