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Kinetics of PET alcoholysis using deep eutectic solvents for DOTP production

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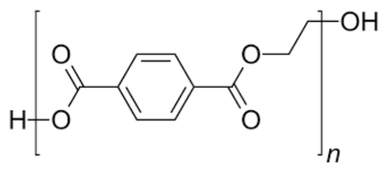
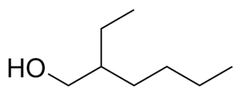
INTRODUCTION

- Plasticiser
- Green
- Non-toxic

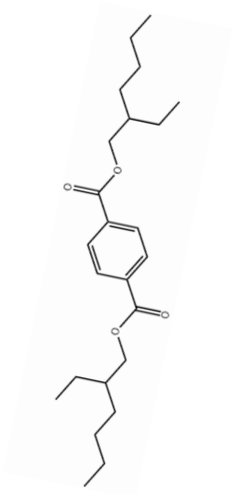


PET



2-ethylhexanol

ChCl/ZnAc anhydrous



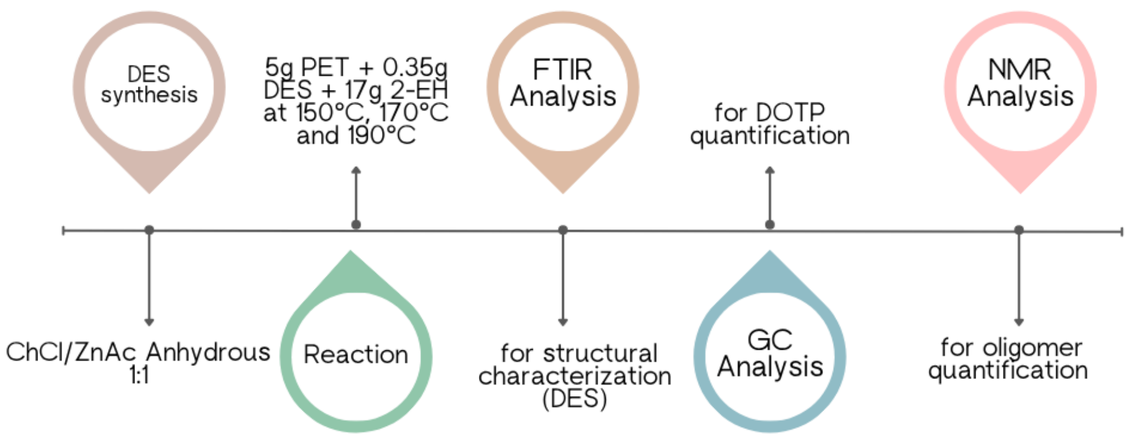
dioctyl terephthalate (DOTP)

- Literature reports a first order reaction [1].
- Model is done based on PET conversion only.
- However, the model does not correlate well with the DOTP concentration data.

AIMS

To develop a kinetic model that can explain not only PET degradation, but also DOTP concentration.

METHOD



Reported kinetic model:

$$PET \xrightarrow{k} DOTP$$

Proposed kinetic model:

$$PET \xrightarrow{k_1} Oligos \underset{k_{-2}}{\overset{k_2}{\rightleftarrows}} DOTP$$

Adapted From [2].

RESULTS & DISCUSSION

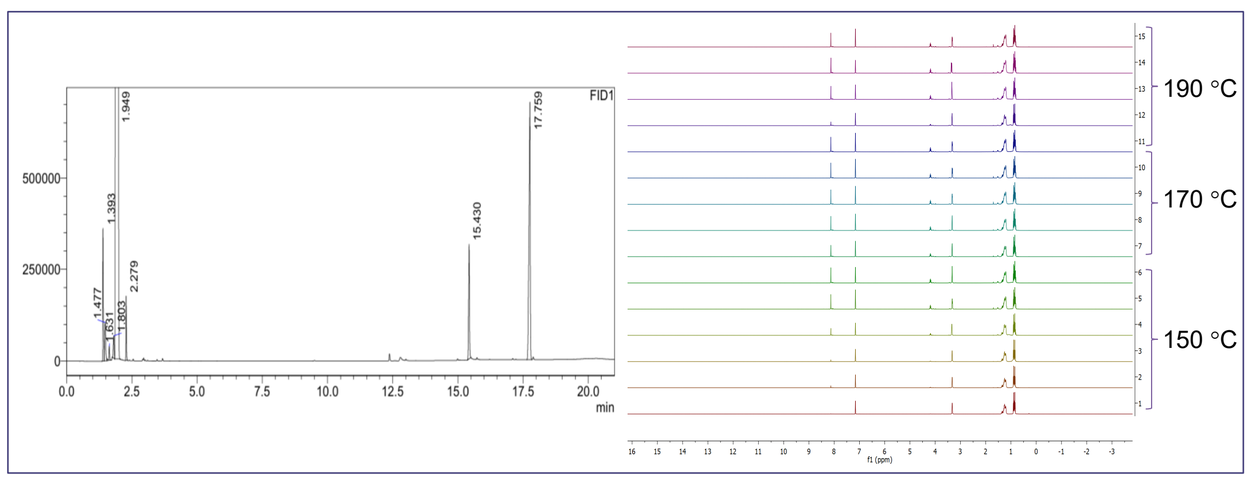


Figure 1. GC (left) and H^+ NMR (right) spectra.

