Temperature Response of the
Ultra-High Throughput Mutational Spectrometer

by

Timothy W. Suen

SUBMITTED TO THE DEPARTMENT OF MECHANICAL ENGINEERING IN
PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE OF

BACHELOR OF SCIENCE IN MECHANICAL ENGINEERING

AT THE

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

JUNE 2005

©2005 Timothy W. Suen. All rights reserved.

The author hereby grants to MIT permission to reproduce
and to distribute publicly paper and electronic
copies of this thesis document in whole or in part.

Signature of Author ____________________________

Department of Mechanical Engineering
May 9, 2005

Certified by ____________________________

Ian W. Hunter
Hatsopolous Professor of Mechanical Engineering
Thesis Supervisor

Accepted by ____________________________

Ernest G. Cravalho
Professor of Mechanical Engineering
Chairman, Undergraduate Thesis Committee, Mechanical Engineering
Temperature Response of the Ultra-High Throughput Mutational Spectrometer

by

Timothy W. Suen

Submitted to the Department of Mechanical Engineering on May 10, 2005 in Partial Fulfillment of the Requirements for the Degree of Bachelor of Science in Mechanical Engineering

ABSTRACT

The Ultra-High Throughput Mutational Spectrometer is an instrument designed to separate mutant from wild type DNA through capillary electrophoresis. Since this technique uses the melting point of the molecule to distinguish between sequences of base pairs, temperature control is crucial to the success of the device. The purpose of this analysis is to characterize the temperature response of the instrument, taking into account the heat dissipated by the 10,000 capillaries in the system during electrophoresis.

Analytical models, finite element analysis, and physical models were used to predict the steady state response of the system to heat generated by capillary electrophoresis. The analytical models estimated a steady state offset of 0.2 K for water at $3.3 \times 10^{-4} \text{ m}^3/\text{s}$ (20 L/min) and 1.0 K for water at $6.7 \times 10^{-5} \text{ m}^3/\text{s}$ (4.0 L/min) and predicted that the system would reach steady state within several seconds. Finite element analysis determined that the gel inside the capillaries would have a steady state offset of 0.24 K. The physical system, which simulated the Joule heating of the capillaries using an immersion heater, yielded a steady state offset of 0.24 K at $3.3 \times 10^{-4} \text{ m}^3/\text{s}$ and 0.65 K at $6.7 \times 10^{-5} \text{ m}^3/\text{s}$, but the settling time in both cases was on the order of 500 s. This discrepancy is due to the fact that many aspects of the physical system, including the thermal mass of the instrument, heat loss through convection, and the PID temperature controller in the circulator, were not taken into consideration in the theoretical analysis.

Pressure drop and vortex shedding were also calculated for the instrument. Finite element analysis determined the pressure drop to be 18.55 Pa. Vortex shedding does not occur, because the operating conditions of this instrument are below the critical Reynolds number.

Thesis Supervisor: Ian Hunter
Title: Hatsopolous Professor of Mechanical Engineering
Acknowledgements

I would like to thank Professor Ian Hunter, Dr. Bryan Crane, Michael Del Zio, Dr. Andrew Taberner, Jim Lin, and Craig Forest for their help with this project.
Table of Contents

1.0 Introduction ............................................................................................................................. 5
2.0 Experimental Method ............................................................................................................... 6
  2.1 Apparatus ............................................................................................................................ 6
  2.2 Procedure ............................................................................................................................. 8
3.0 Theoretical Analysis ................................................................................................................ 8
  3.1 Heat Transfer ...................................................................................................................... 8
    3.1.1 Conservation of Energy ............................................................................................... 9
    3.1.2 Heat Exchanger Analysis .......................................................................................... 10
    3.1.3 Control Volume Model .............................................................................................. 11
    3.1.4 Finite Element Analysis ............................................................................................. 16
  3.2 Pressure Drop .................................................................................................................... 18
    3.2.1 Tube Bank Correlation ............................................................................................. 18
    3.2.2 Finite Element Analysis ............................................................................................. 19
  3.3 Vortex Shedding ................................................................................................................ 20
    3.3.1 The Critical Reynolds Number ................................................................................. 20
    3.3.2 Strouhal Correlation .................................................................................................. 21
    3.3.3 Transverse Vibration of a Thin Uniform Beam ...................................................... 22
    3.3.4 Finite Element Analysis ............................................................................................. 25
4.0 Results and Discussion .......................................................................................................... 26
  4.1 Circulator Temperature Control ..................................................................................... 26
  4.2 Constant Temperature ..................................................................................................... 27
  4.3 Ramped Temperature ...................................................................................................... 30
  4.4 Constant Temperature with Heater ................................................................................ 31
  4.5 Ramped Temperature with Heater ................................................................................. 33
5.0 Conclusion and Recommendations ..................................................................................... 36
Appendix A: Scan Characteristics and RTD Calibration ....................................................... 37
Appendix B: MATLAB Code for Control Volume Model ...................................................... 39
References .................................................................................................................................... 43
1.0 Introduction

In spite of the resources dedicated to genetic research over the past decade, researchers have met with limited success identifying the specific alleles responsible for common diseases. Although certain rare disorders, such as sickle-cell anemia and cystic fibrosis, have been traced back to single alleles or several alleles in a single gene, the genetic basis of more common ailments is not well understood.

Current research suggests that these diseases may have at their root more complex mechanisms, such as imperfect penetrance, polygenic causation, and multigenic multiallelic causation [1]. In the case of imperfect penetrance, each allele has only a modest individual effect on the development of the disorder and its influence may be subject to other genes as well as environmental factors [2]. Polygenic causation requires specific combinations of alleles over several genes to take effect, while multigenic multiallelic causation attributes disorders to low-frequency alleles, possibly distributed across many genes [1]. Verifying the presence of imperfect penetrance or polygenic causation requires thousands of samples, because distinctions must be made between relatively small differences in the allelic frequencies of the general and afflicted populations. Multigenic multiallelic causation can not be established without at least a hundred thousand subjects. Thus, in order to identify any of these scenarios with statistical significance, a very large number of samples must be collected and analyzed.

Although gene sequencing is considered the gold standard in genomic research, various gel electrophoresis techniques have been developed to separate genetic variants at a fraction of the cost. These procedures exploit the fact that DNA denatures under certain conditions, such as exposure to heat or urea [3]. The specific temperature under which a molecule of DNA denatures, however, varies depending on its nucleotide sequence. Furthermore, different domains in a fragment of DNA typically denature at different melting points depending on the hydrogen bonds between the base pairs. If that fragment is held at a temperature between the melting points of two domains, it will travel much more slowly through a sieving medium due to its partially melted state [4]. Even single base changes can significantly alter the equilibrium between the faster unmelted form and the slower partially melted intermediate, such that the original and mutated fragments no longer spend the same fraction of time in each state. The differing speeds at which unmelted and partially melted molecules move through the gel allow capillary electrophoresis to distinguish between mutant and wild type sequences of DNA.

Current instrumentation [5], containing up to 384 capillaries, has the ability to identify causative alleles in candidate genes. Since there are approximately 40,000 genes in the human genome, those under investigation must be chosen with care. With a 10,000 capillary instrument, however, throughput would be increased by more than 25-fold and all alleles in the patient population could be compared at once, avoiding completely the need to select candidate genes. Craig Forest in the BioInstrumentation Laboratory at MIT is currently working to develop and implement this Ultra-High Throughput Mutational Spectrometer (UTMS) [6].

Critical to the success of the UTMS is controlling the temperature of the capillaries. Unless the temperature of the gel is between the melting point of the wild type and mutant DNA, capillary electrophoresis will not be able to distinguish between the two samples. While earlier studies [4, 7] have used constant denaturing conditions for gel electrophoresis, more sophisticated techniques create a temperature gradient in the gel to ensure that differences in the thermodynamic stability of the DNA can be detected. This gradient can either be spatial, by
establishing a linear temperature profile along the length of the gel [8], or temporal, by ramping the temperature of the entire system during the run [3,9,10]. Due to its relative ease of implementation, the temperature gradient in the UTMS takes place over time. Cycling the temperature of the samples during gel electrophoresis has the added advantage that multiple samples may be injected into the same capillary at periodic intervals to further increase throughput of the instrument [2].

The purpose of this analysis is to aid the design of a temperature control system for the UTMS. Analytical and finite element models were developed to predict the temperature of the DNA in the capillaries and the pressure drop through the capillary array, given the fluid and thermodynamic properties of water and air. Vortex shedding was also considered to ensure that the vibration of the capillaries would not be in resonance with their natural frequencies. The results from the heat transfer model were then tested against a physical model of the system in which an immersion heater was used to simulate the constant heat flux generated by Joule heating of the capillaries during electrophoresis.

2.0 Experimental Method

This investigation seeks to characterize the temperature response of the capillary-containing component of the UTMS. Six resistive thermal device (RTD) elements along the side of the instrument measure the temperature of the water inside the system while a screw plug immersion heater simulates the heat flux from the grid of capillaries to be placed in the instrument. A circulator heats, cools, and pumps the water through the system. The system response to the heater was measured for different pump speeds as well as for ramped and constant temperature conditions.

2.1 Apparatus

The instrument shown in Figure 1, which was constructed by Michael Del Zio and Jiengju Lin, holds the 100-by-100 grid of capillaries while allowing heat transfer fluid to be pumped through the array. The instrument consists of six blocks, each of which is roughly 50 mm thick and has eight holes drilled into the side, as shown in Figure 2, for holding flow straighteners and temperature sensors [11]. The PolyScience Model 9601 Digital Circulator in Figure 3 is used to control the temperature of the water and pump it between the capillaries. The Omega screw plug immersion heater in Figure 4, which is rated at a resistance of 19.2 Ω and a maximum power output of 750 W, generates 255 W of heat, the same amount that would be dissipated by the capillaries under normal operation of the instrument.

