PHYS6017 – Computer techniques for physics

Assignment one:
Simulation of Heat Diffusion in a Computer Heat Sink

KAY, Arthur - Student ID: 35347465

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Objective

This assignment uses a computational model to examine thermal diffusion through a computer heat sink. Specifically, a Monte Carlo simulation is used to explore how different materials affect cooling performance. The assignment demonstrates how computer-based methods can be used to model thermal transport and evaluate the performance of engineering components.

Background theory

Thermal energy propagates from regions of higher to lower temperature according to the heat diffusion equation. In its simplest form, the temperature field $T(\mathbf{x}, t)$ satisfies

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T, \tag{1}$$

where α is the thermal diffusivity of a material. The Laplacian, $\nabla^2 T$, represents the sum of the second spatial derivatives of temperature, measuring how much the temperature at a point differs from its average in the surrounding area, driving heat flow from hotter to cooler regions until equilibrium. Materials with a larger value of α transport heat more efficiently, allowing thermal energy to spread more rapidly away from a localised heat source.

The highest temperature reached is also dependent on the injection rate Q, which models the power generated by an electronic component at a localised hotspot. A larger value of Q corresponds to a higher rate of energy input into the system. For a given material and heat injection rate, the system evolves in time until it reaches a steady state temperature, at which point the heat input is balanced by heat loss.

1 Method

Heat diffusion is simulated by tracking the stochastic motion of a large number of independent heat packets. Each packet performs a random walk on a two-dimensional grid, representing microscopic heat flow. Individual trajectories of heat packets are random, whereas averaging over many packets produces smooth temperature distributions.

A random walk reproduces the diffusion equation because the probability distribution of many independent heat packets approaches a Gaussian distribution whose variance grows linearly with time. For diffusion in two dimensions, the mean-squared displacement satisfies:

$$\langle r^2(t) \rangle = 4\alpha t \tag{2}$$

where the factor of 4 corresponds to the two independent spatial directions on a square lattice.

In the discrete random-walk model, a heat packet moves by a distance Δx at each time step Δt. To control the diffusivity for different materials, a move probability p is introduced. At each time step, a heat packet moves to a randomly chosen neighbouring lattice site with probability p and remains stationary with probability $1 - p$. This modifies the discrete mean-squared displacement to:

$$\langle r^2 \rangle \approx p\, n (\Delta x)^2 \tag{3}$$

Equating this with the continuum result ($4\alpha t$) yields the relation:

$$p = \frac{4\alpha\, \Delta t}{(\Delta x)^2} \tag{4}$$

This equation fixes the move probability uniquely for a given thermal diffusivity α.

Example Calculation: Move Probability for Copper

Based on equation (4), using the simulation parameters for the sink grid size and the material properties of copper from Table 2:

- Thermal diffusivity: $\alpha = 1.1 \times 10^{-4}\,\mathrm{m^2 s^{-1}}$
- Time step: $\Delta t = 0.002\,\mathrm{s}$
- Grid spacing: $\Delta x = 0.002\,\mathrm{m}$

the move probability for copper is as follows:

$$\begin{aligned} p &= \frac{4 \times (1.1 \times 10^{-4}\,\mathrm{m^2 s^{-1}}) \times (0.002\,\mathrm{s})}{(0.002\,\mathrm{m})^2} \\ p &= \frac{8.8 \times 10^{-7}\,\mathrm{m^2}}{4.0 \times 10^{-6}\,\mathrm{m^2}} \\ p &= 0.22 \end{aligned}$$

1.1 Heat Loss Mechanisms

Two mechanisms are used to model heat loss in the simulation: stochastic surface convection and absorbing boundary conditions.

Surface Convection: Stochastic surface convection is introduced to simulate Newton's Law of Cooling from the face of the heat sink. At every time step, each heat packet is subject to a uniform removal probability (P_{conv}), representing the likelihood of thermal energy dissipating into the ambient air before reaching the grid boundaries.

Absorbing Boundaries: Absorbing boundary conditions are maintained at the plate edges, ensuring that any residual energy diffusing to the edge of the domain is removed from the system.

