Simulation-based Study of Graphene-water Nanofluid flow through Microchannel Heatsink

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Abstract. This study presents a CFD analysis of the laminar flow of graphene-water nanofluid through a Silicon microchannel heatsink using commercial software ANSYS FLUENT. The microchannel has a rectangular cross-section of given dimensions, and the base of the heatsink is subjected to a constant heat flux. Simulations of the coolant flow are performed at different fluid inlet velocities for nanoparticle concentrations of 0%, 3% and 6% in the base fluid-Water. Results for temperature and pressure distributions in the microchannel heatsink are presented. The cooling performance of the MCHS improves significantly by increasing the flow velocity and enhancing the nanoparticle concentration in the coolant.

Keywords. microchannel, nanoparticle, base fluid, thermal conductivity, cooling.

1. Introduction
The electronics industry has witnessed some phenomenal advancements in the past few decades. However, this progress has been made possible only because of continuous improvements in thermal management technologies that have ensured that the systems work steadily- by removing the high heat generated by the devices.

The path-breaking work of Tuckerman and Pease [1] has given rise to extensive research and development of the microchannel heat sink (MCHS) as a viable device for electronic cooling [2–4]. MCHS comes in handy in micro-level MEMS devices, micro-fluidics and sensitive applications such as micro drug delivery- where the extremely small area of heat dissipation creates significant challenges for the structural and thermal stability of the device and hampers its longevity. For nearly two decades now, research in this domain has focussed on enhancing heat transfer in an MCHS for improvement in cooling performances. Chai et al. conducted a numerical investigation on heat transfer enhancement in a silicon MCHS having offset ribs on sidewalls under laminar flow conditions and inferred that the proposed MCHS model displays better cooling performance than a smooth MCHS [5]. Besides modification of microchannel geometry, heat transfer can also be enhanced by employing nanofluids as coolants in the microchannel. Nanofluids are produced when nanoparticles are suspended in

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conventional heat transfer fluids, and they exhibit better thermal conductivity than the base fluids [6]. Lee and Mudawar experimentally investigated the performance of a microchannel heatsink using Al₂O₃-water nanofluid and demonstrated an enhancement in the single-phase heat transfer coefficient, particularly in the laminar flow domain [7]. Al-Baghdadi et al. performed the CFD analysis of some metal-oxide containing water-based nanofluids flowing through a Silicon MCHS in the range of 100<Re<900 and made a thorough investigation on physical parameters such as pressure drop across the microchannel, temperature distributions in the computational domain, etc. for each nanofluid [8].

Graphene is a carbon allotrope with a special 2-D crystal structure that provides it with excellent electrical and thermal properties [9]. The use of graphene as nanoparticles has found much attention in recent times [10]. Several experimental investigations have confirmed the suitability of graphene-water nanofluid as an effective coolant in various systems [11,12]. In this paper, the cooling performance of graphene-water nanofluid in a Silicon MCHS is studied using commercial CFD software ANSYS FLUENT by simulating the laminar flow of the coolant through the microchannel. Various performance measures such as temperature distributions and pressure drops across the microchannel are investigated for different nanoparticle concentrations in the base fluid.

2. Model Description

![Figure 1. 3D Model of Microchannel Heatsink.](image)

| Table 1. Dimensions of Microchannel Heatsink. |
|-----------------------------------------------|
| Length                        | Dimension (m) |
|-----------------------------------------------|
| Length of the MCHS (L)          | 0.01           |
| Height of the MCHS (H₉)         | 0.00035        |
| Width of the MCHS (W₉)          | 0.0002         |
| Height of the Microchannel (H)  | 0.0002         |
| Width of the Microchannel (W)   | 0.0001         |

Figure 1 shows a diagram of the rectangular microchannel heatsink along with the orientation, and Table 1 presents the dimensions. The MCHS is made of Silicon and the same MCHS model has been used by
Al-Baghdadi et al. in their study as well [8]. For easy computation, we consider only a single microchannel for fluid flow. A 3D model of the microchannel heatsink is created in Autodesk Fusion 360 and then exported to the CFD software, where the simulations are carried out.

3. Numerical Modelling

3.1. Conservation Equations

The numerical model presented in this study assumes a laminar, single-phase flow of incompressible fluid across a microchannel and negligible effect of gravity. Thus, the steady-state Navier-Stokes equations can be used to obtain solution [8].

