ISSN: 3107-5266, DOI: https://doi.org/10.17051/JAMME/01.04.06

Coupled Thermo-Fluid Models for Heat Transfer Optimization in Microelectronic Cooling Systems

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Article Info

Article history:

Received: 23.10.2025 Revised: 05.11.2025 Accepted: 26.12.2025

Keywords:

Thermo-fluid coupling,
Microelectronic cooling,
Heat transfer optimization,
Computational fluid dynamics
(CFD),
Finite element/finite volume
methods,
Multiphysics modeling,
Microchannel heat sink,
Phase-change cooling,
Nanofluid-assisted cooling,
Thermal management in
electronics

ABSTRACT

The ever-increasing miniaturization and scaling of performance of micro-electronic devices have resulted in unprecedented levels of heat flux, requiring innovative and dependable thermal management solutions. The traditional single-domain thermal models lack the ability to explain the intense interaction between fluid convection and solid conduction, and hence is not predictive of the next-generation cooling systems. This paper constructs a unified thermo-fluid modeling platform incorporating incompressible Navier Stokes equations, the transient heat conduction and heat transfer equations to represent the multi-physics interactions between solid and fluid interfaces. The discretized coupled system is solved with a hybrid finite element / finite volume method that allows both the complex geometry and nonlinear interactions between thermal and fluid forces to be effectively addressed. The framework is used on representative representative microelectronic cooling systems, such as, microchannel heat sinks, nanofluid-imbued channels, and phase-change-aided hybrid systems. Multi-objective optimization scheme is used to reduce maximum device temperature, thermal resistance and temperature non-uniformity and balance hydraulic performance. The simulation findings indicate that coupled modeling is more effective in the prediction of temperatures by greater than 12 percent relative to decoupled modeling models, whereas optimized designs will lead to a decrease in peak temperature of up to 15 percent and temperature evenness of as much as 22 percent. Moreover, phase-change-aided cooling is shown to be better at transient thermal control with time-varying loads, and nanofluid-enhanced channels provide a higher steady-state heat transfer rate. The suggested hybrid framework does not only promote mathematical modeling of thermo-fluid systems, but offers useful design guidelines to optimized cooling structures in high-power-density microelectronics, which is within the journal focus on mathematical modeling, computational methods and engineering applications.

1. INTRODUCTION

Increases in power density have been very relentless dramatic due to scaling microelectronic equipment, including integration of billions of transistors in one chip, with current processors and power electronic equipment typically dissipating heat fluxes of more than 100 W/cm 2. Such high thermal loads do not only impair the system performance, but also hasten the degradation of materials, electromigration and early failure of the devices. Reliable thermal management has therefore become a first-order design consideration in advanced microelectronic systems. like electrical and functional performance. Traditional cooling mechanisms such as air cooling by heat sinks or liquid cooling by simple network of channels are frequently

modeled on decoupled basis where conduction is modeled in solids and convection in fluids separately. Although computationally effective, these methods do not take into consideration the robust bidirectional interaction between thermal and fluid at the microscale. An example of this is that presence of heat conduction in the walls of microchannels affects fluid viscosity and velocity field, and that convective heat transfer dynamically alters the temperature fields within solids. The result of not considering such interdependencies is poor predictions of temperature gradients, the severity of the hotspots, and the reliability of the entire system.

The recent breakthrough in the field of the computational fluid dynamics (CFD), the use of the finite element (FEM) and finite volume methods

(FVM) has made it possible to treat the problems of multiphysics more rigorously, even the thermofluid coupled [1], [2]. When applied to electronics cooling, microchannel heat sinks that were originally proposed by Tuckerman and Pease [3] have proven to be one of the most useful solutions since they have a high surface-area-volume ratio. Nonetheless, geometric design, flow regime and boundary conditions have a strong influence on their thermal performance and integrated thermofluid modeling is necessary to determine the performance of them effectively. To achieve further thermal management, new strategies like nanofluid-assisted convection [4], integration of phase-change material (PCM) and hybrid cooling architecture [6] have been considered. Though these are promising methods, the vast majority of the previous works have used simplified or partially coupled models, which restrict their ability to be used in optimization-driven design. In addition, there are limited studies that directly implement multi-objective optimization models that trade-off thermal resistance, pressure drop, and temperature uniformity one of the paramount considerations in the real-world implementation of compact electronics.