Temperature is measured by thin film platinum resistive thermal device (RTD) elements, such as the one shown in Figure 5, rated at 1/3 DIN B with a nominal resistance of 100 Ω and an alpha of 0.00385. The exposed wires were waterproofed with lacquer and the insulated wires with heat shrink tubing. Teflon thread tape is wrapped around the RTD wires, allowing them to screw directly into the holes in the blocks. Four wires connect each element to an Agilent 34901A 20-Channel Multiplexer, which is plugged into the Agilent 34970A Data Acquisition Switch Unit on top of the circulator in Figure 3. A custom application written in Visual Basic reads data from the switch unit using a Virtual Instrument Software Architecture (VISA) application programming interface with the Standard Commands for Programmable Instruments (SCPI) command set via a GPIB-USB-B cable.
Figure 1: Water is pumped through the instrument to cool the array of capillaries within. A screw plug immersion heater mounted through the top is being used to simulate the heat flux that would be generated by the capillaries.

Figure 2: One of the six blocks that make up the instrument. The holes in the side hold the RTD elements and allow the flow straighteners to be held by setscrews.

Figure 3: A PolyScience Model 9601 Circulator controls the temperature of the water entering the instrument and has pump speeds from $2.8 \times 10^{-5}$ to $3.3 \times 10^{-4}$ m$^3$/s.

Figure 4: An Omega screw plug immersion heater simulates the constant heat flux of the capillaries with a power output of 255 W at 70 V DC.

Figure 5: Temperature is measured with RTD elements rated at 1/3 DIN B. Two wires are connected to each end of the RTD for a four-wire resistance measurement.
2.2 Procedure

Temperature measurements were taken from the seven RTD elements at average intervals of 4.83 s per scan or 0.69 s per reading, integrating over 20 power line cycles or nominally 0.333 s per reading. Scan speeds and the standard deviation of the RTD elements at each speed are listed in Appendix A. The RTD elements were calibrated by placing them in the reservoir of the circulator, and taking measurements for 10 minutes with the circulator at 50 °C, 55 °C, and 60 °C. The actual temperature is taken as the average reading from the RTD elements, not as the temperature on the digital display of the circulator. The calibration parameters used for linear interpolation are also listed in Appendix A.

The maximum heating and cooling rate of the circulator between 50 °C and 60 °C was obtained by cycling the circulator between the two temperatures and connecting the pump inlet directly to the pump outlet. To determine how the temperature of the instrument changes with the entry temperature of the heat transfer fluid, six of the RTD elements were installed in the instrument while the seventh remained in the circulator reservoir. The temperature of the water in the instrument and in the circulator was measured while setting the circulator to a constant 50 °C and 60 °C and then cycling the temperature between 50 °C and 60 °C. The pump was set at 3.3×10⁻⁴ m³/s (20 L/min) and the heater was turned off for these baseline measurements.

For the step response of the system to heat generation during capillary electrophoresis, the circulator reservoir was kept constant at 50 °C while the heater was supplied with 70.0 V DC or 255 W. Temperature measurements were taken at pump speeds of 6.7×10⁻⁵, 1.3×10⁻⁴, and 3.3×10⁻⁴ m³/s (4.0, 7.5, and 20 L/min) using two different configurations of the sensors in the instrument. To determine the system response when the inlet temperature of the water was increasing or decreasing, the circulator was set to cycle from 50 °C to 60 °C at 3.3×10⁻⁴ m³/s with the heater outputting 255 W. Before each run, the heater was turned off and the water in the circulator and in the instrument was allowed to equilibrate for at least 10 minutes.

3.0 Theoretical Analysis

The primary purpose of this thesis is to determine the temperature response of the capillaries, given the properties of the heat transfer fluid and other system parameters. Conservation of energy, heat exchangers, and control volumes were used to analyze heat transfer between the capillaries and the fluid. The pressure drop across the capillary array was also calculated, since it affects the velocity of the fluid and determines the size of the pump needed in the instrument. When fluid flow is disrupted by cylinders, vortex streets trail in their wake, generating vibrations that have to potential to cause structural failure if in resonance with the natural frequencies of the system. To determine whether the capillaries are subject to this problem, the possibility of vortex shedding in this instrument was examined. Finite element analysis was used to supplement the analytical models in each of these areas.

3.1 Heat Transfer

Heat transfer analysis was performed using conservation of energy, heat exchangers, control volumes, and finite element analysis. Conservation of energy provides a simple but useful estimate of the temperature of the heat transfer fluid exiting the system at steady state. Heat exchanger analysis extends that calculation to yield the average temperature of the gel at steady state. The control volume model gives a time-dependent temperature profile of the
capillaries and the heat transfer fluid flowing through them, and the finite element analysis provides a visualization of the steady state temperature distribution over the entire cross section of the instrument, including both the fused silica and gel in each capillary as well as the water flowing over the capillaries.

3.1.1 Conservation of Energy

At steady state, the instrument is neither gaining nor losing energy. As a result, the thermal energy absorbed by the fluid leaving the system must be equal to the heat dissipated by the capillaries during electrophoresis. This energy balance is given by

$$\dot{E}_{\text{system}} = N_{\text{tubes}}A_{\text{tube}}q'' - \rho V_{\text{fluid}} c_{p, \text{fluid}} (T_{\text{fluid, out}} - T_{\text{fluid, in}}) = 0,$$

where $N_{\text{tubes}}$ is the number of capillaries in the system, $A_{\text{tube}}$ is the outer surface area of each capillary, $q''$ is the heat flux per unit area on the outer surface of the capillaries, $\rho$ is the density of the fluid, $V_{\text{fluid}}$ is the volumetric flow rate, and $c_{p, \text{fluid}}$ is the specific heat.

When a typical electric field of 10,000 V/m is applied to a 300 mm capillary during electrophoresis, a current of approximately 9 μA is induced in the gel [12]. This gives a constant heat flux of 72.5 W/m$^2$ over the outer surface of the capillaries for a total power output of 270 W across 10,000 capillaries.

The top half of Table 1 gives the volumetric flow rate necessary to maintain a specified temperature change based on conservation of energy in the instrument. Conversely, the temperature differential is calculated from volumetric flow rate in the bottom half. Using water as the heat transfer medium, a 0.2 °C increase in the temperature of the heat transfer fluid can be maintained with a flow rate of 3.3×10$^{-4}$ m$^3$/s and a 1 °C increase with a flow rate of 6.5×10$^{-5}$ m$^3$/s. Air requires an increase of almost four orders of magnitude to 0.268 m$^3$/s in order to maintain a 1 °C temperature differential, although the mass flow rate, which is inversely proportional to the heat capacity, is only four times that of water. Since the equipment used to blow air is so different from that used to pump water, however, the mass and volumetric flow rates are not entirely comparable.

Table 1: Temperature change and volumetric flow rate based on conservation of energy. In the top half, volumetric flow rate is calculated from a given temperature change. In the bottom half, this energy calculation has been made in reverse. The properties of water and air have been evaluated at 55 °C, which is at the center of the expected operating range of 50 °C to 60 °C.

<table>
<thead>
<tr>
<th>Fluid</th>
<th>Density (kg/m$^3$)</th>
<th>Heat Capacity (J/kg/K)</th>
<th>Temperature Change (K)</th>
<th>Mass Flow Rate (kg/s)</th>
<th>Volumetric Flow Rate (m$^3$/s)</th>
<th>Volumetric Flow Rate (L/min)</th>
<th>Flow Velocity (m/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>water</td>
<td>985.69</td>
<td>4183</td>
<td>0.2</td>
<td>0.323</td>
<td>3.3×10$^{-4}$</td>
<td>19.65</td>
<td>0.0109</td>
</tr>
<tr>
<td>water</td>
<td>985.69</td>
<td>4183</td>
<td>1</td>
<td>0.065</td>
<td>6.5×10$^{-5}$</td>
<td>3.93</td>
<td>0.0022</td>
</tr>
<tr>
<td>air</td>
<td>1.0677</td>
<td>1008</td>
<td>1</td>
<td>0.268</td>
<td>0.25</td>
<td>15051</td>
<td>8.36</td>
</tr>
<tr>
<td>water</td>
<td>985.69</td>
<td>4183</td>
<td>0.20</td>
<td>0.329</td>
<td>3.3×10$^{-4}$</td>
<td>20</td>
<td>0.0111</td>
</tr>
<tr>
<td>water</td>
<td>985.69</td>
<td>4183</td>
<td>0.98</td>
<td>0.066</td>
<td>6.7×10$^{-5}$</td>
<td>4</td>
<td>0.0022</td>
</tr>
<tr>
<td>air</td>
<td>1.0677</td>
<td>1008</td>
<td>1.51</td>
<td>0.178</td>
<td>0.17</td>
<td>10000</td>
<td>5.56</td>
</tr>
</tbody>
</table>
The circulator used in this system has a duplex pump, which provides both pressure and suction at flow rates of $6.7 \times 10^{-5} \text{ m}^3/\text{s}$ (4.0 L/min) and $3.3 \times 10^{-4} \text{ m}^3/\text{s}$ (20 L/min). At steady state, the difference between the temperature of water at the inlet and outlet of the instrument is estimated to be $0.98 \, \degree C$ when the pump is at $6.7 \times 10^{-5} \text{ m}^3/\text{s}$ and $0.20 \, \degree C$ at $3.3 \times 10^{-4} \text{ m}^3/\text{s}$. The temperature of the gel inside the capillaries, however, cannot be determined from this energy balance and must be at least as high as the temperature of the fluid cooling it.