1.2 Temperature Scaling and Conductivity

To relate the microscopic packet density $\rho(x, y)$ to macroscopic temperature, the model incorporates the material's thermal conductivity (κ). While the random walk speed is governed by thermal diffusivity (α), the steady-state temperature magnitude is inversely proportional to conductivity. Therefore, the final output is scaled according to the relation:

$$T(x, y) \propto \rho(x, y) \times \left(\frac{\alpha}{\kappa}\right) \tag{5}$$

This normalization corrects for the specific heat capacity of different materials (ρc_p). For example, low conductivity materials limit heat removal, leading to higher steady-state temperatures.

Simulation

The heat sink is modelled as a square two-dimensional plate of width $L_x = L_y = 0.025\,\mathrm{m}$, discretised into a uniform grid with spacing $\Delta x = 0.002\,\mathrm{m}$, corresponding to a 12×12 grid. A central circular hot spot of radius $R = 0.006\,\mathrm{m}$ (three grid cells) was used to represent continuous heat generation by a processor. The values were chosen so that the random-walk model reproduces diffusion.

The total simulation time was $t_{\max} = 10.0\,\mathrm{s}$, corresponding to 5000 time steps. Each time step was fixed at $\Delta t = 0.002\,\mathrm{s}$. The simulation time was sufficient for the system to reach a quasi–steady state, in which heat injection at the hotspot is approximately balanced by diffusive transport, surface convection, and heat loss at the absorbing boundaries.

Material and Physics Parameters

The thermal diffusivity α was varied to represent different metals, spanning the range 1.9×10^{-5} to $1.7 \times 10^{-4}\,\mathrm{m^2\,s^{-1}}$ (steel to silver). In the random-walk formulation, the values correspond to move probabilities in the range $p \approx 0.12$ to 0.68, while keeping Δx and Δt fixed.

To simulate forced convection consistent with a standard computer fan, a convection probability of $P_{conv} = 0.004$ (0.4% chance of removal per step) was applied. This value was empirically calibrated to ensure the steady-state temperature of copper was aligned with standard industrial operating conditions ($\approx 50°C$).

Monte Carlo Parameters

The Monte Carlo model used a total of $N = 1500$ heat packets. Heat was injected continuously at the hotspot at a rate $Q = 5$–25 packets per time step, allowing the dependence of the steady-state temperature on heat input to be examined.

In the simulation, randomness is introduced through the microscopic motion of individual heat packets. At each time step, packets perform a random walk by selecting a direction at random, which collectively reproduces the physical process of diffusion. To ensure the results are reliable, simulations are repeated using different random seeds. While this leads to different individual packet paths, the overall statistical behavior remains the same. Increasing the number of heat packets N reduces random noise, approximately scaling as $1/\sqrt{N}$.

Results

Effect of material on steady-state hotspot temperature

To investigate the influence of material properties, simulations were performed for multiple materials while keeping the sink geometry, boundary conditions, and heat injection rate fixed. Figure 1 compares the steady-state hotspot temperature for silver, copper, and steel at $Q = 20$ packets per step.

Copper has the lowest steady-state temperature. Although silver spreads thermal energy faster than copper due to its high diffusivity, it has a lower heat capacity and, therefore, experiences a larger temperature rise for every unit of heat stored. Steel reaches a steady-state temperature significantly higher than silver and copper due to its low thermal conductivity. This causes heat to accumulate near the hotspot, providing less opportunity for convection throughout the heat sink and less heat absorption at the boundaries.

This reflects the dominant role of **thermal conductivity** (κ) in the steady state. The lower conductivity of steel means that heat is spread less quickly across the heat sink and to the boundaries, causing lower levels of convection and boundary absorption. The stochastic convection term (P_{conv}) removes heat from packets before they reach the boundary, but only from areas of the sink that have been reached by heat.

