



Quantum Computing Applications for Compact Heat Exchanger Design and Assessment

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Abstract

This paper explores possible implementations of quantum computing technologies, namely the quantum annealing and the quantum walk search algorithm, to solve fluid dynamics problems related to the design and assessment of compact heat exchangers for aeronautical environmental control and thermal management systems, as well as several other science and engineering applications, e.g. oil and gas refinery process. The purpose of this paper is to introduce two alternative implementations to the already assessed numerical resolution of Navier–Stokes equations or the resolution of analog quantum mechanical problem, highlighting how the use of quantum annealing and a classification algorithm (quantum walk search algorithm) can be implemented for the resolution of a lumped-characteristic analytical model of the heat transfer inside a compact heat exchanger, also in case of two-phase refrigerant fluid, for the use during design phase of environmental control system, e.g. provide the design engineers with a relatively simple and quick to use tool, which provides a reasonable result with an easily interpretable physical meaning. We start with a simple two-phase flow within a single-pass mini-channel heat exchanger, describing the mathematical formulation of the problem followed by a simplified implementation of the proposed quantum approaches, highlighting the main procedures of the calculation as well as the practical implications, advantages and disadvantages of the proposed method, e.g. a limited number of CFD simulations are required to evaluate air side heat transfer coefficient and pressure drop for particular designs within the defined design space, and the specific hardware required to implement the quantum process.

Keywords Quantum computing · Heat transfer · Compact heat exchanger · Aeronautical environmental control system · Multiphase flows · Computational methods

1 Introduction

In aeronautics, the term Environmental Control System (ECS) of an aircraft identifies the system associated with aircraft thermal management [1, 2]. It includes equipment dedicated to ventilation, heating, cooling, humidity control (also ensuring air recirculation and the supply of fresh air), and possibly pressurization of aircraft zones [3–5]. These

include human occupied compartments as well as cargo compartments and electronic equipment compartments [1, 6–9].

The thermal management is achieved with the use of heat exchangers [1, 2, 5], i.e., equipment designed for efficient heat transfer from one fluid to another, without mixing them. In aeronautical applications, due to the weight and dimensions constraints, this type of equipment is required to be characterized by high heat transfer area to volume ratio, large heat transfer coefficients, small flow passages, and, eventually, laminar flow. This type of heat exchanger is commonly called “compact” heat exchanger. Compact heat exchangers pack a large amount of heat transfer surface area, higher than 400 m²/m³ in case of liquid-to-liquid or phase change heat exchangers, a value higher than the one obtained in other type of heat exchangers, like “fins and tube” or “shell and tube” models [5], [5, 7–9].

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A subclass of the compact heat exchangers are the Micro-channel heat exchangers (MCHXs), [5, 9–12], which are characterized by tubes with hydraulic diameters in the range of a few hundred micrometers to a few millimeters. MCHXs are compact and exhibit superior heat transfer performance owing to an enhanced surface area to volume ratio and the increased effect of surface tension and shear forces on heat transfer at the microscale. Other benefits of MCHXs include decreased air-side pressure drop, lower refrigerant charge when compared with conventional finned-tube heat exchangers, and an all-aluminum body that helps reduce weight.

Owing to the smaller tube and port size, and the use of two-phase refrigerant fluid in the refrigeration cycle, the modeling of heat exchangers can be done analytically with the use of lumped characteristics and experimental/historical correlations, or with the use of expensive numerical models, especially for complete and/or large-scale models, relegating the numerical assessment at the verification phase of a frozen configuration.

Because, on other hands, economical access to powerful microprocessors and high-performance GPU has paved the way for the evolvement of Computational Fluid Dynamics (CFD) during the design phase, it is reasonable to investigate new technologies that could potentially allow a decrement of computational cost, or, in other words, an increment of computational power, allowing the design engineers to evaluate more detailed solutions in an early stage of project development. A relatively new technology is the quantum computing, which is addressed in this paper, this technology being quite promising also for the thermofluid-dynamics applications [13–15].

2 Quantum Computing

2.1 Quantum Computing as a Promising Flexible Technology

Quantum computing is, currently, a very active field of study and development, with expected applications in various fields ranging from the classical computer science problem, like cryptography and search problem, to engineering application, like structural optimization [16] and mechanical dynamics [17], but additional applications in different fields have been identified and developed [18], also for pure financial investments [19].

Fluid dynamics, traditionally described by the Navier–Stokes equation (NSE), by their simplified formulations like the Euler’s equations, or by the Lattice–Boltzmann equation (LBE), is notoriously difficult to be fully simulated on a classical computer at a large Reynolds number (Re), because the high-Re turbulent flow involves length and time scales over a wide range of orders of magnitude. The

computational cost is related to the Reynolds number itself, roughly $\mathcal{O}(Re^3)$ operations for the direct numerical simulation of NSE (DNS), and it results unaffordable in the pure design phase of common engineering applications, thus simplified methods have been introduced to reduce the computational costs (e.g., introducing a turbulence model) [13, 20].

Indeed, several approaches have been proposed for the solutions of CFD problems with the use of quantum computing devices, as summarized in [13–15, 21], being the rationale of the development the estimated scalability of quantum computing [22] or the analogy between fluid dynamic equation with a formally similar quantum system, e.g. the Euler’s equations with the Hydrodynamic Schrödinger equation (HSE) [20] or the analogy between Lattice Boltzmann equation with Dirac equation in the Dirac–Majorana formulation.

A review of the current state-of-the-art of quantum computing applied to computational fluid dynamics has been consequently carried out, highlighting how the technology is promising but still in an early stage of development, [13, 14, 23, 24] and strictly related to the contingent problem to be solved, which can heavily affect not only the scalability/feasibility of the quantum algorithm but also the goodness of the results: preliminary results show that the quantum algorithms are able to achieve reasonable results under heavy simplifications, i.e., limitation of nonlinear terms, [14, 15, 24, 25], or under the application of quite specific physical problem (e.g., inviscid fluids), thus a generalized multipurpose procedure is far to be identified.

2.2 Quantum Computing Fundamentals

A quantum computer is a dedicated device that harnesses quantum mechanical system properties like superposition, interference, and entanglement to manage information and perform calculations, acting on elementary information entities called “*qubits*”, the quantum equivalent of classical computer bits [13]. Since the smallest nontrivial Hilbert space is two-dimensional, a qubit describes a state in the simplest possible quantum system, i.e., it is a quantum system described by a two-dimensional Hilbert space, whose state can take any value of:

$$|\psi_i\rangle = a|\Psi_0\rangle + b|\Psi_1\rangle \quad (1)$$

where $\{|\Psi_0\rangle, |\Psi_1\rangle\}$ is the orthonormal basis for a two-dimensional vector space, usually, $\{|0\rangle, |1\rangle\}$, while a and b are complex numbers that satisfy the normalization rule $|a|^2 + |b|^2 = 1$ and encode the probabilities of the outcomes of a measurement in the selected basis. It follows that the actual value of a qubit can be known only after a measurement, and, before any measurement, the qubit is in a superposition of fundamental states.

Please note that a quantum computer can elaborate many qubits at once, i.e. a quantum state defined by:

$$|\psi\rangle_n = |\psi_n\rangle \otimes |\psi_{n-1}\rangle \otimes \cdots \otimes |\psi_1\rangle \otimes |\psi_0\rangle \quad (2)$$

From a physical point of view, these qubits can be made up of any object that obeys the laws of quantum mechanics, such as electrons or other charged particles, polar molecules, quantum gases, superconducting circuits, or electromagnetic radiation (e.g., polarized light).

The evolution of a quantum mechanical system can be represented by the application of transformations to the original state. These transformations are usually represented by unitary matrices:

$$|\psi_n\rangle = [A_n][A_{n-1}] \cdots [A_0]|\psi_0\rangle \quad (3)$$

Programming a quantum computer consists in the process of designing and assembling sequences of operations and instructions to manipulate a quantum system for a desired outcome. Since a way to design these sequences consists in the use of dedicated gates, analog the classical logic gates, the resulting sequence is usually referred as “quantum circuit”, thus, the algorithmic approach (see the next paragraph) is also known as circuitual approach. On other hand, it is possible to define a quantum architecture without a logical circuit layout (i.e., a circuit based on the logic gates), for example in the case of quantum simulator and quantum annealing architecture (whereas however the evolution of the system can be described as usual with the quantum operators and its Hamiltonian).

