Modeling Two Phase Fluid Flow in High Speed Counter Current Chromatography

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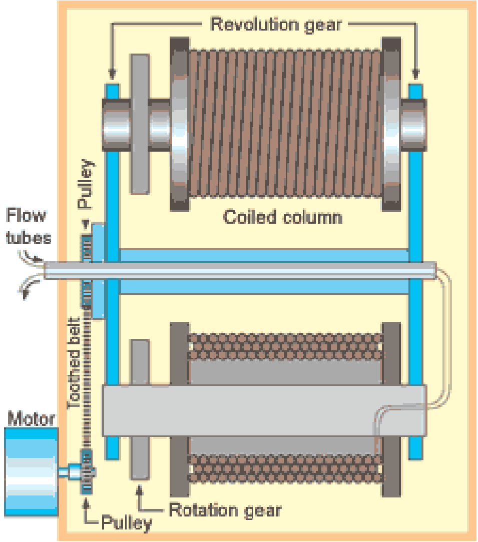
High Speed Counter Current Chromatography (HSCCC)

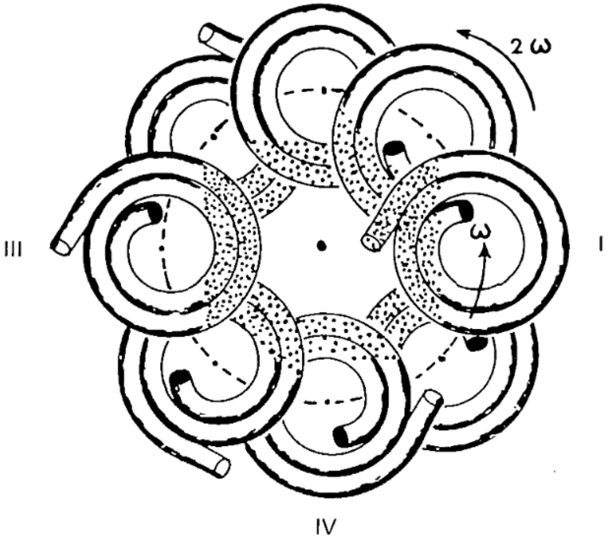
- **Device for liquid chromatography developed by Yoichiro Ito in the late 1970s.**
- **HSCCC utilizes centrifugal forces to flow two immiscible fluids past one another with high interfacial area as well as rapid mixing and settling.**
- **Lack of understanding regarding fluid dynamics in HSCCC presents a challenge for characterizing and optimizing performance.**



HSCCC Schematic

D. Filmore, *Today's Chemist at Work,* July 2001

Manufactured HSCCC



Hypothesized HSCCC Mixing

Y. Ito and W. Conway, *Analytical Chemistry*, 17:1, 65-143 (1986).

Objectives

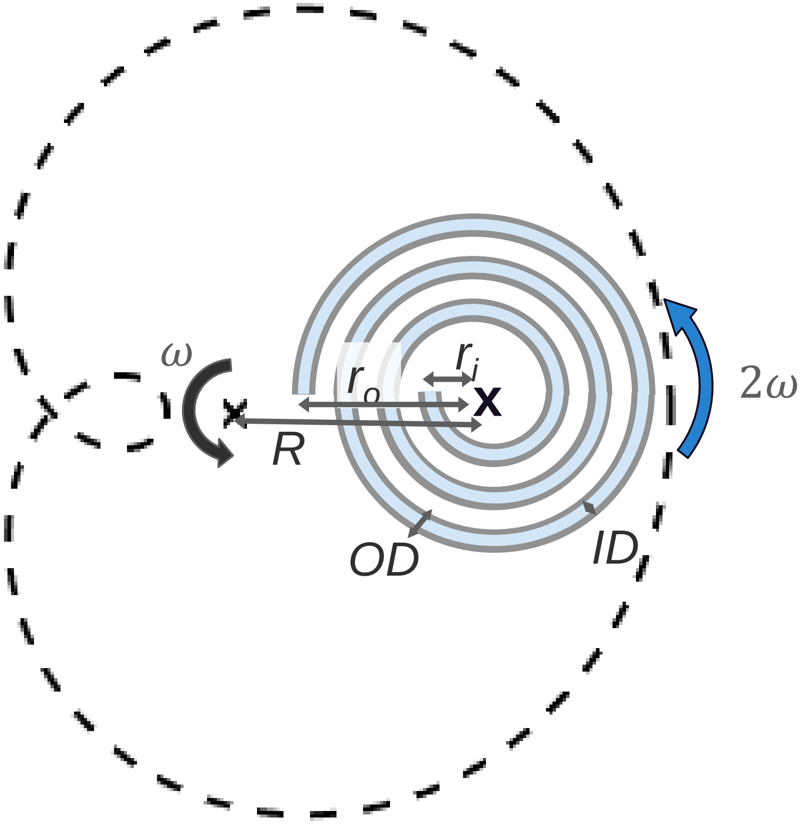
COMSOL Multiphysics model developed to help answer the following questions:

- Where do mixing and settling occur in the column?
- What form does mixing take?
- What is the phenomena governing mixing behavior?

With continued studies the parameterized model may lead to insights including:

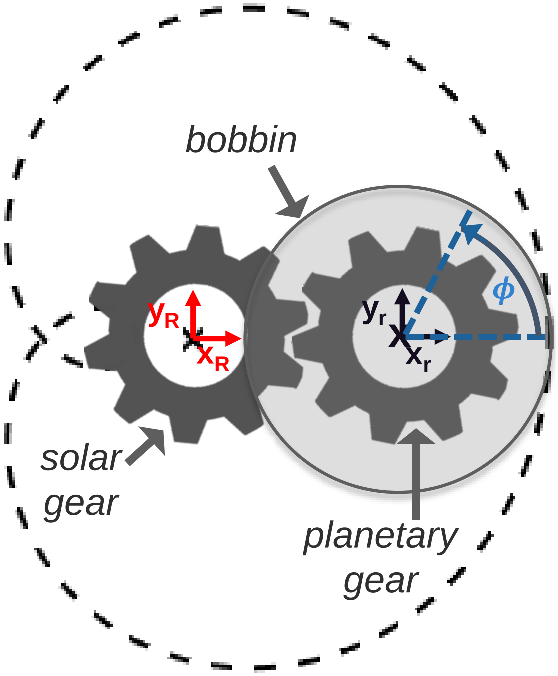
- How does the coil geometry affect mixing and settling performance?
- How do physical properties of fluids affect mixing and settling performance?

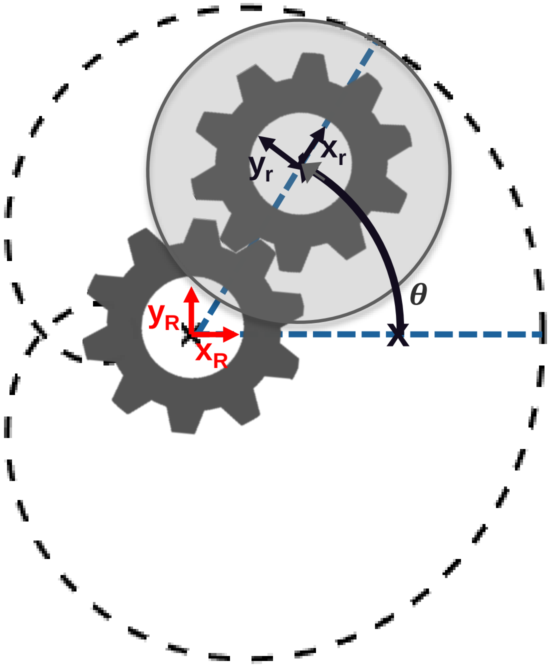
Model Parameterization



Parameter	Value	Units
Geometric Parameters		
Solar radius, *R*	100	mm
Inner planetary radius, r_i	57.0	mm
Outer planetary radius, r_o	76.2	mm
Channel inner diameter, *ID*	3.20	mm
Channel outer diameter, *OD*	6.40	mm
Operational Parameters		
Rotational speed,	800	RPM
Fluid Properties		
Aqueous density, $_{aq}$	1.00	g/cc
Aqueous viscosity, $_{aq}$	1.00	cP
Organic density, $_{org}$	0.75	g/cc
Organic viscosity, $_{org}$	1.34	cP
Interfacial tension, $_{int}$	30.0	mN/m

