# Study of Esterification Reactions in a Batch Reactor:

## Modeling the Industrial Synthesis of Benzoic Acid and Biodiesel

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## What exactly is esterification?

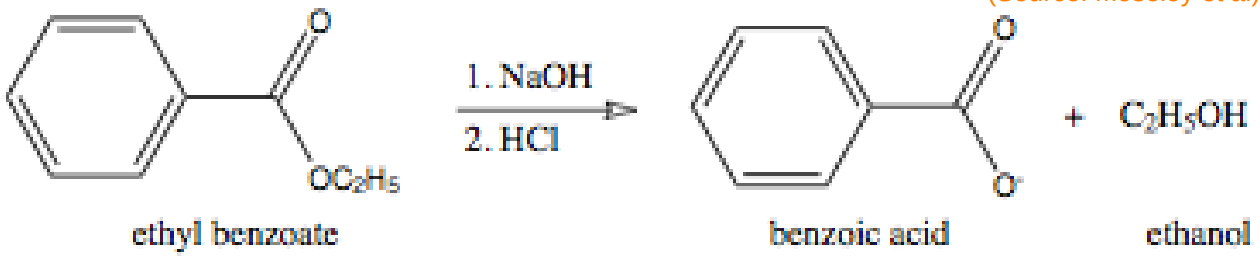
- Addition/removal of ester functional group to/from a molecule

## So, what's an ester?

- Functional group with the general formula R-CO-OR'
- Often scented

# De-esterification

(Source: Moseley et al)




- Motivation: Use the de-esterification of ethyl benzoate to benzoic acid as a model for the synthesis of APIs in a batch reactor
- Objective: Calculate the rate constant, k

# The Rate Constant (k)

$$R = k[EB]^2$$

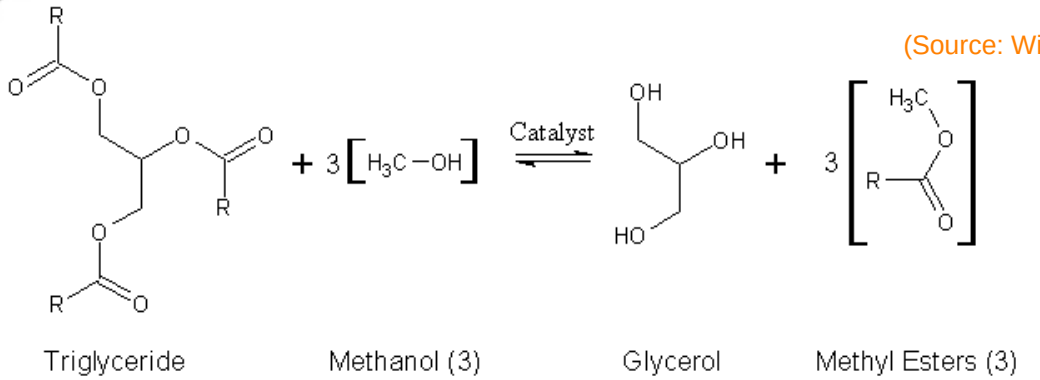
$$[EB] = \frac{[EB]_0}{1+[EB]_0 kt}$$

[EB] = Ethyl Benzoate concentration
$[EB]_0$ = concentration at t=0

- Describes how quickly a reaction proceeds
- Units vary depending on rate law
- Completely describes reaction on any scale

# Transesterification

(Source: Wikipedia)




- Motivation: Produce biodiesel by the transesterification of palm oil in batch reactor
- Objective: Calculate the % yield of the produced biodiesel

# Batch Reactor

- Multitude of sizes, functions, features
- Ours:
  - Closed system
  - Stirrer
  - Temperature controlled
  - Water jacket
  - Sampling tray
  - Condenser

**Why are these important?**

# Experimental Design

Batch Reactor

Add all ingredients except ethyl benzoate

Allow temperature to equilibrate, add ethyl benzoate

Take samples at designated times

Quench samples w/ HCl, record time

Agitate in vortex

Titrate sample, record ethyl benzoate concentration

Enter data into Solver, calculate k

# Experimental Design

Batch Reactor

Transesterification

Allow reaction to run overnight

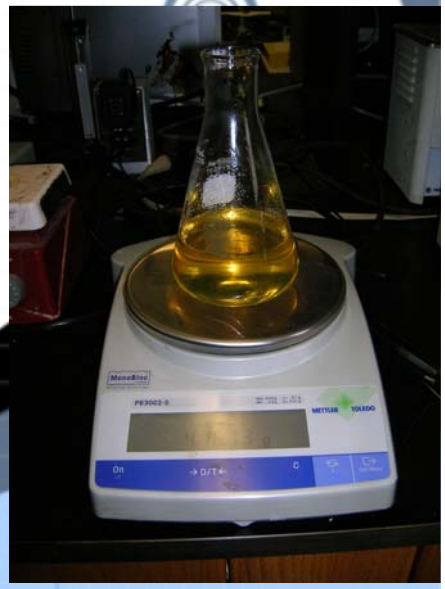
Turn off stirrer, allow products to separate