The current quantum computers architecture applicable to the resolution of CFD problem can be summarized as follows, [21, 23, 26]:

- Quantum computers circuits or gates
- Adiabatic quantum computers, or quantum annealing
- Topological quantum computers
- Measurement-based quantum computers

Beside the hardware on which the quantum computer is based, and starting from the above-mentioned models, three main families of approaches can be envisioned to solve fluid mechanics problems, namely:

- the algorithmic methods, focused on the development of numerical algorithms to be run on quantum computers, and the results are usually displayed as the most probable solutions,
- the analogue techniques, i.e. the “design” of a quantum system able to “mimic” the physical problem, evolving in time and reaching a minimum energy state which is the required solution,

and, last and not least,

the development of machine learning codes for quantum computers, which, however, can be implemented in combination with the above-mentioned methods.

The rationale of this taxonomy, displayed in the following Fig. 1 and being rearranged from Bharadwaj and Sreenivasan’s taxonomy [21] and extended to include

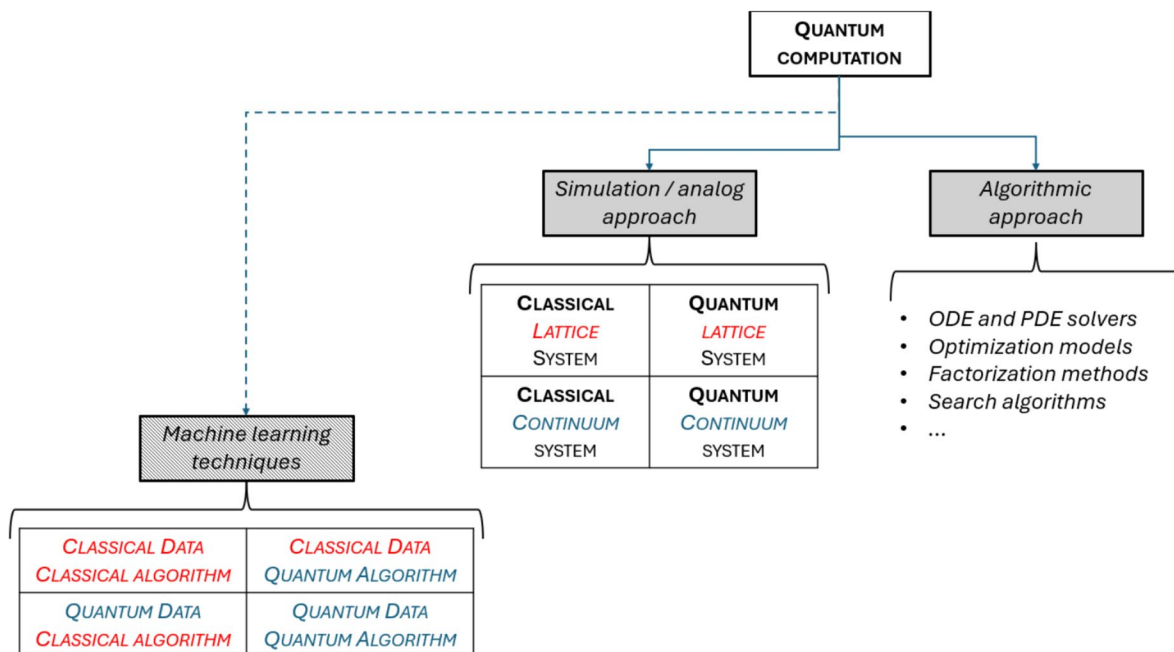
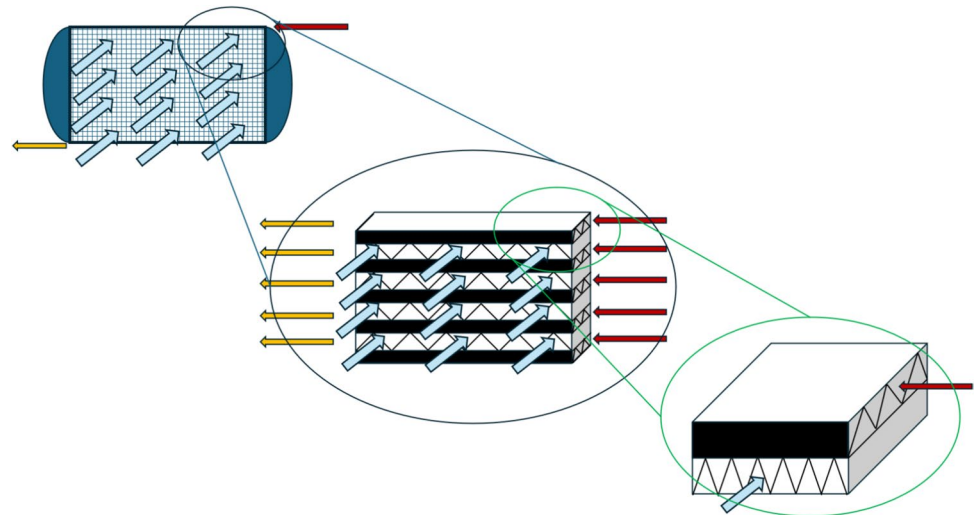


Fig. 1 Classification of problems based on possible QC methods, rearranged from Bharadwaj and Sreenivasan’s taxonomy [21]

Fig. 2 heat exchanger discretization process (cross flow heat exchanger), adapted from [11]



machine-learning techniques, relies on the main conceptual approach used to solve the fluid-dynamics problems, i.e.:

- develop a quantum computing algorithm, i.e. a sequence of unitary operators that will be applied to the quantum mechanical system at its initial state and perform measurement at the end of the evolution.
- The identification of a quantum mechanical system that behaves like the fluid dynamic system, i.e., both systems can be formally described by the same equations.
- Adopt a machine learning framework in which the classical inner solver has been modified to be executed on a quantum computer.

The purpose of this paper is to introduce two alternative implementations to the previous “traditional” ones, in particular the use of quantum annealing and a classification algorithm (quantum walk search algorithm) for the resolution of a lumped-characteristic analytical model of a compact heat exchanger. In fact, within the possible quantum technologies that could be applied to engineering problems, quantum annealers (QAs) are well suited to evaluate the minimum state of a Hamiltonian quadratic potential and thus applicable to engineering problems that can be reformulated in terms of optimization or minimal energy search [27, 28], whereas the quantum walk algorithm can be adapted to find physically informed results, as described in this paper and in other relevant researches [29–33].

3 Background

3.1 Governing Equations – Heat Exchanger Lumped Elements Model

Within the numerical methods for the simulation of heat exchangers it is possible to recall the methods based on the

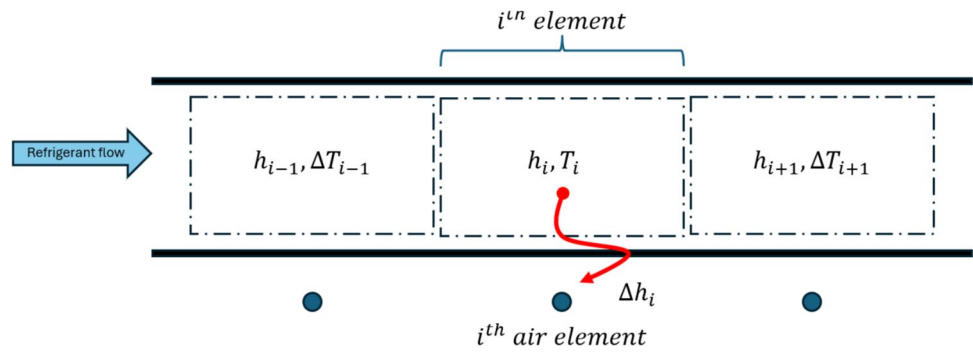
spatial discretization of the channels and the development of a lumped parameter model, also applicable to applications with two-phase fluids, used in several fields, like nuclear reactor analysis [2, 5, 10, 11, 23, 34–37].

Each heat exchanger channel is discretized (see Fig. 2) in a finite element whose properties are described by internal enthalpy and by the rate of exchange with the surrounding environment, and eventually by the pressure drop across the element itself. The model has been developed under the following hypothesis:

- the thickness of the exchanger wall is small as compared to its other two dimensions,
- steady state phenomena,
- working fluids are not mixed,
- known inlet conditions and mass flow rate.
- in the elements,
 - fluid temperatures assumed to vary only along flow lengths,
 - heat transfer coefficients (e.g., surface configurations, heat transfer areas) on both sides constant and uniform throughout the exchanger’s finite element (see 3.2),
- No heat transfer has been considered between the exchanger and the surrounding (i.e., heat transfer occurs only within the working fluids).

The model here considered is a simplified version of that described by Ranganayakulu and Seetharamu [11], Jiang, Aute and Radermacher [37], Macchitella, Colangelo e Starace [36]: the main idea is to characterize each element with averaged enthalpy and a lumped heat transfer mechanism (i.e., a constant heat transfer coefficient across the finite

Fig. 3 Finite element schematics



element), with the two-phase modifications proposed by Lee at al. [10] (as seen in Fig. 3).

The relationship between each finite element is constructed with a set of linear algebraic equations, being, basically, the outlet of an element the inlet of the subsequent element, and the variation of internal enthalpy is related to the heat exchange with the external air flow, i.e., to the thermal gradient, the exposed surface area, and the convection heat transfer coefficient:

$$\Delta h_i = f(\Delta T_i, A_s, h_s) \quad (4)$$

The classical mathematical model consists in the iterative resolution of an algebraic system [10, 11] based on the conservation of energy, the variation of internal enthalpy being balanced by heat exchange with the cold airflow, i.e.:

$$\Delta Q = \sum \dot{m}_i \Delta h_i \quad (5)$$

Or, equivalently,

$$\Delta Q - \sum \dot{m}_i \Delta h_i = 0 \quad (6)$$

with $\Delta Q \doteq \dot{m}(h_n - h_0)$ the variation of enthalpy across the heat exchanger.

3.2 Heat Transfer Parameters Identification

The heat associated with the convective phenomena can be rewritten as:

$$\Delta h_i = f(\Delta T_i, A_s, h_s) = g(A_s, h_s) \cdot \Delta T_i \quad (7)$$

The function $g(A_s, h_s)$ is a function of geometry, the surface finishing, and the fluid-dynamic parameters like turbulence, boundary layer shape, volume fraction, and viscosity. Thus, the governing equations seen in the previous paragraph 3.1 include these functions, usually defined by constant coefficients or expressed through nonlinear relationships.

Consequently, additional correlations related to the actual heat exchangers configuration (like geometry, operating conditions, surface finishing, etc.) are required. The method,

here proposed, relies on the knowledge of these parameters that, basically, can be retrieved with several possible approaches, among which it is possible to list:

1. The use of already known heat exchanger data, e.g., provided by heat exchanger manufacturers or historical applications [1], eventually analyzed with advanced techniques like neural networks [38].
2. The development of a reduced geometrical and mathematical model, to be numerically solved:
 - o The use of traditional CFD tools can be envisioned to retrieve the heat transfer coefficient for the given element shape, with a campaign of virtual experiments for the given element and given combination of temperature and conditions. Because the dimensions of the finite elements are limited, the CFD computational cost is quite limited and well below the effort required to simulate the complete heat exchanger. In fact, traditionally, CFD has been already employed [2] for the several studies in various types of heat exchangers, e.g., fluid flow maldistribution, fouling, pressure drop and thermal analysis, both in the design and the optimization phase. Different turbulence models available in general purpose commercial CFD tools, i.e. standard, realizable and RNG $k - \epsilon$ RSM, and SST $k - \omega$ in conjunction with velocity–pressure coupling schemes such as SIMPLE, SIMPLEC, PISO, etc. can be adopted to carry out the simulations.
 - o The use of quantum algorithms or approaches to solve the numerical simulations based on a CFD mathematical model, e.g., resolution of the algebraic linear system obtained by discretization of Navier–Stokes equations or their simplified version, or the Lattice Boltzmann method, as discussed and summarized in [13–15, 22, 24, 39, 40], the latter being quite promising in the field of heat exchangers operation (i.e., very slow speed), also for two phases operations [13].

4 Proposed Quantum Procedures

4.1 Fixed-Point Arithmetic-Based Conversion of Decimal to Binary Variables

The first step required in the proposed quantum procedures (as well as in every quantum procedure based on binary arithmetic) is the conversion of real numbers into their binary expression, since an adiabatic quantum annealer solves problems posed as unconstrained binary optimization problem, the linear algebraic system in real variables must be converted into an optimization problem with binary variables (i.e., the QUBO problem) [27, 41]. The same step is required for the quantum walk search algorithm where both enthalpy distribution configurations and enthalpy variations are expressed in binary form.

This conversion can be easily done during the preprocessing phase, where the generic quantity u_i can be expressed in binary form with a precision n as:

$$u_i \simeq \sum_{j=0}^n 2^{j_0-j} q_j \Rightarrow \mathbf{u} = \mathbf{A}_b^d \mathbf{q} \quad (8)$$

The precision n required for each procedure is described in the following paragraphs, but it can be easily understood that n shall be large enough to achieve a reasonable conversion of the quantities u_i . For example, if $0 \leq u_i < N$, and it is necessary to have at least D significant decimals,

$$\begin{cases} j_0 = \log_2 N - 1 \\ n = j_0 + D + 2 \end{cases} \quad (9)$$

Please note that the maximum number that could be described is equal to:

$$u_{i,max} = 2^{j_0-1} - 2^{D+1} \quad (10)$$

4.2 Quantum Annealing Approach (Quadratic Unconstrained Binary Optimization)

The quadratic unconstrained binary optimization method (QUBO), also known as *unconstrained binary quadratic program* or *UBQP*, is a combinatorial optimization problem with several applications in various fields, from finance to engineering. Typically, the QUBO problem is set in the form:

$$\min_{x \in S} f_A(x) \text{ where } f_A(x) = x^T A x = \sum_{i=0}^{n-1} \sum_{j=i}^{n-1} A_{ij} x_i x_j \quad (11)$$

Or extended to include additional boundary conditions:

$$f(x) = \sum_i v_i x_i + \sum_{i=0}^{n-1} \sum_{j=i}^{n-1} A_{ij} x_i x_j + \gamma \quad (12)$$

where S represent the binary discrete set $\{0,1\}^n$ and A is a n -by- n square, symmetric matrix of coefficients. The QUBO problem consists of finding a binary vector x_s that is minimal with respect to f_A . Since the QUBO formulation is remarkably close to the Ising spin glass problem, the QUBO problems are reasonable candidates for their implementation and resolution using Quantum Annealing hardware of other Ising machines, such as Fujitsu's Digital Annealer [42].

Thus, the algebraic system describing the thermodynamical problem can be rewritten in a binary form as:

$$\mathbf{A}^d \mathbf{q} = \mathbf{b} \quad (13)$$

where the extended matrix \mathbf{A}^d includes the original matrix \mathbf{A}_b and the conversion factors from real number to binary elements seen in the previous paragraph 4.1.

The least form of the previous linear system assumes the formulation:

$$\tilde{q} = \min_q |\mathbf{A}^d \mathbf{q} - \mathbf{b}|^2 \quad (14)$$

The form of the objective function is thus the QUBO form that the annealer can take as input:

$$f(q) = \sum_i v_i q_i + \sum_{i < j} w_{ij} q_i q_j + \gamma + \sum_{i < j} g_{ij} q_i q_j \quad (15)$$

Being v_i and w_i respectively the weights associated with each logical qubit and the coupling strengths between two logical qubits of the problem that defines its energy landscape:

$$\begin{aligned} v_i &\doteq \sum_j A_{ji}^d (A_{ji}^d - 2b_j) \\ w_{ij} &= 2 \sum_k A_{ki}^d A_{kj}^d \end{aligned} \quad (16)$$

Although the terms $\sum_{i < j} g_{ij} q_i q_j$ is used to introduce additional restrictions on the QUBO formulation, to reinforce the implementation of physical laws, for example the continuity of the thermal gradient. These constraints can be formulated as a penalty term that evaluates to zero when certain constraints are satisfied and returns a positive value otherwise.

Please note that all the states returned by the annealer are collected along with the number of occurrences of each state, i.e. QUBO returns all possible solution states achieved by the hardware, thus a strategy to select a solution must be indicated. However, once a particular solution state is selected, the solution must be transformed from binary to real type, with the already seen transformation $u_i \simeq \sum_{j=0}^n 2^{j_0-j} q_j$.

4.2.1 Proposed Improved QUBO Approach

The above described QUBO approach requires the fixed-point arithmetic conversion, being the unknown quantities q_i the expression of the enthalpy inside the i^{th} element and the temperature gradient across the element. For a single-phase refrigerant, there is no issue expressing enthalpy in terms of temperature or vice versa, but for two-phase fluid, where evaporation or condensation occurs, the relationship between enthalpy and temperature cannot easily be encoded.

The QUBO approach here proposed helps to overcome this issue and, furthermore, it improves the computational efficiency and avoids increasing the number of qubits required for its resolution.

This approach has been inspired by the salesman problem or the minimization of the risk in financial investment (portfolio optimization) [28], exploiting the binary formulation of the input vector q and providing a quick and robust solution, that, coupled with inherent physical meaning, makes this approach a powerful and intuitive tool for design engineers, especially in the preliminary design phase, where the heat exchanger geometry is not fully developed and a “quick and dirt” approach is required to compare several possible solutions.

The idea consists in the discretization of the possible range of enthalpy that the overall heat exchanger could expect, in N_d discrete values. In a rough approach, if no other considerations can be used to simplify the problem, it can be easily identified as the range between the maximum and the minimum values of enthalpy of the two fluids.

The vector of the unknown solution for the i^{th} element is thus given by a sequence of N_d qubits that describe the index of this range of enthalpy for each element, i.e., the nonzero qubit of the vector identifies the enthalpy of that finite element. Overall, this method requires only $N_e \cdot N_d$ qubits.

The energy balance can be accordingly written with this approach, in a very straightforward manner: the energy balance is still given by the sum of the qubits q_{nd} , where the parameter a_{nd} is the heat exchange coefficient associated with the nd^{th} possible enthalpy, while b_{nd} are the terms describing the enthalpy jump over the whole exchanger (in fact, b_{nd} are zero except for the first and the last element).

$$H_e(q_{nd}) = \left(\sum_{n=0}^{N_e-1} \sum_{d=0}^{N_d-1} a_{nd} \cdot q_{nd} - \sum_{n=0}^{N_e-1} \sum_{d=0}^{N_d-1} b_{nd} \cdot q_{nd} \right)^2 = \left(\sum_{n=0}^{N_e-1} \sum_{d=0}^{N_d-1} c_{nd} \cdot q_{nd} \right)^2 \quad (19)$$

In addition, it is possible to easily introduce additional constraints or boundary conditions, e.g. the fact that only one qubit can be nonzero is described by the following constraint.

$$H_\gamma(q_{nd}) = \sum_{n=0}^{N_e-1} \left(1 - \sum_{d=0}^{N_d-1} q_{nd} \right)^2 \quad (18)$$

where q_{nd} is the binary identification of the d^{th} enthalpy in the n^{th} element. The function $H_\gamma(q_{nd})$ implements the rule that only **one** enthalpy configuration is allowed for each element.

In addition,, it is possible to introduce other constraints like the continuity of the enthalpy variation, with the mixed terms:

$$H_\delta(q_{nd}) = \sum_{n_0=0}^{N_e-1} \sum_{d_0=0}^{N_d-1} \sum_{n_1=n_0+1}^{N_e-1} \sum_{d_1=d_0+2}^{N_d-1} q_{n_0 d_0} \cdot q_{n_1 d_1} \quad (19)$$

Or the inlet property element ($q_{n_0,d}$):

$$H_0(q_{nd}) = \sum_{d=0}^{N_d-1} \alpha_0 \cdot q_{n_0,d} \begin{cases} \alpha_0 = 0 & \text{for the required inlet enthalpy index} \\ \alpha_0 = 1 & \text{otherwise} \end{cases} \quad (20)$$

The purpose of the quantum (digital) annealer is to minimize the Hamiltonian function:

$$H_{QUBO} = \lambda_e \cdot H_e + \lambda_\gamma \cdot H_\gamma + \lambda_\delta \cdot H_\delta + \lambda_0 \cdot H_0 \quad (21)$$

This formulation allows easy implementation for quantum annealer, keeping its physical meaning for design engineer and it can be easily retrieved.

The lagrangian multiplier λ_i reinforce the relative weight of the above laws.

4.3 Quantum Gate-Based Approach (Quantum Walk Search Algorithm)

However, it is possible to solve the lumped model with the application of a quantum search algorithm, extending the subset-sum problem [31, 43–45]. As done previously, it is possible to discretize to a range of possible enthalpies with a finite number of qubits, repeated for each finite element. Neglecting pressure drops to simplify the process exposition, every element has thus associated with heat dissipation: the sum of all dissipations shall equal the total change

in internal enthalpy. Within all the possible configurations, the solution consists in the configuration which minimizes the difference between enthalpy changes and heat transfer. The process can be extended including the pressure drops

inside the elements, introducing additional qubits required to solve the problem.

The schematic of the proposed circuit, based on an iterative quantum walk search (QWS) algorithm, is shown in the following figure. The “solution marking” box (identified by the block identified by the label $U_f(\sum \Delta h_i)$) represent the evaluation of the energy balance within the possible configurations and its purpose is to “mark” the optimal configuration which nullify the energy unbalance, evaluated through the ancillary qubits $|\psi_f\rangle$ (Fig. 4).

In the simplified form here described, the “solution marking box” can be coded as a simple adder of finite enthalpy changes, activated (“controlled” in quantum computing terminology) by the element’s configuration. It is worth noting that the number of qubits used to discretize the enthalpy changes shall be sufficient to cover the maximum sum of the enthalpy variations and that there is a sufficiently discrete granularity to guarantee a combination. In addition, the “solution marking box” could be extended to include the pressure drop information as well as other physical laws (e.g., the enthalpic variation must be decreasing).

The other boxes represent the quantum walk search (QWS) algorithm proper functions, i.e., the state initializations H , the controlled Grover diffusion operators $-C_0$ (triggered by the “marked” solution) and C_0 , probability generators, as well as the controlled transition gate T , operating on the solution qubits $|\psi_r\rangle$ and additional ancillary qubits, $|\psi_c\rangle$.

Compared with the traditional quantum walk search approach for the subset problem, or the previously described quantum annealing approach, where the solution space is represented by the index of the optimal configuration, an additional coding technique can be envisioned to reduce the computational effort and the number of qubits involved: the present proposal consists in representing the possible configurations by a reduced number of qubits:

assuming, for sake of simplicity, that the enthalpy range is divided into n discretized values, the classical solution is a vector of n qubits, $|\psi_i\rangle = \{0 \dots 1 \dots 0\}$, where the unity represent the desired solution (for the i th element), as seen in the previous paragraph for the QUBO solution. The proposed algorithm, otherwise, represent the n discretized values in binary values, thus requiring only $\log_2(n)$ qubits. Please consider that the total number of qubits required for the resolution of the problem also in this case is equal to the product of n times the number of elements in which the heat exchangers is discretized.

As said, the number of elements and the number of enthalpy configurations, however, shall thus be carefully identified to achieve a good discretization and, at the same time, minimize the total number of qubits involved in the simulation. With four qubits, for example, it is possible to discretize the enthalpy range in 16 possible values, which leads, in the case studied, a minimum enthalpy variation of, roughly, 10 kJ/(kg•K).

From an engineering point of view, for the example assessed, eight qubits are able to discretize the enthalpy variation inside the elements with a reasonable degree of precision, as well as the total enthalpy variation: considering a frigorific cycle with the exit of compression at 21 bar and 70 °C, the corresponding enthalpy is 436.17 kJ/(kg•K), while, assuming a perfect and ideal heat exchanger in which the exit temperature equals the incoming fresh air temperature (55 °C), the exiting enthalpy is 287.185 kJ/(kg•K), with a maximum total variation of 149 kJ/(kg•K), a value covered by eight qubits, since max. enthalpy variation that can be described in binary form equals 255 kJ/(kg•K).

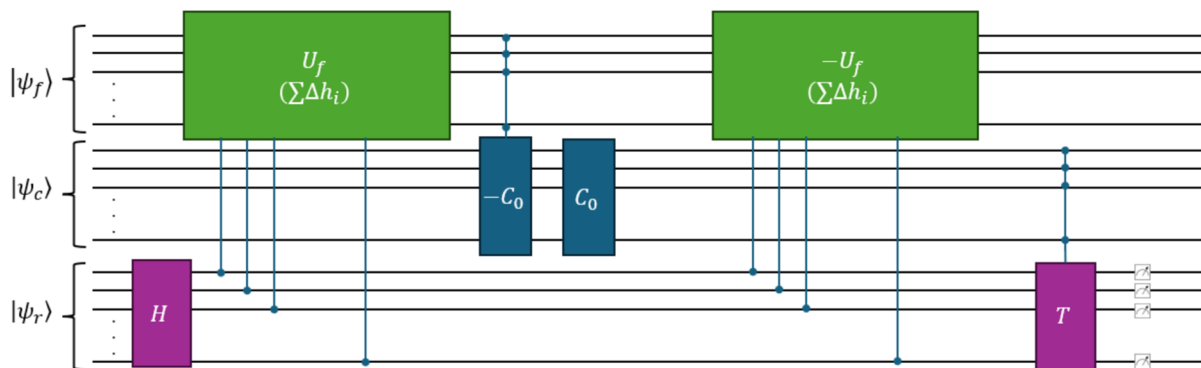


Fig. 4 Proposed quantum walks search algorithm, developed to find energy balanced configuration, and based on subset search problem algorithm

