Computational Fluid Dynamics of Capillary Sample Flow

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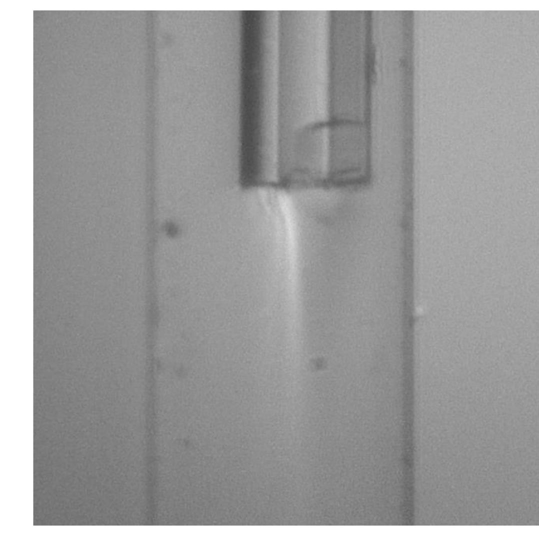

Goals

Improve the sample detection sensitivity of the Supercontinuum Rapid Excitation-Emission Matrix (ScREEM) Laser Fluorescence Apparatus through Computational Fluid Dynamics (CFD) analysis of the sample flow concentration.

- Maximize sample concentration at the fluorescing zone by varying sample flow rate and sheath flow rate
- Better understand flow patterns near fluorescing zone
- Optimum detection zone will be determined and evaluated after considering physical constraints of the assembly and the varying sample concentration along the length of the sample volume.

