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NUMERICAL OPTIMIZATION OF ADVANCED MONOLITHIC MICROCOOLERS FOR HIGH HEAT FLUX MICROELECTRONICS

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ABSTRACT

This study considers the optimization of a complex micro-scale cooling geometry that represents a unit-cell of a full heat sink microstructure. The configuration consists of a channel with a rectangular cross section and a hydraulic diameter of $100\ \mu\text{m}$, where the fluid flows between two cooling fins connected by rectangular crossbars ($50 \times 50\ \mu\text{m}$). A previous investigation showed that adding these crossbars at certain locations in the flow can increase the heat transfer in the microchannel, and in the present work we perform an optimization to determine the optimal location and number of crossbars. The optimization problem is defined using 12 discrete design parameters, which represent 12 crossbars at different locations in the channel that can either be turned off and become part of the fluid domain, or turned on and become part of the solid domain. The optimization was done using conjugate heat transfer computational fluid dynamics (CFD) simulations using Fluent 15.0. All possible 4096

configurations were simulated for one set of boundary conditions. The domain was discretized using about 1 million nodes combined for the fluid and solid domains and the computational time was around 1 CPU hour per case. The results show that further improvements in heat transfer are feasible at an optimized pressure drop. The results cover a range of pressure drops from 25 kPa to almost 90 kPa and the heat transfer coefficient varies from 60 to 120 kW/m²K. The configurations on the Pareto front show the trend that crossbars closer to the maximal fluid-solid interface result in a more optimal performance than crossbars positioned farther away. In addition to performing simulations for all possible configurations, the potential of using a genetic algorithm to identify the configurations that define the Pareto front was explored, demonstrating that a 80% reduction in computational time can be achieved. The results of this study demonstrate the significant increase in performance that can be obtained through the use of computational tools and optimization algorithms for the design of single phase cooling devices.

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NOMENCLATURE

Roman

c_p	specific heat capacity at constant pressure	$[J/kgK]$
D_h	hydraulic diameter	$[m]$
h	heat transfer coefficient	$[Wm^{-2}K]$
k	thermal conductivity	$[Wm^{-1}K^{-1}]$
P	pressure	$[kg/ms^2]$
q	heat flux under the solid slab	$[W/m^2]$
q_w	wall heat flux at the interface	$[W/m^2]$
T	temperature	$[K]$
u	velocity	$[m/s]$
U_∞	bulk velocity	$[m/s]$
x, y, z	Cartesian coordinates	$[m]$

Greek

ρ	density	$[kg^1m^{-3}]$
μ	dynamic viscosity	$[Pa^1s^1]$
ij	Einstein'sche summation convention	

Acronyms

CFD	Computational Fluid Dynamics
CHT	Conjugate Heat Transfer
GaN	Gallium nitride
SiC	Silicon Carbide
SIMPLE	Semi Implicit Pressure Linked Equations
NSGAI	Nondominated Sorting Genetic Algorithm II
TIM	Thermal Interface Material

Super- and Subscripts

f	fluid
s	solid
w	wall quantity
∞	free stream quantity

INTRODUCTION

To ensure further development of high performance electronic systems, innovative cooling techniques should be developed [1] [2]. Since the first design for microchannel heat sinks has been proposed [3] and investigated [4], significant efforts have been made to enhance the conventional designs consisting of long channels that run parallel to the heated base [5], but the development of advanced micro-channel heat sinks has been constrained by fabrication limitations. Recently, new manufacturing techniques are enabling fabrication of monolithic, complex micro-scale structures, thus creating significant potential for optimizing the geometrical configuration of the heat sink geometry. Given the large design space in such a geometrical optimization process, computational tools and optimization algorithms

can support converging towards an optimal design.

In a previous study, CFD simulations with conjugate heat transfer have been performed for a reduced model of the entire heat sink micro-structure to enable exploring a wide variety of the design space at a limited computational cost. The reduced model represents a unit-cell and uses periodic boundary conditions to mimic the conditions in the entire cooling manifold. The baseline configuration is a channel with copper fins, and we investigated possible improvements in the efficiency of micro-channel heat sinks by using different geometrical features, e.g., fins, woodpile structures and fins connected by cross-bars. The design using fins with cross-bars was shown to be the most promising configuration, and also poses opportunities for further optimization in terms of the location and the number of cross-bars.

The present investigation addresses this optimization problem using similar unit-cell CFD simulations with conjugate heat transfer. A multi-objective optimization problem is defined to maximize the heat transfer, while minimizing the pressure drop in the channels. 12 discrete design parameters are considered, which represent 12 crossbars at different locations in the channel that can either be turned off and become part of the fluid domain, or turned on and become part of the solid domain. Three different optimization approaches have been considered, a brute force approach, where the 2^{12} configurations were considered, an intuitive approach starting from 12 simulations that each consider a single cross-bar, and a genetic algorithm approach.

