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Title: Microfluidic Liquid-Liquid Contactors

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Microfluidic Liquid-Liquid Contactors

By Quinn McCulloch
06/28/2017

MPA Division Counsel Presentation

LA-UR-16-XXXXX

Outline

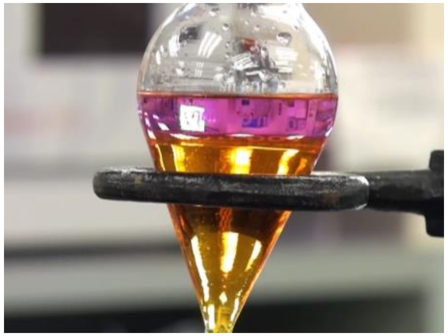
- Liquid-Liquid Extraction
- Traditional LLE
- Microfluidic LLE
- Mastering capillarity
- Screen contactors
  - Modeling
  - Liquid characterization
  - Test flowing
  - Mass transfer
- Future work
- Conclusion

Liquid-liquid extraction

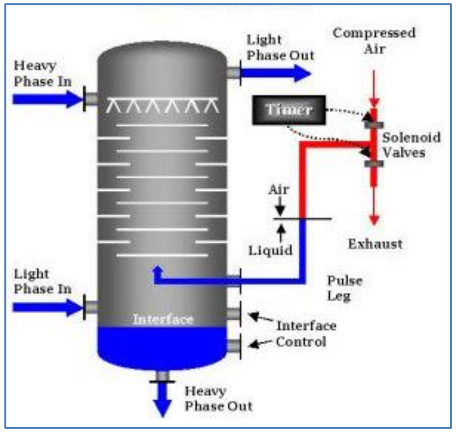
- **LLE** represents a large subset of chemistry where one or more solutes are transferred across an interface between two immiscible liquids.
- **Uses include:** counter-current chromatography, ore processing, petroleum processing, biological purification, water decontamination, vegetable oil production…

Traditional LLE

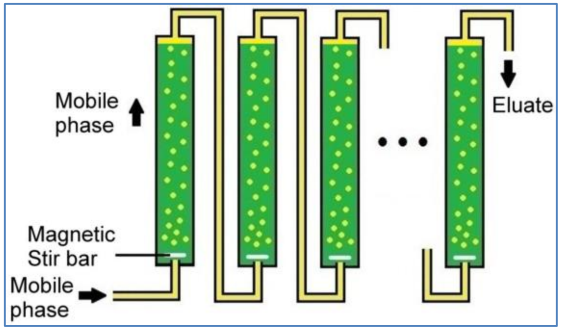
Reaction rates dictated by mixing. Separation relies on buoyancy.
Slow and inefficient, but high throughput.