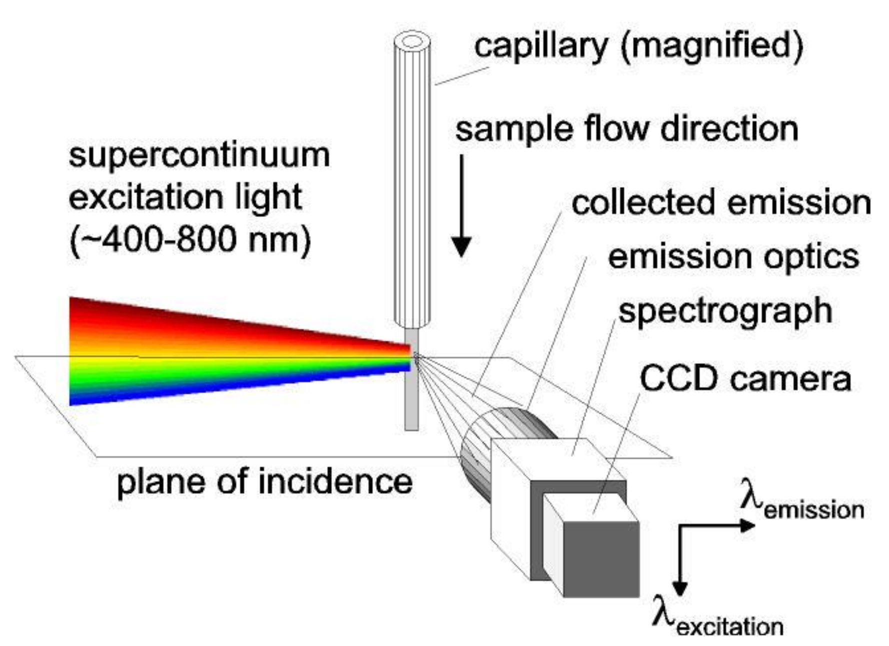

Figure 1. ScREEM Apparatus Schematic

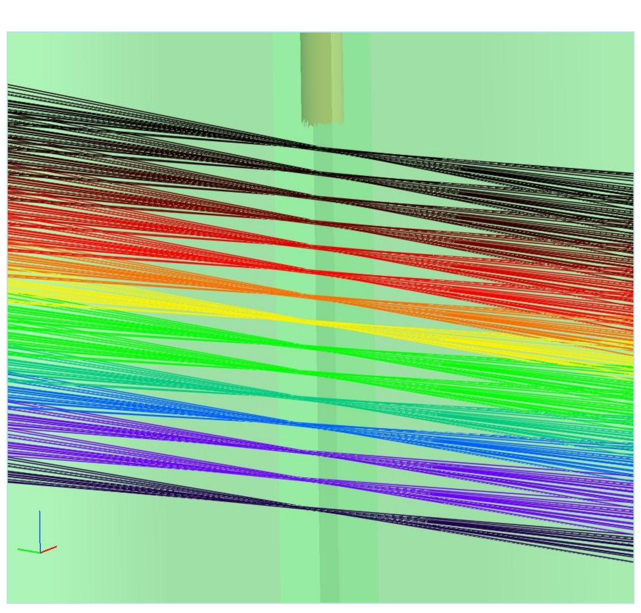

Figure 2. Close-up of Laser Interaction with Detection Zone

Background

The design goal of the ScREEM Laser Fluorescence Apparatus is to adapt the excitation-emission detection method such that it may be applied to capillary electrophoresis sheath-flow detection, allowing rapid and ultrasensitive analysis of biological samples labeled with multiple fluorescent tags (Figure 1).

The input on the ScREEM device is a supercontinuum laser, while the output of the device is an excitation-emission matrix or EEM (Figure 2).

Importance

The sensitivity of the ScREEM design is limited by three basic factors including sample preparation, sample detection, and data analysis.

Sample detection will be improved with increased sample concentration at the detection zone. The limit of detection is determined by the intensity of peaks produced in the EEM. Increasing the sensitivity of the system results in more intense and resolved peaks (Figure 4). These well resolved peaks translate into more accurate results regarding fluorescing species' concentration and type.

Requirements of ScREEM Design:

- Limit of detection less than nanomolar concentrations
- Sample volumes in the nanoliter range
- Detection of multiple fluorescing species

Method

SolidWorks Flow Simulation is a Computational Fluid Dynamics (CFD) software which solves the Navier-Stokes Equations using an iterative technique. The Navier-Stokes Equations are the governing equations for continuous fluids. The CFD technique discretizes the region of interest into Fluid Cells, Partial Cells, and Solid Cells. Flow parameters are changed iteratively until a predefined goal is reached. The goals are convergence criteria based on desired flow parameters such as velocity. For example, the goal criteria may be a change in velocity of less than 5% of the current velocity value between iterations. Iteration continues until all convergence goals are met.

Navier-Stokes Equation for Incompressible Fluids:

$$\frac{\partial \boldsymbol{V}}{\partial t} + (\boldsymbol{V} \cdot \boldsymbol{\nabla})\boldsymbol{V} = \boldsymbol{g} - \frac{1}{\rho}\nabla p + \nu \nabla^2 \boldsymbol{V}$$

Where each term is an acceleration, V is the fluid velocity vector, t is time, g is acceleration vector due to gravity, ρ is density, and ν is fluid viscosity.