For the fluid “f”, the equations for mass and momentum conservations respectively are [8]:

\[ \nabla \cdot (\rho_f u) = 0 \]  \hspace{1cm} (1)
\[ (u \cdot \nabla) \rho_f = -\nabla p + \mu_f \nabla^2 u \]  \hspace{1cm} (2)

where \( p \) refers to the pressure (Pa), \( \rho_f \) refers to the fluid density (kg/m³), \( u \) refers to the flow velocity (m/s), and \( \mu_f \) refers to the dynamic viscosity (kg/m s) of the fluid.

The energy equation for the fluid is [8]:

\[ u \cdot \nabla T = \frac{k_f}{\rho_f C_p} \nabla^2 T \]  \hspace{1cm} (3)

where \( k_f \) denotes the fluid’s thermal conductivity (W/m K), \( T \) denotes the temperature (K) and \( C_p \) refers to the specific heat capacity (J/kg K) of the fluid.

For the solid “s”, energy equation is [8]:

\[ k_s \nabla^2 T = 0 \]  \hspace{1cm} (4)

where \( k_s \) denotes the thermal conductivity of the solid (W/m K).

3.2. Thermophysical Properties

Table 2. Thermophysical properties of Water and Graphene.

| Fluid   | Density \( \rho \) (kg/m³) | Specific Heat \( C_p \) (J/kg K) | Thermal Conductivity \( k \) (W/m K) | Dynamic Viscosity \( \mu \) [kg /m s] |
|---------|-----------------------------|----------------------------------|-------------------------------------|--------------------------------------|
| Water   | 996.7                       | 4180                             | 0.608                               | 0.000855                             |
| Graphene| 2267                        | 75                               | 4000                                |                                      |

Fluid properties at 300 K.

Table 3. Thermophysical properties of Silicon.

| Material | Density \( \rho \) (kg/m³) | Thermal conductivity \( k \) (W/m K) | Specific Heat \( C_p \) (J/kg K) | Young’s modulus \( Y \) (Pa) | Thermal Expansion \( \alpha \) (1/K) | Poisson’s Ratio |
|----------|-----------------------------|-------------------------------------|----------------------------------|----------------------------|-------------------------------------|----------------|
| Silicon  | 2329                        | 130                                 | 700                              | 170e⁹                       | 2.6e⁹                              | 0.28            |

The temperature-correlated equation of density (kg/m³) for water is obtained from the Best-Fit Curve, extrapolating from Density variation with Temperature data [13].

\[ \rho_{bf} = 999.9 + 0.0556(T-273.15) - \left( 8 \times 10^{-3} \right)(T-273.15)^2 + \left( 6 \times 10^{-5} \right)(T-273.15)^3 - \left( 2 \times 10^{-7} \right)(T-273.15)^4 \]  \hspace{1cm} (5)
The equations for specific heat capacity (J/kg K), thermal conductivity (W/m K) and dynamic viscosity (kg/m s) respectively for water are as follows [8]:

\[ C_{p_{bf}} = 8959.9 - 40.535(T-273.15) + 0.11243(T-273.15)^2 - 1.014 \times 10^{-4}(T-273.15)^3 \] (6)

\[ k_{bf} = -0.58166 + 6.3556 \times 10^{-3}T - 7.964 \times 10^{-6}T^2 \] (7)

\[ \mu_{bf} = 2.414 \times 10^{-5} \frac{247.8}{10^{1.146}} \] (8)

The thermophysical properties of the base fluid are considered at the inlet temperature of 300K to resemble real-life conditions closely.

The thermophysical properties of Water at 300 K and graphene are shown in Table 2 [14]. For the nanofluid “nf”, the equations of its thermophysical properties are as follows [15]:

\[ \rho_{nf} = (1-\phi) \rho_{bf} + \phi \rho_{np} \] (9)

\[ C_{p_{nf}} = \frac{(1-\phi) C_{p_{bf}} + \phi C_{p_{np}}}{\rho_{nf}} \] (10)

\[ k_{nf} = k_{bf} \frac{k_{np} + 2k_{bf}-2\phi(k_{bf}-k_{np})}{k_{np} + 2k_{bf}+\phi(k_{bf}-k_{np})} \] (11)

\[ \mu_{nf} = \frac{\mu_{bf}}{(1-\phi)^{2.5}} \] (12)

where \( \phi \) denotes the volume concentration of nanoparticles “np” in the coolant.

The current study involves Silicon as heatsink material. Table 3 states the thermophysical properties of Silicon.