The following section describes the computational model for the considered geometry, the governing equations, the boundary conditions and the numerical solution methods to solve for the conjugate heat transfer problem. Moreover, the optimization algorithm for the topology optimization is explained. The results section first presents the output quantities of interest and a thorough grid dependency study. Finally, the results of the multi-objective optimization problem are presented.

DESCRIPTION OF COMPUTATIONAL MODEL

Geometry description and material properties

Figure 1 shows the baseline geometry, which consists of two cooling fins that define an empty channel with a rectangular cross section and a hydraulic diameter of $100 \mu m$. The channel and the copper fins are $460 \mu m$ long, the fins are $300 \mu m$ high. An inlet and an outlet section of $200 \mu m$ and $300 \mu m$ length, respectively, have been added to the computational domain to avoid influencing the flow through the channel by the inlet or outlet boundary conditions.

The heat is distributed from the gates in the GaN layer (See Fig. 1) with a surface of $2 \times 160 \mu m$ through the SiC layer with a thickness of $100 \mu m$ and the stress relieving TIM and

epotek layers with respective thicknesses of 4 and 10 μm . The epotek layer is in contact with the coolant and the heat dissipating copper fins. The working fluid is water. The fluid and solid conductivities are summarized in Table 2. Figure 2 shows sketches of the baseline geometry (2(a)) and the cross bars (see Fig. 2(b)). The overall dimensions of the investigated geometries are identical. The squared crossbars are bars connecting the cooling fins with a 50 μm diameter (the minimal feature size restricted by manufacturing constraints) meant to increase the cooling surface area and to accelerate and redirect the flow towards the hotspot.

TABLE 1. MATERIAL PROPERTIES.

material	conductivity [W/mK]
GaN	$214.17 - 0.1623T$
SiC	$1259 - 4.1734T + 0.0038T^2$
TIM	314
epotek	30
copper	387.6
water	0.6

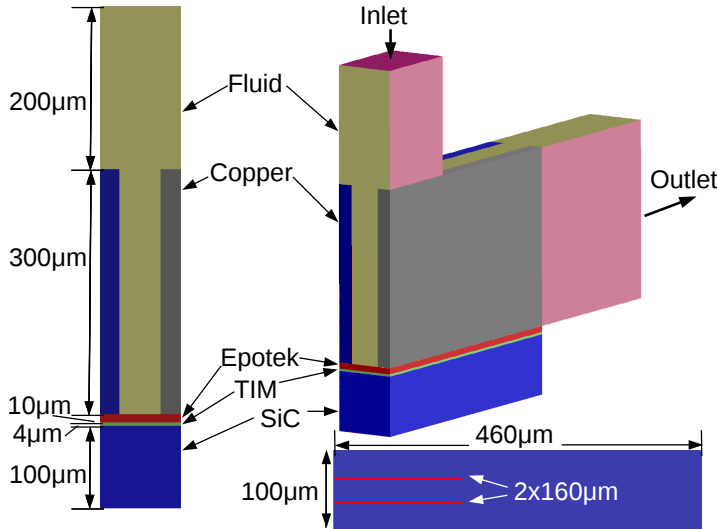


FIGURE 1. GEOMETRY OF SINGLE CELL MODEL

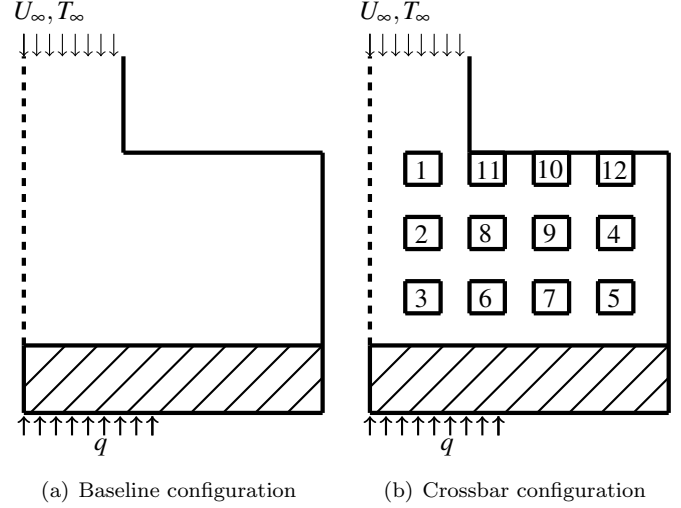


FIGURE 2. SKETCHES OF INVESTIGATED GEOMETRIES.

Governing Equations

Previous studies have demonstrated that the macroscale Navier-Stokes equations and energy equations sufficiently describe the flow and heat transfer in microchannel heat sinks [6] [7]. The fluid flow and the heat transfer in the fluid and solid domain are therefore governed by the following equations [8]:

- the continuity equation:

$$\frac{\partial}{\partial x_j}(\rho u_j) = 0, \quad (1)$$

- the momentum equation:

$$\frac{\partial}{\partial x_j}(\rho u_j u_j) = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\mu_f \frac{\partial u_i}{\partial x_j} \right), \quad (2)$$

- the energy equation for the fluid domain:

$$\frac{\partial}{\partial x_j}(\rho u_j C_p T_f) = \frac{\partial}{\partial x_j} \left(k_f \frac{\partial T_f}{\partial x_j} \right), \quad (3)$$

- the energy equation for the solid domain:

$$0 = \frac{\partial}{\partial x_j} \left(k_s \frac{\partial T_s}{\partial x_j} \right). \quad (4)$$

Boundary Conditions

A constant heat flux was prescribed at the bottom of the solid on the two gates (Fig. 1), with $2.46 \times 10^9 \text{ W/m}^2$.

All other solid outer walls were assumed to be adiabatic. In the fluid domain, no-slip conditions were applied on the interfaces to the solid domain and on the fluid top boundary. A coupled wall boundary condition was used to compute the temperature at the solid-fluid interface walls. Dealing with a steady state problem in fluid and solid domain, the conjugate heat transfer was solved with a monolithic coupling approach as provided by the ANSYS Fluent software, thus assuring continuity of temperatures and heat fluxes at the fluid-solid interfaces:

$$T_s = T_f, \quad (5)$$

$$k_s \left(\frac{\partial T_s}{\partial n} \right) = k_f \left(\frac{\partial T_f}{\partial n} \right). \quad (6)$$

Symmetry boundary conditions were applied on the front and the inlet and outlet region side walls (see Fig. 1). A constant pressure outlet condition was applied on the outlet set to 1 bar. The mass-flow at the inlet was set to 3.7781×10^{-5} kg/s with an inlet temperature of 343K. (see Table 2). The minimal convergence criterion was set to 10^{-5} for the continuity and momentum equation and to 10^{-8} for the energy equation.

TABLE 2. SIMULATION PARAMETERS.

parameter	value
single cell mass flow rate	3.7781×10^{-5} kg/s
single cell heat flux at the gate	$2.46 \cdot 10^9$ W/m ²
Inlet temperature	343 K

METHODS

Fluid Solver

The numerical simulations solved the incompressible three-dimensional steady-state Navier-Stokes and energy equations, with the Reynolds number remaining low enough to consider a laminar flow, being lower than 480. The conjugate heat transfer problem was solved using the simulation software ANSYS Fluent 15.0 [9]. The code uses the finite volume method to solve the governing equations of fluid flow and heat transfer in the fluid and solid domain. The SIMPLE algorithm was employed to treat the coupling between the pressure and the velocities. All discretization schemes used were of second order. The ANSYS meshing mode was used to set up the computational model and to generate the grids.

Optimization

Three different optimization methods have been used and evaluated as described in the following sections.

Brute force approach The design space is defined by 12 crossbars, which each have a binary parameter ('ON' or 'OFF') associated with them. This leads to a total of 2^{12} , or 4096 possible geometrical configurations. Using a brute force approach, all possible cross-bar configurations were simulated.

Intuitive approach The intuitive optimization first investigated the influence of each individual crossbar on the cooling performance. Subsequently, it was tried to combine the best individual crossbar configurations. This approach was a first attempt to perform a topology optimization with a significantly improved computational efficiency, but it lacks the ability to account for interactions among different crossbars.

Evolutionary algorithm approach A multi-objective evolutionary algorithm (MOEA) [10] [11] [12] [13] was used for the optimization. A genetic algorithm [14] [15], more specifically, a so-called Nondominated Sorting Genetic Algorithm II (NSGAI) [16] was used, implemented in the in-house developed optimization code CADO of the Von Karman Institute for Fluid Dynamics (VKI). For details on the algorithm and the implementation, the reader is referred to [17] and [18]. The used genetic algorithm is based on the idea of natural selection, using the principle of the survival of the fittest. In the present case, each individual (one specific channel geometry) has 12 properties, i.e., each cross bar can be turned on or off (in this case it becomes part of the fluid domain). This leads to a discrete optimization problem, where the 12 design parameters can each be represented by one bit (1 or 0). Each individual is therefore defined by a binary string with 12 digits that represent the 12 crossbars. For instance, the binary string 100010111001 represents a geometry in which the crossbars labeled 1,5,7,8,9 and 12 in Fig.2(b) are present. The initial population consists of a certain amount of individuals, which are randomly selected. After evaluating the performance of each individual in the initial population using the CFD simulations, the best individuals are considered for reproduction as parent individuals.

RESULTS

The following section first presents the definition of the output quantities of interest. Subsequently, it presents the

results for the mesh dependency study and finally, the results for the channel optimization, comparing the efficiencies of different optimization strategies.

Output quantities of interest

The quantities used in the following sections are the maximal temperature at the gate T_{max} , the temperature at the interface from solid to fluid T_w , the pressure drop from inlet to outlet of the fluid domain ΔP and the heat transfer coefficient h . The heat transfer coefficient is a frequently used engineering parameter during the thermal design. It is derived from Newton's law of convection:

$$q = h(T_w - T_\infty), \quad (7)$$

with the the free-stream temperature T_∞ .

Mesh description and grid dependency study

A fully structured hexahedra mesh was constructed, using global and local size functions to adjust the mesh size as needed. Special care was taken to resolve the very thin solid layers, in particular the GaN surface where the heat flux was imposed. The coarsest mesh, M1, contained one cell at this surface. Mesh M2 contained two and mesh M3 four cells. The grid influence on the solutions was checked on those three different meshes on the crossbar geometry. Table 4 summarizes the mesh properties. Figure 3 shows the values for the maximal temperature at the gates, for the maximal temperature at the interface surface between fluid and solid domain, pressure drop inside the channel and the heat transfer coefficient for the different meshes. While a significant change of the results from mesh M1 to mesh M2 is still visible, further increasing the mesh resolution does not change the results considerably. Thus, to keep a balance between computational time and prediction accuracy mesh M2 was chosen for the following studies.

Crossbar configuration optimization

The objective of the optimization was to minimize the pressure drop inside the channels, while minimizing the maximal temperature at the gates. The two objectives lead to a multi-objective optimization. These two objectives conflict and no single optimal solution exists, rather, a so-called Pareto front with non-dominated solutions is present.

Brute force optimization Figure 5 shows the results of the brute force optimization, obtaining a full set of the population with the temperature as a function of the pressure drop. Figure 5 further indicates a subset of the Pareto

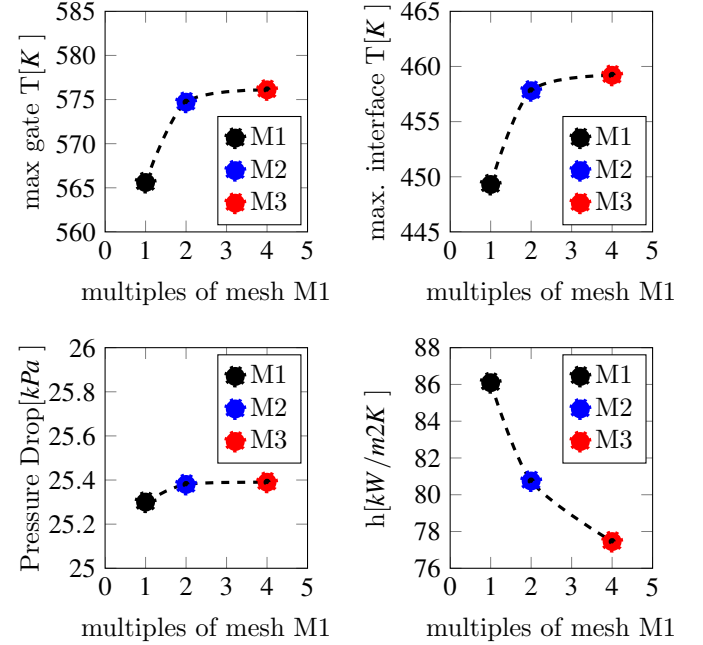


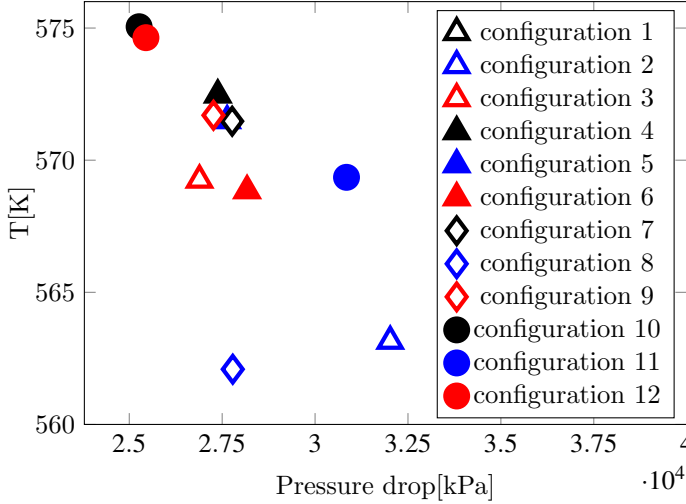
FIGURE 3. MESH DEPENDENCE STUDY.

front, configurations A-L, which Fig. 6 and Fig. 7 detail. Starting with configuration A on the Pareto front, which is the baseline configuration, the efficiency of the cooling increases until configuration L. A first reason for an increased heat transfer is the increased wetted surface area that is added with each crossbar (see Table 3). Further going along the Pareto front, configuration (B) has one more single crossbar added. Intuitively, one would expect that the first single crossbar on the Pareto front is positioned close to the hot spot, while configuration (B) has its crossbar positioned more towards the middle of the channel, where the path for the conducted heat is longer. The reason for this positioning is the higher velocity in the middle that is further increased with the crossbar leading to an enhanced heat transfer coefficient, especially in a region that was part of a recirculation zone in the baseline configuration of the fluid and has, now, largely increased. This increase in heat transfer coefficient also overcompensates the small decrease of the heat transfer coefficient in the wake of the crossbar of configuration (B). As Fig. 7 shows, adding the bottom left crossbar in configuration (D) increases the heat transfer coefficient to a smaller amount.

Intuitive optimization The results of the brute force optimization allowed investigating more efficient optimization approaches. First, an intuitive approach was explored, where in the first step the influence of each individual cross

TABLE 3. EXTRA SURFACE AREA.

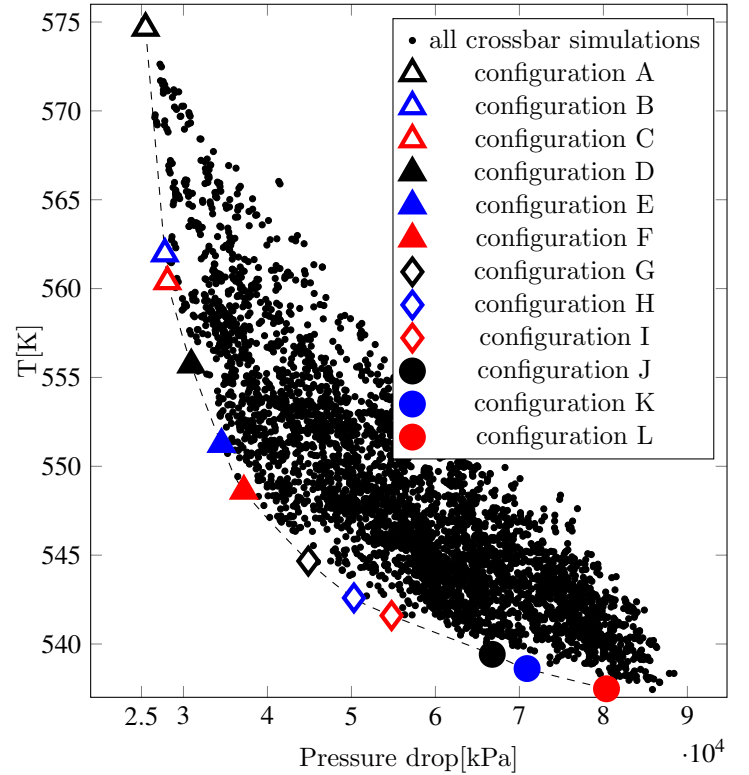
geometry	baseline	crossbar
surface area	$3.22 \times 10^{-8} m^2$	$3.22 - 3.49 \times 10^{-8} m^2$
difference compared to baseline	-	0 - 8.4%

**FIGURE 4.** 12 SINGLE CROSSBAR SIMULATIONS., CONFIGURATION 1 CORRESPONDS TO ONLY CROSS-BAR 1 IN FIG. 2(b) TURNED ON, CONFIGURATION 2 CORRESPONDS TO ONLY CROSS-BAR 2 IN FIG. 2(b) TURNED ON, etc.

bar on the cooling performance was investigated (Fig. 4). Subsequently, the configurations that are on the Pareto front of this first population can be combined to determine optimal configurations. This approach can indeed identify members that are on the Pareto front on the entire population shown in Fig. 5. For instance, combining configuration 8, which is already on the Pareto front for the entire population, with configuration 3 leads to another member on the Pareto front. Adding crossbar 9 to this combination will generate another optimal design. The drawback of this approach is that not all the members of the Pareto front can be identified. In addition, this approach would overestimate the benefit that could be gained by adding crossbars 10 and 12, which are part of the Pareto front for the individual crossbars, but are positioned far away from the hot spot and do not influence the flow significantly.

Optimization with genetic algorithm With the previously described genetic algorithm, the efficiency could be improved while also maintaining the result of the previous

Pareto front. The crossover probability for the present case, i.e., the probability for the parents genes to be crossed with another parent for the next generation, was set to 80%. The mutation probability, the likelihood of an inherited property to change from one generation to another, which is used to avoid that the algorithm gets stuck in local minima, was set to 8.3%. This gives an individual with 12 binary parameters a likely chance that one of his properties changes. Figure 8 compares the entire population of the brute force approach with the population that results from the genetic algorithm. It is apparent that the used algorithm reduced the computational time by more than 80%, and all but one member of the brute force Pareto front have been identified. The population for each generation contained 24 individuals, with 33 computed generations.

**FIGURE 5.** 4096 CROSSBAR SIMULATIONS

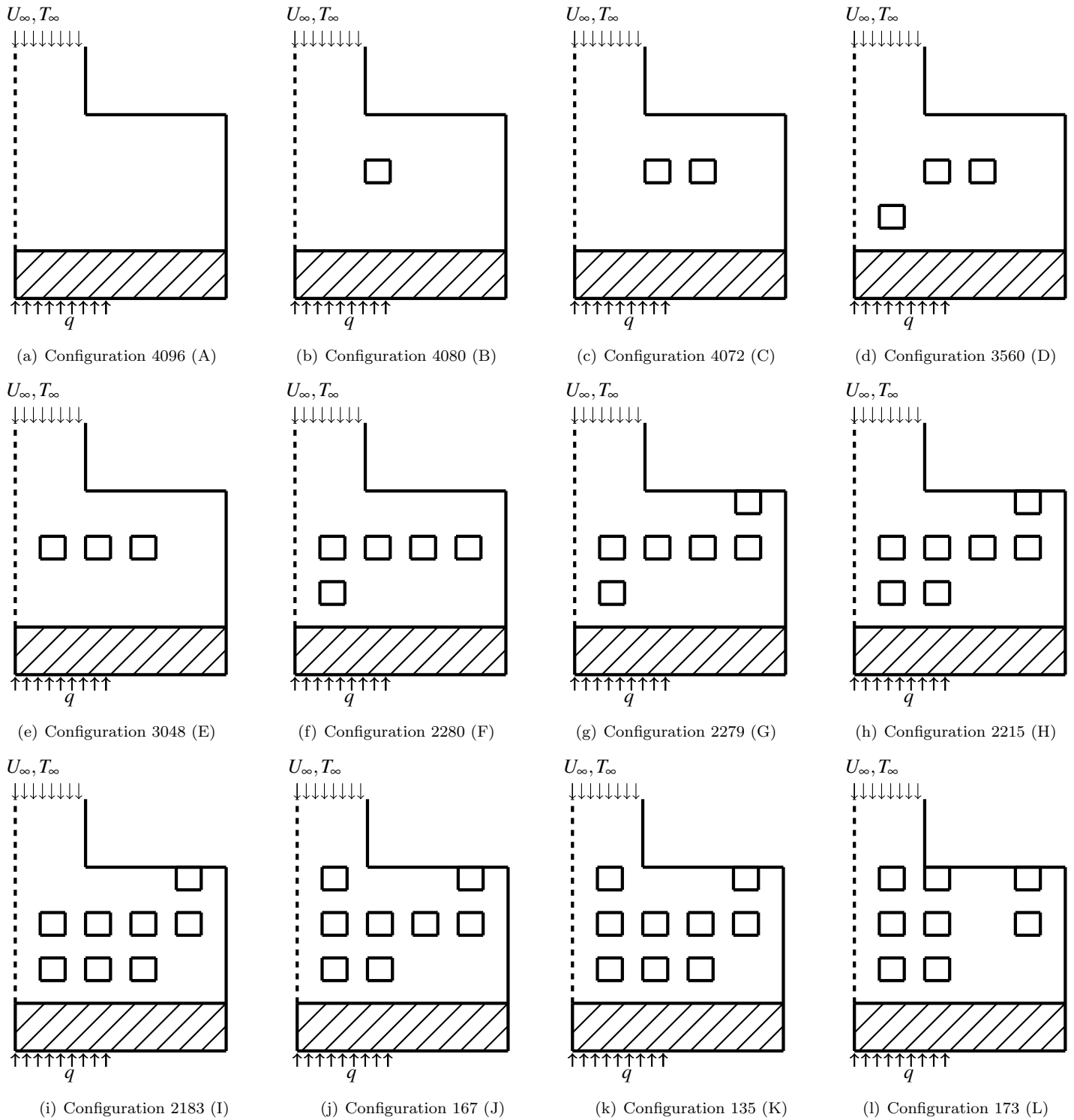


FIGURE 6. CROSSBAR CONFIGURATION SKETCHES.

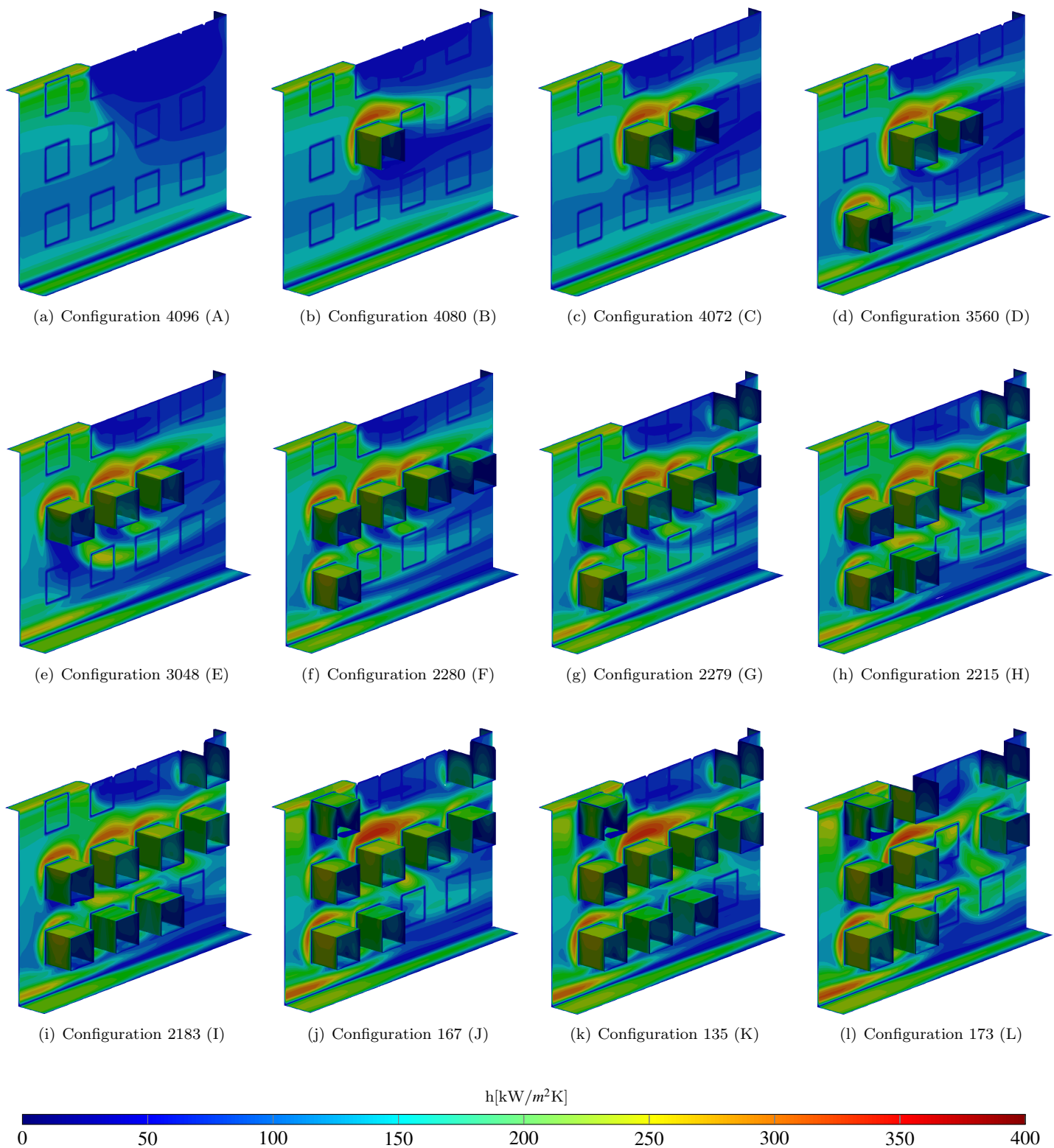


FIGURE 7. HEAT TRANSFER COEFFICIENT CONTOUR PLOTS FOR CROSSBAR CONFIGURATIONS.

