Charaterizing Biomass Feedstock Transport Properties Using State of the Art Imaging and Computational Techniques

Meagan F. Crowley1, Hariswaran Sitaraman2, Jordan Klinger3, Francois Usseglio-Viretta4, Nicholas E. Thornburg5, Nick Brunhart-Lupo6, M. Brennan Pecha1, Yidong Xia3, and Peter N. Ciesielski1


Abstract

The microstructure of lignocellulosic biomass determines heat and mass transfer during conversion processes. We present a novel method for characterizing the transport properties of biomass using advanced imaging and computational techniques. The microstructure of two woody feedstocks, red oak and Douglas fir, before and after pyrolysis, is revealed using X-ray computed tomography (XCT). Transport properties are calculated from the XCT images, and principal permeability tensors are calculated using an immersed boundary-based finite volume solver to model gas flow through the geometries. We observe that the permeabilities of native biomass are distinctly anisotropic, however, this anisotropy is greatly reduced after pyrolysis.

Methods

- 3D pore microstructure of native and pyrolyzed red oak and Douglas fir imaged using X-ray Computed tomography and software reconstruction
- 1mm³ sub-volumes imported into Mesoflow, a compressible finite-volume solver developed on the AMReX library. (Zhang et al, 2019) for CFD simulations
- Permeability was computed from simulations using the Navier-Stokes momentum balance:
  \[ \frac{\partial \mathbf{p}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{p} = -\nabla \cdot \mathbf{F} + \mathbf{S} \]
  (1)
  \[ \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \frac{1}{ho} \nabla \cdot \mathbf{F} + \mathbf{S} \]
  (2)
- The equations are closed using ideal gas law, total energy, and Newtonian fluid assumption:
  \[ P = \rho RT \]
  \[ \rho = \frac{\partial \mathbf{p}}{\partial \mathbf{u}} + \frac{1}{2} \mathbf{u} \cdot \nabla \mathbf{u} \]
  \[ \varepsilon = \frac{\partial \mathbf{u}}{\partial \mathbf{p}} \]
- Void fraction, tortuosity calculated using the open-source software tool MATBOX:
  \[ \varepsilon = \frac{1}{N} \sum_{k=1}^{N} \varepsilon_k \text{with } \varepsilon_k = \begin{cases} 1 & \text{if } \varepsilon_k \in \text{phase } k \\ 0 & \text{if } \varepsilon_k \notin \text{phase } k \end{cases} \]
- The tortuosity, \( \tau \), along direction \( i \) is solved for according to Equation 9:
  \[ \frac{\partial \mathbf{u}_i}{\partial x_i} = \varepsilon \frac{\partial \mathbf{u}_0}{\partial x} \]

Table 1. Calculated permeability tensors for each sample. All values in units of m².

<table>
<thead>
<tr>
<th>Property</th>
<th>Native Red Oak</th>
<th>Pyrolyzed Red Oak</th>
<th>Native Douglas Fir</th>
<th>Pyrolyzed Douglas Fir</th>
</tr>
</thead>
<tbody>
<tr>
<td>Void Fraction</td>
<td>0.73</td>
<td>0.87</td>
<td>0.66</td>
<td>0.77</td>
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<tr>
<td>Longitudinal tortuosity factor</td>
<td>1.13</td>
<td>1.16</td>
<td>1.26</td>
<td>1.08</td>
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<tr>
<td>Radial tortuosity factor</td>
<td>2.47</td>
<td>1.29</td>
<td>16.7</td>
<td>1.99</td>
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<tr>
<td>Tangential tortuosity factor</td>
<td>6.00</td>
<td>1.39</td>
<td>38.5</td>
<td>4.02</td>
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<tr>
<td>Longitudinal effective diffusivity multiplier</td>
<td>0.62</td>
<td>0.75</td>
<td>0.52</td>
<td>0.71</td>
</tr>
<tr>
<td>Radial effective diffusivity multiplier</td>
<td>0.29</td>
<td>0.67</td>
<td>0.04</td>
<td>0.38</td>
</tr>
<tr>
<td>Tangential effective diffusivity multiplier</td>
<td>0.12</td>
<td>0.62</td>
<td>0.02</td>
<td>0.19</td>
</tr>
</tbody>
</table>

Table 2. Calculated void fraction, directional tortuosity factors of the void phase, and directional effective diffusivity multipliers of each species before and after pyrolysis.

Results & Discussion

- Microstructure is species-specific (Ciesielski et al 2015)
  - Native red oak = fine pore structure of fiber cells with large-diameter vessel cell channels characteristic of hardwoods
  - Native Douglas fir = highly regular pore structure with arrays of axial tracheids characteristic of softwoods.
- Longitudinal direction is the dominant avenue for mass and heat transport in both native Douglas fir and red oak samples
- highest permeability and lowest tortuosity = path of least resistance
- Thermal treatment affects microstructure of both species:
  - pore structure degrades
  - void volume increases
  - directional anisotropy reduces
- These trends are reflected in the reduction in the directional anisotropy for void fraction, tortuosity, and permeability in both Douglas fir and Native oak samples.
- The values for permeability, tortuosity, and void fraction can be a useful touchstone for the bioenergy community to improve the fidelity of conversion models by explicitly including species-specific transport properties.

Figure 1. Diagram of XCT workflow. (a) Initial particle, native red oak photograph. (b) Raw image slice from XCT radiograph. (c) 3D reconstruction of the full particle from the raw images. (d) Cropped sub-volume used for numerical analysis and calculation of material properties.

Figure 2. Sub-volumes of each sample with longitudinal, radial, and tangential slices. (a) Native red oak sub-volume, (b) Pyrolyzed red oak sub-volume, (c) Native Douglas fir sub-volume, (d) Pyrolyzed Douglas fir sub-volume, Longitudinal slices of (e) Native red oak, (f) Pyrolyzed red oak, (g) Native Douglas fir, (h) Pyrolyzed Douglas fir, Radial slices of (i) Native red oak, (j) Pyrolyzed red oak, (k) Native Douglas fir, (l) Pyrolyzed Douglas fir, Tangential slices of (m) Native red oak, (n) Pyrolyzed red oak, (o) Native Douglas fir, (p) Pyrolyzed Douglas fir. All scale bars 400μm length.

Figure 3. Steady state visualizations of permeability simulations for native and pyrolyzed Douglas fir and red oak XCT sub-volumes. In each case, pressure gradients were applied to only one of the longitudinal, radial, or tangential directions. Velocity magnitudes below 10⁴ are not visualized, hence the partial renditions for native red oak in the radial and tangential directions.

References: