Characterizing the diffusion of select natural oils into wax systems with transmission Fourier-transform infrared spectroscopy

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INTRODUCTION

- Diffusion can be described as the rate of change in concentration of diffusant with respect to time.
- The diffusion coefficient or diffusivity parameter, D, is a proportionality constant unique to a system which can characterize the speed of the diffusion process.
- Units for diffusivity are in $\frac{m^2}{s}$.
- A larger diffusion coefficient means the diffusant moves more quickly through the substrate.
- The Beer-Lambert law states that as concentration of an analyte increases, so does the light absorbance of that substance. Thus, infrared absorbance can be used to measure the concentration of diffusant in a system.
- Collection of the infrared spectra of a system in timed increments can measure the change in absorbance in the bands characteristic to the diffusant, and by extension monitor the concentration.
- Plotting the maximum absorbance of the diffusant bands will give a diffusion curve that shows the concentration of the diffusant increasing and leveling out when the system equilibrizes.[1]
- Determining the slope of the initial steady rise of concentration of diffusant can give the diffusivity of the system.[2]
- Wax composition is detailed in Table 1.
- Limonene is a naturally occurring non-planar, non-polar molecule. The structure of limonene is shown in Fig. 1.

Table 1. *Wax composition by wax.*

Wax	Composition
Paraffin wax	Petroleum-derived hydrocarbon chains[3]
Beeswax	Hydrocarbon chains, fatty acids, esters[4]
Carnauba wax	Aliphatic esters and diesters[5]

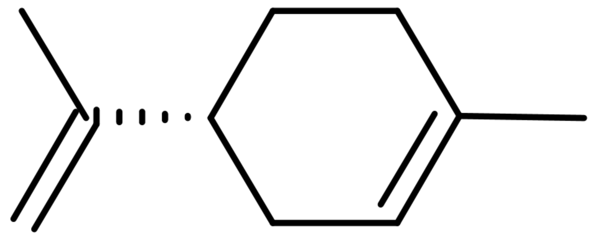

Figure 1. *The structure of limonene.*

METHODS

- There are three waxes used in this project, paraffin wax, carnauba wax, and beeswax.
- The diffusant used in every trial was limonene.
- The waxes were melted onto a cut glass microscope slide and topped with a similarly sized glass pane to allow the transmitted light to penetrate the system.
- After the introduction of limonene, a spectrum was collected every 15 minutes using a Bruker INVENIO FT-IR coupled with a Hyperion 3000 microscope.
- The background spectrum for each system was the spectrum of the two glass panes without wax between them.