Table 1 Experimental results

| Refrigerant fluid | Inlet temperature | Inlet Pressure | Outlet temperature | Inlet Enthalpy | Outlet Enthalpy | Air side | Air Inlet temperature |
|-------------------|-------------------|----------------|--------------------|-------------------|-------------------|----------|-----------------------|
| - | [°C] | [bar] | [°C] | $kJ/(kg \cdot K)$ | $kJ/(kg \cdot K)$ | - | [°C] |
| R134a | 69.64 | 21.00 | 65.5 | 436.174 | 296.40 | Air | 55 |

Table 2 Numerical Results – Outlet Enthalpy

| Experimental Enthalpy | QUBO Enthalpy (23 elements) | QUBO Enthalpy (46 elements) | QWS Enthalpy |
|-----------------------|-----------------------------|-----------------------------|-------------------|
| $kJ/(kg \cdot K)$ | $kJ/(kg \cdot K)$ | $kJ/(kg \cdot K)$ | $kJ/(kg \cdot K)$ |
| 296.40 | 297.12 | 297.12 | 287.17 |

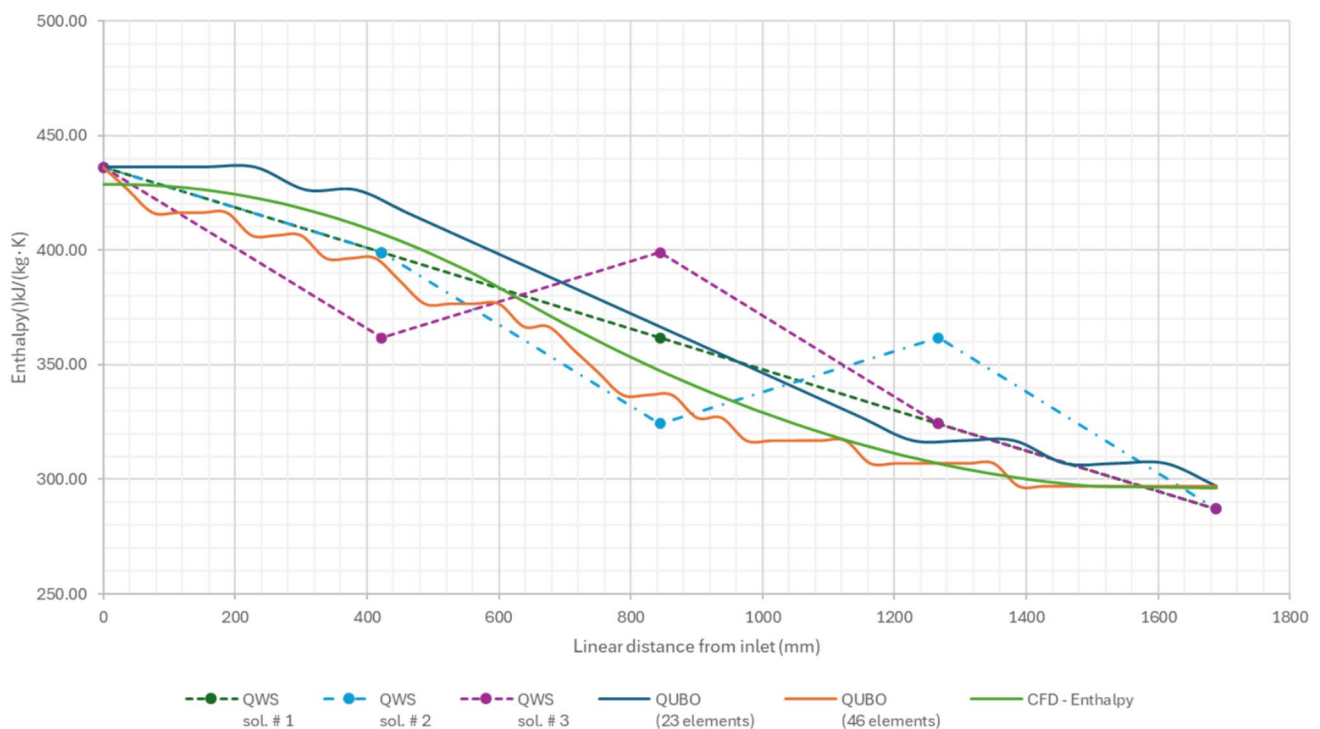
4.4 Results

4.4.1 Problem Overview

The proposed models have been validated considering a single-pass crossflow heat exchanger in the operating conditions described in the following Table 1, which summarizes the inlet conditions as well as the outlet conditions experimentally retrieved. Enthalpy values are displayed in Table 2.

The heat transfer coefficients implemented in the quantum algorithms have been retrieved with a finite volume sub model using ANSYS® CFX solver.

An unsteady (transient) numerical simulation has been executed also to have an additional result to be compared with which obtained with quantum computing approach. A simplified model has been developed with the ANSYS® CFX suite implementing the Lee model for evaporation and condensation, i.e. a model based on the volume fraction approach and the mass transfer between the phases [46–48]. Comparison between results obtained with the proposed quantum approaches and traditional computational fluid dynamics are displayed in the following Figs. 5 and 6, respectively for enthalpy distribution across the heat exchanger and the refrigerant volume fraction.

**Fig. 5** Enthalpy results

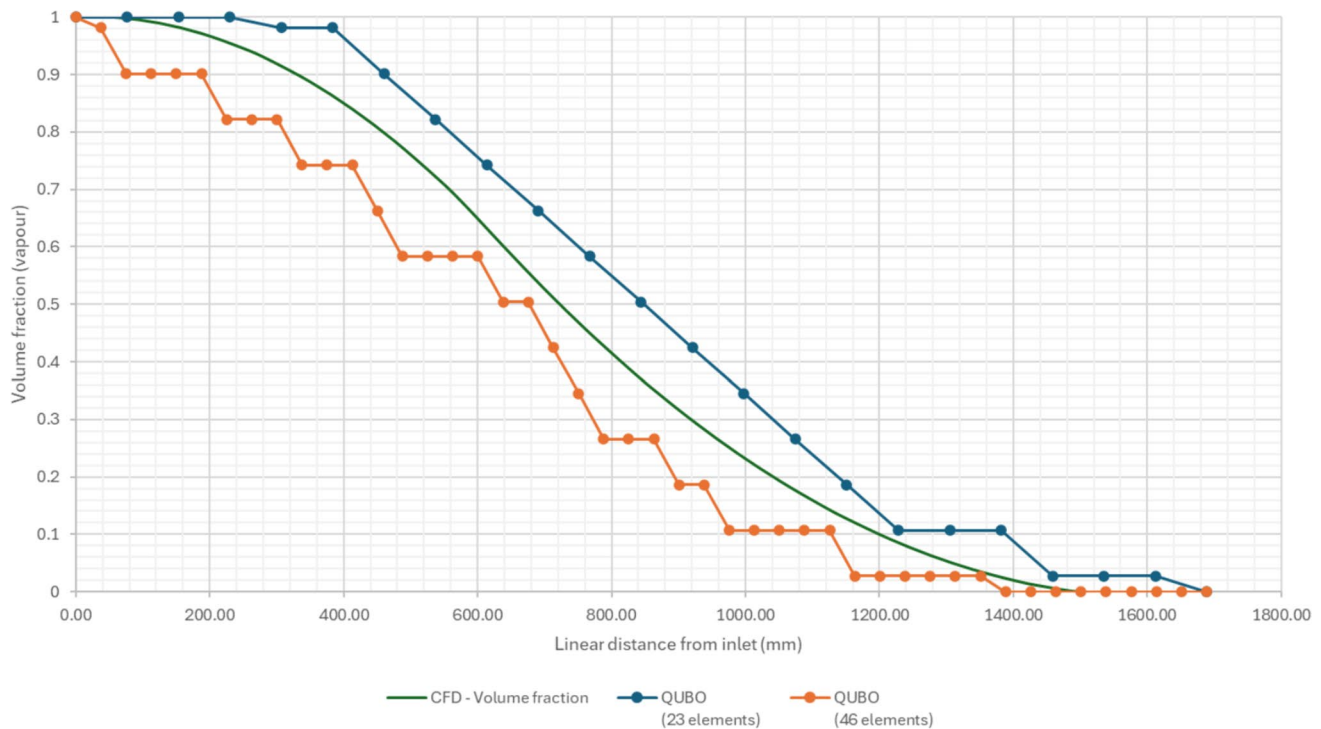


Fig. 6 Volume fraction results

4.4.2 QUBO Results

The model used for validating the QUBO model consists in a discretization of sixteen enthalpy values, while the heat exchanger has been modeled with twenty-three finite elements. This proof of concept has been carried out with a limited range of finite elements to have a direct comparison with the Quantum Walk Search approach; the latter being limited by the number of available qubits.

