

Heat Transfer in Crossflow Heat Exchangers for Application with Microreactors

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Abstract: The development and employment of microreactors, with built-in heat exchangers, has rapidly expanded both the research in and the production of new and exotic chemicals through the exploration of difficult, complex and highly exothermic reaction systems. This paper explores methods of improving the heat transfer coefficient in a crossflow heat exchanger as might be employed in conjunction with such an experimental or production microreactor.

This model demonstrates that the rate of heat transfer in a crossflow heat exchanger can be made significantly larger, in this case by a factor of 26, through structural enhancement and appropriate materials selection in the design and modeling phase.

Keywords: heat transfer, heat exchangers, crossflow, chemical microreactors, temperature control.

1. Introduction

The development and employment of microreactors, with built-in heat exchangers, has rapidly expanded both the research capability in and the production volume of new and exotic chemicals by facilitating the exploration of new, difficult, complex and highly exothermic reaction systems. Such exothermic reactions, for research exploration and/or production development, can now be readily characterized (modeled) and then utilized without extreme concern for any excessive, unexpected energy releases (explosions) during the reaction process. Only the normal observation of careful procedures and the application of First Principle Techniques need to be applied to ensure that the experiment is fully and carefully modeled.

This paper explores a new methodology that facilitates the improvement of the heat transfer coefficient in crossflow heat exchangers through the application of appropriate materials selection and geometry configuration in the modeling and

simulation phase of the crossflow heat exchanger during the microreactor system development. Exploration of the chemistry occurring in the microreactor is not discussed herein. A typical microreactor/heat exchanger configuration is shown in Figure 1, where the microreactor is shown on top of the heat exchanger block.

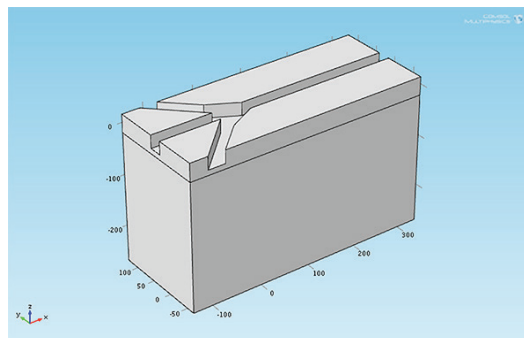


Figure 1. Typical Microreactor and Crossflow Heat Exchanger Geometric Configuration

2. Heat Exchanger Theory

The study of heat and heat transfer has a long history. The relationship of pressure (P) to volume (V) in a gas:

$$PV = k \quad (1)$$

Where: k = constant.

Robert Boyle first published this law in 1662 {1}.

The relationship of pressure (P) to temperature (T) in a gas:

$$\frac{P_1}{T_1} = \frac{P_2}{T_2} \quad (2)$$

Where the subscripts 1 & 2 indicate the different states. Joseph Louis Gay-Lussac first published this law in 1809 {2}.

These laws were combined with the work of Amedeo Avogadro on the number of molecules (moles) (n) in a volume (V) of gas, published in 1811 {3}.

$$\frac{V_1}{n_1} = \frac{V_2}{n_2} \quad (3)$$

Johannes Diderik van der Waals examined the ideal gas law:

$$PV = nRT \quad (4)$$

and decided that it needed to be compensated for the inter-particle interaction forces. He used the pressure, temperature, and volume of a gas at the critical point and developed an equation {4} that would be valid for any gas.

$$\left(P + \frac{n^2 a}{V^2} \right) (V - nb) = nRT \quad (5)$$

Where: a = attraction factor
b = volume excluded factor

In 1910, he was awarded the Nobel Prize for his discovery.

Joseph Fourier published his equation for heat flow by conduction in 1822 {5}:

$$\vec{q} = k \Delta T \quad (6)$$

Where: \vec{q} = local heat flux
k = thermal conductivity
 ΔT = temperature gradient

Drawing upon this basis, heat exchanger theory currently comprises four (4) fundamental modes of energy transfer. They are:

Advection = transfer through motion and/or momentum {6}.

Conduction - Diffusion = transfer by direct contact, using Fourier's Law {7}.

Convection - Diffusion = transfer by fluid motion and contact {8}.

Radiation = transfer of energy by emission {9}.

3. Use of COMSOL Multiphysics

The models developed in this study are derivatives of the Cross-Flow Heat Exchanger {10} model shipped in the COMSOL Models Library. In the models herein, the substrate geometry is modified. Two (2) additional layers are added and the material copper is used in the

center region, instead of stainless steel. Figure 2 shows the basic geometry of this set of models. Each of these models now comprise four (4) layers total, with two (2) relatively thick layers in the center of the geometry and two (2) thin layers, one (1) on the top and one (1) on the bottom.