### 3.1.2 Heat Exchanger Analysis

In order to determine the average temperature of the gel at steady state, the instrument was modeled as a heat exchanger in which the heat transfer fluid is the cold fluid and the gel is the hot fluid. In heat exchangers, the heat flux is the product of the overall heat transfer coefficient $U$, the surface area $A$, and the log mean temperature difference $\Delta T_{\text{lm}}$:

$$ q = UA\Delta T_{\text{lm}}. \tag{2} $$

Assuming that convection from the capillaries to the heat transfer fluid and conduction in the walls of the capillaries are the limiting modes of heat transfer, $UA = \frac{1}{h_o \pi D_o L + \frac{\ln(D_o/D_i)}{2\pi k L}}$, \tag{3}

where $h_o$ is the average convection coefficient over the outer surface of the capillaries, $k$ is the thermal conductivity of the fused silica, $D_o$ is the outer diameter of the capillaries, $D_i$ is the inner diameter, and $L$ is the length. The convection coefficient of the capillaries was calculated based on a procedure in Gnielinski, Zukauskas, and Skrinska [13] for tube banks and using the Nusselt number correlations from Churchill and Bernstein [14].

Since the temperature of the gel, which was taken as the hot fluid in the heat exchanger, remains constant, the log mean temperature difference is

$$ \Delta T_{\text{lm}} = \frac{(T_{\text{gel}} - T_{\text{fluid, in}}) - (T_{\text{gel}} - T_{\text{fluid, out}})}{\ln \left( \frac{T_{\text{gel}} - T_{\text{fluid, in}}}{T_{\text{gel}} - T_{\text{fluid, out}}} \right)} = \frac{T_{\text{fluid, out}} - T_{\text{fluid, in}}}{\ln \left( \frac{T_{\text{gel}} - T_{\text{fluid, out}}}{T_{\text{gel}} - T_{\text{fluid, in}}} \right)}, \tag{4} $$

where $T_{\text{gel}}$ is the average temperature of the gel and $T_{\text{fluid, in}}$ and $T_{\text{fluid, out}}$ are the temperatures of the heat transfer fluid entering and exiting the instrument.

Because the rate of heat transfer from the gel to the heat transfer fluid is one to two orders of magnitude larger than the heat flux from electrophoresis, the log mean temperature difference is only $0.024 \, \text{K}$ for water at $3.3 \times 10^{-4} \text{ m}^3/\text{s}$ and $0.035 \, \text{K}$ for water at $6.7 \times 10^{-5} \text{ m}^3/\text{s}$. As a result, the average temperature of the gel $T_{\text{gel}}$ is almost exactly equal to $T_{\text{fluid, out}}$. The results of this analysis are shown in Table 2.
Table 2: Heat exchanger analysis of the gel and heat transfer fluid. The average gel temperature is the same as the exit temperature of the fluid, because the rate of heat transfer is much larger than the heat flux of the capillaries.

<table>
<thead>
<tr>
<th>Fluid</th>
<th>Entry Temp (°C)</th>
<th>Flow Rate (m³/s)</th>
<th>Fluid Velocity (m/s)</th>
<th>Re</th>
<th>Nu</th>
<th>$\dot{h}$ (W/m²/K)</th>
<th>UA (W/K)</th>
<th>Gel Temp (°C)</th>
<th>Exit Temp (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>water</td>
<td>50</td>
<td>$3.3\times10^{-4}$</td>
<td>0.0111</td>
<td>11.5</td>
<td>4.34</td>
<td>7063</td>
<td>1.11</td>
<td>50.20</td>
<td>50.20</td>
</tr>
<tr>
<td>water</td>
<td>50</td>
<td>$6.7\times10^{-5}$</td>
<td>0.0022</td>
<td>2.3</td>
<td>2.16</td>
<td>3520</td>
<td>0.78</td>
<td>50.98</td>
<td>50.98</td>
</tr>
<tr>
<td>air</td>
<td>50</td>
<td>0.17</td>
<td>5.56</td>
<td>175.7</td>
<td>8.70</td>
<td>618</td>
<td>0.21</td>
<td>51.49</td>
<td>51.49</td>
</tr>
</tbody>
</table>

3.1.3 Control Volume Model

Control volumes around the capillaries and the water, as shown in Figure 6, were used to determine the transient response of the system. For simplicity, the fused silica and gel in each capillary are treated as a lumped thermal mass, which is valid if heat transfer from convection between the capillaries and the fluid is much slower than conduction through the gel and the capillary walls. Otherwise, the temperature of the capillaries will be higher than predicted and heat transfer will take place slower than predicted. The only modes of heat transfer taken into consideration are convection between the capillaries and the fluid and constant heat generation in the capillaries.

In Figure 6, the control volume containing the capillary gains energy through Joule heating and loses energy through convection to the fluid. The rate of temperature change in the capillary is the sum of these two energy transfers:

$$\frac{dT_{i,\text{cap}}}{dt} = \frac{-\bar{h}\left(\frac{T_{i-1,\text{fluid}} + T_{i,\text{fluid}}}{2} - T_{i,\text{cap}}\right) + \dot{q}}{C_{\text{cap}}}$$

where $T_{i,\text{cap}}$ is the temperature of the capillary, $T_{i-1,\text{fluid}}$ and $T_{i,\text{fluid}}$ are the temperatures of the fluid as it enters and exits the fluid control volume, $\bar{h}$ is the average convection coefficient of the capillary bank, $\dot{q}$ is the rate of heat generation, and $C_{\text{cap}}$ is the heat capacity. The convection coefficient of the tube bank was calculated as before.

The control volume enclosing the fluid around the capillaries must also take into account fluid entering and leaving the system:

$$\frac{1}{2}\left(\frac{dT_{i-1,\text{fluid}}}{dt} + \frac{dT_{i,\text{fluid}}}{dt}\right) = \frac{\rho \dot{V} c_{\text{fluid}} T_{i-1,\text{fluid}} - \bar{h}\left(\frac{T_{i-1,\text{fluid}} + T_{i,\text{fluid}}}{2} - T_{i,\text{cap}}\right) - \rho \dot{V} c_{\text{fluid}} T_{i,\text{fluid}}}{\rho \dot{V} c_{\text{fluid}}}$$

where $V$ is the volume of the region, $\dot{V}$ is the volume flow rate, $\rho$ is the density of the fluid, and $c_{\text{fluid}}$ is the heat capacity of the fluid.

In the step response to the heater, fluid entering the instrument is kept constant at 50 °C. The initial temperature of the capillaries and the fluid already inside the instrument is also 50 °C. Since an electric potential is being applied to the capillaries, they increase in temperature until the rate of convection matches the internal heat flux and Equation 1 is satisfied at steady state.
Figure 6: Two control volumes are used for this analysis. One encloses the capillaries and the other encloses the fluid around the capillaries. The capillaries undergo constant heat generation and forced convection to the fluid. The temperature of the control volume around the fluid is taken as the average of the inlet and outlet temperatures.

Figures 7 and 8 plot the temperature profile of the capillaries in water at $3.3 \times 10^{-4} \text{ m}^3/\text{s}$ (20 L/min) and in air at $0.17 \text{ m}^3/\text{s}$ (10,000 L/min) respectively based on Equations 5 and 6 for the step response. Air at $0.17 \text{ m}^3/\text{s}$ takes 7.5 times as long as water at $3.3 \times 10^{-4} \text{ m}^3/\text{s}$ to reach steady state. As shown in Table 3, water at $3.3 \times 10^{-4} \text{ m}^3/\text{s}$ has a 1% settling time of 0.79 s, with a steady state temperature of 50.20 °C for the last row of capillaries. At $6.7 \times 10^{-5} \text{ m}^3/\text{s}$ (4.0 L/min), the settling time is 2.90 s and the temperature is 50.98 °C. The temperature of each capillary at steady state is approximately proportional to its row number, which agrees with the energy calculations. The temperature offset of capillary 50 at steady state is roughly half that of capillary 100, because the fluid flowing around capillary 50 has come in contact with only half the capillaries and gained only half the energy of the fluid at capillary 100.

If the entry temperature of the heat transfer fluid can be controlled independently of the capillaries and the fluid already in the instrument, a step input from the circulator can be imposed on the system, in addition to the step input from the Joule heating that occurs during electrophoresis. Figure 9 shows the response of the capillaries when the water temperature is stepped to 60 °C from an initial system temperature of 50 °C. In Figure 10, water at 50 °C is being pumped into a system with an initial temperature of 60 °C. Tables 4 and 5 list the temperatures of the capillaries in rows 50 and 100 at steady state, which have the same offset from the fluid temperature as that calculated for the step response to electrophoresis. The settling times of 1.14 s, 3.75 s, and 8.52 s for water at $3.3 \times 10^{-4} \text{ m}^3/\text{s}$, water at $6.7 \times 10^{-5} \text{ m}^3/\text{s}$, and air at $0.17 \text{ m}^3/\text{s}$ respectively are 30% to 45% greater than those in Table 3, where the fluid and system start off at the same temperature.
Figure 7: Temperature profile of step response to electrophoresis with the water and capillaries at 50°C.

Figure 8: Temperature profile of step response to electrophoresis with the air and capillaries at 50°C.

Table 3: Step response to electrophoresis with the fluid and capillaries at 50°C.

<table>
<thead>
<tr>
<th>Fluid</th>
<th>Initial Temp (°C)</th>
<th>Fluid Temp (°C)</th>
<th>Flow Rate (m³/s)</th>
<th>Fluid Velocity (m/s)</th>
<th>$\bar{h}$ (W/m² K)</th>
<th>Settling Time (s)</th>
<th>Tube 50 (°C)</th>
<th>Tube 100 (°C)</th>
<th>Exit Temp (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>water</td>
<td>50</td>
<td>50</td>
<td>$3.3 \times 10^{-4}$</td>
<td>0.0111</td>
<td>7034</td>
<td>0.79</td>
<td>50.11</td>
<td>50.20</td>
<td>50.19</td>
</tr>
<tr>
<td>water</td>
<td>50</td>
<td>50</td>
<td>$6.7 \times 10^{-5}$</td>
<td>0.0022</td>
<td>3494</td>
<td>2.90</td>
<td>50.50</td>
<td>50.98</td>
<td>50.97</td>
</tr>
<tr>
<td>air</td>
<td>50</td>
<td>50</td>
<td>0.17</td>
<td>5.56</td>
<td>617</td>
<td>5.94</td>
<td>50.84</td>
<td>51.56</td>
<td>51.47</td>
</tr>
</tbody>
</table>
Figure 9: Temperature response to step input of inlet water from 50°C to 60°C.