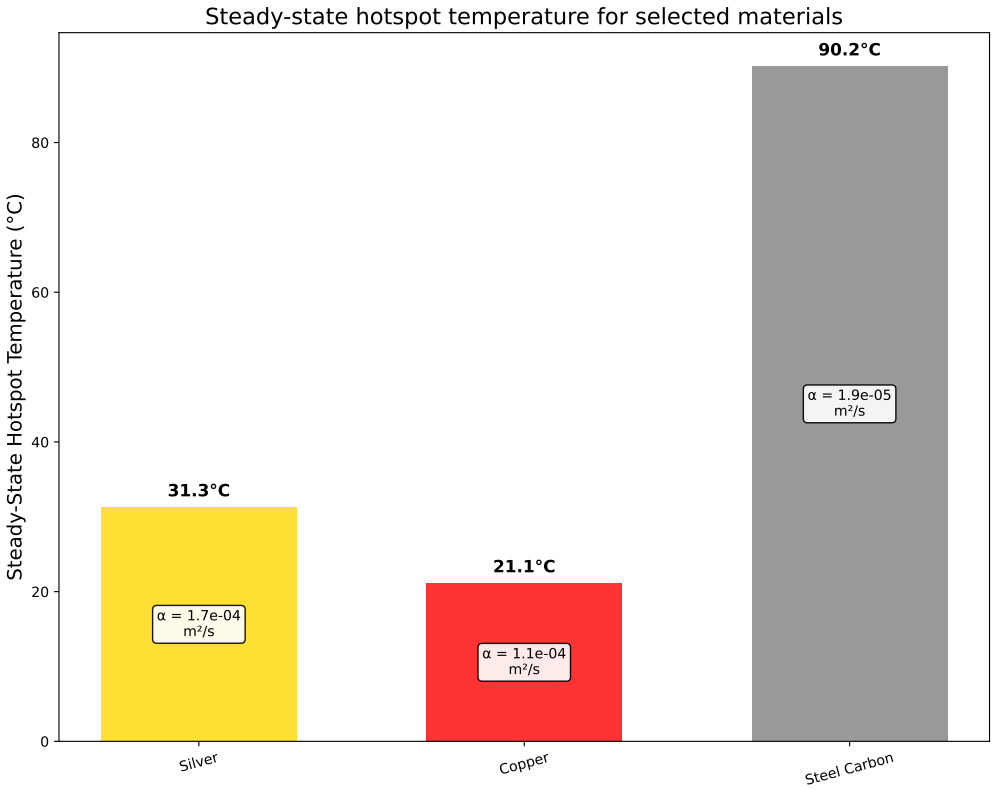

Figure 1: Comparison of steady-state hotspot temperature for silver, copper, and steel at $Q = 20$ packets per step.

Full steady-state hotspot temperatures for all simulated materials are reported in Appendix A. The remainder of the Results section focuses on copper as a representative heat-sink material, due to its industrial use and high thermal diffusivity.

Steady-state behaviour of copper

Figure 2 shows the evolution of the hotspot temperature for a simulation using copper The temperature initially rises rapidly as heat accumulates near the source and then approaches a plateau in which heat injection is balanced by diffusive transport and heat loss at the absorbing boundaries.