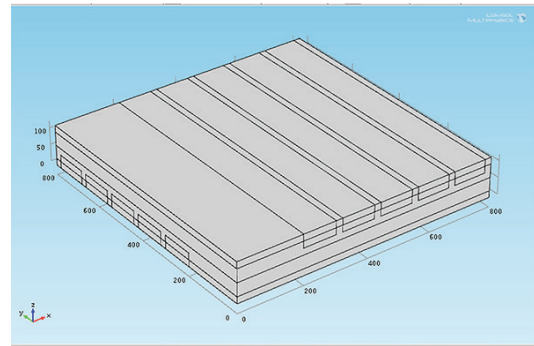


Figure 2. Modified Crossflow Heat Exchanger Geometric Configuration

4. Crossflow Heat Exchanger Geometry Construction

Figure 3 shows the Model Builder tree for the new crossflow heat exchanger geometry developed herein.

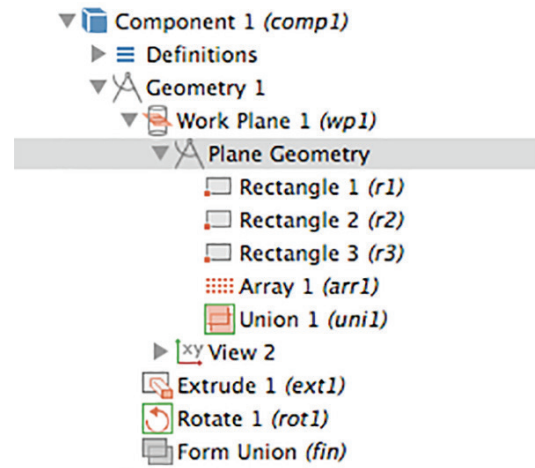


Figure 3. Model Builder Tree for the Crossflow Heat Exchanger New Geometric Configuration

Rectangle 1 forms the bottom layer. It has a width of 800 μm , a height of 20 μm , is corner referenced with no offset ($x_w=0, y_w=0$).

Rectangle 2 forms the second layer. It has a width of 800 μm , a height of 40 μm , is corner referenced with a vertical offset ($x_w=0$, $y_w=20$).

Rectangle 3 forms the channels. It has a width of 100 μm , a height of 40 μm , is corner referenced with a horizontal offset ($x_w=200$, $y_w=0$). Rectangle 3 is employed with the Array build and has an x_w size of 5 and an y_w size of 1. Also, the Array build has an x_w displacement of 120 μm and an y_w displacement of 0.

Once the array is built, the geometry can be Extruded 800 μm . After the Extrude, a Rotate command is used to duplicate and invert the base geometry. The final complete configuration is as shown in Figure 2.

4. Crossflow Heat Exchanger Materials Configurations

This model comprises three materials employed in different configurations, as shown in Figure 4.

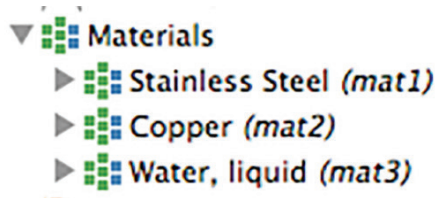


Figure 4. Model Builder Tree for the Crossflow Heat Exchanger Materials Configuration

The properties for the Stainless Steel are entered by the modeler and are Thermal conductivity ($k = 15 \text{ W}/(\text{m}^*\text{K})$), Density ($\rho = 7800 \text{ kg}/\text{m}^3$), and Heat capacity ($C_p = 420 \text{ J}/(\text{kg}^*\text{K})$). The properties for the Copper and the Water are obtained from the built-in materials library.

The materials are configured differently in the all Stainless Steel and Stainless Steel and Copper models. Figure 5 shows the configuration of the Stainless Steel (blue layers) in the top and bottom layers.

Figure 6 shows the configuration of the Copper center cores (blue layers).

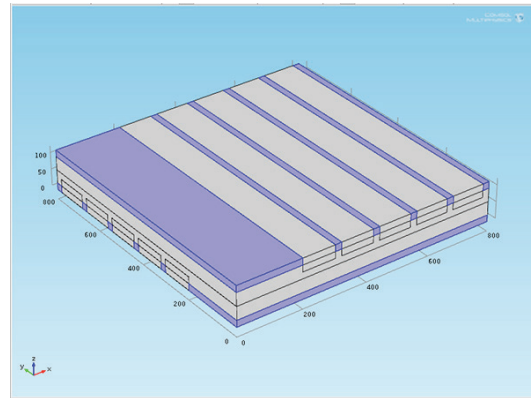


Figure 5. Crossflow Heat Exchanger Materials Stainless Steel Configuration, Top & Bottom Layers.