Figure 10: Temperature response to step input of inlet water from 60°C to 50°C.

Table 4: Step input of inlet water from 50°C to 60°C.

<table>
<thead>
<tr>
<th>Fluid</th>
<th>Initial Temp (°C)</th>
<th>Fluid Temp (°C)</th>
<th>Flow Rate (m³/s)</th>
<th>Settling Time (s)</th>
<th>Tube 50 (°C)</th>
<th>Tube 100 (°C)</th>
<th>Exit Temp (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>water</td>
<td>50</td>
<td>60</td>
<td>3.3×10⁻⁴</td>
<td>1.14</td>
<td>60.11</td>
<td>60.20</td>
<td>60.19</td>
</tr>
<tr>
<td>water</td>
<td>50</td>
<td>60</td>
<td>6.7×10⁻⁵</td>
<td>3.75</td>
<td>60.50</td>
<td>60.98</td>
<td>60.97</td>
</tr>
<tr>
<td>air</td>
<td>50</td>
<td>60</td>
<td>0.17</td>
<td>8.52</td>
<td>60.87</td>
<td>61.61</td>
<td>61.52</td>
</tr>
</tbody>
</table>
Table 5: Step input of inlet water from 60°C to 50°C.

<table>
<thead>
<tr>
<th>Fluid</th>
<th>Initial Temp (°C)</th>
<th>Fluid Temp (°C)</th>
<th>Flow Rate (m³/s)</th>
<th>Settling Time (s)</th>
<th>Tube 50 (°C)</th>
<th>Tube 100 (°C)</th>
<th>Exit Temp (°C)</th>
<th>Max Temp (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>water</td>
<td>60</td>
<td>50</td>
<td>3.3×10⁻⁴</td>
<td>1.15</td>
<td>50.11</td>
<td>50.21</td>
<td>50.20</td>
<td>60.07</td>
</tr>
<tr>
<td>water</td>
<td>60</td>
<td>50</td>
<td>6.7×10⁻⁵</td>
<td>3.75</td>
<td>50.50</td>
<td>51.00</td>
<td>50.99</td>
<td>60.56</td>
</tr>
<tr>
<td>air</td>
<td>60</td>
<td>50</td>
<td>0.17</td>
<td>8.39</td>
<td>50.84</td>
<td>51.61</td>
<td>51.50</td>
<td>60.43</td>
</tr>
</tbody>
</table>

When the temperature of the fluid is dropped from 60 °C to 50 °C in Figure 10, the capillaries actually heat up briefly, because the incoming fluid at 50 °C has not yet replaced the warmer fluid already in the system. As listed in Table 5, the final row of capillaries will reach maximum temperatures of 60.07 °C in water at 3.3×10⁻⁴ m³/s, 60.56 °C in water at 6.7×10⁻⁵ m³/s, and 60.43 °C in air at 0.17 m³/s.

Unless the fluid in the instrument is isolated from the fluid in the circulator, however, it is very difficult to create the conditions needed for a step response. This is especially true with the apparatus being used for this experiment, since all the fluid is connected and the pump can not be disabled without turning off the temperature control as well. Furthermore, since the heat capacity of the fluid is large relative to the maximum power of the heating coils in the circulator, a large temperature gradient can not be created within the system. Based on the measurements in Figures 27 and 28, the maximum rate of temperature change is 0.0083 K/s from 50 °C to 60 °C and -0.0106 K/s from 60 °C to 50 °C. The response to these ramped inputs at a pump rate of 3.3×10⁻⁴ m³/s is shown in Figures 11 and 12. The temperatures listed for the capillaries and the exit and entry temperatures are taken at the 1% settling time of the temperature offset. Since the change in temperature of the heat transfer fluid is so slow, the settling times are very close to those listed in Table 3, where the fluid and the system start off at the same temperature. The temperature offsets of the capillaries from the fluid inlet temperature are also very close at about 0.2 K for water at 3.3×10⁻⁴ m³/s, 1.0 K for water at 6.7×10⁻⁵ m³/s, and 1.6 K for air at 0.17 m³/s. These offsets are slightly higher when the temperature of the fluid is being decreased than when it is being increased, partly because the rate of cooling is faster than the rate of heating, but also because the fluid must counteract the constant heat flux in the capillaries.

Figure 11: Temperature response to ramped input of inlet water at 0.0083°C/s.

Figure 12: Temperature response to ramped input of inlet water at -0.0106°C/s.
Table 6: Ramped input of inlet water from 50°C to 60°C.

<table>
<thead>
<tr>
<th>Fluid</th>
<th>Fluid Temp (°C)</th>
<th>Initial Temp (°C)</th>
<th>Flow Rate (m³/s)</th>
<th>Settling Time (s)</th>
<th>Entry Temp (°C)</th>
<th>Tube 50 (°C)</th>
<th>Tube 100 (°C)</th>
<th>Tube 100 Offset (K)</th>
<th>Exit Temp (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>water</td>
<td>50 to 60</td>
<td>50</td>
<td>3.3×10⁻⁴</td>
<td>0.79</td>
<td>50.01</td>
<td>50.11</td>
<td>50.20</td>
<td>0.19</td>
<td>50.20</td>
</tr>
<tr>
<td>water</td>
<td>50 to 60</td>
<td>50</td>
<td>6.7×10⁻⁵</td>
<td>2.90</td>
<td>50.02</td>
<td>50.51</td>
<td>50.98</td>
<td>0.96</td>
<td>50.98</td>
</tr>
<tr>
<td>air</td>
<td>50 to 60</td>
<td>50</td>
<td>0.17</td>
<td>5.97</td>
<td>50.05</td>
<td>50.88</td>
<td>51.58</td>
<td>1.53</td>
<td>51.49</td>
</tr>
</tbody>
</table>

Table 7: Ramped input of inlet water from 60°C to 50°C.

<table>
<thead>
<tr>
<th>Fluid</th>
<th>Fluid Temp (°C)</th>
<th>Initial Temp (°C)</th>
<th>Flow Rate (m³/s)</th>
<th>Settling Time (s)</th>
<th>Entry Temp (°C)</th>
<th>Tube 50 (°C)</th>
<th>Tube 100 (°C)</th>
<th>Tube 100 Offset (K)</th>
<th>Exit Temp (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>water</td>
<td>60 to 50</td>
<td>60</td>
<td>3.3×10⁻⁴</td>
<td>0.78</td>
<td>59.99</td>
<td>60.10</td>
<td>60.20</td>
<td>0.21</td>
<td>60.19</td>
</tr>
<tr>
<td>water</td>
<td>60 to 50</td>
<td>60</td>
<td>6.7×10⁻⁵</td>
<td>2.89</td>
<td>59.97</td>
<td>60.48</td>
<td>60.98</td>
<td>1.01</td>
<td>60.97</td>
</tr>
<tr>
<td>air</td>
<td>60 to 50</td>
<td>60</td>
<td>0.17</td>
<td>6.04</td>
<td>59.94</td>
<td>60.82</td>
<td>61.59</td>
<td>1.65</td>
<td>61.49</td>
</tr>
</tbody>
</table>

3.1.4 Finite Element Analysis

A finite element analysis was performed to obtain the temperature profile of the capillary array at steady state. A cross-section of the instrument was modeled in ANSYS using the FLUID141 2-D fluid-thermal element [15]. To save computing time and power, only five columns were used in the simulation, and the velocity in the horizontal direction on the left and right sides of the model were constrained to zero due to symmetry. Water enters the system at 50 °C and 0.011 m/s, which corresponds to 3.3×10⁻⁴ m³/s, and a zero pressure constraint has been imposed at the top of the columns, where the fluid leaves the system. The gel at the center of the capillaries has the same material properties as water and generates heat at a power density of 5.1 MW/m³.

The nodal solution for temperature after 50 iterations is shown in Figure 13. As expected, temperature is close to linear along the length of the column. The steady state temperature at the center of the final row of capillaries is 50.237 °C, an offset 20% higher than that predicted by the control volume model. The discrepancy exists, because the heat transfer resistance of conduction through the capillary wall is not negligible, as assumed under lumped thermal capacitance. Since the heat generated from electrophoresis must be conducted to the surface of the capillary before it can be removed by convection, the gel is perceptibly warmer than the fused silica. Based on the data plotted in Figure 14 for the horizontal profile of a capillary in the last row, the temperature of the fused silica rises from 50.212 °C to 50.226 °C between the outer surface and the inner surface and the temperature of the gel increases from 50.230 °C at the capillary wall to 50.237 °C at the center. The temperature of water leaving the system ranges from 50.193 °C in between two capillaries to 50.212 °C at the surface of a capillary. This temperature gradient also manifests in the vertical temperature profile shown in Figure 15. The hottest points are at the center of the capillaries, while the temperature of water in between drops to 0.03 K lower than that of the gel. The temperature profile has positive slope, because the water is heating up as it passes through the capillaries.
Figure 13: Steady state temperature profile of the capillary array. The full model is on the left, several sections have been magnified in the center, and the contour scale is on the right.

Figure 14: Temperature profile in the horizontal direction across the last capillary.
Figure 15: Temperature profile across the first five rows of capillaries.

3.2 Pressure Drop

Two of the most important factors in a fluid system are the flow velocity and the pressure drop. The pressure differential was estimated with a correlation from Zhukauskas and Ulinskas [16] and computed using finite element analysis.