Separatory funnel: omicsonline.org



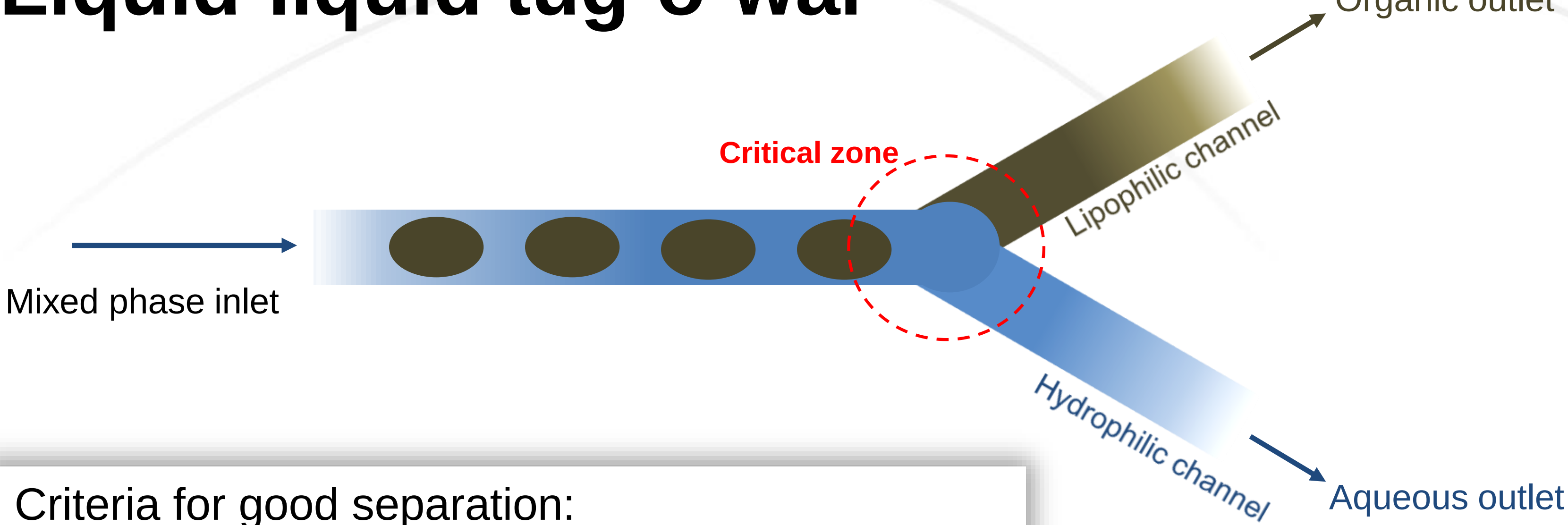
Pulsed column: modularprocess.com



CCC: mdpi.com

HSCCC: www.tu-braunschweig.de

Liquid-liquid tug-o-war



Criteria for good separation:

$$P_{cap} \gg \Delta P_{hyd}$$

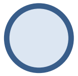
where,

$$P_{cap} = \frac{\gamma \cos\theta}{r}, \quad \text{and} \quad \Delta P_{hyd} = Q \sum_n \left[\frac{k_n L_n}{r_n^4}\right].$$

NNSA National Nuclear Security Administration
Los Alamos NATIONAL LABORATORY EST.1943

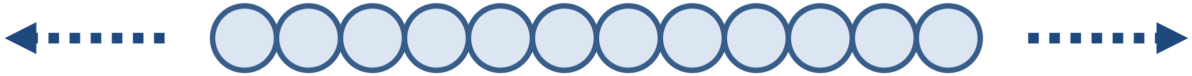
A new architecture

Cross section of microfluidic device:



Single capillary

$$\Delta P \propto \frac{1}{r^4}$$

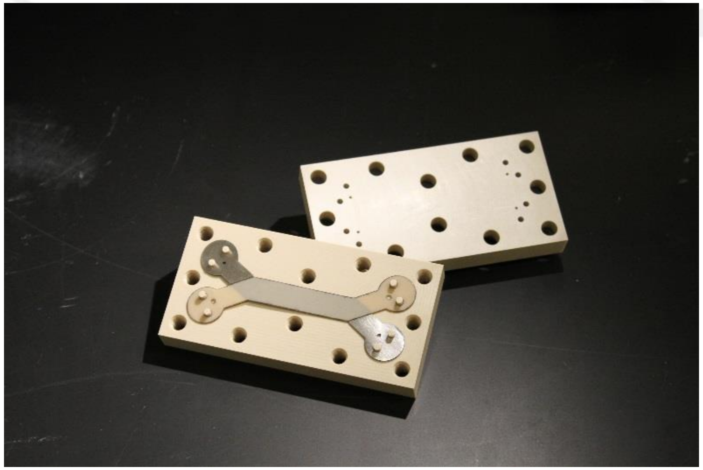


Numerous capillaries

$$\Delta P_{hyd} \propto \frac{1}{nr^4}$$

Screen contactors

- Wettable screens provide high surface to volume ratio necessary for capillary action
- Two screens are used: one hydrophilic, the other lipophilic
- Screens are 70 microns thick, which maintains micrometer length scales
- ***Scalable***
  - Screens may be layered/interleaved indefinitely to improve liquid throughput
- Parallel flow and countercurrent flow schemes are achievable

