Chapter 9

Modeling and Simulation of Heat Transfer Phenomena

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Additional information is available at the end of the chapter

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1. Introduction to modeling and simulation of heat transfer

> “Heat transfer is a discipline of thermal engineering that concerns the generation, use, conversion, and exchange of thermal energy and/or heat between physical systems. Heat transfer is classified into various mechanisms, such as heat conduction, convection, thermal radiation, and transfer of energy by phase changes. Engineers also consider the transfer of mass of differing chemical species, either cold or hot, to achieve heat transfer. While these mechanisms have distinct characteristics, they often occur simultaneously in the same system” [1].

In recent times, numerical modeling and simulation techniques have been increasingly applied to the problems of heat transfer. Various studies have been carried out utilizing the basic techniques and their modifications and/or customized variants to customize, operate, test, evaluate, optimize and judge the performance of experimental systems and actual engineering problems. Problems particularly related to engineering issues in the fields of energy [2], oil and gas, metallurgy [3], chemical, process and reaction engineering, fuel cell technologies, manufacturing technologies [2], nanotechnology [4, 5], and aerospace have been extensively studied.

This chapter enlists, describes, explains and elaborates with examples these techniques as applied to problems and practical scenarios of heat transfer.

2. Basic techniques of modeling and simulation

Modeling and simulation, like any other field of science and technology has some certain basic techniques using which all practices are carried out. These are the foundation stones on which the building of modeling and simulation practices and procedures is built.

2.1. Introduction

Various techniques have evolved in modeling and simulation since its inception [6] for the solution of technical and engineering problems, ranging from ancient Roman military techniques to classical analog methods to modern Runge – Kutta method and Monte Carlo techniques. [7]. The history of modeling and simulation dates back to ancient times. It was first used by ancient Romans to simulate the actual war conditions in areas of peace to train its soldiers to fight in areas where they have never been. These war games were based upon very well and adequately designed models. Later, techniques of modeling and simulation were used by artists and scientists to test their designs of statuary or edifices during the age of the Renaissance (1200 – 1600 C.E). The renowned Leonardo da Vinci, extensively made use of techniques of modeling and simulation to test and validate his models in art, military, and civil works. [7]. Chess, also known as the world's first war game and its evolution in to a computer game is a result of rigorous use of techniques of modeling and simulation [8]. Similarly, war games (a technique of modeling and simulation) were used in Europe (Prussia, modern-day northeastern Germany) and same was used by Army Corps of Engineers in the United States [9]. In technical fields, the first successful use is reported in the production and use of "Link Flight Simulator", which was patented in 1929 by the American Edward Link. [10]. SAGE – semi, automated ground environment (1949);, MEW – Microwave early warning (1950) [11];, "Whirlwind", MIT, *Cape Cod System (1953)* were also important milestones in modeling and simulation. Ranging from days of the Cold War to the war in Iraq (1991), more advanced techniques were used to develop more realistic and real-world-scenario war games. Following this increasingly well designed simulation centers were opened at various universities and institutions in the United States and the world to better research the areas of modeling and simulation, develop new models, improve existing ones, and develop applications, as a result of which various new techniques/methods of modeling and simulation were formulated [11].

2.2. Energy minimization

Energy minimization (also called energy optimization or geometry optimization) methods are numerical procedures for finding a minimum on the potential energy surface/state starting from a higher energy initial structure/state [1, 14]. These are extensively used in chemistry, mathematics, computer science, image processing, biology, metallurgical engineering, materials science, mechanical engineering, chemical engineering, electrical engineering etc. to find the stable/equilibrium states of molecules, solids, and items. Extensive studies have been carried out in various fields making use of energy minimization techniques to formulate models highlighting the importance, significance, and use of this method in modeling and simulation and solution of engineering problems.

Levitt [12] used energy minimization to formulate solutions of protein folding. The potential energy functions used are detailed and include terms that allow bond stretching, bond angle bending, bond twisting, van der Waals' forces, and hydrogen bonds. A unique feature of the methods used includes easy approach for restrained energy minimization work (including all terms) to anneal the conformations and reduce their energies further. The methods used were very versatile and were proposed to be applicable for building models of protein conformations that have low energy values and obey a wide variety of restraints. Recently, Micheletti and Maritan, [13] also used energy minimization methods to formulate solutions of protein design. They went a step further in their approach, and defined actual real-world scenarios and formulated alternative design strategies based upon correct treatment of free energy. Sutton [14] presented the use of energy minimization methods to determine the solution of atomic structures and solute concentration profiles at defects in elemental solids and substitutional alloys as a function of temperature. He used mean field approximation, rewrote free energy, used Einstein models and auto-correlation approximation and showed that the better statistical averaging of the auto-correlation approximation leads to better temperature – and concentration – dependent pair interactions. His formula was fairly simple and effective. Lwin [15] used spreadsheets to solve chemical equilibrium problems by Gibbs energy minimization.

Similarly, Olga Veksler during her PhD thesis at Cornell University [16] presented the use of energy minimization techniques in computer vision problems. She developed algorithms for several important classes of energy functions incorporating everywhere smooth, piecewise constant and piecewise smooth priors. These algorithms primarily rely on graph cuts as an optimization technique. For a certain everywhere smooth prior, an algorithm based on finding the exact minimum by computing a single graph cut was developed. For piecewise smooth priors, two approximate iterative algorithms, computing several graph cuts at each iteration, were developed and for certain piecewise constant prior, same algorithms were used along with a new one which finds a local minimum in yet another move space. The approach was quite effective on image restoration, stereo, and motion. [16]. Similar studies were carried out later as well to further test and evaluate energy minimization in computer vision [17, 19]. Nikolova [20] explained the use of energy minimization methods in the field of image analysis and processing. Onofrio and Tubaro applied the same to the problem of three-dimensional (3D) face recognition [21]. Standard [22] explained the use of energy minimization to determine the states for a molecule in chemistry; he explained that the geometry of molecule is changed in a stepwise fashion so that the energy is reduced to lowest minimum.

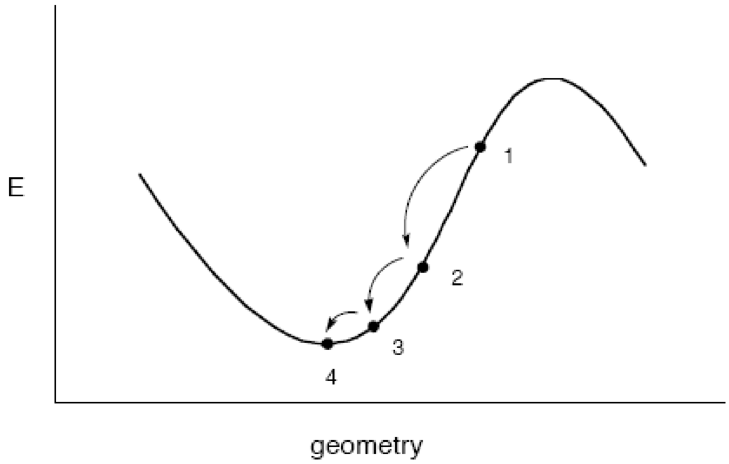

Figure 1. Graphical representation of energy minimization process [22]

Figure 1 shows energy minimization process for a molecule in steps. "*Most energy minimization methods proceed by determining the energy and the slope of the function at point 1. If the slope is positive, it is an indication that the coordinate is too large (as for point 1). If the slope is negative, then the coordinate is too small. The numerical minimization technique then adjusts the coordinate; if the slope is positive, the value of the coordinate is reduced as shown by point 2. The energy and the slope are again calculated for point 2. If the slope is zero, a minimum has been reached. If the slope is still positive, then the coordinate is reduced further, as shown for point 3, until a minimum is obtained*". [22]

There are other methods for actually varying the geometry to find the minimum [22]. Many of these, which are used to find a minimum on the potential energy surface of a molecule, use an iterative formula to work in a step wise fashion. These are all based on formulas of the following type:

$$x_{new} = x_{old} + correction \tag{1}$$

where, x_{new} is value of the geometry at the next step, x_{old} is geometry at the current step, and *correction* is some adjustment made to the geometry.

2.2.1. Newton Raphson method

"*The Newton-Raphson method is the most computationally expensive per step of all the methods utilized to perform energy minimization. It is based on Taylor series expansion of the potential energy surface at the current geometry*" [22]. The equation for updating the geometry is a modification of eq. [1]:

$$x_{new} = x_{old} - \frac{E'\left(x_{old}\right)}{E''\left(x_{old}\right)}. \tag{2}$$

The correction term depends on both the first derivative (also called the slope or gradient) of the potential energy surface at the current geometry and also on the second derivative (also called the curvature). The Newton Raphson method involves fewest steps to reach the minimum.