3.2.1 Tube Bank Correlation

The pressure drop in the array of capillaries was calculated from a formula for tube banks given by Zhukauskas and Ulinskas [16]:

\[
\Delta P = N \chi \left( \frac{\rho V_{\text{max}}^2}{2} \right) f,
\]

where \( N \) is the rows of tubes, \( \chi \) is a correction factor, \( \rho \) is the density of the fluid, \( f \) is the friction factor, and \( V_{\text{max}} \) is the maximum velocity of the fluid, which is given by

\[
\frac{V_{\text{max}}}{V_0} = \frac{S_T}{S_T - D}.
\]

The correction factor \( \chi \) is 1 for an aligned tube bank with equal transverse and longitudinal spacing. The friction factor \( f \) is a function of the Reynolds number and the longitudinal pitch \( P_L \), which is 2.48 for the given spacing between the capillaries. Since the friction factor was extrapolated off a chart, the pressure differentials calculated in Table 8 are only accurate to 50%.

Table 8: Pressure drop through the capillary array.

<table>
<thead>
<tr>
<th>Fluid</th>
<th>Flow Rate (m³/s)</th>
<th>Fluid Velocity (m/s)</th>
<th>( R_{e_{\text{max}}} )</th>
<th>( f )</th>
<th>( \Delta P ) (Pa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>water</td>
<td>( 3.3 \times 10^{-4} )</td>
<td>0.0111</td>
<td>14.7</td>
<td>1.5</td>
<td>26</td>
</tr>
<tr>
<td>water</td>
<td>( 6.7 \times 10^{-5} )</td>
<td>0.0022</td>
<td>2.9</td>
<td>3.0</td>
<td>3.4</td>
</tr>
<tr>
<td>air</td>
<td>0.17</td>
<td>5.56</td>
<td>202</td>
<td>0.3</td>
<td>1387</td>
</tr>
</tbody>
</table>
3.2.2 Finite Element Analysis

As shown on the profile of the capillary array in Figure 16 and on the graph of pressure against distance in Figure 17, water pressure drops linearly with distance along the length of the column. The pressure gradient for the entire column is 18.55 Pa. In Figure 18, the pressure of the water increases from 18.491 Pa in between capillaries to 18.622 Pa at the center of a capillary. Low-pressure boundary layers are visible around the cylinders in Section A of Figure 16.

Figure 16: Steady state pressure profile of the capillary array. The full model on the left and Section A use the same contour scale. The contours in Section B are more closely spaced.

Figure 17: The pressure of the fluid between the capillaries is directly proportional to the distance it has traveled along the column.
3.3 Vortex Shedding

Vortex shedding describes the phenomenon that occurs when a bluff body obstructing fluid flow leaves eddies in its wake [17]. The vortex streets generate alternating forces along the top and bottom of the body, causing it to vibrate perpendicular to fluid flow. These vibrations can lead to failure if they are in resonance with the natural frequency of the structure. In this instrument, the capillaries may be at risk if their structural frequency matches the frequency of vortex shedding. The vortex shedding frequencies of water and air and the natural frequency of a capillary modeled as thin uniform beam are calculated to ensure that there is no overlap between the two. Finite element analysis is again used to confirm the analytical results.

3.3.1 The Critical Reynolds Number

Below the critical Reynolds number, the wake of a bluff body does not develop into periodic instabilities [17]. Instead, flow behind the cylinder is symmetric, with steady recirculation regions on each side of the wake. Flow profiles of a smooth tube in the laminar steady regime and the laminar vortex shedding regime are depicted in Figures 19 and 20. Past studies have cited critical Reynolds numbers of 40 [18], 49 [17], and 47 [19]. Thus, there is no possibility of vortex shedding with the current apparatus, which uses a heat transfer fluid of water at a flow rate of $3.3 \times 10^{-4}$ m$^3$/s and Reynolds number of 8.6.
3.3.2 Strouhal Correlation

Based on a critical Reynolds number of 49, the capillaries will experience vortex shedding once the flow rate of water exceeds $0.0019 \, \text{m}^3/\text{s}$ (117 L/min). The frequency of vortex shedding is given by the Strouhal number

$$St = \frac{f D}{U},$$

(9)

where $f$ is the frequency, $D$ is the diameter of the bluff body, and $U$ is the free-flow velocity of the fluid. Williamson and Brown [20] developed the following correlation for the Strouhal number in terms of the square root of the Reynolds number:

$$St = A + B/\sqrt{Re} + C/Re$$

(10)

From Equations 9 and 10, the capillaries will generate vortices at 20 Hz when the flow rate is $0.0019 \, \text{m}^3/\text{s}$. The frequency of vortex shedding is plotted against the volume flow rate of water in Figure 21.

If air is used as the heat transfer fluid, however, the Reynolds number will be at least an order of magnitude higher to maintain a comparable degree of heat transfer and the frequency of vortex shedding will have to be taken into consideration. The frequency of vortex shedding in air is plotted in Figure 22.

Figure 21: Vortex shedding frequency against volume flow rate of water.
3.3.3 Transverse Vibration of a Thin Uniform Beam

The vibration modes were determined by modeling the capillaries as thin uniform beams. The capillaries were taken as hollow tubes of fused silica, and the effects of the gel were neglected completely.

The thin uniform beam takes into account the distribution of both mass and elasticity while neglecting rotary inertia and shear of the element [21]. Moment balances about the beam element shown in Figure 23 yield the equation

$$\frac{\partial^4 y}{\partial x^4} + \left( \frac{\rho A}{EI} \right) \frac{\partial^2 y}{\partial t^2} = 0,$$

where $\rho$ is the density of the beam, $A$ is the cross-sectional area, $E$ is the Young’s modulus, and $I$ is the moment of inertia. Since the deflection of the beam is harmonic with time for normal
modes of vibration,

\[ y = X \left( B_1 \sin \omega t + B_2 \cos \omega t \right), \]  

(12)

where \( X \) is a time-independent function that determines the shape of the vibration mode. Substituting Equation 12 into Equation 11 gives

\[ \frac{\partial^4 X}{\partial x^4} = \left( \frac{\rho A}{EI} \right) \omega^2 X = \lambda^4 X, \]  

(13)

where

\[ \lambda^4 = \frac{\rho A \omega^4}{EI}. \]  

(14)

Based on Equation 13, the general solution for the beam shape is

\[ X = C_1 \cos \lambda l + C_2 \sin \lambda l + C_3 \cosh \lambda l + C_4 \sinh \lambda l. \]  

(15)

The boundary conditions for a beam that is pinned at both ends are

\[ X(0) = X(l) = 0 \quad \text{and} \]

\[ \frac{d^2 X}{dx^2}(0) = \frac{d^2 X}{dx^2}(l) = 0, \]  

(16a)

and those for a beam that is clamped at both ends are

\[ X(0) = X(l) = 0 \quad \text{and} \]

\[ \frac{dX}{dx}(0) = \frac{dX}{dx}(l) = 0. \]  

(17a)

Solving for \( \lambda \) yields

\[ \sin \lambda l = 0, \]  

(18)

for the pinned-pinned boundary conditions and

\[ \cos \lambda l \cosh \lambda l = 1, \]  

(19)

for the clamped-clamped boundary conditions. Figure 24 plots the first and second natural modes of vibration, which were obtained by solving Equations 18 and 19 for \( \lambda l \) and substituting the material characteristics of the capillaries into Equation 14.

If the beam is in tension, an additional force must be taken into account, resulting in

\[ EI \frac{\partial^4 y}{\partial x^4} - T \frac{\partial^2 y}{\partial x^2} + \rho A \frac{\partial^2 y}{\partial t^2} = 0. \]  

(20)

The general solution for Equation 20 is

\[ X = C_1 \cos \alpha_1 t + C_2 \sin \alpha_1 t + C_3 \cosh \alpha_2 t + C_4 \sinh \alpha_2 t, \]  

(21)

and the boundary conditions for both the pinned-pinned and clamped-clamped cases remain the
same, as described by Equations 16 and 17. The natural frequencies of a 300-mm capillary in tension are plotted in Figure 25.

Since the primary vibration modes of the capillaries are 10 Hz under pinned-pinned conditions and 23 Hz under clamped-clamped conditions for a 300-mm capillary, it is unlikely for the natural frequency of the system to be in resonance with the vortex shedding frequency of air, which starts above 700 Hz. If water is used in the system at a volume flow rate greater than 0.0019 m³/s, however, the vortex shedding frequency will be close to 20 Hz and the potential for resonance to cause unwanted effects must be considered. Depending on the velocity of the water, it may be necessary to add structural supports to the capillary array or apply tension to the capillaries themselves such that their natural frequency is well above the vortex shedding frequency of the water in the system.

Figure 24: Natural modes of vibration of a capillary in pinned-pinned and clamped-clamped end conditions.
Figure 25: Natural modes of vibration of a capillary in tension. The natural frequency increases with tension.

3.3.4 Finite Element Analysis

The velocity solution to the finite element model is shown in both vector and contour plots in Figure 26. Since the fluid between the capillaries is moving very slowly, there is little opportunity for vortex shedding in the wake directly behind the capillaries. Nor is a recirculation region present, as suggested in Figure 19. Vibrations may still be a concern if the flow around the capillaries is in any way periodic. This information, however, can not be determined from a steady state analysis.

Figure 26: Steady state velocity profile of the capillary array. The two images on the left are vector plots and the image on the right is a contour plot. All three use the same contour scale.
4.0 Results and Discussion

The purpose of the physical model is to determine how the temperature of the system can be controlled by the fluid entering the instrument and how it is influenced by the heat dissipated during electrophoresis. Thus, baseline experiments must first be conducted in which the temperature of the inlet is constant or changing without the effect of the heater. When the temperature of the water entering the instrument is held at a constant temperature of approximately 50 °C, the temperature of the water inside the instrument is about 0.2 K lower. When the inlet temperature is being increased, the system temperature is 0.40 K lower, and when the inlet temperature is being decreased, the system temperature is 0.34 K higher than the inlet. Contrary to the predictions made in the analysis, it takes roughly 300 s for the rate of temperature change in the instrument to catch up with that of the reservoir, and achieving equilibrium can take up to 900 s.