Remove top layer (biodiesel) using peristaltic pump

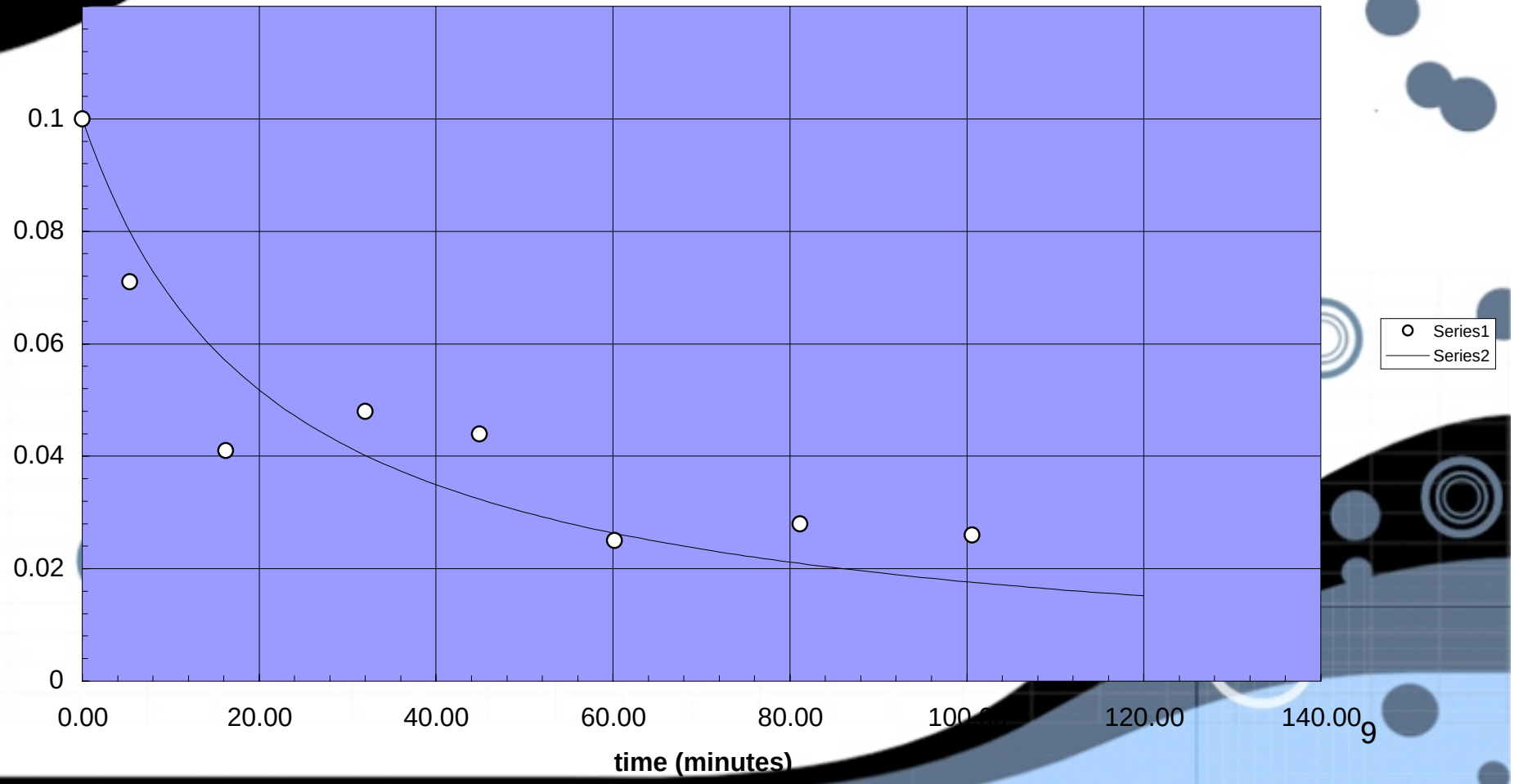
Use vacuum filtration system to purify biodiesel

Pass purified biodiesel through evaporator

Measure volume of final biodiesel product



# Results: Ethyl Benzoate



# Results: Biodiesel

- 92.8g biodiesel (filtered and evaporated)
  - 5% removed each time
- 115 mL (using average density)
- % Yield: 23.0%
  - Excess methanol prevented complete reaction (density)

# Why is all of this important?

- Familiarity with esterification
- Familiarity with batch reactors
- API production model
- Alternative energy

# Conclusions

- Our k value confirms Moseley's rate constant
- Successful production of biodiesel from palm oil
- Presence of water --> de-esterification
- Lack of water --> transesterification

# Conclusions (continued)

- Industrial esterification reactions can be accurately modeled on a small scale
- Problems with biodiesel
  - Shelf life
  - Cold flow properties
  - Not domestically producible on large scale

# Future Work: Biodiesel

- Moseley-like experiment with different conditions
- CSTR
- Soybeans? Vegetable? Other Oils!
  - Yields?
  - Energy efficiency?

# Future Work: Ethyl Benzoate

- Repetition, Repetition, Repetition
- Confirm Moseley's results
- Different Reactors
- Different reactants --> Real API synthesis

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# Questions?

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