2.2.2. Steepest descent method

This is a method which relies on an approximation. In this method, the second derivative is assumed to be a constant.

$$x_{new} = x_{old} - \gamma E'\left(x_{old}\right) \tag{3}$$

where γ is a constant. In this method, the gradient at each point is again calculated. Because of the approximation, it is not efficient, so more steps are required to find the minimum. [22]

2.2.3. Conjugate gradient method

"In this method, the gradients of the current geometry are first computed. Then, the direction of the largest gradient is determined. The geometry is minimized along this one direction (this is called a line search). Then, a direction orthogonal to the first one is selected (a 'conjugate' direction). The geometry is minimized along this direction. This continues until the geometry is optimized in all the directions". [22]

2.2.4. Simplex method

In the Simplex Method, the energies at the initial geometry and two neighboring geometries on the potential energy surface are calculated (points A, B, and C in Fig. 2).

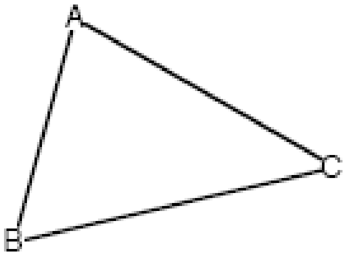

Figure 2. Schematic of Simplex Method implementation (three points)

"The point with the highest energy of the three is noted. Then, this point is reflected through the line segment connected to the other two (to move away from the region of high energy). For example, if the energy of point A is the highest out of the three points A, B, and C, then A is reflected through line segment BC to produce point D." (Fig. 3)

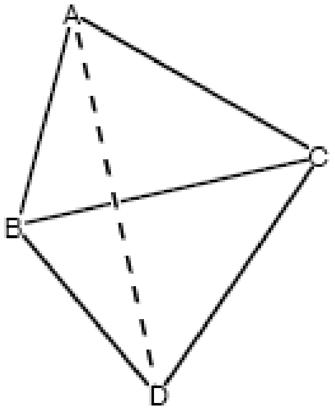

Figure 3. Simplex Method (four points)

"In the next step, the two original lowest energy points (B and C) along with the new point D are analyzed. The highest energy point of these is selected, and that point is reflected through the line segment connecting the other two. The process continues until a minimum is located" [22]. As a result, it is the least expensive in CPU time per step. However, it often requires the most steps.

2.3. Molecular Dynamics (MD) simulations

Molecular dynamics (MD) is a technique in which physical movements of atoms and molecules is simulated using computers. In this the atoms and molecules are allowed to interact for a period of time, giving a view of the motion of the atoms. MD simulation circumvents the problem of finding the properties of complex molecular systems by using numerical methods. In the most common version, the trajectories of molecules and atoms are determined by numerically solving Newton's equations of motion for a system of interacting particles [1, 23]. This is one of the two main families of simulation techniques [23]. The results of molecular dynamics simulation can be used in various fields such as thermodynamics, biology, chemistry, materials science and engineering, statistical mechanics and nanotechnology [1, 24, 25].

van Gunsteren, [26] explained in detail about methodology, applications and prospective of molecular dynamics in chemistry. He effectively explained molecular dynamics in terms of choosing unavoidable assumptions, approximations and simplifications of the molecular model and computational procedure such that their contributions to the overall inaccuracy are of comparable size, without affecting – significantly the property of interest. *"He further postulated and argued that the aim of computer simulation of molecular systems is to compute macroscopic behavior from microscopic interactions giving the reason that the main contributions a microscopic consideration can offer are (1) the understanding and (2) interpretation of experimental results, (3) semi – quantitative estimates of experimental results, and (4) the capability to interpolate or extrapolate experimental data into regions that are only difficultly accessible in the laboratory"* [26]. His methodology was good, accurate and in detail for explaining molecular dynamics. A similar study is also conducted by McKenzie [27]. Karplus and McCammon [28] extensively reviewed the use of molecular dynamics as applied to biomolecules. Their study encompasses all aspects of application of computational techniques for solving structure, folding, internal motion, conformational changes, etc., of biomolecules and problems. A similar study was carried by Kovalskyy et al. [29] in which they used molecular dynamics for the study of structural stability of HIV – 1 Protease under physiological conditions.

Kupka [30] applied molecular dynamics in computer-based graphic accelerators. He proposed an algorithm consisting of CPU and GPU parts, The CPU part is responsible for streams preparations and running kernel functions from the GPU part, while the GPU part consists of two kernels and one reduce function.