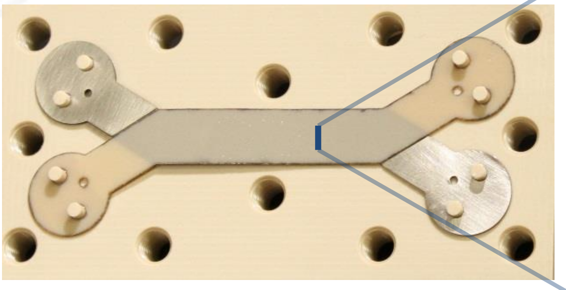


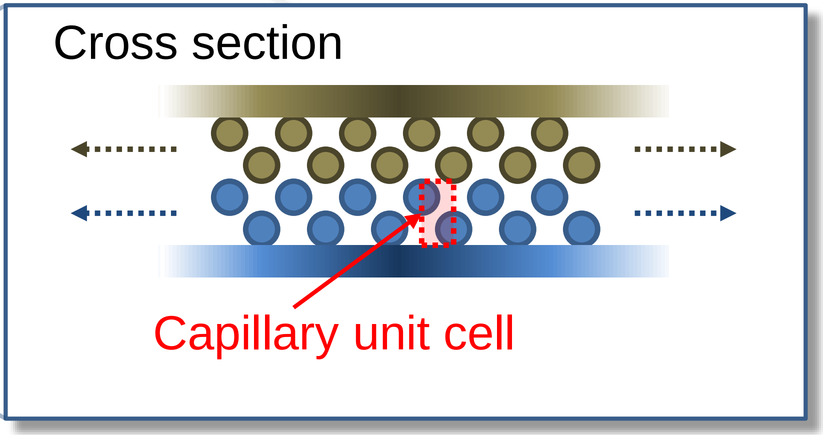
Open housing

Layers

Modeling

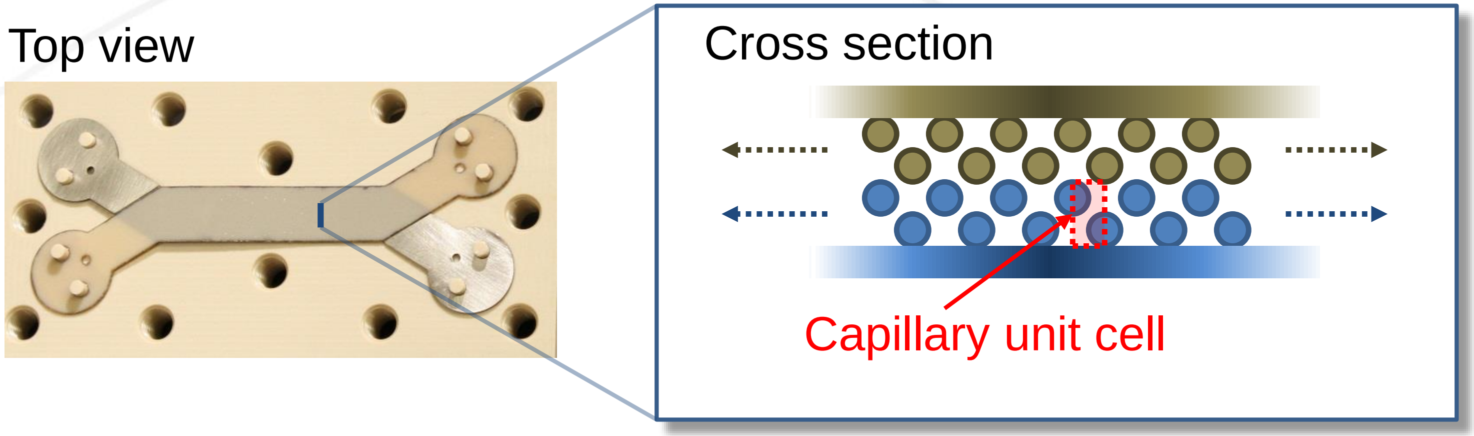
Top view





- The geometry of a mesh screen is difficult to model exactly, but…
- A screen has a repeating structure of n capillary unit cells
- Two unknown quantities are used to predict capillarity
  - The number of capillaries, n
  - The effective capillary radius, r
- Other quantities are directly measurable: $(\mu, \gamma, \theta_{adv}, \theta_{rec}, SFE)$