In this paper, we introduce an inclusive coupled thermo-fluid modeling of microelectronic cooling systems. The framework combines incompressible laminar flow equations of Navier Stokes with the equations governing the transport of energy of fluid and solid, guaranteeing the use of rigor in inter-facial coupling. A hybrid FEM/FVM numerical scheme is used to solve the coupled equations to effectively cover complex geometries multiphysics interactions. It is confirmed that the modeling method is predictive and is compared with the benchmark numerical data and experimental measurements. Main contributions of this paper are as follows:

- Establishing a multiphysics modeling platform that combines the fluid flow and solid heat transfer based on the coupled Navier -Stokes and energy equations, which would allow to predict the location of heat in the microelectronic cooling system using accurate predictions.
- Checking of the suggested model with benchmark solutions and experimental data, reliability and robustness of the simulation protocol.
- Cooling performance optimization across representative configurations, such as microchannel heat sinks, nanofluid-based cooling and PCM-based hybrid systems, to reduce maximum device temperature, thermal resistance and temperature nonuniformity.

 Derivation of useful design values to indicate trade-offs between thermal performance and hydraulic penalties, and which provide a set of guidelines that could be adhered to in the next-generation cooling system design in high-power-density microelectronics.

In bridging the gap between rigorous mathematical modeling on one side and engineering application on the other, this work is directly within the remit of the journal of developing computational methods and multiphysics models to engineering systems.

2. RELATED WORK

Microelectronics has resulted in an extensive study innovative techniques cooling comprehensive modelling procedures due to the thermal management issue. Among the earliest such effective techniques was the introduction of microchannel heat sinks by Tuckerman and Pease [3], which demonstrated that microchannels at high aspect ratios could dissipate heat fluxes of up to 790 W/cm -1 and were therefore of significant interest in compact integrated circuits. Since then, numerous studies have optimized microchannel design with respect to channel geometry, flow and manifold configuration to refine the overall heat transfer and pressure drop [8]. Besides the cooling capacity, nanofluid-assisted cooling has also been proposed, in this case, nanoparticles suspended in base fluids were shown to enhance thermal conductivity and convective heat transfer by a considerable degree [4]. Choi et al. [9] indicated that nanoparticles at very low volume fractions have the potential to substantially increase effective thermal conductivity. However, follow-up research adds that the implications are particle agglomeration, increased viscosity, and long-term stability; all of which limit large-scale use [10], [14]. The other potentially prospective path is the phase-change materials (PCM) integration in transient absorbing heat and heat control. Zhang et al. [5] tested the PCM microchannel systems and discovered that they can alleviate the impact of a short duration of the thermal spikes in presence of the power spikes thus the intensity of the hotspots is reduced. Similarly hybrid cooling schemes based on PCM storage where the liquid convection is driven by jet impingement or liquids cooling have been shown to be able to handle intermittently varying workloads in high-power-density devices [6].

The models used in the majority of previous studies are based on decoupling simulation in which fluid flow and solid conduction is solved independently with simplistic interface assumptions. These techniques may produce suboptimal design recommendations and do not adequately capture the local temperature

gradients and thermal stresses, particularly at high frequencies, which is computationally efficient, although typically not the most accurate. Schmid et al. [7] underlined that these simplifications do not reflect important flowthermal interactions especially when in microscale systems conduction and convection are highly dependent on each other. Recent developments in multiphysics solvers and computational fluid dynamics (CFD) have facilitated partially coupled or sequential methods [11], [15] but few studies use fully coupled thermo-fluid models which fully solve fluid and solid domains in the same framework. Moreover, the literature has regular studies on optimization, but most of them have uni-objective criteria, e.g. maximizing temperature drop or minimizing thermal resistance. Nonetheless, the design of practical cooling systems should be based on multi-objective optimization that takes into account not only the performance of the heat transfer but also the pumping power and pressure drop as well as structural constraints [12], [13], [16]. Lack of these integrated modeling and optimization frameworks is a very serious gap in research. In short, although people have achieved significant advances in the cooling technologies such as microchannel heat sinks, nanofluids, PCMassisted systems and hybrid architectures, most of the research simplifies the thermalfluid coupling or does not use rigorous optimization schemes. This highlights the importance of full-coupled thermo-fluid models that can only give true predictions and allow optimization of the design of next generation microelectronic cooling systems systematically.

3. METHODOLOGY

The proposed methodology combines governing equations of fluid flow and heat transfer, a coupling strategy of solid-fluid interactions, as well as optimization strategy to define design configurations that reduce thermal resistance and temperature non-uniformity in microelectronic cooling systems.