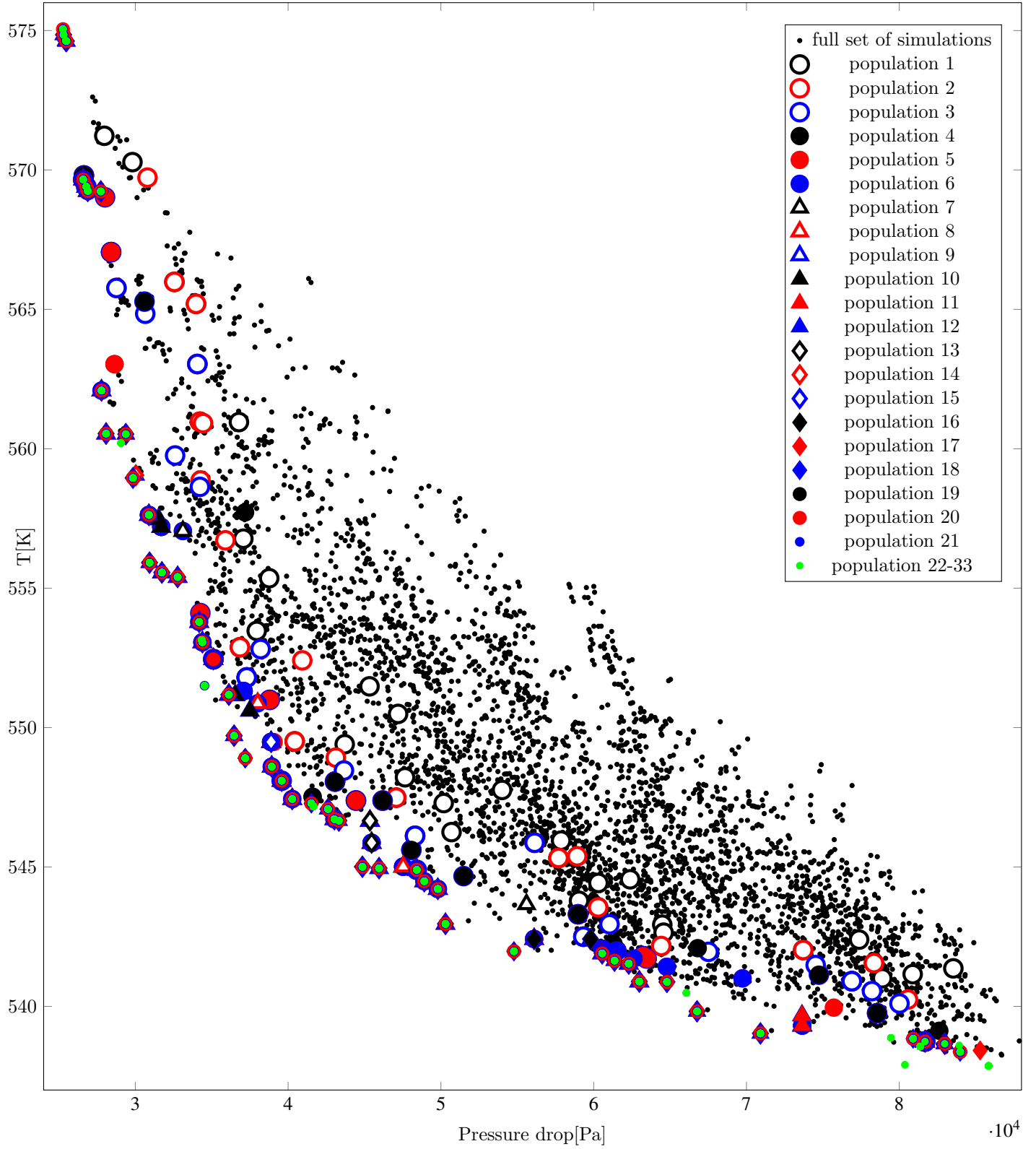


FIGURE 8. NSGA2 crossbar optimization. Crossover probability: 0.8. Mutation probability: 0.0833. Size of each population: 24 individuals.

CONCLUSIONS

Conjugate heat transfer CFD simulations have been used to solve a multi-objective optimization problem formulated to determine optimal geometrical configurations for a micro-scale heat sink. The objective is to maximize the heat transfer while minimizing the pressure, and the CFD simulations solve the three-dimensional laminar flow and heat transfer in different unit-cell geometries representative of a complete heat sink design. The unit cell consists of a rectangular channel defined by fins that can be connected by crossbars. 12 discrete design parameters were considered, representing 12 crossbars at different locations in the channel that can either be turned off and become part of the fluid domain, or turned on and become part of the solid domain. Three optimization principles have been investigated and compared to each other: (1) a brute-force optimization, simulating the full set of possible individuals, (2) an intuitive optimization, and (3) a genetic algorithm (NSGAI). Based on the brute-force approach a large amount of configurations that define the Pareto front and provide optimized cooling configurations for the micro-channel heat sink was identified. Using the intuitive optimization only a small number of individuals on the Pareto front was recovered, but the advantage of this approach is its very limited computational cost. The most promising approach was shown to be the genetic algorithm, which identified the entire Pareto front at only 20% of the computational cost of the brute-force approach.

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