The proposed code has been run using Fujitsu's proprietary software development kit (SDK) called *dadk* [41], developed for the Fujitsu's *Digital Annealer Unit (DAU)*, a custom application-specific integrated circuit (ASIC) hardware architecture realized using conventional CMOS technology, dedicated to the solution of large and complex combinatorial optimization problems in form of QUBOs [42].

The results obtained are in line with the expected classical values and the required computational time (in the virtual environment) is roughly comparable with the time required by analytical solutions on classical hardware, thus, it is reasonable to estimate a speed-up once the code is executed on a real quantum computer. Indeed, the computational time is order of magnitude lower than the time required by the

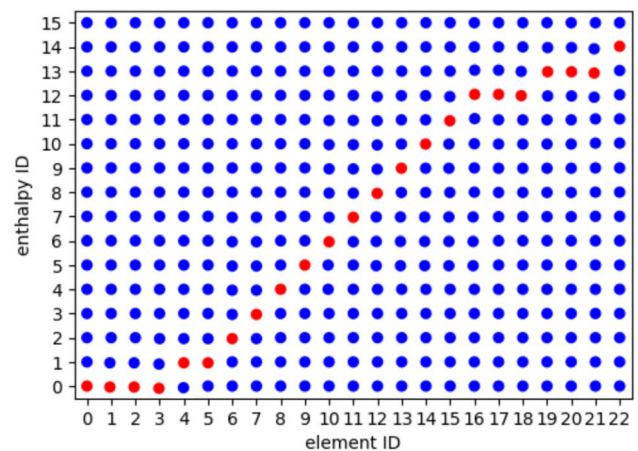


Fig. 7 Result obtained for a reduced-size model using QUBO optimization

thermal transient analysis executed with the ANSYS CFX® program.

A simulation with a more refined model has been carried out considering forty-six elements. The results, displayed in Figs. 7 and 8, confirm the results obtained with the reduced model, within limits due to the intrinsic probabilistic nature of the method.

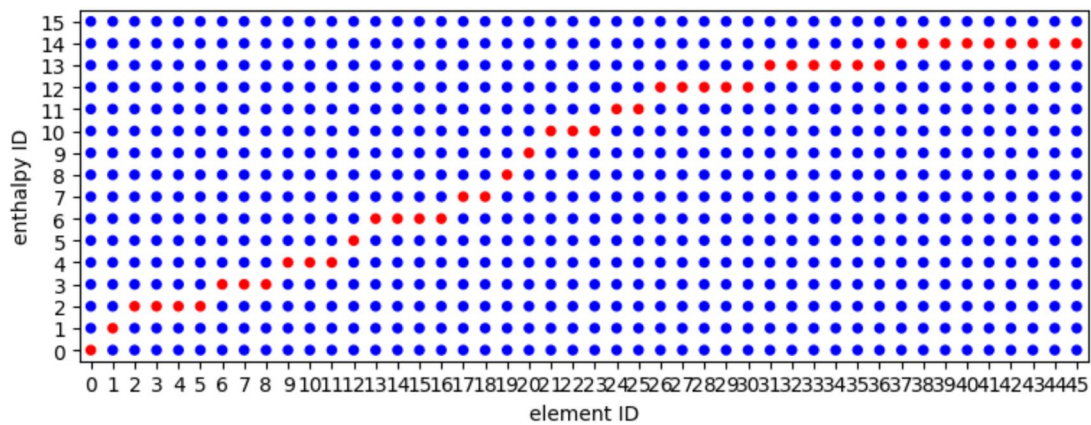


Fig. 8 Result obtained for a more refined model using QUBO optimization

Despite the heavily simplified and discretized enthalpy range, introduced to reduce the size of the model, the algorithm is able to retrieve a physically reasonable result (i.e., continuous variation of enthalpy and a final enthalpy consistent with the experimental results). Indeed, the proposed method and algorithm can be extended to various types of

heat exchangers (parallel flows, counters flows, crossflows, two passes), and the parameters q_{nd} can be used to describe both enthalpies range that temperature ranges, as well as other parameters, offering a very flexible tool for design engineers.

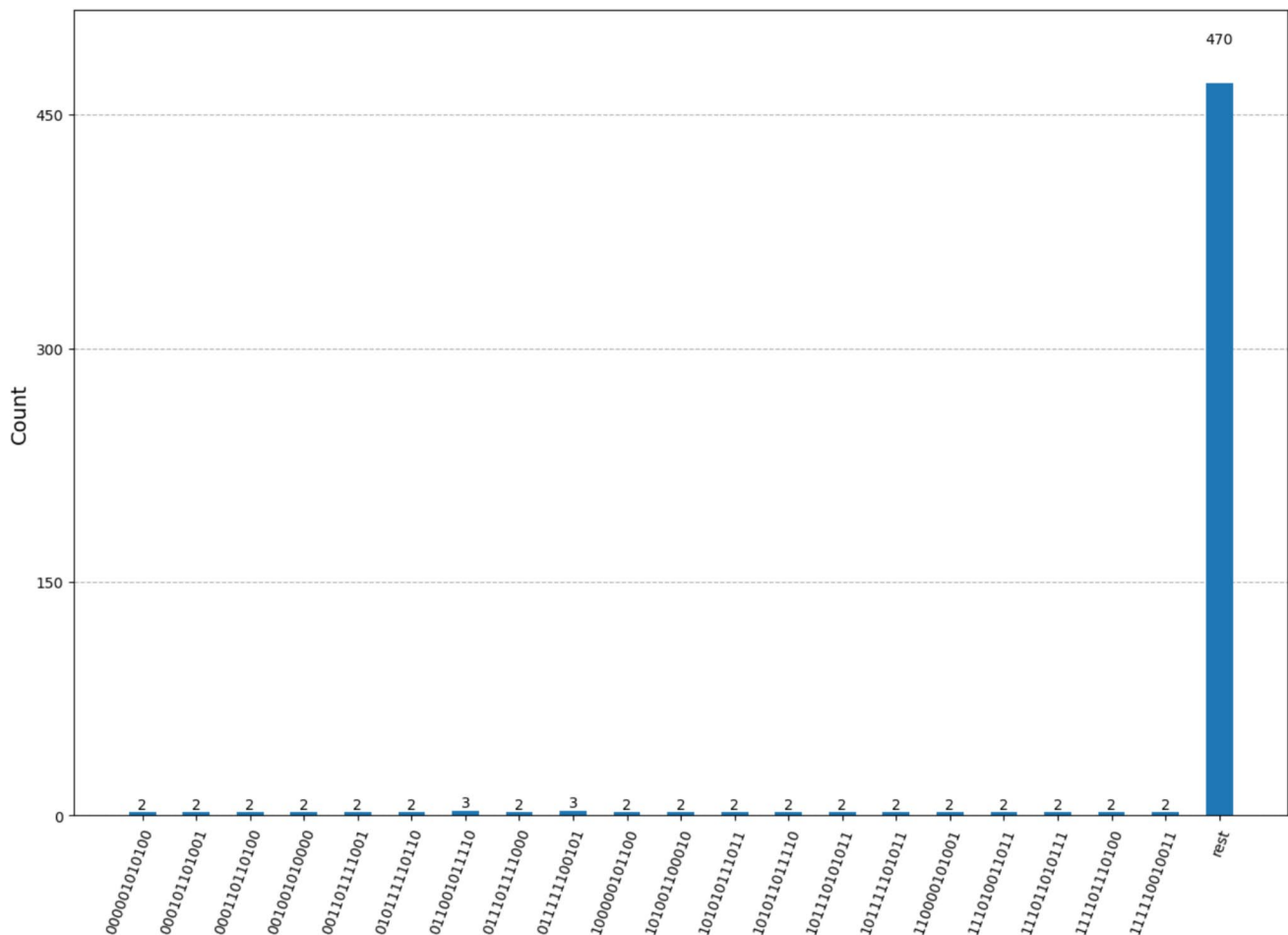


Fig. 9 Frequencies distribution for simplified heat exchanger with four elements – 1 search algorithm iterations (top 20 frequencies)

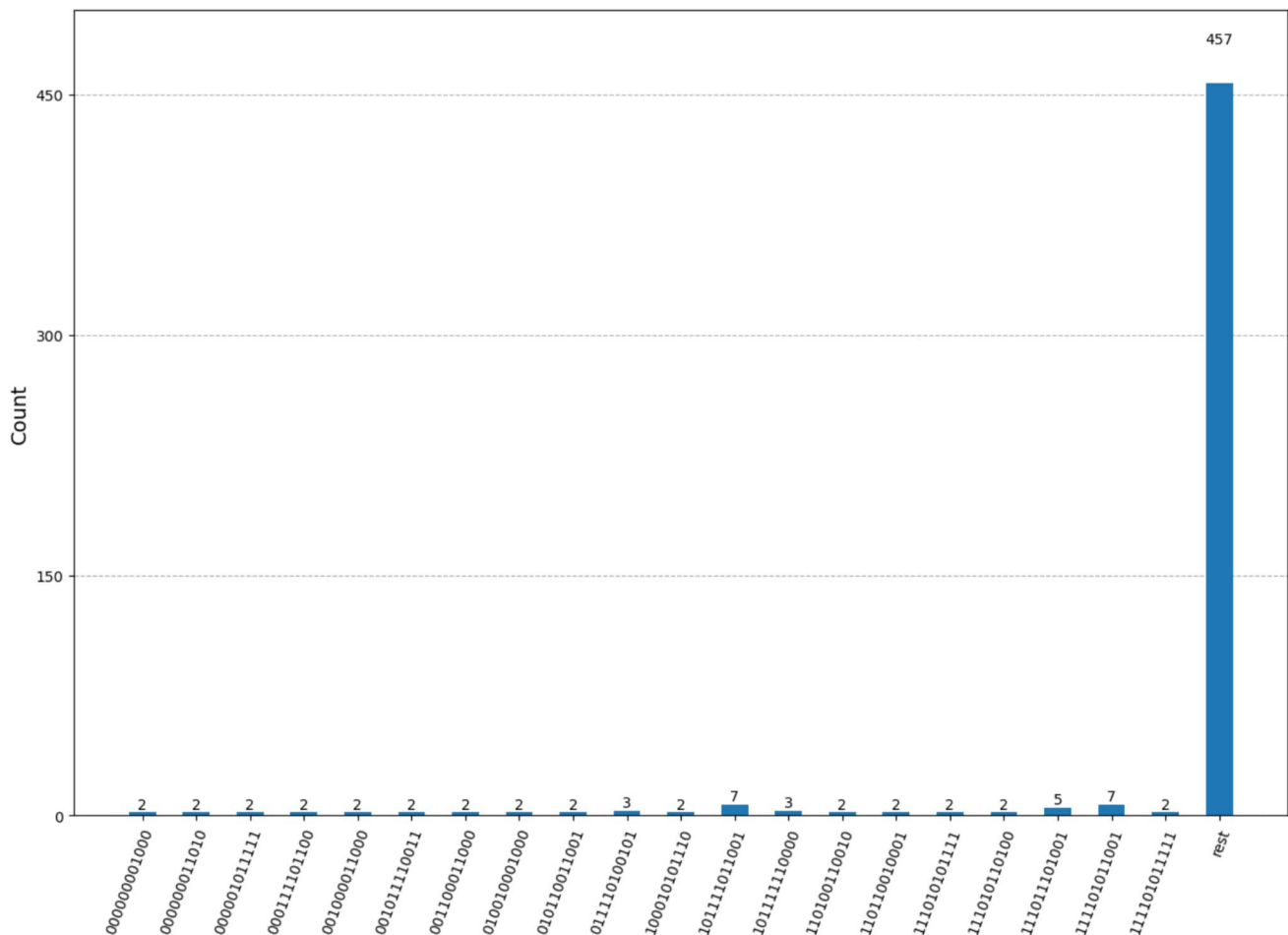


Fig. 10 Frequencies distribution for simplified heat exchanger with four elements – 3 search algorithm iterations (top 20 frequencies)

4.4.3 Quantum Walk Search (QWS) Results

Proof of concept has been carried out with a very rough model to keep the total number of qubits limited, using a division in four macro elements of the heat exchanger, with the enthalpy discretized by three qubits, without any other type of constraints. This heavy simplification is due to the opportunity to run the proposed code on the most available quantum backend provided by the IBM *Qiskit*® Software Development Kit [49], which allows only 32 qubits at maximum. Please also note that, even if a qubit is not formally used, its presence affects (and it is affected by) the other qubits. This detail should be kept clearly in mind when a quantum circuit is designed and a backend shall be chosen, because the presence of unused qubits could hinder the resolution.

Regarding the proposed code for a very reduced configuration, the algorithm is able to identify three possible configurations that satisfy the energy balance (i.e., the only boundary condition wired into the “circuit”). The non-univocity of the solution is strictly related to the rough discretization and the absence of other constraints (e.g., the C_2 continuity of thermal gradient), i.e., the algorithm identifies all the possible paths that are congruent to energy balance.

Figures 9, 10, 11, 12 show the results of the code written in Qiskit, for different “iterations” of the circuit, the results expressed in terms of frequencies of occurrence of the enthalpy configurations, i.e., how many times one of the possible configurations has triggered the search mechanism. It is important to note several things:

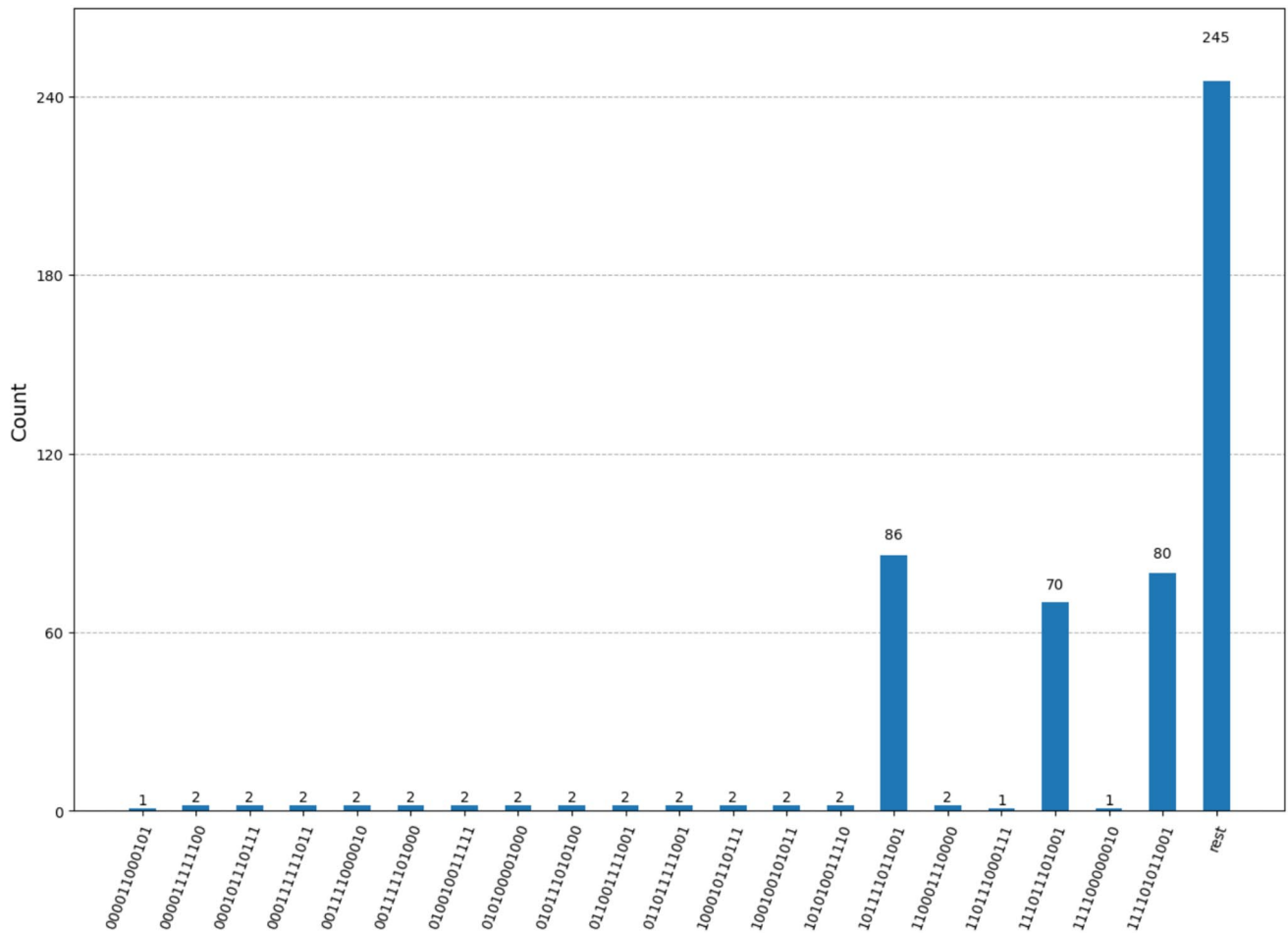


Fig. 11 Frequencies distribution for simplified heat exchanger with four elements – 10 search algorithm iterations (top)