Modeling



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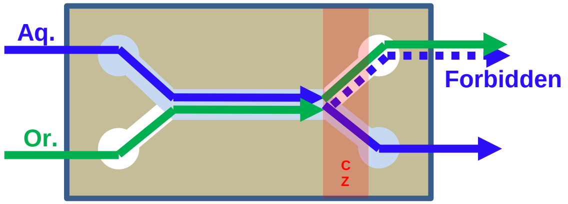
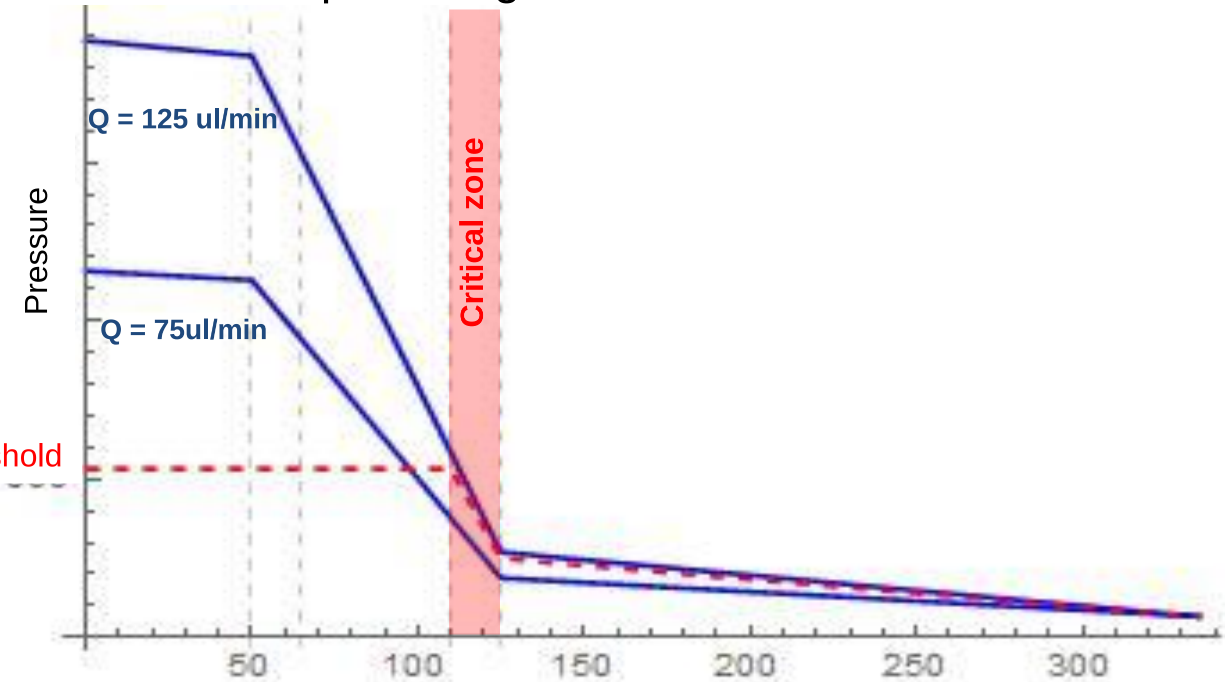
Model results: parallel flow