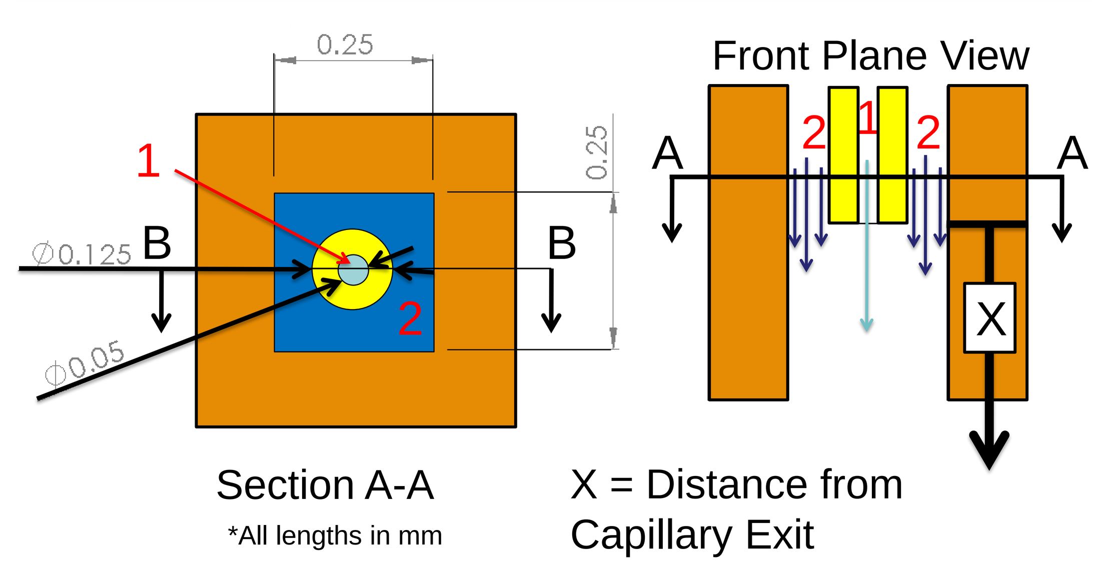

Figure 3. Sample Flow Area 1 (Cyan), Sheath Through Area 2 (Blue), Capillary Tube (Yellow) and Walls (Orange)

Assumptions

Several modeling parameters have to be assumed in order to run CFD. These parameters strongly influence the results of the simulations and must be consistent with the actual model conditions.

- Internal Flow Analysis
- Incompressible Fluid
- Mesh size used throughout Analysis:
  - 30,188 Fluid Cells,
  - 29,404 Partial Cells
- Flow Model Geometry – See Figure 3.
  - All walls considered Smooth and Fully Insulated
- Initial Conditions
  - Fluid Filling reservoir - Volume Ratio
    - 1 Sheath Fluid: 0 Sample Fluid
  - Standard Temperature
- Boundary Conditions
  - Sample Volumetric Flow Rate Varied
  - Sheath Volumetric Flow Rate Fixed at 0.3125 mm^3/s
- Constant Flow Rate
- Atmospheric Pressure at flow outlet
- Sample and Sheath Flow Modeled as Water
- Symmetry Over Front Plane B-B