### 3.3. Procedure and Boundary Conditions

#### Table 4. Inlet and Boundary Conditions.

| Coolant                | Graphene-water |
|------------------------|----------------|
| Inlet Fluid Temperature \( T_{f,in} \) [K] | 300            |
| Outlet gauge pressure [Pa] | 0              |
| Inlet velocity of coolant \( u_{in} \) [m/s] | 1.3; 2.5       |
| Concentration of nanoparticles \( \phi \) | 0, 3, 6 vol%   |
| Heat Flux on MCHS Bottom wall \( q \) [W/m²] | \( 10^6 \)    |

The Finite Volume Method is implemented in the present study to discretize the governing equations which are solved using ANSYS FLUENT 2021 R2. The important inlet and boundary conditions employed are summarized in Table 4. The two different inlet velocities fall within 100<Re<500 for both the base fluid and the nanofluids and hence constitute laminar flow through the microchannel. For the same inlet velocity and boundary conditions, performances of graphene-water nanofluid at various nanoparticle concentrations are analyzed and compared.
The Reynolds number of the fluid flow is defined as:

\[ Re = \frac{\rho_f u_m D_h}{\mu_f} \]  

(13)

where \( D_h \) refers to the microchannel’s hydraulic diameter (m) and \( u_m \) refers to the fluid inlet velocity (m/s).

Here, the hydraulic diameter for the rectangular microchannel is:

\[ D_h = \frac{2WH}{W+H} \]  

(14)

where \( W \) denotes the microchannel’s width (m) and \( H \) indicates the microchannel’s height (m).

### Table 5. Grid Independence Test.

| Elements | Nodes  | Relative error |
|----------|--------|----------------|
| MESH-1   | 800000 | 912912         |
| MESH-2   | 900000 | 1018017        | 0.004421726 |
| MESH-3   | 100000 | 1123122        | 0.002119347 |
| MESH-4   | 110000 | 1228227        | 0.001222145 |
| MESH-5   | 120000 | 1333332        | 0.000781618 |

The 3D Model is linearly meshed. The grid independence of the solution is established by executing several simulation trials using base fluid water for a fluid inlet velocity of 1.3 m/s. Table 5 lists the relative error \( \left( \frac{\Delta P_{\text{mesh}(n)} - \Delta P_{\text{mesh}(n-1)}}{\Delta P_{\text{mesh}(n)}} \right) \) calculated for 5 different meshes. MESH-4 is chosen, which contains 1100000 elements and 1228277 nodes. It is found to provide good resolution, yet it is economical in terms of processing time. SIMPLE Algorithm is selected for implementing Pressure-Velocity coupling. The computational domain is initialized with the inlet boundary conditions before commencing the iterative process. For spatial discretization of energy and momentum equations, a second-order upwind scheme is chosen. For achieving solution convergence, a residual of \( 1.0 \times 10^{-6} \) is selected for the continuity, velocity and energy equations.

### 3.4. Model Validation

For validating the model, the Average Nusselt Numbers of the simulated model using water at distinct flow Reynolds Numbers within the laminar domain are compared with the results experimentally obtained by Chai et al. [5].

The average Heat Transfer Coefficient (W/m\(^2\) K) and Nusselt Number respectively are [5]:

\[ h = \frac{q_A_{\text{hot}}}{A_{\text{con}}(T_w, \text{area} - T_{f,m})} \]  

(15)
where the applied heat flux upon the bottom wall of the MCHS (W/m²) is denoted by \( q \), \( A_{\text{bot}} \) denotes the silicon bottom wall area (m²), \( A_{\text{con}} \) denotes the inner wall-fluid contact area, \( k_{f,m} \) indicates the mass-average thermal conductivity of the fluid, \( T_{w,\text{area}} \) denotes the area-weighted temperature of the MCHS bottom wall (K) and \( T_{f,m} \) indicates the mass-average temperature of the base fluid domain.

Figure 2. Comparison of Average Nusselt Numbers: Current results using Water as fluid through the microchannel versus experimental results.

Figure 2 clearly indicates that the simulation results are in reasonable agreement with the experimentally obtained results.

4. Results and Discussion

| Table 6. Numerical Results. |
|----------------------------|
| Inlet velocity, \( u_{m} \) [m/s] | Fluid | Volume Fraction \( \phi \) (in %) | Pressure Drop \( \Delta P \) [Pa] | Fluid outlet temperature, \( T_{f,\text{out}} \) [K] | Maximum wall temperature, \( T_{w,\text{max}} \) [K] |
|-----------------|--------|----------------|----------------|----------------|----------------|
| Water           | 0      | 20501.651      | 318.463        | 337.566        |
| 1.3 Water + Graphene | 3      | 22075.858      | 319.008        | 336.701        |
| Water + Graphene | 6      | 23826.222      | 319.587        | 335.988        |
Influence of Nanoparticle concentration on Pressure Drop

Table 6 clearly suggests that nanofluids display greater pressure drop (Pa) across the microchannel than the base fluid at the same coolant inlet velocity. When the nanoparticle concentration in the coolant is increased, the pressure drop also increases. Pumping power (W) is required to steadily drive the flow of coolant in the microchannel and is given by:

$$P_{\text{pump}} = u_m \cdot \Delta P \cdot A_{cs}$$

(17)

where $A_{cs}$ denotes the area of cross-section of the rectangular microchannel ($m^2$), $\Delta P$ denotes the pressure drop across the microchannel (Pa). Therefore, the pumping power increases on increasing the concentration of nanoparticles in the coolant.