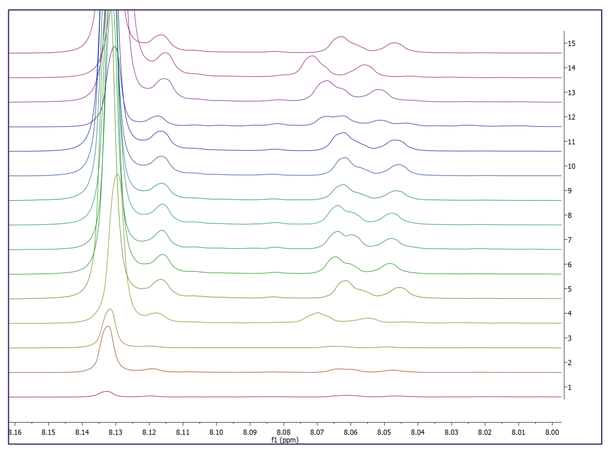


Figure 2. NMR spectrum showing stable oligomer presence.

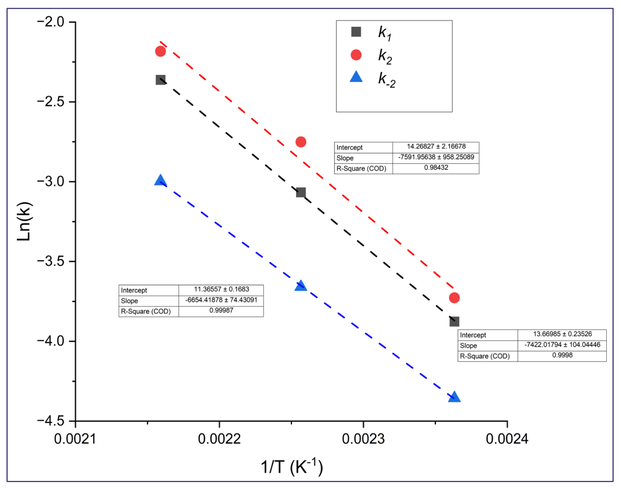


Figure 3. Arrhenius plots for proposed kinetic model.

Table 1. Activation energies.

Model		Ea, kJ/(mol K)
Proposed	k_1	61.7
	k_2	63.1
	k_{-2}	55.3
Reported	k	95.0
Reported (this work data)	k	82.9

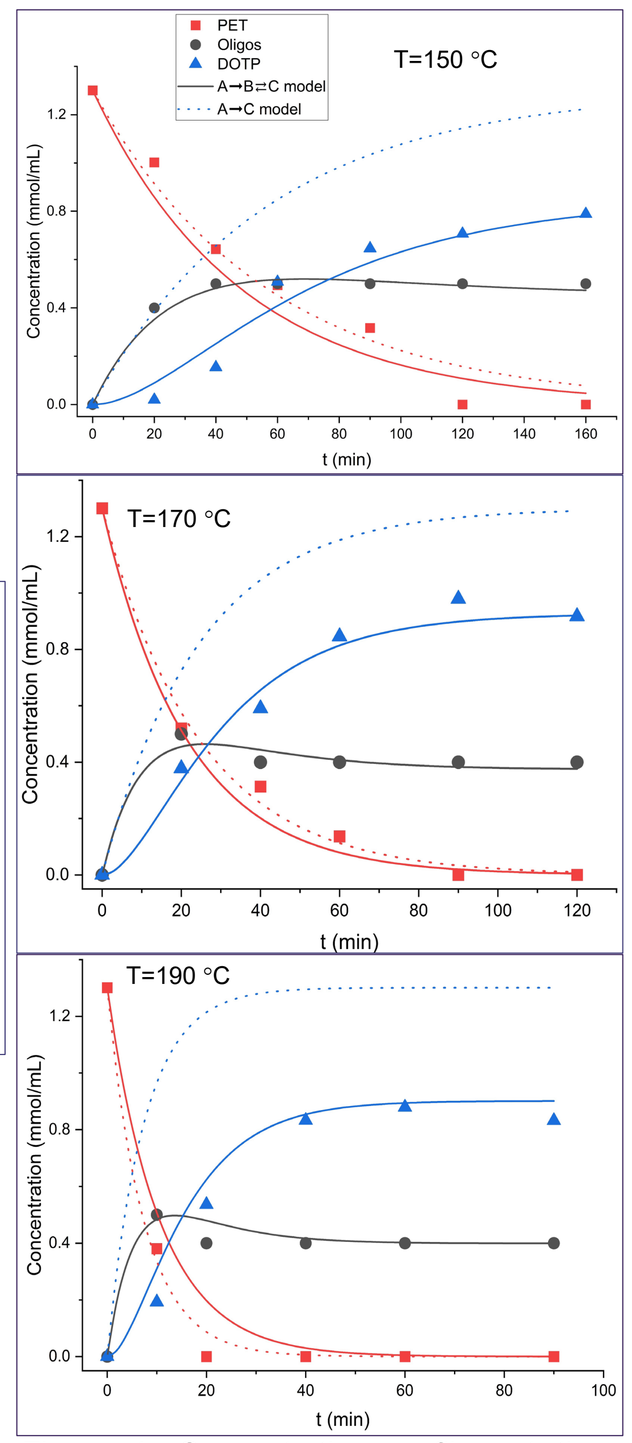


Figure 4. Concentration profiles at three different temperatures showing the proposed model being a better fit of the DOTP data. Oligomers data are potential data based on the model.

CONCLUSION

The formation of DOTP from PLA most likely follows a two-step consecutive reaction where the second step is a reversible reaction.

REFERENCES

[1] Zhou L, Lu X, Ju Z, Liu B, Yao H, Xu J, et al. (2019). Alcoholysis of polyethylene terephthalate to produce dioctyl terephthalate using choline chloride-based deep eutectic solvents as efficient catalysts. Green Chemistry, 21 (4): 897.

[2] Román-Ramírez LA, McKeown P, Jones MD and Wood J (2019). Poly(lactic acid) degradation into methyl lactate catalyzed by a well-defined Zn(II) complex. ACS Catalysis, 9 (1): 409.