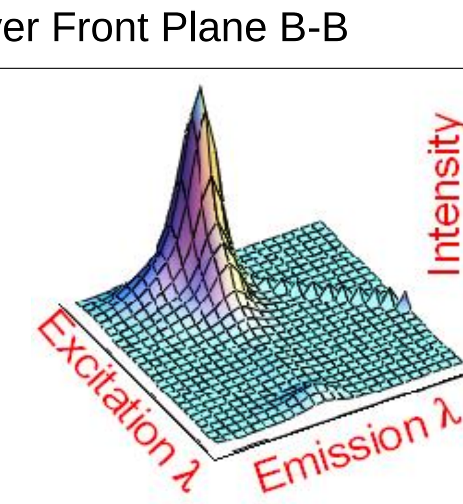

Figure 4. Excitation Emission Matrix (EEM) data output from high-speed CCD

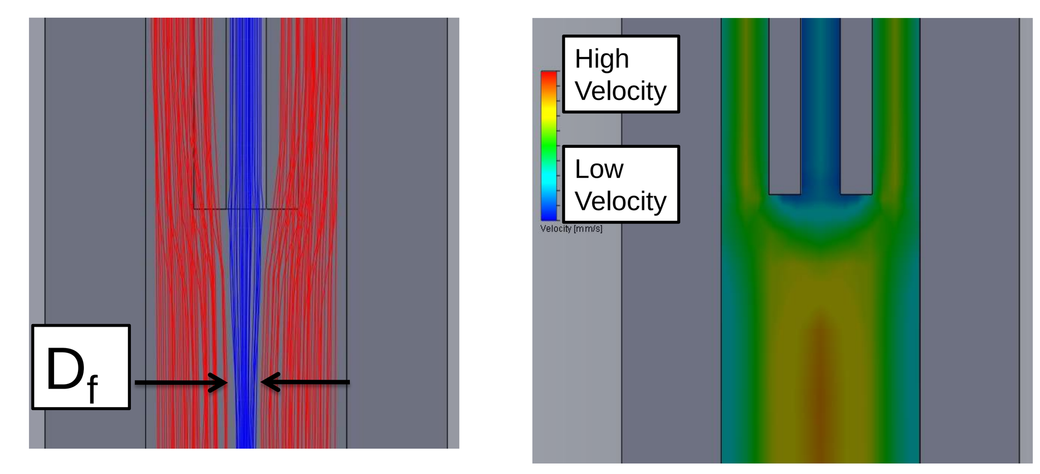

Figure 5. CFD Plots of Streamlines & Velocity Contours

Results & Discussion

SolidWorks Flow Simulation CFD analyses were created for 6 different capillary sample flow rates ranging from .3125 mm^3/s down to .003125 mm^3/s as shown below in Figure 5 with respective velocities of 47 mm/s down to 17mm/s at the detection zone.

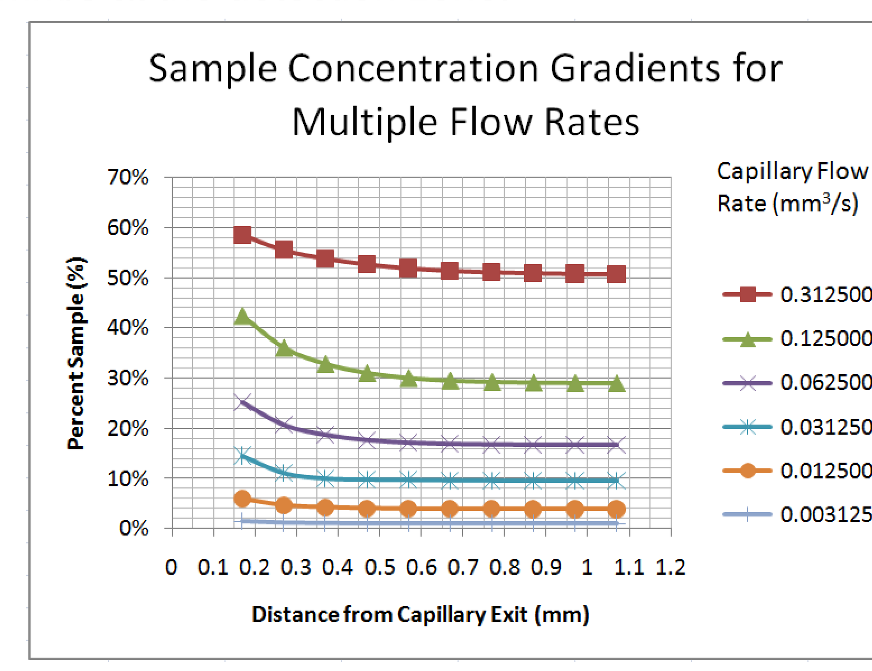

Figure 6. Flow Rate Comparison

As shown a significant amount of dilution occurs regardless of capillary flow rate, however concentration levels off after the flow is .5 mm from the capillary exit. The largest flow rate results in the highest percent sample, 59%. D_f, the focused diameter, was smallest with the lowest flow rate of .003125 mm^3/s with D_f= 23 μm.

Conclusion

The CFD simulations produced by SolidWorks Flow Simulation helped clarify flow patterns acting in the detection region. A tradeoff between focused diameter and sample concentration was observed. Additionally, a major source of sample concentration reduction was determined to be caused by the squared edges of the modeled capillary.

Future Work:

- Validation of results through physical testing
- CFD of Capillary with rounded or chamfered tip
- Validation of Rounded Capillary by etching Capillary and running physical tests

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References

- Granger, Robert Alan. "The Navier-Stokes Equations." *Fluid mechanics* . New York: Holt, Rinehart, and Winston, 1985. 203-208. Print.
- Dassault Systemes, SolidWorks Flow Simulation. "Governing Equations." *SolidWorks Flow Simulation 2009 Technical Reference* 1 (2009): 2-37. Print.