Derivation of Gravitational Forces





Position in Solar Coordinates

$$x_R = R\cos(\omega t) + r\cos(2\omega t + \phi)$$

$$y_R = R\sin(\omega t) + r\sin(2\omega t + \phi)$$

Acceleration in Solar Coordinates

$$a_{x,R} = -R\omega^2\left(\cos(\omega t) + 4\beta\cos(2\omega t + \phi)\right)$$

$$a_{y,R} = -R\omega^2(\sin(\omega t) + 4\beta\sin(2\omega t + \phi))$$

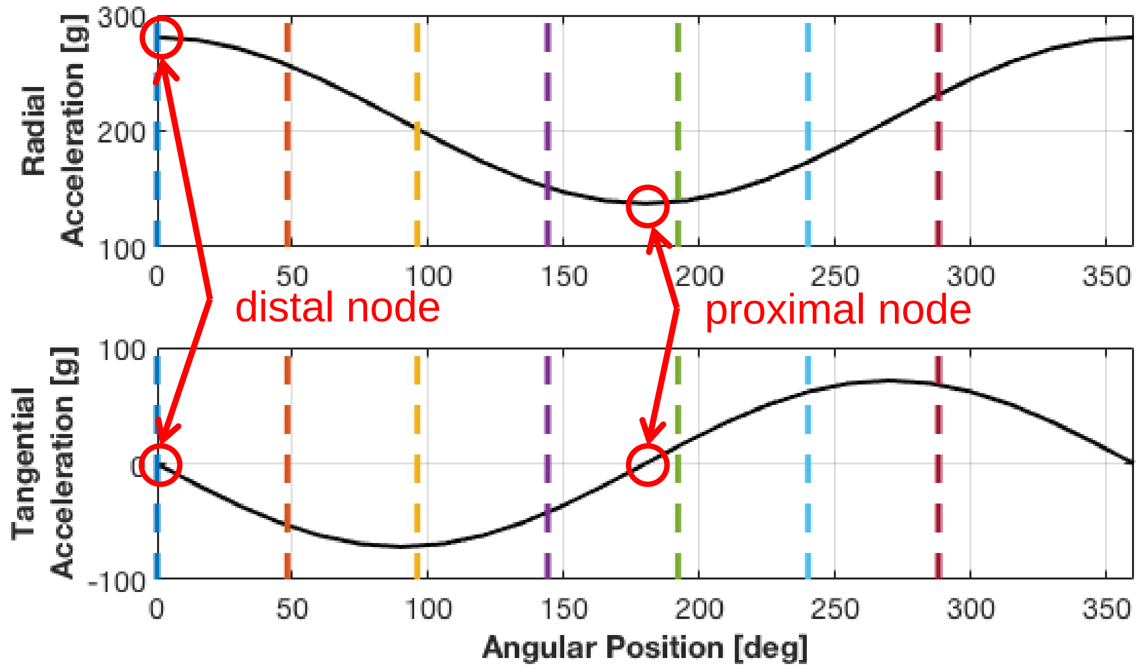
Acceleration in Planetary Coordinates

$$a_{x,r} = a_{x,R}\cos(2\omega t) + a_{y,R}\sin(2\omega t)$$

$$a_{y,r} = -a_{x,R}\sin(2\omega t) + a_{y,R}\cos(2\omega t)$$

P. Wood et al. *Journal of Liquid Chromatography* 24:11-12, 1629-1654 (2001).

Derivation of Gravitational Forces



Tangential acceleration changes direction at the **highest** (distal) and **lowest** (proximal) points for radial accelerations.