Pressure drops through Screen Contactor



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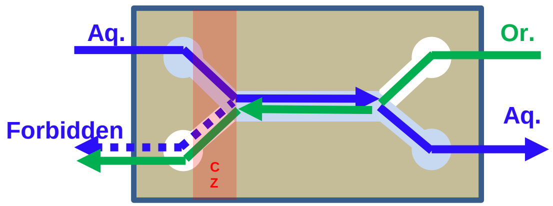
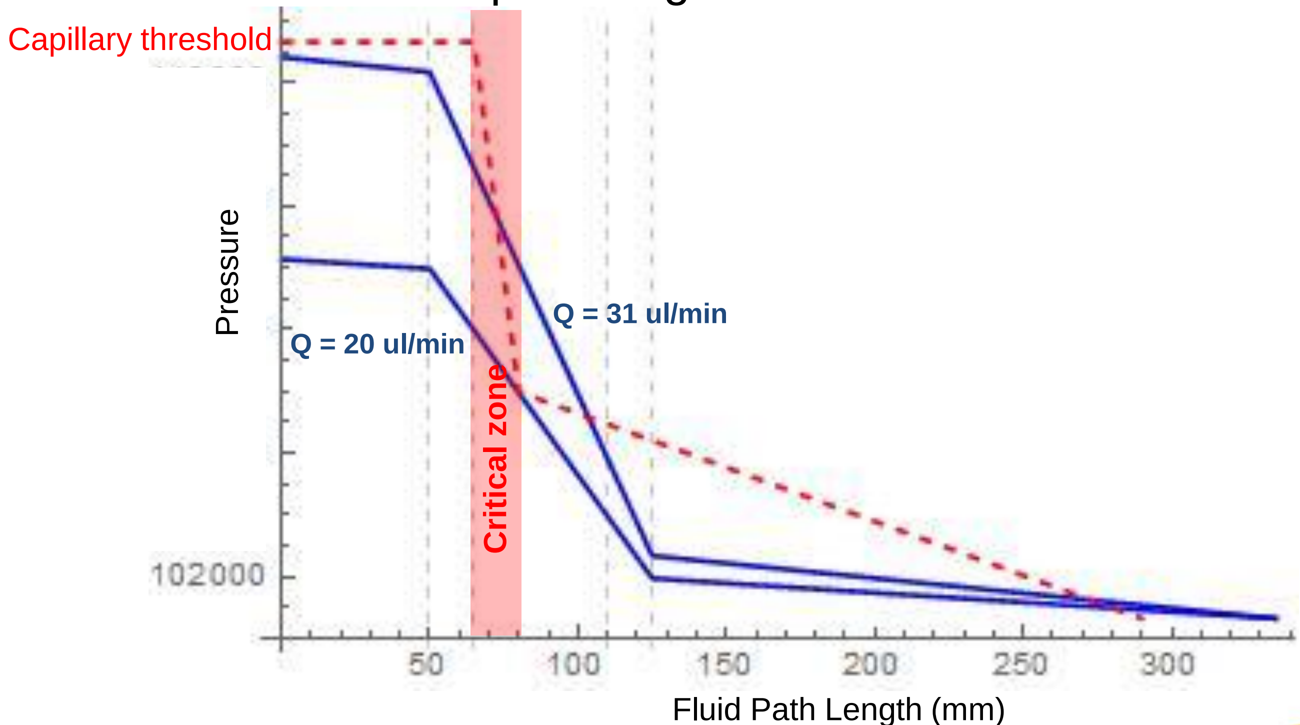
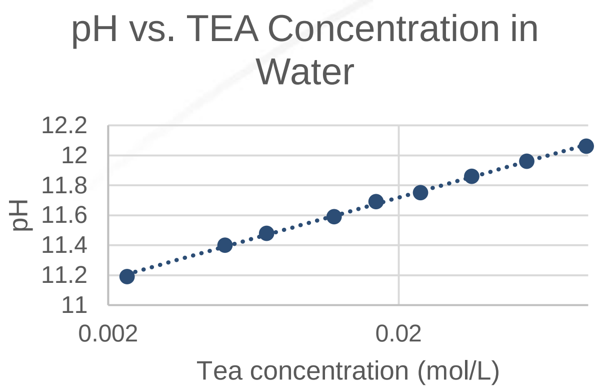
Model results: countercurrent flow