A very nice study about molecular dynamics simulation for heat transfer problems is given by Maruyama [31]. He also applied MD simulations to the problem of heat conduction of finite length single walled-carbon nanotubes [32]. The measured thermal conductivity did not converge to a finite value with increase in tube length up to 404 nm, but an interesting power law relation was observed.

Wang and Xu applied MD techniques to problems of heat transfer and phase change during laser matter interaction [33]. They irradiated argon crystal by a picoseconds pulsed laser and investigated the phenomena using molecular dynamics simulations. Result reveals transition region, superheating, and rapid movement of solid-liquid interface and vapors during phase change. Lin and Hu [34] applied the same techniques to the problems of ablation and bio heat transfer in bimolecular systems and biotissues and developed a new model.

Krivtsov, [35] discussed the problems of heat conductivity in monocrystalline materials with defects via molecular dynamics simulation. *"It was shown that in ideal monocrystals the heat conductivity is not described by the classical conductivity theory. For the crystals with defects for the big enough specimens the conductivity obeys the classical relations and the coefficient (β) describing the heat conductivity is calculated. The dependence of the heat conductivity on the defect density, number of particles in the specimen, and dimension of the space is investigated"* [35]. The obtained dependencies increase with time: almost linear in two dimensional (2D) cases and nonlinear in one-dimensional (1D) and (3D) (with positive time derivative in 1D case, and with negative time derivative in 3D case).

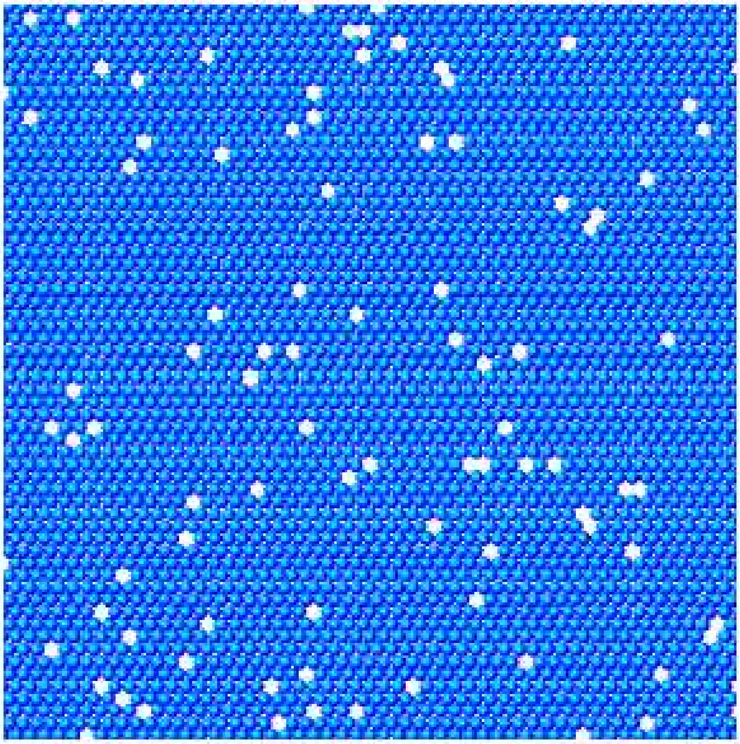

Figure 4. An element of 2D monocrystal with predefined distribution of defects.[35]

He also applied the same technique for determining and simulating the mechanical properties of polycrystals as well earlier. [36]. Recently, Steinhauser applied molecular dynamics simulation technique to various condensed matter forms [37]. He showed how semi flexibility or stiffness of polymers can be included in the potentials describing the interactions of particles in proteins and biomolecules. For ceramics he modeled the brittle failure behavior of a typical ceramic and simulated explicitly the set-up of corresponding high-speed impact experiments. It was shown that this multiscale particle model reproduces the macroscopic physics of shock wave propagation in brittle materials very well while at the same time allowing for a resolution of the material on the microscale.

2.4. Monte Carlo (MC) simulations

Monte Carlo (MC) methods/simulations are a set of simulation techniques that rely on repeated random sampling to compute their results. They are often used in computer simulations of physical and mathematical systems. These are also used to complement theoretical derivations. Monte Carlo methods are especially useful for simulating systems with many coupled degrees of freedom, such as fluids, disordered materials, strongly coupled solids, and cellular structures. They are widely used in business (calculation of risk), mathematics, (evaluate multidimensional definite integrals), Space exploration, and oil exploration (predictions of failures, cost overruns and schedule overruns) [1, 38].