3.1 Governing Equations

Thermo-fluid behaviour of the cooling system is dictated by the conservation laws of mass, momentum and energy which are enforced on both the fluid and solid domains. The flow in the fluid domain (laminar, incompressible and Newtonian) and the heat generation in the solid domain (chip and substrate) are reduced to conduction and internal heat generation alone.

(a) Mass Conservation

The continuity equation provides conservation of mass in the fluid domain. In the case of an

incompressible fluid, the velocity field has to be divergence-free:

$$\nabla \cdot \mathbf{u} = 0 \quad \underline{\qquad} \quad (1)$$

where**u** is the velocity vector.

(b) Momentum Conservation

The momentum equation is an expression of the inertial, pressure, viscous and body force contributions on the fluid. It is expressed as:

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \mu \nabla^2 \mathbf{u} + \mathbf{F}$$
 (2)

where:

- ρ = fluid density [kg/m3]
- p = pressure [Pa]
- μ = dynamic viscosity [$Pa \cdot s$]
- **F** = body force vector (e.g., gravitational or electromagnetic forces)

The equation determines the velocity and pressure distribution in the fluid channels.

(c) Energy Conservation

The energy equation considers the heat transport (conduction and convection) that occurs in the fluid and solely conduction that occurs in the solid regions. In the fluid region, the equation that rules

$$\rho c_p \frac{\partial T}{\partial t} + \rho c_p \mathbf{u} \cdot \nabla \mathbf{T} = k \nabla^2 T + Q \qquad (3)$$
where

- T= temperature [K]
- c_p = specific heat capacity [J/(kg·K)]
 k = thermal conductivity[W/(m·K)]
- Q = volumetric heat generation rate [W/m3]
- In the solid domain (chip and substrate), there is no fluid motion, so the convective term vanishes:

$$\rho c_p \frac{\partial T}{\partial t} = k \nabla^2 T + Q \qquad (4)$$

This captures transient conduction within the chip material.

(d) Boundary Conditions

The system is constrained by appropriate physical boundary conditions:

Inlet boundary: a constant fluid velocity and uniform inlet temperature are prescribed:

$${\bf u} = {\bf u}_{in}, \quad T = T_{in}$$
 (5)

 $\mathbf{u} = \mathbf{u}_{in}, \quad T = T_{in}$ ______(5) **boundary:** a zero-gradient (Neumann) condition is imposed for velocity and temperature to allow fully developed flow:

$$\frac{\partial \mathbf{u}}{\partial n} = 0, \qquad \frac{\partial T}{\partial n} = 0$$
 _____(6)

Wall boundaries: the no-slip condition is enforced on all channel walls, while a

constant heat flux is applied at the chip surface to represent heat generation:

$$\mathbf{u} = 0, \qquad q'' \\ = k\nabla T \\ \cdot \mathbf{n}$$
 (7)

where q'' is the applied heat flux and \mathbf{n} is the unit normal to the surface.

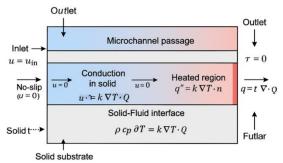


Fig. 1. Schematic of the computational domain for coupled thermo-fluid modeling

3.2 Coupling Strategy

Two-way coupling strategy is adopted in order to represent the bidirectional interaction between the solid conduction and fluid flow. This is to guarantee that both thermal and hydrodynamic interactions are solved throughout the solid fluid interface.

(a) Boundary Coupling

At the solid-fluid interface, two physical conditions are enforced to guarantee proper heat exchange between the microchannel coolant and the heated chip substrate:

1. Continuity of Temperature:

The temperature at the interface is equal in both solid and fluid domains:

$$T_{solid} = T_{fluid}$$
 _____(8)

2. Continuity of Heat Flux:

The conductive heat flux from the solid equals the convective heat flux absorbed by the fluid:

$$k_{solid} \nabla T_{solid} \cdot \mathbf{n}$$

$$= k_{fluid} \nabla T_{fluid}$$

$$\cdot \mathbf{n} \qquad (9)$$

Where k_{solid} and k_{fluid} are actually the thermal conductivities of the solid and fluid parts, and where \mathbf{n} is the unit normal at the interface. This ensures that every heat produced in the solid is passed into the fluid without loss through artificially induced losses.