RESULTS AND DISCUSSION

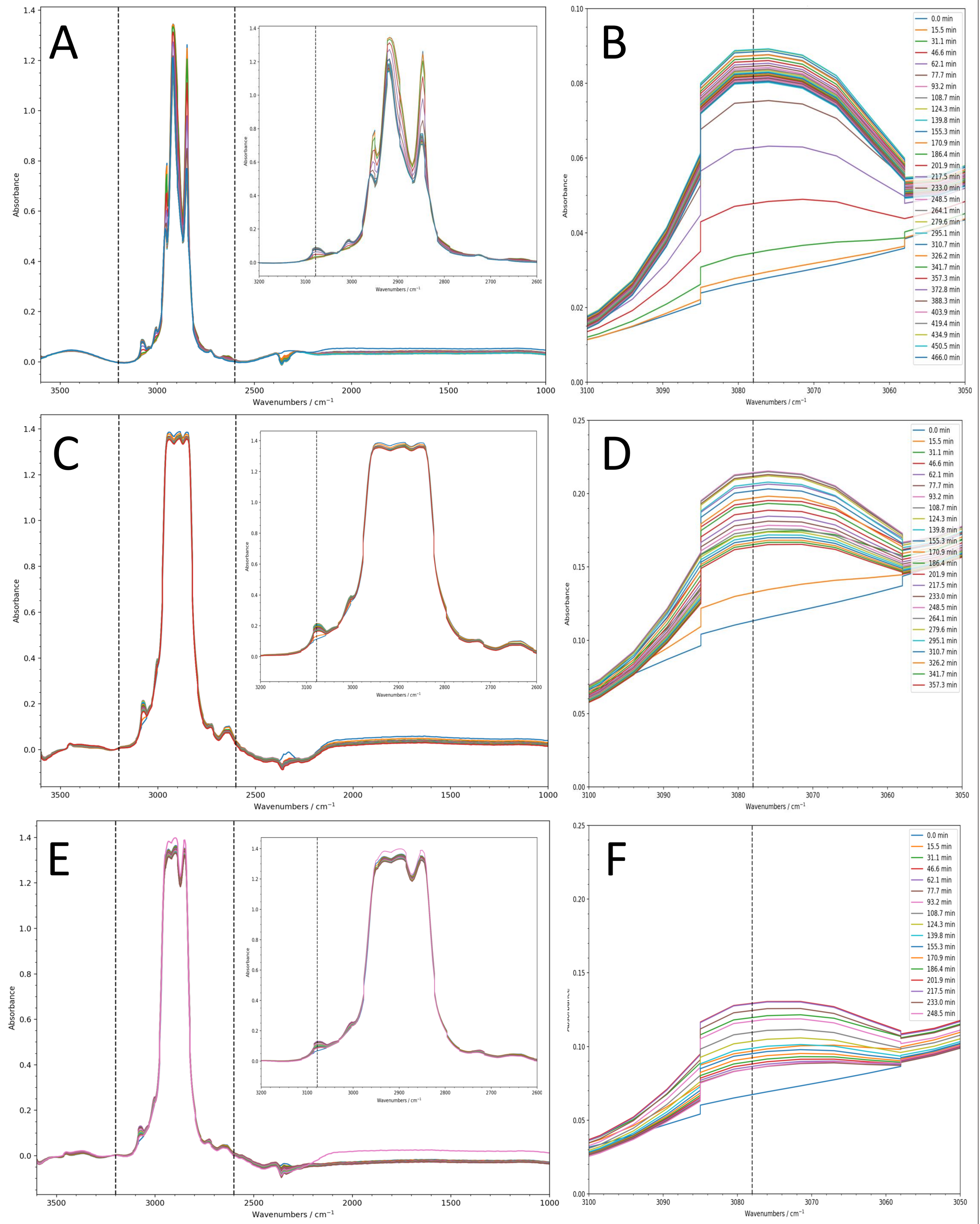

Figure 2. *The overlaid IR spectra of measurements taken 15 minutes (900 s) apart.* ***A)*** *The limonene/paraffin wax system full IR spectra with inlaid zoomed region.* ***B)*** *The changing limonene absorption band in limonene/paraffin wax.* ***C)*** *The limonene/beeswax system full IR spectrum with inlaid zoomed region.* ***D)*** *The changing limonene absorption band in limonene/beeswax.* ***E)*** *The full limonene/carnauba wax system full IR spectra with inlaid zoomed region.* ***F)*** *The changing limonene absorption band in limonene/carnauba wax.*

RESULTS AND DISCUSSION

- The "fingerprint" right-side region of the spectra acquired is hidden by the absorbance of IR light by glass (Figs. 2A, 2C, 2E).
- Limonene has an infrared absorbance band around 3100 cm^{-1}, which is still visible and lies outside the glass absorbance region, shown in Figs. 2B,2D, 2F. This band was used to track concentration over time.
- The maximum absorbance for the absorbance band is marked by the vertical line at 3079 cm^{-1} shown in Figs. 2B, 2D, 2F.