When the heater is on, the system temperature is 0.24 K, 0.43 K, and 0.65 K higher than the reservoir temperature at pump speeds of $3.3 \times 10^{-4} \text{ m}^3/\text{s}$, $1.3 \times 10^{-4} \text{ m}^3/\text{s}$, and $6.7 \times 10^{-5} \text{ m}^3/\text{s}$ respectively. The rise time is about 350 s. When the inlet temperature is increasing, the temperature inside the instrument is 0.06 K lower than the reservoir temperature. The system temperature is 0.67 K higher when the reservoir is being cooled. The rise time is only 300 s, but equilibrium can take up to 900 s.

4.1 Circulator Temperature Control

The temperature profile within the instrument depends in large part on the equipment used to control the temperature of the water entering the system. In order to determine the maximum rate of heating and cooling in the reservoir, the temperature of the circulator was cycled between 50 °C and 60 °C. Based on the results in Figures 27 and 28, the temperature of the reservoir can increase at a maximum rate of 0.0083 K/s and decrease at a maximum rate of 0.0108 K/s. Cooling occurs more quickly, because the refrigeration unit in the system is more powerful than the heating coils and because heat from the reservoir is dissipated into the cooler ambient air. As the temperature of the reservoir approaches the target temperature of the system, the PID controller slows down the heating or cooling to a much more gradual rate. Once the temperature of the reservoir is within one degree of the target, the system may take over 300 s to reach steady state, as was the case when the reservoir was cooled to 50 °C in Figure 29.

![Figure 27: Temperature profile of the circulator reservoir while heating from 50°C to 60°C.](image)
4.2 Constant Temperature

In this section, the temperature of the water in the circulator was held constant by the temperature controller while being pumped through the instrument at $3.3 \times 10^{-4}$ m$^3$/s. The temperature readings from the RTD elements, which are located in a vertical line along the side of the instrument as shown in Figure 30, are plotted in Figure 31. During this run, the controller was set to 50.00 °C, but the temperature of the reservoir was 49.57 °C and the RTD elements in
the instrument averaged 49.36 °C, with a range from 49.18 °C to 49.44 °C. It is uncertain how much of the variation in the readings can be attributed to real differences in temperature, however. Although the RTD elements have standard deviations of only 0.004 K to 0.009 K when placed in the reservoir at constant temperature during calibration, their resistances may drift over time or under other influences. The results from RTD 1, in particular, are somewhat suspect. Based on Figure 30, RTD 1 appears to experience lower temperatures and greater variations in temperature than the other RTD elements; however, it also gave the lowest reading and had the highest standard deviation during calibration in the reservoir. Likewise, it is difficult to draw conclusions from Figure 32, since there is no clear trend in the graph and the variation between the RTD elements may be within their range of uncertainty. Nevertheless, it seems evident from Figure 31 that the temperature of the water in the instrument is on average 0.2 K lower than the temperature of the reservoir and that the RTD elements in the instrument experience more variation in temperature than the one in the reservoir.

In a closed system, the temperature of the water in the instrument should be exactly the same as the temperature of the water in the reservoir at steady state, if it is not gaining or losing energy. In this case, however, the instrument may be losing heat to the environment through its aluminum walls. Some heat may be lost through the rubber tubing as well, cumulatively bringing the temperature down by 0.2 K.

Figure 30: Temperature measurements of the water inside the system were taken with the RTD elements in a vertical line along the side of the instrument. Water flows into the system from the lower left corner through flow straighteners that run the length of the instrument and out of upper right corner, such that the RTD elements are downstream of the heater.
Figure 31: Temperature profile of the instrument with inlet temperature constant at 50°C.

Figure 32: Average temperature of the RTD elements in the instrument.
4.3 Ramped Temperature

The temperature profile of the instrument was obtained by ramping the inlet temperature from 50 °C to 60 °C and back again. The system response during the temperature rise is shown in Figure 33, and the difference between the average temperature of the RTD elements in the instrument and the temperature of the reservoir is plotted in Figure 34. While the temperature of the reservoir is increasing at 0.0040 K/s, the instrument temperature reaches a constant temperature offset of 0.40 K after about 200 s. Once the reservoir temperature begins to level off at 60 °C, the temperature offset drops to 0.19 K. It takes the system 300 s for the offset to reach 0.19 and another 700 s before full equilibrium is achieved.

The cooling in Figure 35 occurs at a rate of 0.0067 K/s. During cooling, the average temperature of the RTD elements in the instrument reaches 0.34 K above the reservoir temperature in about 200 s. This temperature offset, which is plotted in Figure 36, drops to 0.12 K once the reservoir approaches steady state at 50 °C. The drop from 0.34 K to 0.12 K takes place over 400 s and equilibrates after about 900 s.
4.4 Constant Temperature with Heater

After a system has reached equilibrium, the heater is set to 70 V or 255 W in a step response. Figure 37, which is a graph of the temperature response, suggests that the higher the position of the RTD element, the lower the temperature and the smaller the offset. Figure 38 plots the average difference in temperature between the water temperature inside the instrument and the water temperature in the reservoir. Based on Figure 38, the offset between the system temperature and the inlet temperature reaches a steady state after about 350 s. Since the reservoir temperature continues to drop, however, the absolute temperatures do not reach steady state until after 500 s.

The average steady state offset is 0.24 K at $3.3 \times 10^{-4}$ m³/s, 0.43 K at $1.3 \times 10^{-4}$ m³/s, and 0.65 K at $6.7 \times 10^{-5}$ m³/s. The relation between lower pump speeds and higher steady state temperatures is illustrated by Figure 39. Figures 39 and 40 also suggest that temperature along the length of the instrument decreases with height. There is a lot of overlap between the temperatures of the first four RTD elements, but the fifth one is significantly lower than the other four and the sixth is significantly lower than the fifth.

![Figure 37: Temperature profile of the response to a step input from the heater at $3.3 \times 10^{-4}$ m³/s.](image-url)
Figure 38: Average temperature offset of the instrument from the reservoir in the response to a step input from the heater at $3.3 \times 10^{-4}$ m$^3$/s.

Figure 39: Steady state temperature profile in response to a step input from the heater at different pump speeds.
4.5 Ramped Temperature with Heater

Since it may be necessary to sweep through a range of temperatures during electrophoresis, it is also necessary to characterize the temperature response of the instrument to a changing water inlet temperature with a step response from the heater. Figure 41 plots the temperature response when the heater is dissipating energy at 255 W and water entering the instrument is being heated at a rate of 0.0056 K/s from 50 °C to 60 °C. Figure 42 is the temperature difference between the average RTD element in the instrument and the RTD element in the reservoir. It takes roughly 300 s for the rate of change in temperature of the system to reach that of the reservoir, at which point the temperature inside the instrument is 0.06 K less than that of the reservoir. Once the reservoir temperature levels off, another 500 s is required to reach the steady state offset of 0.27 K.

When the temperature is decreasing at 0.0053 K/s, the system takes 300 s to reach a constant offset of 0.67 K, as shown in Figures 43 and 44. As the reservoir temperature approaches 50 °C, the temperature of the water inside the instrument takes 500 s to reach an offset of 0.33 K and roughly 900 s to equilibrate completely.
Figure 41: Temperature profile of instrument in response to a step input from the heater with inlet temperature increasing from 50°C to 60°C.

Figure 42: Average temperature offset from the reservoir in the response to a step input from the heater with inlet temperature increasing from 50°C to 60°C.
Figure 43: Temperature profile of instrument in response to a step input from the heater with inlet temperature decreasing from 60°C to 50°C.

Figure 44: Average temperature offset from the reservoir in the response to a step input from the heater with inlet temperature decreasing from 60°C to 50°C.
5.0 Conclusion and Recommendations

Analytical models, finite element analysis, and physical models were used to predict the temperature response of the instrument to changes in the temperature of the water entering the system and to heat generated by capillary electrophoresis. The analytical models estimated a steady state offset of 0.2 K for water at $3.3 \times 10^{-4}$ m$^3$/s (20 L/min) and 1 K for water at $6.7 \times 10^{-5}$ m$^3$/s (4 L/min) and predicted that the system would reach steady state within several s. Finite element analysis calculated that the gel inside the capillaries would have a steady state offset of 0.24 K. The physical system yielded a steady state offset of 0.24 K at $3.3 \times 10^{-4}$ m$^3$/s and 0.65 K at $6.7 \times 10^{-5}$ m$^3$/s, but the settling time in both cases was on the order of 500 s. Factors in the physical system not considered in the theoretical models, such as convection to the environment, account for at least part of this discrepancy. Relative to the physical system, the analytical models were very simplistic and neglected the effects of important components, such as the circulator reservoir.

There are many ways to improve the analytical models. First of all, the thermal mass of the aluminum in the instrument, convection from the instrument to the environment, and conduction within the capillary walls can be taken into account. Heat transfer within the reservoir should also be modeled in order to optimize the PID controller or replace it with something else. The heating and cooling capacity of the circulator should allow the system to come to steady state much more quickly than observed in this analysis. In addition, fluid flow through the instrument needs to be studied to ensure that flow is indeed uniform across all the capillaries. Finite element analysis would be one approach to this problem.

The experimental procedure would also benefit from some changes. A better method of calibrating the RTD elements needs to be implemented so that there is no question whether temperature differences are due to bias errors or actually exist in the system. In addition, some of the RTD element should be placed in different locations. For example, one RTD element at the inlet to the instrument and one at the exit could be used to calculate the change in thermal energy over time. Likewise, flow sensors in the instrument would provide valuable information. There were also some problems with the software. Since the software had difficulty saving a lot of data points, the RTD elements were sampled much more slowly than desired.

ANSYS calculated a pressure drop of 18.55 Pa, which is reasonably close to my analytical calculation of 26 Pa. The only way to get a more accurate number would be to test it out on a real system.