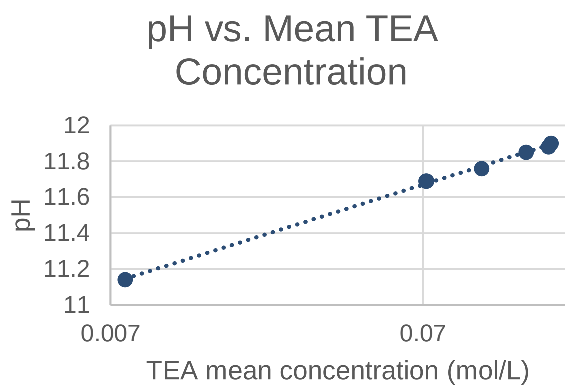


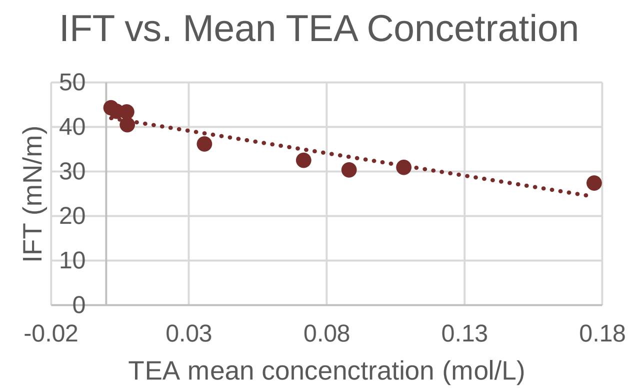
Pressure drops through Screen Contactor



Surrogate chemical system: water/TEA/n-Decane



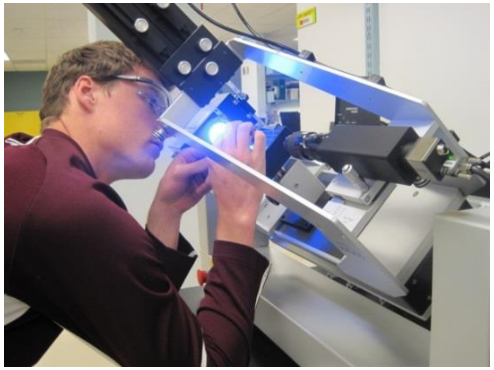




Contact angles on Stainless steel and PEEK

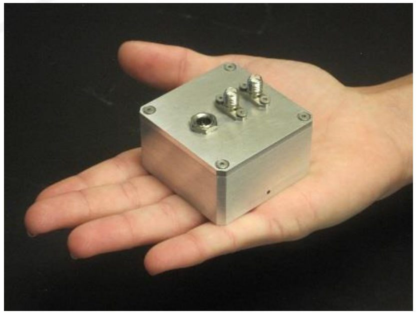
Stainless			
Bulk	**Drop**	**CA adv.**	**CA rec.**
Water	n-Decane	180	180
n-Decane	Water	83.64 (+- 12.04)	0

PEEK			
Bulk	**drop**	**CA adv.**	**CA rec.**
Water	n-Decane	90.44 (+- 1.74)	32.97 (+- 1.27)
n-Decane	Water	138.33 (+- 0.91)	91.56 (+- 0.95)

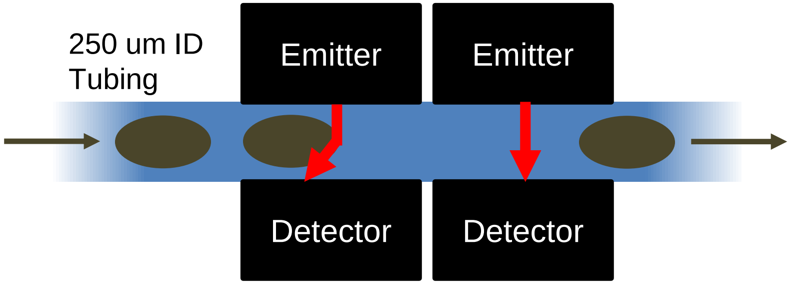


Mass Transfer Model of Triethylamine across the n-Decane/Water Interface Derived from Dynamic Interfacial Tension Experiments
Michael Fricke and Kai Sundmacher. Langmuir **2012**, 28, 6803-6815