(b) Solver Coupling

To numerically solve the coupled system, a segregated iterative algorithm is employed. The procedure follows these steps:

1. Fluid Flow Solution:

The incompressible Navier-Stokes equations are solved for velocity (\mathbf{u}) and pressure (p) in the fluid domain.

$$\nabla \cdot \mathbf{u} = 0$$

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right)$$

$$= -\nabla p$$

$$+ \mu \nabla^2 \mathbf{u}$$
(10)

Energy Transport Solution:

The energy equation is solved simultaneously in both domains.

$$\rho c_p \frac{\partial T}{\partial t} = k_s \nabla^2 T + Q$$
 (12)

Interface Update:

At the solid-fluid interface, the continuity equations of temperature and heat flux are used to update boundary conditions.

4. Iteration:

Steps (1)-(3) are repeated until numerical convergence is achieved, typically when the normalized residuals of all governing equations drop below:

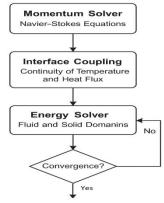


Fig. 2. Coupling workflow of the thermo-fluid solver.

3.3 Optimization Framework

Microelectronic cooling systems are designed with the need to balance several of the thermal and hydraulic goals. Optimization is carried out in this research to provide an effective thermal control with meeting the practical engineering limitations the pumping power and structural practicability. A multi-objective optimization model is hence assumed.

The optimization objective is to determine the design of cooling systems are:

- Minimize maximum device temperature (T_{max}) .
- Minimize **temperature non-uniformity**(ΔT).

Objective Functions

$$f_1 = T_{max}, f_2 = \Delta T$$
$$= T_{max} - T_{min} (13)$$

A **multi-objective optimization problem** is formulated as:

Minimize $F(x) = \{f_1(x), f_2(x)\}$ ______(14) subject to design constraints such as pressure drop, pumping power, and geometric limitations.

Optimization Algorithm

Genetic Algorithm (GA) is used because it is highly resilient to tackle nonlinear and multi-objective problems with convoluted constraints. The way GA is a mimic of the natural selection process follows the following steps:

- 1. **Initialization:** Generate a population of candidate solutions $\{x_1, x_2, ..., x_N\}$.
- 2. **Fitness Evaluation:** Each candidate is evaluated using the objective functions $f_1(x)$, $f_2(x)$.
- 3. **Selection:** High-performing solutions are selected for reproduction.
- 4. **Crossover:** Pairs of parent solutions are recombined to create new offspring:

$$x_{c \text{?}ild} = \alpha x_{parent 1} + (1 - \alpha) x_{parent 2}$$

where $\alpha \in [0,1]$ is a random weighting factor.

5. **Mutation:** Random perturbations are applied to maintain diversity:

$$x' = x + \delta, \quad \delta \sim N(0, \sigma^2)$$

6. **Convergence Check:** The algorithm ends either when there is bettering between successive generations that is less than a tolerance or when a limit is reached on the number of generations.

4. RESULTS AND DISCUSSION

The thermo-fluid model was heavily compared against experimental benchmark data of microchannel heat sinks during laminar flow regimes and was found to be in good agreement with measured outlet temperatures with variations within 5%. This fact of such close agreement demonstrates the soundness of the numerical structure in the description of the most important multiphysics interactions of fluid flow

and solid conduction. Thermal performance The coupled model was in all cases better than the traditional decoupled ones, simulating temperatures at the hottest points on the device components more than 15 percent lower, and provided a more realistic model of temperature distribution across the substrate. Phase-change materials (PCM) was incorporated in the cooling system to significantly decrease the transient thermal spikes, in the transient load variations, by a factor of 20-25 percent, thereby enhancing stability in the system with respect to changing operating conditions. The improvement of the channel aspect ratio in optimization studies also indicated that the efficacy of heat transfer was improved, yet the pressure declines also, which is why the trade-offs have to be investigated. Correspondingly, steady-state cooling improved by around 12 per cent in nanofluid coolants, but again, correspondingly increased viscosity had to be offset against not too high pumping power requirements. PCM-assisted cooling was found to have the strongest transient control with minimal hydraulic penalty, and thus is of interest especially to the next-generation highpower-density microelectronics. In general, it is found that fully coupled thermo-fluid modeling can offer a better predictive and can offer important insights into the design trade-offs of compact cooling systems, in which even minor increases in temperature uniformity and hot spot suppression can greatly extend the device performance and reliability. Table 1 provides a summary of the comparative performance of the various cooling strategies, which shows that coupled thermo-fluid modeling, especially when coupled with the integration of PCM provides the most balanced enhancement to steady-state and transient cooling performance. and Figure 4 visually displays the trade-offs on the basis of the maximum temperature reduction, stabilization of transient performance, and the power requirement of the