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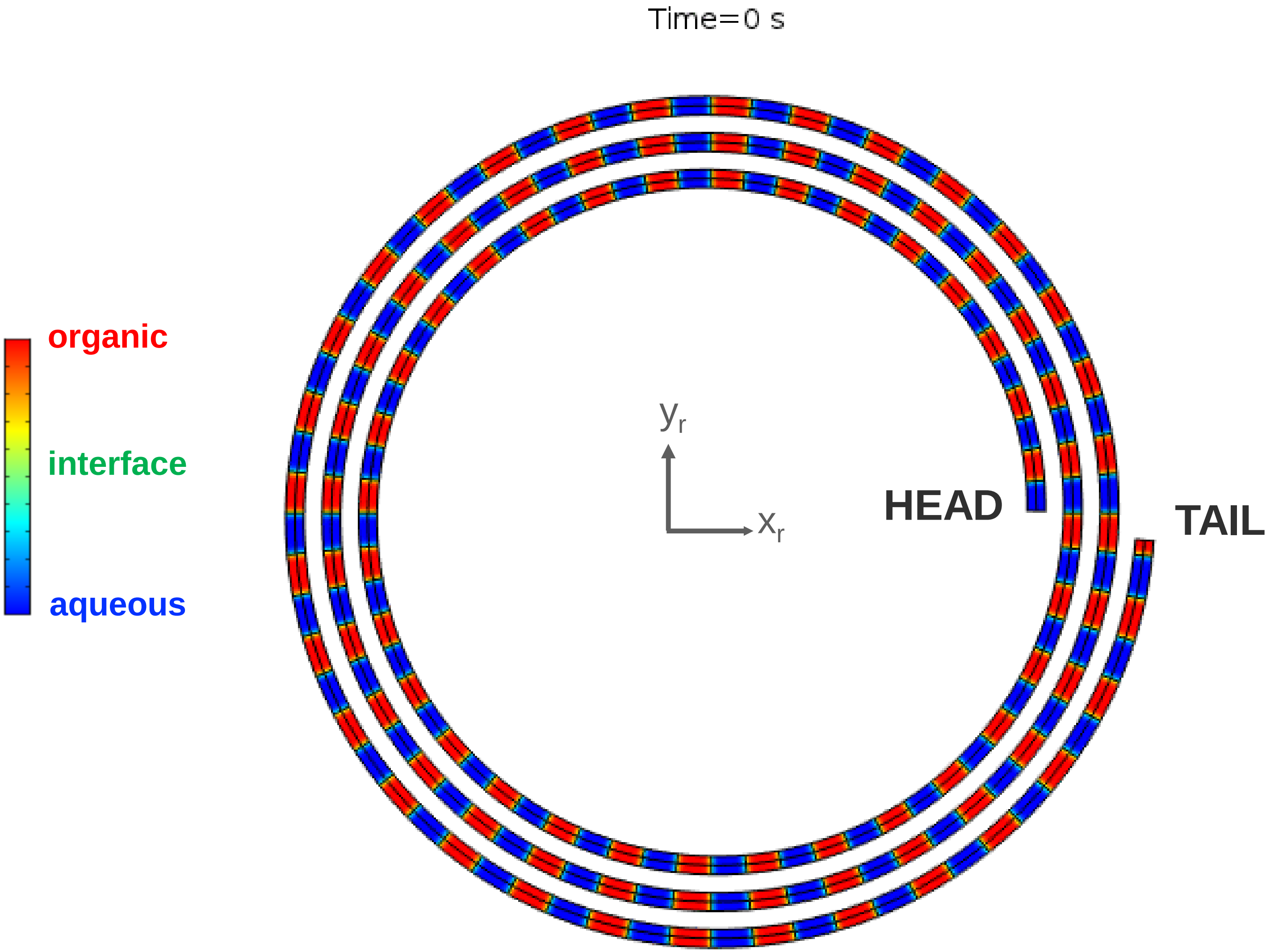
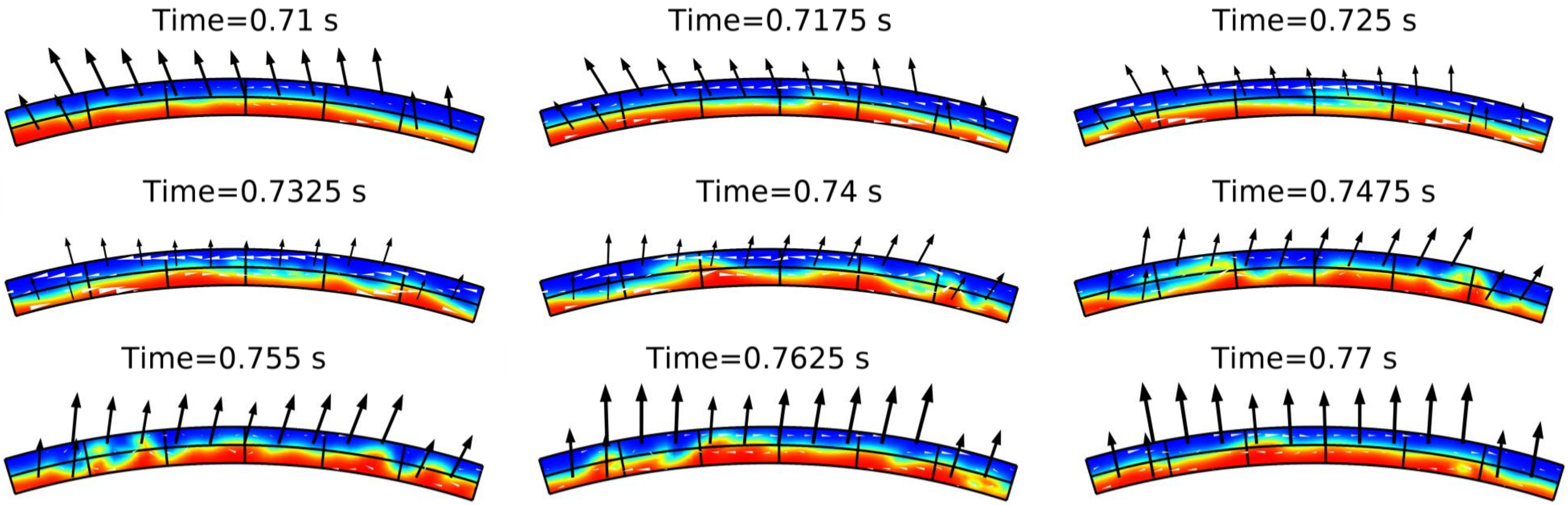
Accelerations are applied as body forces changing in time with respect to column position in planetary coordinates.



Centrifugal forces cause higher density phase to move to the outer diameter of the coil and be forced to column tail.

Mixing takes place in the form of waves, initiated at the node closest to the solar axis, where radial force is low and flows reverse directions due to change in tangential force.

Separation occurs in the node located furthest away from the solar axis, where radial force is highest.



Conclusions and Future Work

A computational fluid dynamics model has been developed using COMSOL Multiphysics to study mixing and settling behavior of High Speed Counter Current Chromatography

- Mixing and settling zones are found to be governed by the rapidly changing tangential force at alternatively high and low radial force.
- Mixing takes place in the form of waves as the heavy phase backs up into itself with the change of tangential direction.
- Separation occurs as the heavy phase is pushed to the outer wall at high radial accelerations with a net velocity of greatest magnitude towards the column tail.

Understanding the driving forces of HSCCC fluid dynamics is critical to achieving optimized, stable flows in the machine.

- Future work will focus on parametric studies of column geometry and fluid properties to determine optimal operating conditions.
- Validation of simulations with experimental data will be critical as high speed imaging of fluid flows becomes attainable.

Thank you!

Questions?

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