LASER INDUCED POROUS GRAPHENE SPONGE

Capstone Spring 2015

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Motivation and Background
Motivation

Oil spills significantly impact:
• Wildlife habitats
• World economics
• Ecosystems
• Human Life
# Current Technology

<table>
<thead>
<tr>
<th>Polyurethane</th>
<th>Spongy graphene</th>
<th>CNT</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1" alt="Original sponge" /></td>
<td><img src="image2" alt="Coated sponge" /></td>
<td><img src="image3" alt="Image3" /></td>
</tr>
</tbody>
</table>

- **Polyurethane**
  - 30 grams of oil per gram of polymer
  - Selectivity if coated
  - Environmentally harmful
  - Complex processing for selectivity
  - High volume needed

- **Spongy graphene**
  - 70 grams of oil per gram of graphene
  - Excellent selectivity
  - Very expensive
  - Not scalable manufacturing
  - Very low density
  - Poor mechanical properties

- **CNT**
  - 80 grams of oil per gram of CNT
  - Excellent selectivity
  - Very expensive
  - Complex, resource intensive processing
  - Very low density

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Laser-Induced Graphene

- Laser ablation of polyimide
- Controllable properties
- Cost effective and scalable

$\lambda \approx 10.6 \, \mu m$
Design Goals
Main Objective:
Design a LIG sponge for oil sorption

Design Goals:
- Develop atomistic model to understand nanoscale interaction of oil-graphene
- Develop model to understand bulk fluid flow of oil through porous graphene
- Determine a relationship between LIG pore size and oil sorption
Technical Approach: Nanoscale Modelling
Simulation Design

The image cannot be displayed. Your computer may not have enough memory to open the image, or the image may have been corrupted. Restart your computer, and then open the file again. If the red x still appears, you may have to delete the image and then insert it again.
Simulation Results

[Graph showing atomic distribution with distance [Å], time points at t=0, t=25 fs, and t=1000 fs.]

[Graph showing distance per graphene atom vs. diameter [Å].]

[Graph showing molecules per carbon vs. time [fs], with different pore radii: 16 Å, 13 Å, 7 Å, 4 Å.]
Simulation Results

~600 stretched graphene atoms
Technical Approach:
Fluid Flow Modelling
Fluid Flow Modeling Background

Goal:
Implement Darcy’s Law to understand bulk fluid flow through porous media.

\[
\left( \frac{\partial^2 \Psi}{\partial X^2} + \frac{\partial^2 \Psi}{\partial Y^2} \right) = -\omega \\
U \frac{\partial \omega}{\partial X} + V \frac{\partial \omega}{\partial Y} = \frac{\varepsilon}{Re} \left( \frac{\partial^2 \omega}{\partial X^2} + \frac{\partial^2 \omega}{\partial Y^2} \right) - \frac{\varepsilon^2}{DaRe} \omega - \frac{F \varepsilon^2}{\sqrt{Da}} \| \mathbf{v} \| \omega
\]

Key Assumptions:
- Air omitted from inside porous graphene (space initially empty)
- Effects of gravity are omitted

\( \Psi = \) stream function; \( X, Y = \) coordinates; \( \omega = \) vorticity; \( Da = \) Darcy Number; \( F = \) geometric function; \( U, V = \) interstitial velocity components; \( \varepsilon = \) porosity; \( Re = \) Reynolds Number; \( \mathbf{v} = \) velocity vector;
(all variables are dimensionless)
Results From Fluid Flow Modelling

![Diagram showing fluid flow models with low and high conditions](image-url)
Technical Approach: Experimentation
Experimental Procedure

1. Weigh original sample (LIG+PI)
2. Place sample partially in octane
3. Weigh saturated sample
4. Subtract for mass of LIG
5. Weigh remainder of PI
6. Exfoliate graphene from PI
Experimental Findings

Graphene wetting characteristics

- Verified oleophilic behavior
- Verified hydrophobic behavior

Capillary within graphene

- Increases absorption allowing captured gases to exit the system

Linear octane absorption v. time

- Supports graphene sheet spacing is too small for alkane bulk absorption

Water | Octane | Oil

**Linear octane absorption v. time**

![Graph showing linear relationship between oil sorption and time.](attachment:oil_sorption.png)

- Experimental: $y = 0.36x + 3.78$
- $R^2 = 0.8169$
Conclusion
Conclusions

- LIG currently has a lower oil absorption than other carbon-based oil sponge technologies
- Oil sorption is independent of porosity
- The interlayer spacing in the graphene is too small to allow bulk absorption
- Octane layers form over graphene surface
- Current LIG sponge technology has potential if device is open on both sides
Future Work

- Compare oil sorption of LIG with different pore characteristics
- Fabricate ideal design using open backside of LIG
- Test sorption with crude oil
- Investigate mechanical stability during sorption and recovery
- Investigate LIG samples with graphene sheet spacing greater than 3.4 Å
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• UMD Deepthought
• UMD OTC

for their guidance, resources, and time.
## BP Deepwater Horizon Oil Spill

<table>
<thead>
<tr>
<th>Method</th>
<th>Cost</th>
<th>Volume</th>
<th>Selectivity</th>
<th>Recovery</th>
<th>Environmentally Safe</th>
</tr>
</thead>
<tbody>
<tr>
<td>Corexit 9500</td>
<td>~$1 billion*</td>
<td>~21.1 m³*</td>
<td>Yes</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>Polyurethane</td>
<td>$0.513 billion**</td>
<td>~902,000 m³**</td>
<td>No</td>
<td>No</td>
<td>Yes</td>
</tr>
<tr>
<td>CNT sponge</td>
<td>$91.3 billion***</td>
<td>~43,500 m³***</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>LIG sponge</td>
<td>$2.52 billion***</td>
<td>~2,640 m³***</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
</tbody>
</table>

What this table neglects:
- Corexit is dispersant which breaks down oil into smaller pieces to be further broken down by microbes
- Spongy graphene can be reused at least 10 times with >99% capacity
- LIG can approximately retrieve 80% of oil back. In the case of the BP oil spill over $300 million.

* - No specification of oil dispersed  
** - Assumption: polyurethane only absorbed oil  
*** - Assuming each unit of volume is used 10 times  

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<tr>
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<td>Polyurethane</td>
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<td>★★★★★</td>
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