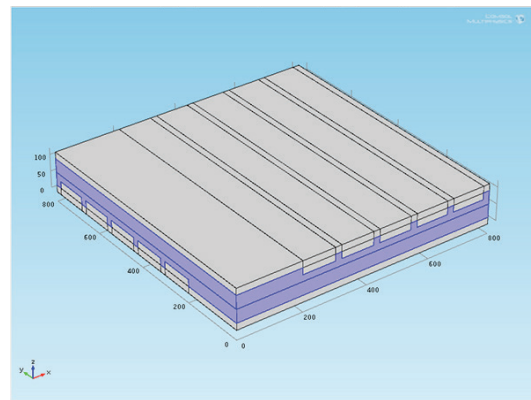


Figure 6. Crossflow Heat Exchanger Materials Copper Configuration, Center Core Layers.

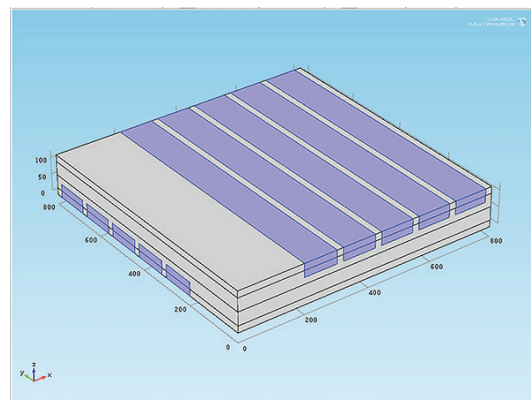


Figure 7. Crossflow Heat Exchanger Materials Water Configuration, Top & Bottom Channels.

Figure 7 shows the configuration of the Water channels (blue layers), top and bottom.

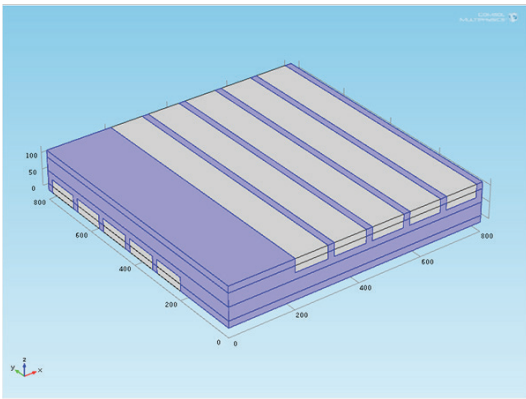


Figure 8. Crossflow Heat Exchanger Materials, All Stainless Steel Configuration.

Figure 8 shows the configuration of the Stainless Steel (blue layers), for the all Stainless Steel Crossflow Heat Exchanger.

5. COMSOL Model Builder Details

Now that the geometry has been configured, the details of the Model Builder Tree need to be added. The first detail that is added is the parametric values. Figure 9 shows the Inlet and Outlet Temperatures and the fluid velocity.

Parameters

| Name | Expression | Value | Description |
|--------|------------|---------------|-------------------------|
| T_cold | 300.0[K] | 300.00 K | Temperature cold stream |
| T_hot | 330.0[K] | 330.00 K | Temperature hot stream |
| u_avg | 2.5[mm/s] | 0.0025000 m/s | Average inlet velocity |

Figure 9. Crossflow Heat Exchanger Parameters, Temperatures and Fluid Velocity.

Next, each Explicit needs to be created to facilitate the correct calculations. Figure 10 shows the combined Explicit collection.

Now, each Conjugate Heat Transfer interface boundary condition needs to be set to facilitate the correct calculations. Figure 11 shows the final Model Builder Tree configuration.

Next, a custom Mesh needs to be created to facilitate the correct calculations. Figure 12 shows the Mesh selection.

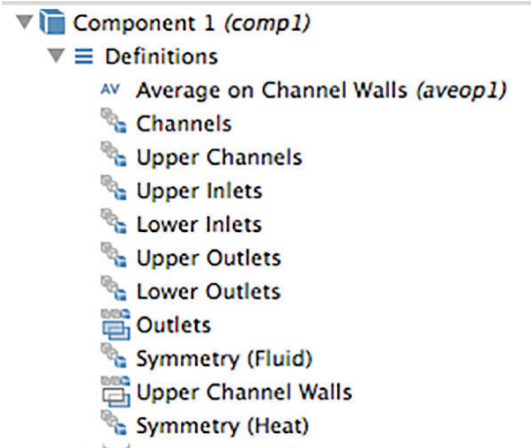


Figure 10. Crossflow Heat Exchanger Explicit Collection.