Unless water is used as the heat transfer fluid at a flow rate of over 0.0019 m$^3$/s (117 L/min), vortex shedding is not a critical concern. ANSYS can be used to model the transient fluid flow, but it is unlikely that vortex shedding will play an important role in the design of this instrument.
Appendix A: Scan Characteristics and RTD Calibration

Table A.1: Scan speeds and RTD standard deviations at 50 °C

<table>
<thead>
<tr>
<th>NPLC</th>
<th>0.02</th>
<th>0.2</th>
<th>1</th>
<th>2</th>
<th>10</th>
<th>20</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time Integrating (s)</td>
<td>0.0003</td>
<td>0.0033</td>
<td>0.0167</td>
<td>0.0333</td>
<td>0.1667</td>
<td>0.3333</td>
</tr>
<tr>
<td>Time Readings (s)</td>
<td>0.028</td>
<td>0.033</td>
<td>0.061</td>
<td>0.090</td>
<td>0.357</td>
<td>0.690</td>
</tr>
<tr>
<td>Time Scanning (s)</td>
<td>0.226</td>
<td>0.265</td>
<td>0.485</td>
<td>0.721</td>
<td>2.855</td>
<td>5.522</td>
</tr>
<tr>
<td>Time Integrating / Time Reading</td>
<td>0.012</td>
<td>0.101</td>
<td>0.275</td>
<td>0.370</td>
<td>0.467</td>
<td>0.483</td>
</tr>
<tr>
<td>RTD 1 σ (K)</td>
<td>0.037</td>
<td>0.018</td>
<td>0.003</td>
<td>0.004</td>
<td>0.004</td>
<td>0.003</td>
</tr>
<tr>
<td>RTD 2 σ (K)</td>
<td>0.035</td>
<td>0.019</td>
<td>0.002</td>
<td>0.002</td>
<td>0.002</td>
<td>0.002</td>
</tr>
<tr>
<td>RTD 3 σ (K)</td>
<td>0.036</td>
<td>0.023</td>
<td>0.003</td>
<td>0.003</td>
<td>0.002</td>
<td>0.002</td>
</tr>
<tr>
<td>RTD 4 σ (K)</td>
<td>0.034</td>
<td>0.020</td>
<td>0.003</td>
<td>0.003</td>
<td>0.003</td>
<td>0.003</td>
</tr>
<tr>
<td>RTD 5 σ (K)</td>
<td>0.044</td>
<td>0.034</td>
<td>0.002</td>
<td>0.003</td>
<td>0.002</td>
<td>0.002</td>
</tr>
<tr>
<td>RTD 6 σ (K)</td>
<td>0.034</td>
<td>0.024</td>
<td>0.002</td>
<td>0.007</td>
<td>0.005</td>
<td>0.005</td>
</tr>
<tr>
<td>RTD 7 σ (K)</td>
<td>0.035</td>
<td>0.024</td>
<td>0.002</td>
<td>0.003</td>
<td>0.002</td>
<td>0.002</td>
</tr>
<tr>
<td>RTD 8 σ (K)</td>
<td>0.039</td>
<td>0.028</td>
<td>0.003</td>
<td>0.003</td>
<td>0.002</td>
<td>0.005</td>
</tr>
<tr>
<td>Average σ (K)</td>
<td>0.037</td>
<td>0.024</td>
<td>0.003</td>
<td>0.003</td>
<td>0.003</td>
<td>0.003</td>
</tr>
</tbody>
</table>

Table A.2: Scan speeds and RTD standard deviations at 60 °C

<table>
<thead>
<tr>
<th>NPLC</th>
<th>0.02</th>
<th>0.2</th>
<th>1</th>
<th>2</th>
<th>10</th>
<th>20</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time Integrating (s)</td>
<td>0.0003</td>
<td>0.0033</td>
<td>0.0167</td>
<td>0.0333</td>
<td>0.1667</td>
<td>0.3333</td>
</tr>
<tr>
<td>Time Readings (s)</td>
<td>0.028</td>
<td>0.033</td>
<td>0.060</td>
<td>0.090</td>
<td>0.356</td>
<td>0.690</td>
</tr>
<tr>
<td>Time Scanning (s)</td>
<td>0.223</td>
<td>0.261</td>
<td>0.481</td>
<td>0.719</td>
<td>2.852</td>
<td>5.518</td>
</tr>
<tr>
<td>Time Integrating / Time Reading</td>
<td>0.012</td>
<td>0.102</td>
<td>0.277</td>
<td>0.371</td>
<td>0.468</td>
<td>0.483</td>
</tr>
<tr>
<td>RTD 1 σ (K)</td>
<td>0.100</td>
<td>0.025</td>
<td>0.007</td>
<td>0.005</td>
<td>0.005</td>
<td>0.006</td>
</tr>
<tr>
<td>RTD 2 σ (K)</td>
<td>0.099</td>
<td>0.027</td>
<td>0.005</td>
<td>0.004</td>
<td>0.004</td>
<td>0.004</td>
</tr>
<tr>
<td>RTD 3 σ (K)</td>
<td>0.101</td>
<td>0.030</td>
<td>0.005</td>
<td>0.004</td>
<td>0.004</td>
<td>0.004</td>
</tr>
<tr>
<td>RTD 4 σ (K)</td>
<td>0.100</td>
<td>0.028</td>
<td>0.006</td>
<td>0.005</td>
<td>0.005</td>
<td>0.004</td>
</tr>
<tr>
<td>RTD 5 σ (K)</td>
<td>0.096</td>
<td>0.038</td>
<td>0.004</td>
<td>0.004</td>
<td>0.003</td>
<td>0.003</td>
</tr>
<tr>
<td>RTD 6 σ (K)</td>
<td>0.100</td>
<td>0.030</td>
<td>0.005</td>
<td>0.004</td>
<td>0.004</td>
<td>0.003</td>
</tr>
<tr>
<td>RTD 7 σ (K)</td>
<td>0.107</td>
<td>0.032</td>
<td>0.006</td>
<td>0.004</td>
<td>0.004</td>
<td>0.003</td>
</tr>
<tr>
<td>RTD 8 σ (K)</td>
<td>0.103</td>
<td>0.034</td>
<td>0.006</td>
<td>0.005</td>
<td>0.006</td>
<td>0.006</td>
</tr>
<tr>
<td>Average σ (K)</td>
<td>0.101</td>
<td>0.030</td>
<td>0.005</td>
<td>0.004</td>
<td>0.004</td>
<td>0.004</td>
</tr>
</tbody>
</table>

Table A.3: RTD calibration characteristics at 50 °C

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Offset (K)</th>
<th>σ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>RTD 1</td>
<td>49.250</td>
<td>0.285</td>
</tr>
<tr>
<td>RTD 2</td>
<td>49.616</td>
<td>-0.081</td>
</tr>
<tr>
<td>RTD 3</td>
<td>49.441</td>
<td>0.093</td>
</tr>
<tr>
<td>RTD 4</td>
<td>49.572</td>
<td>-0.037</td>
</tr>
<tr>
<td>RTD 5</td>
<td>49.502</td>
<td>0.033</td>
</tr>
<tr>
<td>RTD 6</td>
<td>49.675</td>
<td>-0.140</td>
</tr>
<tr>
<td>RTD 7</td>
<td>49.688</td>
<td>-0.153</td>
</tr>
<tr>
<td>Average</td>
<td>49.535</td>
<td>0.0033</td>
</tr>
</tbody>
</table>
Table A.4: RTD calibration characteristics at 55 °C

<table>
<thead>
<tr>
<th>RTD</th>
<th>Temperature (°C)</th>
<th>Offset (K)</th>
<th>σ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>54.184</td>
<td>0.326</td>
<td>0.0040</td>
</tr>
<tr>
<td>2</td>
<td>54.603</td>
<td>-0.093</td>
<td>0.0036</td>
</tr>
<tr>
<td>3</td>
<td>54.398</td>
<td>0.112</td>
<td>0.0037</td>
</tr>
<tr>
<td>4</td>
<td>54.561</td>
<td>-0.051</td>
<td>0.0040</td>
</tr>
<tr>
<td>5</td>
<td>54.487</td>
<td>0.022</td>
<td>0.0033</td>
</tr>
<tr>
<td>6</td>
<td>54.651</td>
<td>-0.141</td>
<td>0.0046</td>
</tr>
<tr>
<td>7</td>
<td>54.685</td>
<td>-0.175</td>
<td>0.0037</td>
</tr>
<tr>
<td>Average</td>
<td>54.510</td>
<td></td>
<td>0.0039</td>
</tr>
</tbody>
</table>

Table A.5: RTD calibration characteristics at 60 °C

<table>
<thead>
<tr>
<th>RTD</th>
<th>Temperature (°C)</th>
<th>Offset (K)</th>
<th>σ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>59.087</td>
<td>0.398</td>
<td>0.0086</td>
</tr>
<tr>
<td>2</td>
<td>59.605</td>
<td>-0.120</td>
<td>0.0050</td>
</tr>
<tr>
<td>3</td>
<td>59.340</td>
<td>0.144</td>
<td>0.0048</td>
</tr>
<tr>
<td>4</td>
<td>59.548</td>
<td>-0.064</td>
<td>0.0042</td>
</tr>
<tr>
<td>5</td>
<td>59.489</td>
<td>-0.004</td>
<td>0.0042</td>
</tr>
<tr>
<td>6</td>
<td>59.640</td>
<td>-0.156</td>
<td>0.0039</td>
</tr>
<tr>
<td>7</td>
<td>59.682</td>
<td>-0.198</td>
<td>0.0040</td>
</tr>
<tr>
<td>Average</td>
<td>59.484</td>
<td></td>
<td>0.0050</td>
</tr>
</tbody>
</table>
Appendix B: MATLAB Code for Control Volume Model

tubebanktemp.m
VdotLmin = 20
capillary.initialT = 60;
fluidfunc = @linearwater2;
tempfunc = inline('60-0.00832*t');
tspan = [0 2];
integrator = @ode15s;
tubefunc = @tubetemp2;