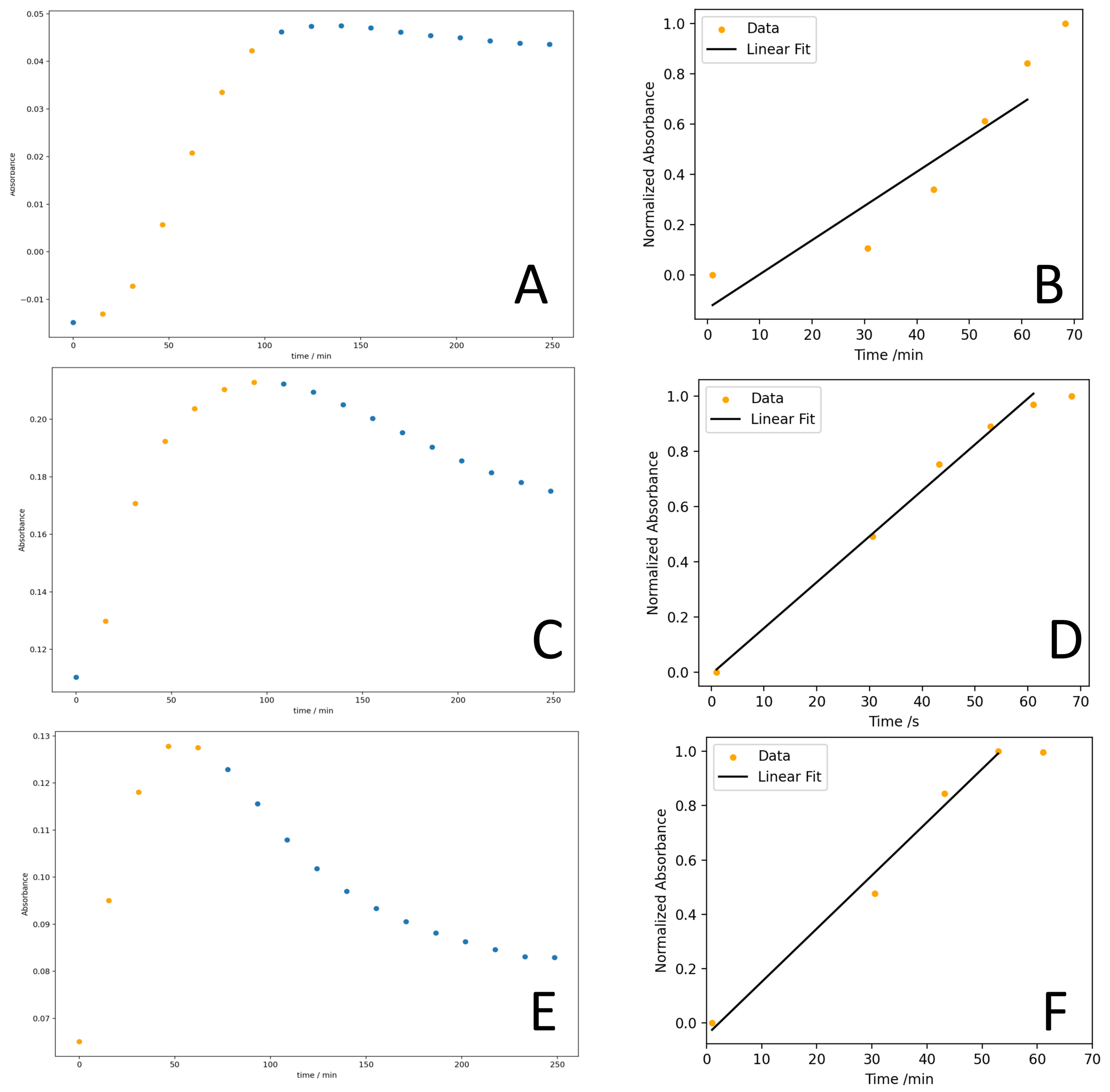

Figure 3. *The diffusion profiles of each limonene/wax system.* ***A)*** *Limonene/paraffin wax diffusion.* ***B)*** *Linear fitting of the initial diffusion in limonene/paraffin wax.* ***C)*** *Limonene/beeswax diffusion.* ***D)*** *Linear fitting of the initial diffusion in limonene/beeswax.* ***E)*** *Limonene/carnauba wax diffusion.* ***F)*** *Linear fitting of the initial diffusion in limonene/carnauba wax.*