- the first is that, given the random nature of quantum computing, it is necessary to execute the circuit a sufficient number of times to purify the result of spurious solutions (i.e. solutions that, due to errors, interference, or other reasons, have triggered the search mechanism).
- The second aspect, intrinsic instead of the type of algorithm chosen, is that the iteration of the search mechanism must be defined a priori, and the iteration cannot be resumed, since, once the measurement has been performed, the quantum state collapses.
- Last but not the least, this rough model helps to identify, from a theoretical point of view, the main limitation of this approach, which is basically related to the discretization issues, namely the possibility that there exists more than one solution or, equivalently, there is no achievable solution (because, due to truncation error, the energy sum is unbalanced and it does not “flip” the coin, i.e., it does not activate the quantum walk algorithm).
- Figs. 9, 10, 11 shows a truncated view of the results, i.e. the twenty most frequent configurations, whereas the other configurations are collected into a lumped single column. It is worthy to notice that the solutions searched could not be identified with a single iteration.
- Fig. 12 shows a complete view of the results diagram as returned by Qiskit program, in order to display also the necessity to post-process the results with additional tools, or, equivalently, plot only the results with the highest frequencies (e.g., the top 20 qubits).

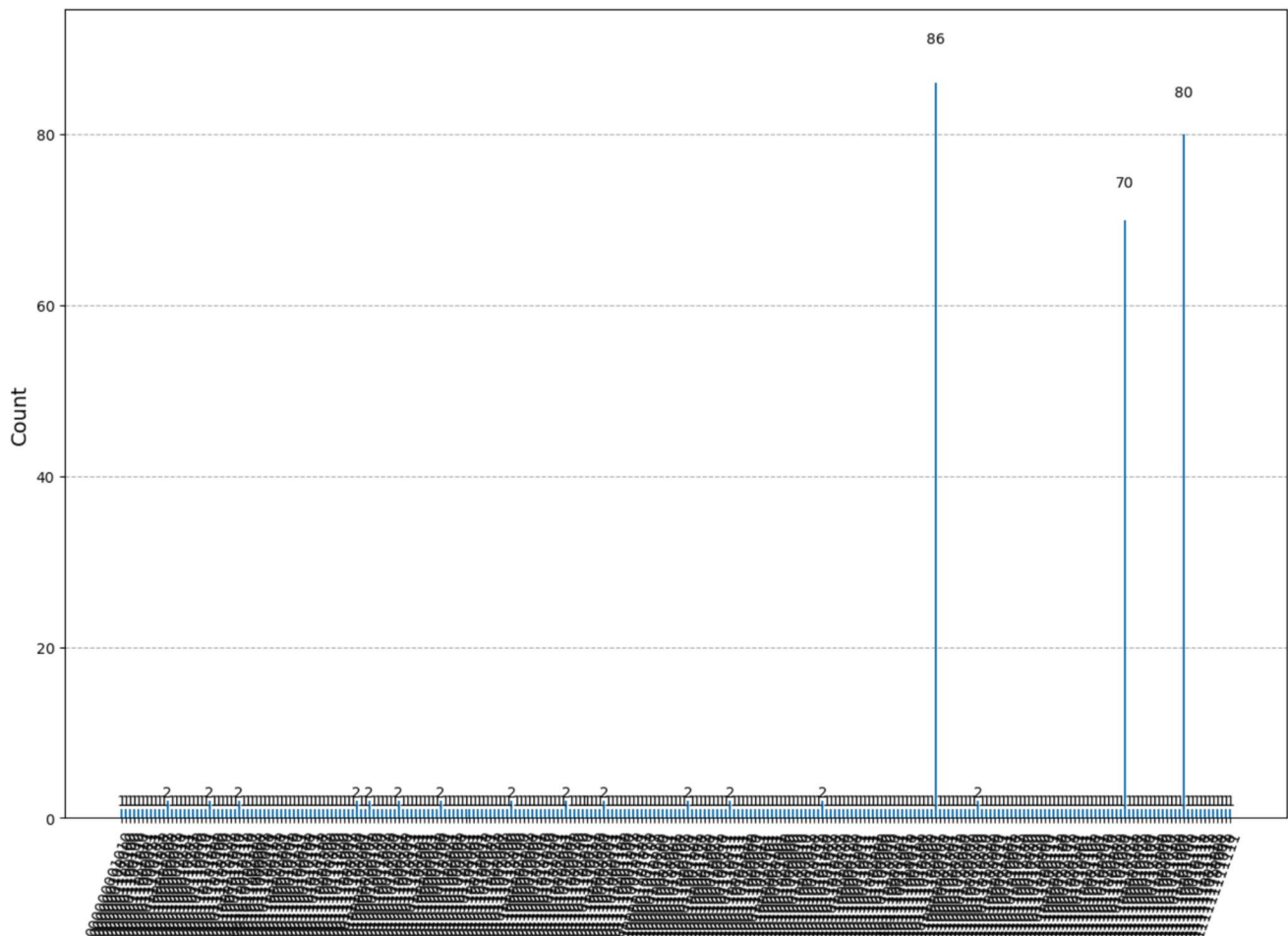


Fig. 12 Frequencies distribution for simplified heat exchanger with four elements – 10 search algorithm iterations (full view)

5 Conclusions

This article, having summarized the traditional approaches that can be envisioned to solve thermofluid mechanics problems of compact heat exchangers with quantum computers, namely the algorithmic or circuital method and the analogue or annealing techniques, has proposed two possible application of quantum computing to the resolution of lumped model for compact heat exchanger, highlighting how this technology has reached a (relatively) low technology readiness level (TRL) [23] but it shows promising applications.

Regarding the technological implementation, the current main limitation is due to the availability of machine with enough qubits to simulate a well-refined lumped model: the total amount of qubits is given by the number of elements,

multiplied by the, the number of qubits for the coins generator (equal to the logarithm of previous number), and, last but not least, the number of qubits used to discretize the enthalpy and the energy variation. A detailed engineering model easily exceeds hundreds of qubits.

When compared with the QUBO methodology, the quantum walks search algorithm seem to be less flexible and, indeed, more prone to truncation errors, even if it results in being more easily implementable, being based on the already established quantum circuits (namely, addition and subtraction, plus the classical coin and transition matrix common to the search algorithm) for the simplified model studied in this paper. However, once it is necessary to introduce more complex physical laws, the supposed simplicity of the method is lacking, whereas the QUBO model allows

the introduction of any physical law expressible in terms of mathematical equations: in fact, the QUBO approach can be easily understood as an implementation of classical optimization algorithms, and the coding activities, even if less straightforward than the search algorithms at first sight, permit the implementation of several physical laws also in an automated way.

Furthermore, the results obtained with the application of these methods show that the quantum approaches are able to achieve (even if under simplifications and hardware limitations) results which are comparable with those obtained with classical numerical or analytical techniques, with the codes running in few minutes also in a virtual environment. However, the number of qubits required to describe a real-life engineering problem hinders the achievement of practical results, at least until affordable quantum computers become available.

Thus, quantum computers technology consists of several very interesting approaches that could be applied in the solution of thermofluid dynamics models of heat exchangers, e.g., it can be considered a key enabling technology, validated in an industrially relevant environment, but under some constraints (e.g., available resources and hardware) and hypothesis (e.g., tailored applications) that show technology limitations, i.e. this technology has a (relatively) low technology readiness level (TRL) and manufacturing readiness level (MRL), respectively 5 and 4 [13–15, 23, 24] but it shows promising applications in thermofluid-dynamics applications [13–15].

6 Conflict of Interests

The authors declare no competing interests.

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Author Contributions G.M. and J.B. conceived of the presented idea. G.M. developed the theoretical formalism and the algorithm, performed the numerical simulations and wrote the main manuscript. J.B. supervised the findings of this work and reviewed the manuscript. All authors discussed the results and contributed to the final manuscript.

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Data availability Data sets generated during the current study and the proof-of-concept codes are available from the corresponding author on reasonable request. The thermodynamics experimental data and heat exchanger geometry, which were used for the current study, are not publicly available.

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