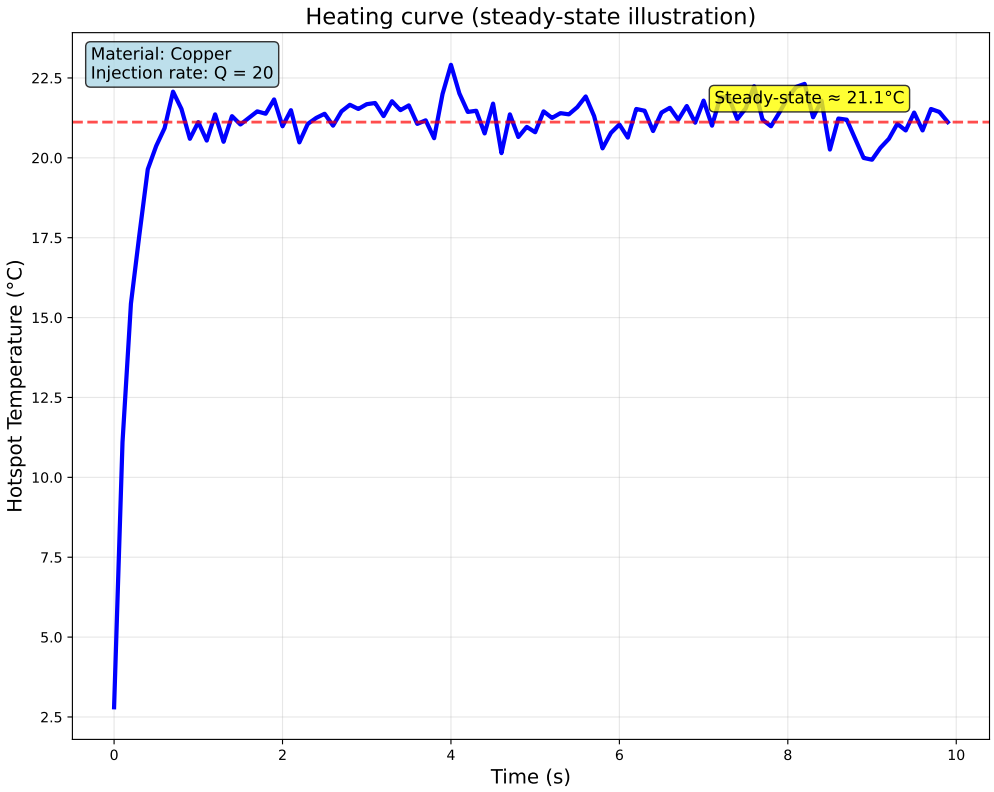

Figure 2: Time evolution of the hotspot temperature for copper at a heat injection rate of $Q = 20$ packets per step.

Spatial temperature distribution

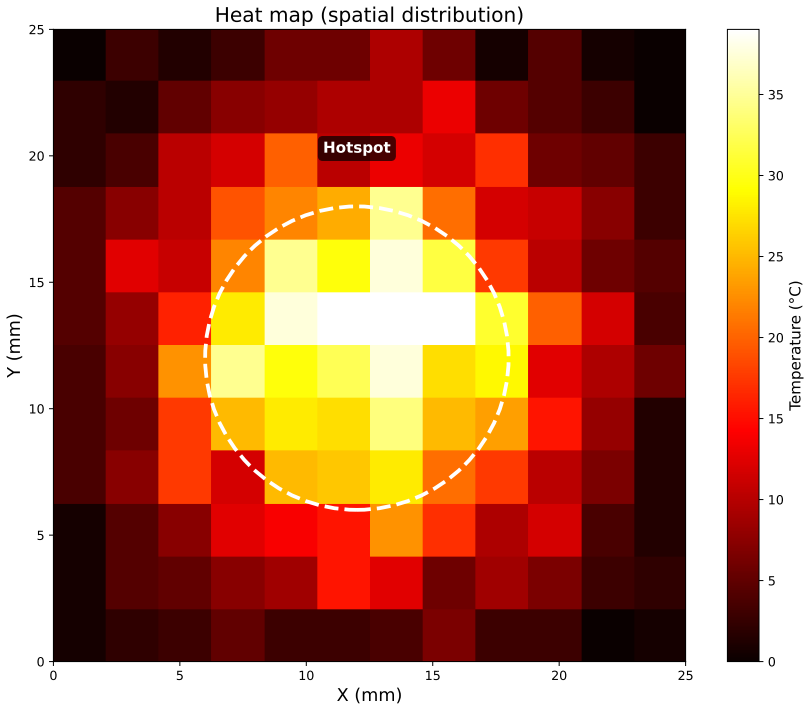

Figure 3: Final two-dimensional temperature distribution for the copper simulation at steady state.

The temperature field exhibits a maximum at the central hotspot, with temperature decreasing smoothly towards the boundaries of the plate. Heat is removed once it reaches the boundaries.