% Assumptions:
% 1. The capillary as lumped thermal capacitance
% 2. Uniform convection coefficient over all tubes

% Capillary dimensions
capillary.ID = 75E-6;
capillary.OD = 403E-6; % 363 +/- 10 um + 2 x 20 um coating
capillary.length = 300E-3; % 2 x 150 mm (standard length)

% Capillary characteristics
silica.rho = 2.2E3; % kg/m^3 from Fused Quartz on MatWeb
silica.cp = 700; % J/kg/K from Fused Quartz on MatWeb
silica.k = 1.7; % W/m/K from Fused Quartz on MatWeb
water.rho = 985.69; % kg/m^3 at T = 55 C
water.cp = 4183; % J/kg/K at T = 55 C
water.k = 0.64926; % W/m/K at T = 55 C
capillary.CPUL = pi/4 * (capillary.OD^2 - capillary.ID^2) * silica.rho * silica.cp ...
+ pi/4 * capillary.ID^2 * water.rho * water.cp;

% Energy dissipated from electrophoresis
voltage = 3000; % 100 V/cm
current = 9E-6;
Qdot = voltage * current;
QdotPUL = Qdot / capillary.length;

% Tube bank dimensions
tubebank.ST = 1E-3;
tubebank.SL = 1E-3;
tubebank.staggered = 0;
tubebank.SD = sqrt(tubebank.ST^2 + tubebank.SL^2);
tubebank.Ntubes = 10000;
tubebank.NT = 100;
tubebank.NL = tubebank.Ntubes / tubebank.NT;

% Fluid characteristics
% range is 50 to 60 C
fluid.velocity = VdotLmin / 1000 / 60 / (tubebank.NT * tubebank.ST * capillary.length)
fluid.initialT = feval(tempfunc, 0);
Ti(1:tubebank.NL*2) = capillary.initialT;
VdotPUL = fluid.velocity * tubebank.ST;

fluid = feval(fluidfunc, fluid.initialT, fluid); % fluid is an input to preserve other associated values
ToutGuess = fluid.initialT + tubebank.NL * QdotPUL / fluid.rho / VdotPUL / fluid.cp;
TMean = (fluid.initialT + ToutGuess) / 2;
surfaceprops = feval(fluidfunc, capillary.initialT);
fluid = feval(fluidfunc, TMean, fluid);
[ReBar, NuBar] = nusseltgnielinski(fluid, surfaceprops.Pr, tubebank, capillary.OD);
hBar = fluid.k * NuBar / capillary.OD
hBarPUL = hBar * pi * capillary.OD;

tic
options = odeset('Refine', 4, 'MaxStep', 0.01);
[T, Y] = feval(integrator, tubefunc, tspan, Ti, options, fluid, fluidfunc, tempfunc, tubebank, capillary, VdotPUL, QdotPUL);
toc

cla
hold on
colors = ['r' 'g' 'b' 'c' 'm' 'y'];
plot(T, Y(:, 1), colors(1))
for i = 1:4
    plot(T, Y(:, i*50-1), colors(i+1))
end
hold off
xlabel('Time (s)')
ylabel('Temperature (°C)')
legend('tube 1', 'tube 25', 'tube 50', 'tube 75', 'tube 100', 0)

Vdot = tubebank.NT * tubebank.ST * capillary.length * fluid.velocity
VdotLmin = Vdot * 1000 * 60
resistance = 100 * 1.0782 * (fluid.velocity * 1E-3 / (1E-3 - capillary.OD)).^ 2 / 2 * 0.2

tubetemp2.m
function dT = tubetemp2(time, T, fluid, fluidfunc, tempfunc, tubebank, capillary, VdotPUL, QdotPUL)
% For Zhukauskas, all properties except Prs are evaluated at the
% arithmetic mean of the fluid inlet and outlet temperatures.
fluid.initialT = feval(tempfunc, time);
fluid = feval(fluidfunc, fluid.initialT, fluid);
TMean = fluid.initialT + tubebank.NL * QdotPUL / fluid.rho / VdotPUL / fluid.cp / 2;
capsurf = feval(fluidfunc, mean(T));

mixingarea = tubebank.ST * tubebank.SL - pi/4 * capillary.OD^2;
TMeanGuess = TMean + 100;
while abs(TMean - TMeanGuess) > 1
    TMeanGuess = TMean;
    fluid = feval(fluidfunc, TMeanGuess, fluid);
    [Remax, NuBar] = nusseltgnielinski(fluid, capsurf.Pr, tubebank, capillary.OD);
    hBar = fluid.k * NuBar / capillary.OD;
    hBarPUL = hBar * pi * capillary.OD;

40
\[
\begin{align*}
\frac{dT(1)}{dt} &= \frac{(h_{\text{BarPUL}} \cdot (\text{fluid.initialT} - T(1)) + Q_{\text{dotPUL}})}{\text{capillary.CPUL}}; \\
\frac{dT(2, 1)}{dt} &= \frac{(\text{fluid.rho} \cdot V_{\text{dotPUL}} \cdot \text{fluid.cp} \cdot (\text{fluid.initialT} - T(2)) - h_{\text{BarPUL}} \cdot (\text{fluid.initialT} - T(1)))}{(\text{fluid.rho} \cdot \text{mixingarea} \cdot \text{fluid.velocity} \cdot \text{fluid.cp})}; \\
\text{for } i = 2: \text{tubebank.NL} & \\
\frac{dT(i*2-1, 1)}{dt} &= \frac{(h_{\text{BarPUL}} \cdot (T(i*2-2) - T(i*2-1)) + Q_{\text{dotPUL}})}{\text{capillary.CPUL}}; \\
\frac{dT(i*2, 1)}{dt} &= \frac{(\text{fluid.rho} \cdot V_{\text{dotPUL}} \cdot \text{fluid.cp} \cdot (T(i*2-2) - T(i*2-1)) - h_{\text{BarPUL}} \cdot (T(i*2-2) - T(i*2-1)))}{(\text{fluid.rho} \cdot \text{mixingarea} \cdot \text{fluid.velocity} \cdot \text{fluid.cp})}; \\
\text{end} \\
T_{\text{Mean}} &= \frac{(\text{fluid.initialT} + T(2 \cdot \text{tubebank.NL}))}{2}; \\
\end{align*}
\]

linearwater2.m
function water = linearwater2(T, varargin)
T = T + 273.15;

if nargin > 1
    water = varargin(1);
end

TRef = [300 305 310 315 320 325 330 335 340 345 350];
rhoRef = 1E3 ./ [1.003 1.005 1.007 1.009 1.011 1.013 1.016 1.018 1.021 1.024 1.027];
cpRef = [4179 4178 4179 4179 4182 4184 4186 4188 4191 4195];
muRef = 1E-6 * [855 769 695 631 577 528 489 453 420 389 365];
kRef = 1E-3 * [613 620 634 640 645 650 656 660 668 668];
PrRef = [5.83 5.20 4.62 4.16 3.77 3.42 3.15 2.88 2.66 2.45 2.29];

i = ceil((T - TRef(1)) / 5);
if i < 1
    i = 1;
elseif i > length(TRef) - 1
    i = length(TRef) - 1;
end

water.rho = rhoRef(i) + (rhoRef(i+1) - rhoRef(i)) * (T - TRef(i)) / (TRef(i+1) - TRef(i));
water.cp = cpRef(i) + (cpRef(i+1) - cpRef(i)) * (T - TRef(i)) / (TRef(i+1) - TRef(i));
water.mu = muRef(i) + (muRef(i+1) - muRef(i)) * (T - TRef(i)) / (TRef(i+1) - TRef(i));
water.k = kRef(i) + (kRef(i+1) - kRef(i)) * (T - TRef(i)) / (TRef(i+1) - TRef(i));
water.Pr = PrRef(i) + (PrRef(i+1) - PrRef(i)) * (T - TRef(i)) / (TRef(i+1) - TRef(i));

nusseltgnielinski.m
function [ReBar, NuBar] = nusseltgnielinski(fluid, Prs, tubebank, OD)
% yields higher Nusselt % relation from A.F. Mills

% Convection constant
vBar = fluid.velocity * tubebank.ST / (tubebank.ST - (pi/4) * OD);
ReBar = fluid.rho * vBar * OD / fluid.mu;
if ReBar * fluid.Pr < 0.2
    NuBar1 = 1 / (0.8237 - log((ReBar * fluid.Pr) ^ (1/2)));
elseif ReBar < 1E4
    NuBar1 = 0.3 + 0.62 * ReBar^(1/2) * fluid.Pr^(1/3) / (1 +
      (0.4/fluid.Pr)^(2/3)) ^ (1/4);
elseif ReBar >= 2E4 & ReBar < 4E5
    NuBar1 = 0.3 + 0.62 * ReBar^(1/2) * fluid.Pr^(1/3) / (1 +
      (0.4/fluid.Pr)^(2/3)) ^ (1/4) * (1 + (ReBar/282000)^(1/2)) ;
elseif ReBar >= 4E5 & ReBar < 5E6
    NuBar1 = 0.3 + 0.62 * ReBar^(1/2) * fluid.Pr^(1/3) / (1 +
      (0.4/fluid.Pr)^(2/3)) ^ (1/4) * (1 + (ReBar/282000)^(5/8))^(4/5);
else
    error('tubebanknusselt2:outofrange', '1E4 < ReBar < 2E4 or ReBar > 5E6',
        ReBar)
end

if tubebank.staggered == 0
    if tubebank.SL / OD >= 1
        psi = 1 - pi / (4 * tubebank.ST / OD);
    else
        psi = 1 - pi / (4 * tubebank.ST / OD * tubebank.SL / OD);
    end
    phi = 1 + 0.7 / psi^1.5 * (tubebank.SL / tubebank.ST - 0.3) /
    (tubebank.SL / tubebank.ST + 0.7) ^ 2;
else
    phi = 1 + 2 / (3 * tubebank.SL / OD);
end
NuBar = NuBar1 * phi;
References


Washington, DC.