Howell [39] explained in detail the use of Monte Carlo method in radiative heat transfer problems. He used the method for computations of complex geometries, configurations, and exchange factors, inverse design, packed beds, and fiber layers, etc., and also explained the use of related algorithms (READ, REM, Markov Chains, etc.). A similar study was also conducted by Zeeb [40] and Kersch (1993) [41]. Modest [42] used various implementations of the backward Monte Carlo method for problems with arbitrary radiation sources. His focus area was backward Monte Carlo simulation. He included small collimated beams, point sources, etc., in media of arbitrary optical thickness and solved radiative heat transfer equation with specified internal source and boundary intensity.

Frijns et al. [43] used Monte Carlo simulation to discuss and solve problems of heat transfer in micro and nanochannels. They proposed and utilized a combination algorithm of Monte Carlo and molecular dynamics simulation to argue about its effectiveness.

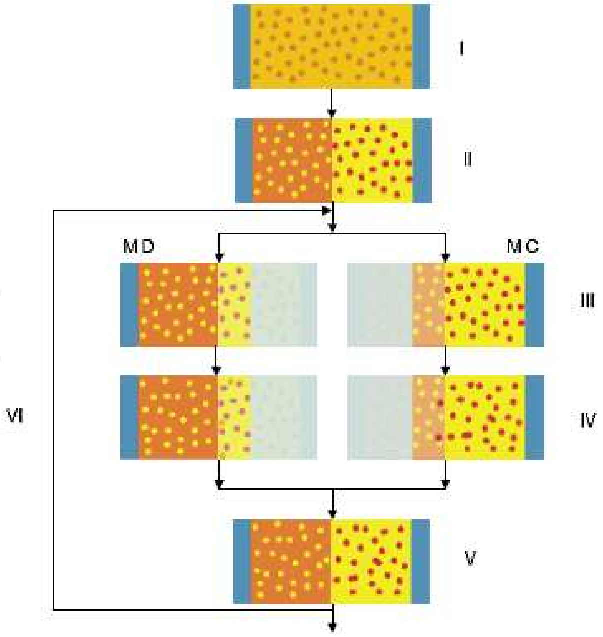

Figure 5. Schematic view of the coupling algorithm. Left: MD steps; right: MC steps. The particles that have been assigned to molecular dynamics have a light color, whereas the MC particles are dark [43]

Steps of performing simulation are: I) define an initial condition. II) Assign particles to MD or MC part. III) Distribute over MD and MC codes. IV) Compute new positions and velocities. V) Update the particles in the buffer layer. VI) Start over with step III.

An extensive use of Monte Carlo in gas flow problems is explained by Wang and co-workers [44, 45, 46]. They used direct simulation MC for simulation of gas flows in MEMS devices. They examined orifice and corner flow using modified DSMC codes and showed that the channel geometry significantly affects the micro gas flow [44]. For orifice flow, the flow separation occurred at very small Reynolds numbers while in corner flow, no flow separation occurred even with a high driving pressure. The results were found to have good agreement with continuum theory and existing experimental data. In a later study, they used the same methods to discuss and solve the problem of gas mixing in micro channels [45]. Very high Knudsen numbers were used. The simulation results show that the wall characteristics have little effect on the mixing length. The mixing length is nearly inversely proportional to the gas temperature. The dimensionless mixing coefficient is proportional to the Mach number and inversely proportional to the Knudsen number. They also extended the use of their codes to heat transfer and gas flow problems in vacuum-packaged MEMS devices [46] and found to have good results in explaining the heat transfer and gas flow behavior on chip surfaces.

2.5. Langevin dynamics

Langevin dynamics is an approach to the mathematical modeling of the dynamics of molecular systems. The approach is characterized by the use of simplified models while accounting for omitted degrees of freedom by the use of stochastic differential equations. [1]. In philosophy, the Langevin equation is a stochastic differential equation in which two force terms have been added to Newton's second law to approximate the effects of neglected degrees of freedom. One term represents a frictional force, the other a *random* force [47]. They are used in biology, chemistry, engineering, etc, to formulate solutions of complex problems. Antonie [48] used LD methods to investigate influence of confinement on protein folding. He used MATLAB to formulate code of equation developed using LD methods. The model developed and then its programming was found effective. A similar type of study was also conducted by Lange et al [49].