- Plotting the absorbance values at this wavenumber verses time yields a diffusion profile which shows the gradual increase in concentration of limonene over time. These profiles are shown in Fig. 3A, 3C, 3E.
- By fitting the data points highlighted in orange linearly, a slope and intercept was determined for each system. The slopes are shown in Table 2.
- According to work by Fieldson and Barbari (1992), the diffusivity of a system can be determined by the slope of the initial diffusion.
- The determined diffusion coefficients are tabulated in Table 2.

RESULTS AND DISCUSSION

- The slowest diffusion was found to be the limonene/paraffin wax system.
- Paraffin wax has the most nonpolar composition and may interact with the limonene molecules more than the more polar waxes like carnauba and beeswax.
- A composite image of the limonene/paraffin wax system was taken by the coupled microscope before and after the limonene diffusion (Fig. 4).

Table 2. *Tabulated slope values and determined diffusion coefficients by system.*

Wax	Slope	D ($\frac{m^2}{s}$)
Paraffin wax	0.0133 ± 0.003	$1.782 \pm 0.1 \times 10^{-11}$
Beeswax	0.015 ± 0.002	$2.659 \pm 0.01 \times 10^{-11}$
Carnauba wax	0.020 ± 0.002	$3.690 \pm 0.02 \times 10^{-11}$

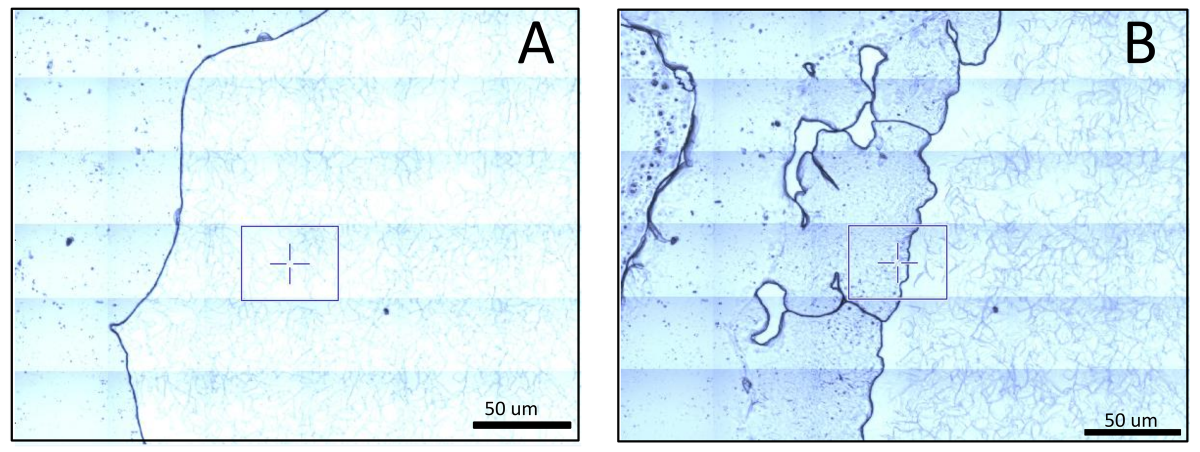

Figure 4. *The images of paraffin wax. The crosshair represents the position of the IR beam path.* ***A)*** *Image of the wax before the introduction of limonene.* ***B)*** *Image of the wax after the diffusion of limonene.*

CONCLUSION

- This experiment determined the diffusion coefficients of three wax and limonene systems by determining the slope of the initial diffusion profiles.
- The future of this project is to expand the characterization of wax and oil systems to other oils.

References

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