Influence of Nanoparticle Concentration on Wall Temperature

For the MCHS, the cooling performance is determined by evaluating the overall thermal resistance (K/W), which is defined as:

$$R_T = \frac{T_{w,max} - T_{f,in}}{q}$$

(18)

where $T_{w,max}$ denotes the maximum wall temperature of the MCHS (K), $T_{f,in}$ represents the fluid inlet temperature. Table 6 suggests that the maximum wall temperature decreases on increasing the nanoparticle concentration in the coolant and consequently, the overall thermal resistance decreases.
4.3. Influence of Nanoparticle Concentration on Coolant Exit Temperature
For a particular fluid inlet velocity, the coolant temperature at the microchannel outlet increases on increasing the nanoparticle concentration.

4.4. Effect of Flow Velocity on Wall Temperature
It is evident from Table 6 that for a given coolant, a higher flow velocity through the microchannel leads to lower wall temperature of the heatsink and hence, the overall thermal resistance decreases.

![Figure 4](image-url)

*Figure 4.* Temperature Gradient of MCHS Bottomwall edge in the outlet plane (i.e. X=L, Y=0) due to inlet velocity 1.3 m/s for (a) Water (b) Graphene(3%)+Water (c) Graphene(6%)+Water.

4.5. Effect of Flow Velocity on Pressure Drop
An increase in flow velocity enhances pressure drop. It is evident from Table 6 that the same nanofluid will induce a more significant pressure drop at a higher fluid velocity.

4.6. Overall Variation in Temperature Distribution
Figure 3 displays the temperature distribution across the axial plane of the MCHS for the flow of base fluid water at an inlet velocity of 1.3 m/s. For both the solid and fluid zones, maximum temperature occurs at the outlet. Similar trends are displayed when nanofluids flow through the microchannel.
Figures 4 and 5 depict the temperature variation in the Silicon bottom wall edge in the outlet plane. Temperatures are minimum at either end of the MCHS (Z=0 and Z= W/2), increase as the centre-line of the bottom wall (Z= W/2) approaches, where it finally attains the maximum wall temperature. As visible, the wall temperature decreases with an increase in nanoparticle concentration in the coolant. Figures 6 and 7 show the temperature variation of the Silicon bottom wall along the length of fluid flow in the X-direction. At the same inlet velocity, the axial bottom wall temperature of the heatsink decreases on increasing the concentration of nanoparticles in water along the length of fluid flow.

![Figure 5](image_url)

**Figure 5.** Temperature Gradient of MCHS Bottomwall edge in the outlet plane (i.e. X= L, Y= 0) due to inlet velocity 2.5 m/s for (a) Water (b) Graphene(3%)+Water (c) Graphene(6%)+Water.

5. **Conclusion**

This study analyses the enhanced heat transfer performance of nanofluids compared to the base fluid in the Silicon MCHS. The enhancement in heat transfer is attributed to a significant improvement in the coolant's thermal conductivity- obtained by adding very small concentrations of nanoparticles in the coolant. The thermal conductivity of the nanofluid containing 6% graphene by volume concentration exceeds the thermal conductivity of water by almost 9.5%. Using nanofluids in the cooling device reduces its thermal resistance and wall temperature- compared to water. Therefore, it is established that the cooling performance of the MCHS gets better on increasing the graphene nanoparticle concentration.
in the coolant. Furthermore, the findings on temperature distribution in the MCHS in this study agree with the results obtained by Farsad et al. [16] using other nanofluids - which reinforces the consistency of this study.

The nanofluid-cooled MCHS presents an efficient device for cooling electronic components. However, it is accompanied by a considerable rise in pressure drop across the microchannel, which increases pumping power requirements. Hence, the future scope of research lies in addressing this limitation and suggesting ways to balance optimum nanoparticle concentration in the coolant with feasible pressure drop, to ensure the best possible cooling performance of the device.

Figure 6. MCHS Bottomwall Temperature Gradient along Flow Length (X) for different fluids at inlet velocity 1.3 m/s.

Figure 7. MCHS Bottomwall Temperature Gradient along Flow Length (X) for different fluids at inlet velocity 2.5 m/s.
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