Dependence on heat injection rate

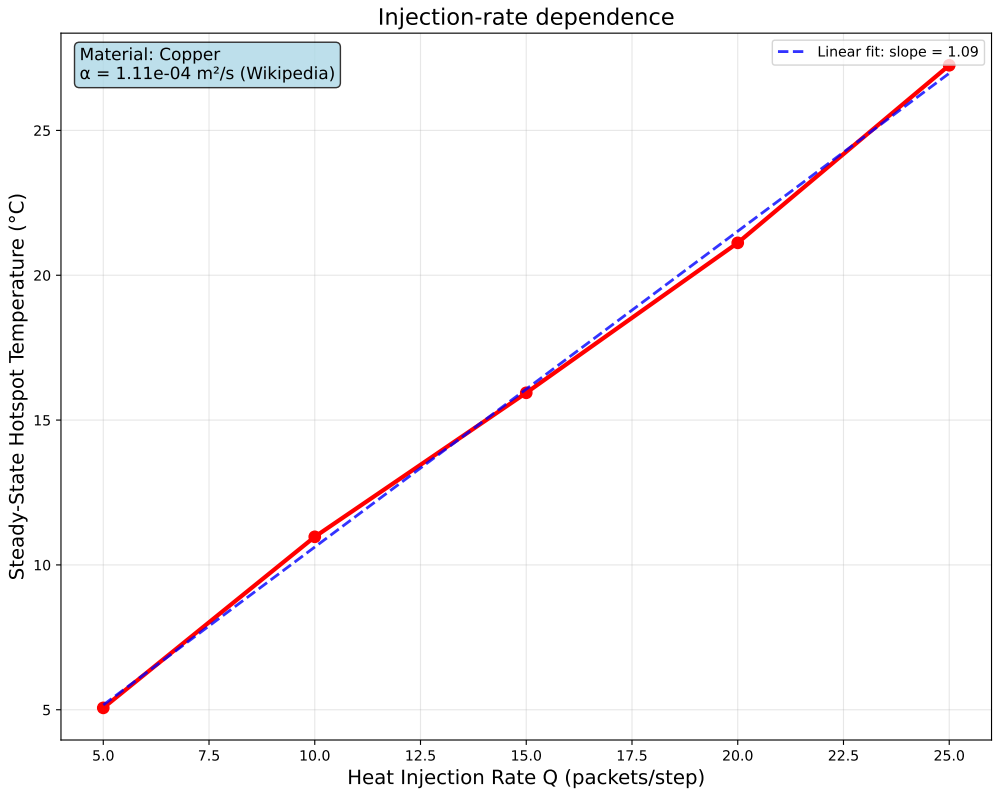

Figure 4: Steady-state hotspot temperature as a function of heat injection rate Q for copper.

As more heat is injected, there is a linear increase in the steady-state temperature as in the model there is no mechanism to prevent the temperature from continuing to rise as power increases.

Discussion

Geometric limitations

An important limitation of the simulation is the simplified 2D geometry of the heat sink as a flat plate. Industrial heat sinks use three-dimensional geometries, including vertical fins, to increase the effective surface area available for convective cooling. The model based architecture of the sink plate could be expanded to three dimensions and more complex designs to provide greater cooling potential.

Boundary condition effects

The use of absorbing boundary conditions at the grid edges ($x = 0, L$) is a simplification. In an industrial heat sink, the plate edges act as insulating or convective interfaces where heat is

largely reflected back into the bulk material (Neumann boundary conditions) rather than instantly removed. By treating the edges as perfect heat sinks that maintain zero temperature, the model artificially accelerates heat loss at the perimeter. Consequently, this assumption likely overestimates the total cooling efficiency, particularly for high-diffusivity materials where heat packets frequently reach the domain boundaries. More complex Neumann boundary conditions could be added to the simulation to better reflect physical conditions.

Hybrid Monte Carlo – deterministic approaches

Monte Carlo techniques have been combined with deterministic conditions to improve model accuracy. For example, Monte Carlo–driven optimisation has been coupled with computational fluid dynamics (CFD) simulations to optimise thermal performance [1] and heat sink design, allowing for the precise modelling of airflow, turbulence, and complex 3D fin geometries.

Conclusion

This project demonstrates that a Monte Carlo random-walk model can be used to study thermal diffusion in a simplified computer heat sink. By interpreting thermal transport as a stochastic diffusion process, the simulation reproduces the expected macroscopic behaviour of heat flow.

The results indicate that while thermal diffusivity (α) governs the rate of heat propagation, thermal conductivity (κ) determines the magnitude of the steady-state temperature. High-conductivity materials are shown to reduce hotspot temperatures by distributing thermal energy across the heat sink volume, which facilitates convective cooling across the effective surface area. Conversely, low-conductivity materials create thermal bottlenecks that limit the total heat loss, regardless of the convective cooling rate.

A Simulation Parameters (Appendix)

Table 1: Fixed simulation parameters

Parameter	Symbol	Value
Plate width	L_x	0.025 m
Plate height	L_y	0.025 m
Grid spacing	Δx	0.002 m
Grid dimensions	$N_x \times N_y$	12×12
Hotspot radius	R	0.006 m (3 cells)
Hotspot centre	(x_c, y_c)	$(6, 6)$ grid cells
Time step	Δt	0.002 s
Total simulation time	$t_{\max}$	10.0 s
Number of steps	N_{steps}	5000
Total packets	N	1500
Random seed	–	42
Boundary condition	–	Absorbing
Output interval	Δt_{out}	10 steps
Snapshots enabled	–	Yes
P_{conv}	–	0.004
T_{amb}	–	21 (approx)

Table 2: Material parameters used in the Monte Carlo simulations. Thermal diffusivity values and thermal conductivity (κ) are representative room-temperature values taken from standard reference tables (Brown, 1958). The equivalent move probability p is computed using $p = 4\alpha\Delta t/(\Delta x)^2$.