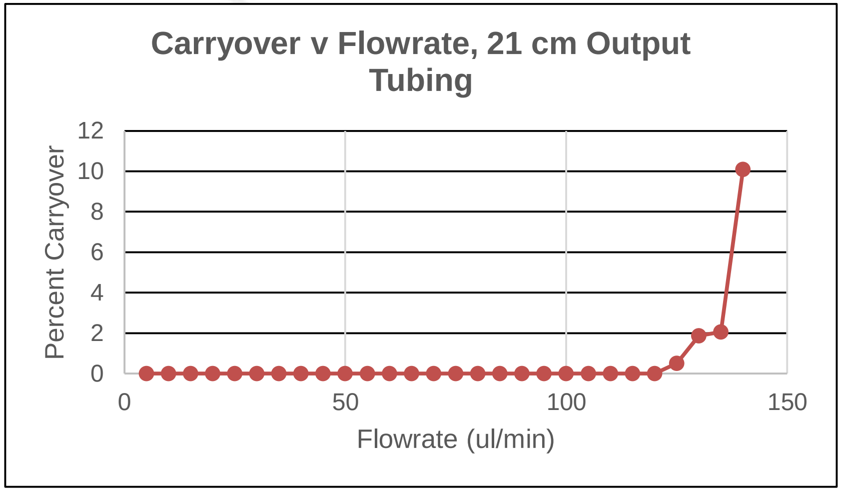
Flow testing using a LANL invention

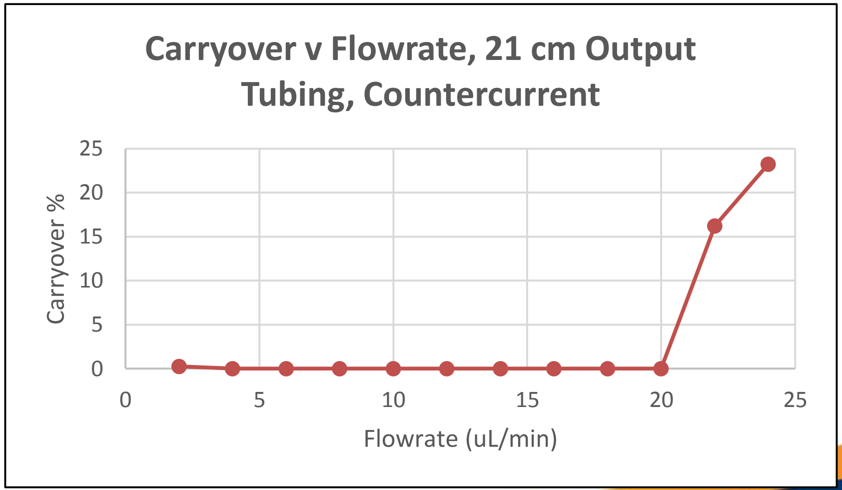


Aluminum case used to house the circuitry for the optical detection system. The length and width of this device are 1.8”, and the overall height is 1.025”.



Invention: pair of commercial, millimeter-scale photo-interrupters are used to monitor phase carryover and flow rate.





Future work

- Provisional patent for Screen Contactors filed
- Planning paper submission on Screen Contactor experiments with water/TEA/n-Decane
- IDEAS submission for optical detectors
- Materials compatibility: replace or surface treat stainless steel
- Upcoming year will be focused on scaling and automation

Conclusions

- A microfluidic contactor for performing LLE has been invented that:
  - Performs efficient separation of immiscible liquid phases
  - Is scalable
  - Can run in parallel or countercurrent modes
  - Can run in forward and reverse directions
- A model has been developed to predict this device's failure
- A surrogate chemical system has been selected to demonstrate mass transfer
- Liquid characterization is underway for H2O/TEA/n-Decane
- An all-optical system has been invented and implemented to monitor carryover and flowrates

A large team effort!

- Began as LDRD-DR in 2013
- Milli and Microfluidic Purification and Recovery (MMPR)

Steve Yarbro, **Becky Chamberlin**, George Goff, Kirk Weisbrod, Brad Skidmore, Casey Finstad, Enkeleda Dervishi, Kevin Boland, John Rowley, David Kimball, Benjamin Manard, Garrison Stevens, John Ahern, Chuck Helma, Diana Decker.

Students: Quintessa Guengerich, Sebastian Litchfield, Eric Auchter, Justin Marquez, Trevor Wacht

Thank you!