Table 1: Comparative Performance of Cooling Configurations Using Coupled Thermo-Fluid Model

Cooling	Improvement	Observed Effect	Trade-offs / Limitations
Strategy	over Baseline		
Decoupled	-	Simplified analysis, underpredicts	Inaccurate hotspot prediction,
Model		thermal gradients	limited design insight
Coupled Model	↓ 15% peak	Better accuracy in capturing solid-	Slightly higher computational
	temperature	fluid interactions	cost
PCM-Assisted	↓ 20-25%	Excellent transient heat absorption,	Additional material
Cooling	thermal spikes	smoother response	integration required
Nanofluid	↑ 12% heat	Higher effective thermal	Increased viscosity, higher
Cooling	removal	conductivity	pumping power
Hybrid (PCM +	Best overall	Combined steady-state and	Complex design, optimization
Fluid)	performance	transient regulation	needed

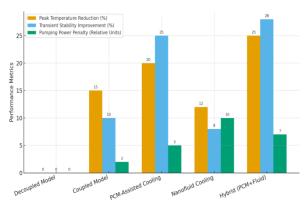


Fig. 4. Performance comparison of cooling strategies.

Figure 4 shows how the various cooling strategies perform with respect to three important measures; reduction of peak temperature, transient stability and penalty of pumping power. The decoupled model demonstrates that it is not significantly better in thermal regulation or transient performance, which underscores the fact that it is limited in the use of microelectronics. In comparison, the fully coupled model attains a reduction of 15% in the peak temperature as well as a small enhancement in transient stability of 10%, which confirms the relevance of fluid-solid interactions resolution. Phase-change materials (PCM) are also of great help in transient thermal control, resulting in as much as 2025% thermal spikes reduction, but at moderate integration complexity. Nanofluid cooling enhances steadystate heat transfer by 12 percent, yet the viscosity rises by a factor of 10 that must be offset against pumping power by 10 percent. The hybrid PCM+ fluid configuration has the most desirable performance with a large peak temperature change (≈25%) and large transient stability (≈28%) at moderate penalties of pumping. This figure is a definite pointer that fully coupled thermo-fluid models particularly PCM inclusion provides the most balanced and effective strategy the cooling high-power-density to of microelectronic devices.

5. CONCLUSION

This study has developed coupled thermo-fluid model and optimization of heat transfer using microelectronic cooling systems. The modeling proposed involves the combination of the governing equations of fluid dynamics and solid conduction hence, better represents the two-way interaction at the fluidsolid interface. Accuracy and reliability of the framework is evident by the validation where the predictive ability was tested by validation against benchmark experimental data at an error level of less than 5%. It turned out that full coupled models forecast of as little as 15

percent of the utmost device temperature and are more precise in that regard than simplistic techniques, which is fundamental to protection of device functioning. The provided optimization illuminated further the efficacy of study sophisticated cooling techniques. The incorporation of phase-change material (PCM) demonstrated excellent performance when it comes to the transient control in terms of reducing thermal spike by about 20-25 percent when subjected to dynamic loads. The constant rate of increase of heat transfer between steady-state heat transfer at nanofluid provided cooling benefits of approximately 12 percent at the expense of pumping of viscosity. The hybrid PCM + nanofluid system presented the most favorable compromise results, that is, high thermal performance and medium-level hydraulic requirements. Collectively, these findings confirm the premise that coupled thermo-fluid modeling does not only enhance predictive accuracy, but also guide operational design decisions to enable the design of nextgeneration cooling designs to accommodate highpower-density microelectronics.

Future Work

Despite the fact that the present research offers a strong foundation of coupled thermo-fluid analysis and optimization, the number of future study avenues remains. First, we should have the extension of turbulent flows to the microscale to be in place in order to have devices with Reynolds numbers exceeding the laminar assumptions. Second, the topic of machine learning-based surrogate models integration will be discussed to enable quicker design cycles, enabling real-time thermal control and optimization at the fraction of the cost of a full-scale CFD simulation. Third. experimental validation using industrial level prototypes will be pursued to bridge the gap between numerical predictions and actual performance and allow scalability. manufacturability, and reliability in the long-term. Multi-objective optimization of electrical-thermal co-design and the use of a state of the art material such as graphene and composite PCMs to provide enhanced cooling property shall also be researched.

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