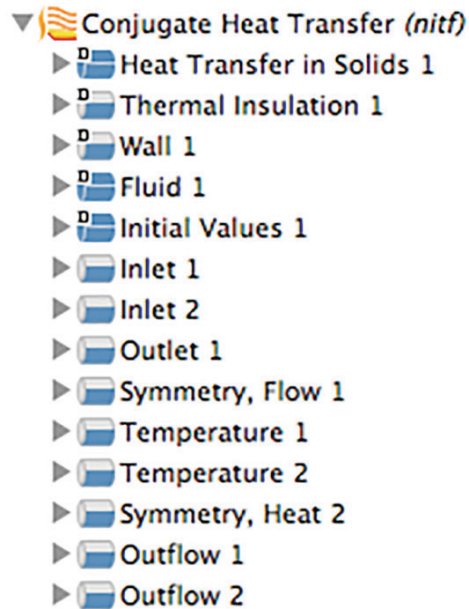


Figure 11. Crossflow Heat Exchanger Conjugate Heat Transfer Model Conditions.

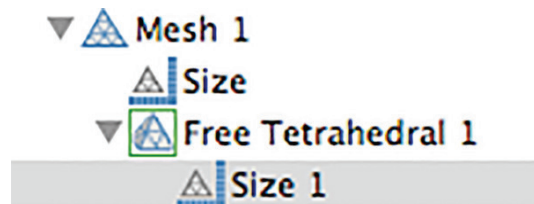


Figure 12. Crossflow Heat Exchanger Mesh Selection.

After Mesh type selection, Figure 13 shows the custom mesh parameter selection.

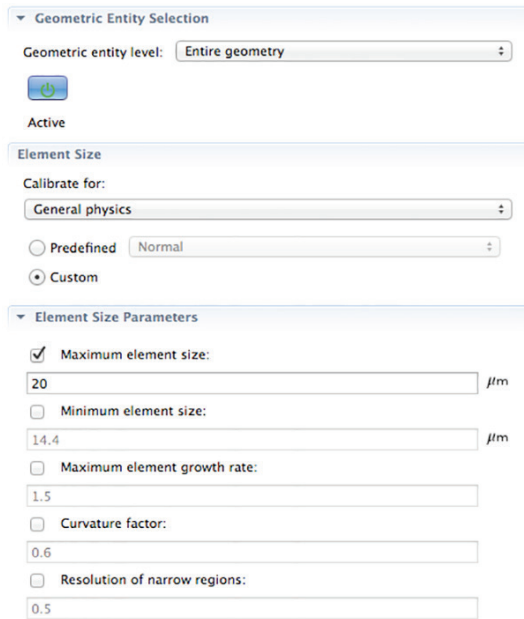


Figure 13. Crossflow Heat Exchanger Custom Element Size.

Figure 14 shows the meshed model geometry.

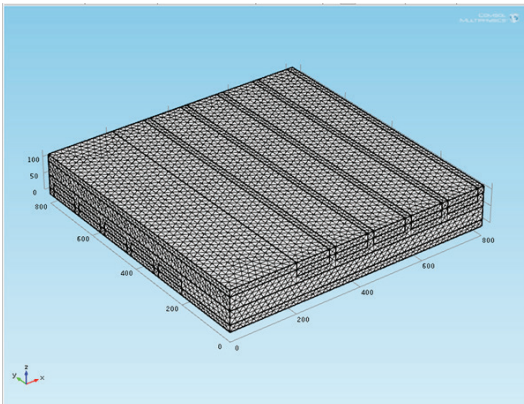


Figure 15. Crossflow Heat Exchanger Meshed Geometry.

6. Results

The computational results of modifying the inner stainless steel volume to copper layers for the

Crossflow Heat Exchanger model is shown in Figure 16.

The incorporation of additional layers of copper in the center of the crossflow heat exchanger geometry increased the heat transfer coefficient by a factor of approximately 26. Figure 16 shows the temperature at the outlets of the modeled crossflow heat exchanger and the calculated heat transfer coefficient ($\sim 30,056 \text{ W}/(\text{m}^2 \text{ K})$) for this structure. The heat transfer coefficient for the all Stainless Steel model is $1560 \text{ W}/(\text{m}^2 \text{ K})$.

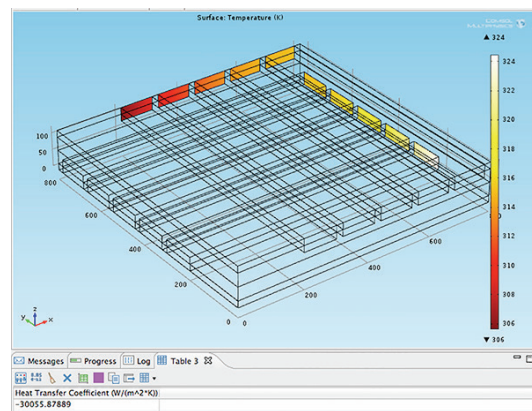


Figure 16. Crossflow Heat Exchanger Outlet Temperatures and Heat Transfer Coefficient.

7. Conclusions

The rate of heat transfer in this crossflow heat exchanger was increased by approximately a factor of 26, through structural and materials design modifications.

8. References

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