Material	**Diffusivity** α $(m^2 s^{-1})$	**Conductivity** κ $(W m^{-1} K^{-1})$	**Heat Capacity** $\rho c_p = \frac{\kappa}{\alpha}$ $(J m^{-3} K^{-1})$	**Move Prob.** p
Silver	1.7×10^{-4}	429	2.52×10^6	0.340
Gold	1.3×10^{-4}	317	2.44×10^6	0.260
Copper	1.1×10^{-4}	401	3.65×10^6	0.220
Aluminium	9.7×10^{-5}	237	2.44×10^6	0.194
Iron	2.3×10^{-5}	80	3.48×10^6	0.046
Steel (Carbon)	1.9×10^{-5}	50	2.63×10^6	0.038

Table 3: Heat injection rates

Q (packets/step)	Purpose
5, 10	Low heat (minimal heating regime)
15, 20	Moderate heat (standard operation)
25, 30	High heat (stress testing)
35, 40	Extreme heat (maximum load)

Table 4: Key constraints and diagnostic relationships.

Quantity	Expression	Typical range
Stability condition	$p = \dfrac{4\alpha\Delta t}{\Delta x^2}$	$p < 1$
Diffusion length	$l_d = \sqrt{\alpha t}$	0.3–0.8 mm
Domain coverage	l_d/L	0.01–0.03

Table 5: Summary of fixed and variable parameters.

Parameter type	Parameters
Fixed	$L_x, L_y, \Delta x, \Delta t, t_{\max}, N,$ seed, boundaries
Variable	Thermal diffusivity α, heat injection rate Q

B Appendix: Results

Steady-state hotspot temperatures

Table 6: Steady-state hotspot temperature T_{steady} (°C) for all materials and heat injection rates Q. Thermal diffusivity values are taken from standard reference data (Wikipedia/Brown, 1958).

Material	$Q = 5$	$Q = 10$	$Q = 15$	$Q = 20$	$Q = 25$
Silver	7.9	15.4	22.8	31.3	39.3
Gold	9.8	19.8	29.6	39.9	52.1
Copper	5.1	11.0	15.9	21.1	27.2
Aluminium	12.5	25.5	38.2	51.6	65.3
Iron	13.1	25.5	37.2	49.7	62.9
Steel (carbon)	23.5	45.3	71.2	90.2	113.8

Time to steady state

Table 7: Estimated time to steady state t_{ss} based on diffusion scaling $t_{\text{ss}} \sim L^2/(4\alpha)$, with $L = 25\,\text{mm}$.

Material	α ($\text{m}^2\,\text{s}^{-1}$)	t_{ss} (s)
Silver	1.7×10^{-4}	0.9
Gold	1.3×10^{-4}	1.2
Copper	1.1×10^{-4}	1.4
Aluminium	9.7×10^{-5}	1.6
Iron	2.3×10^{-5}	6.8
Steel (carbon)	1.9×10^{-5}	8.3

Monte Carlo convergence summary

Table 8: Monte Carlo convergence of steady-state temperature with packet count N.

Material	Packet count N	Mean T_{steady}	Std. dev.	Relative error
Copper	500	21.1	5.00	0.2368
Copper	1000	21.1	3.54	0.1674
Copper	1500	21.1	2.89	0.1367
Copper	2000	21.1	2.50	0.1184
Copper	3000	21.1	2.04	0.0967
Steel (carbon)	500	90.2	5.00	0.0554
Steel (carbon)	1000	90.2	3.54	0.0392
Steel (carbon)	1500	90.2	2.89	0.0320
Steel (carbon)	2000	90.2	2.50	0.0277
Steel (carbon)	3000	90.2	2.04	0.0226

References

[1] R. Busqué, M. Bossio, R. Fabregat, F. Bonada, H. Maicas, J. Pijuan, and A. Brigid, "Hybrid CFD and Monte Carlo-Driven Optimization Approach for Heat Sink Design," *Energies*, vol. 18, no. 11, p. 2801, 2025. doi: 10.3390/en18112801.

[2] M. Brown, "Introduction to Heat Transfer," 3rd ed., McGraw–Hill, New York, 1958.