Quigley [50] discussed the advantages of using LD in constant pressure extended systems and showed it to be effective technique for simulating the equilibrium isobaric–isothermal ensemble. They analyzed canonical ensemble, Hoover ensemble, and Parrinello–Rahman ensemble and showed that despite the presence of intrinsic probability gradients in this system, a Langevin dynamics approach samples the extended phase space in the correct fashion. Wu, Li and Nies [51] applied Langevin dynamics method to the problem of cross-linking into polymer networks. Commercially available software package GROMACS 4.0 was used for simulation. Their study revealed that cross-linking is associated with effects such as changes in thermodynamic stability of reacting mixture or the presence of nanoparticles. This also facilitated the study of macromolecules.

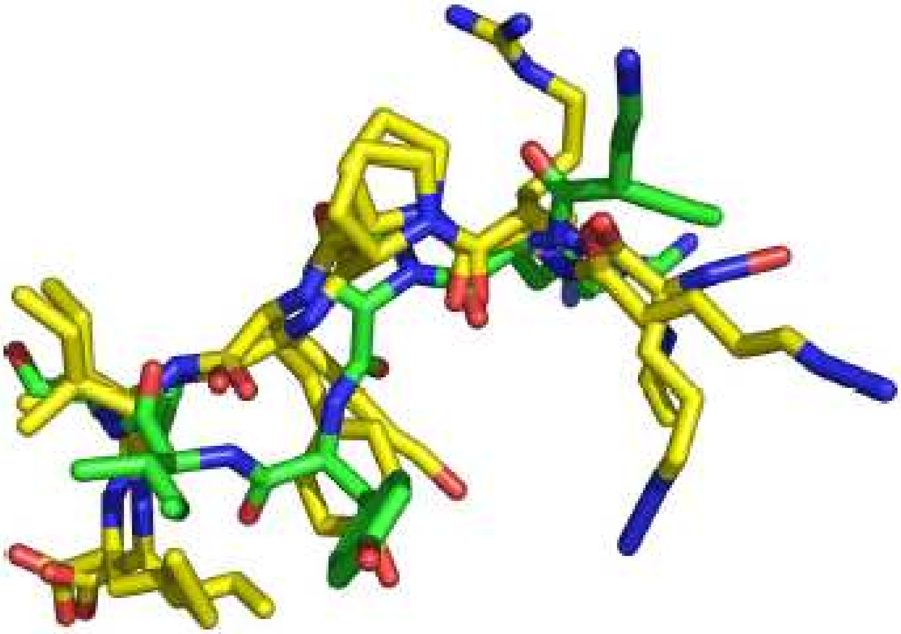

Figure 6. "*Overlay of average neurotensin structures. The relative orientation of the structures minimizes the RMSD between the C _ atoms. The green structure is obtained from state A, and the two yellow structures are obtained from state B. The parts of the side chains that were overly distorted due to the averaging were removed. The N terminus is oriented towards the upper right corner*". [49]

2.6. Normal mode (harmonic) analysis

Normal mode (harmonic) analysis is a method of simulation in which the characteristic vibrations of an energy-minimized system and the corresponding frequencies are determined assuming its energy function is harmonic in all degrees of freedom. Normal mode analysis is less expensive than MD simulation, but requires much more memory [52]. These are extensively used in science and engineering to model, simulate and solve engineering problems. Magyari [53] used this method to examine the convection model of the fully developed flow in a differentially heated vertical slot with open to capped ends. He found that the method is quite transparent and has algebraic and computational efficiency. It is shown that dimensionless temperature field and the velocity field scaled by the Grashof number are characterized by only two physical parameters; also, capped slot is an ideal heat transfer device. Schuyler et al., [54] used the same method to C_α – based elastic network model (C_α – NMA) of protein analysis and "*present a new coarse grained rigid body based analysis (cluster NMA). This new cluster NMA represents a protein as a collection of rigid bodies interconnected with harmonic potentials. This produces reduced degree of freedom (DOF) equations of motion (EOMs), which even in the case of large structures enable the computation of normal modes to be done on a desktop PC*" [54]. This new cluster NMA proved to be very effective for protein analysis. Similar type of studies have been done by Hinson [55] in France and showed that normal mode analysis is advantageous as no sampling is required, enables fast calculations and is simple to use. However, it suffers from the drawback of exhibiting inaccuracies in certain cases and is limited to single-well potentials and thus offers no possibility to study conformational transitions explicitly.

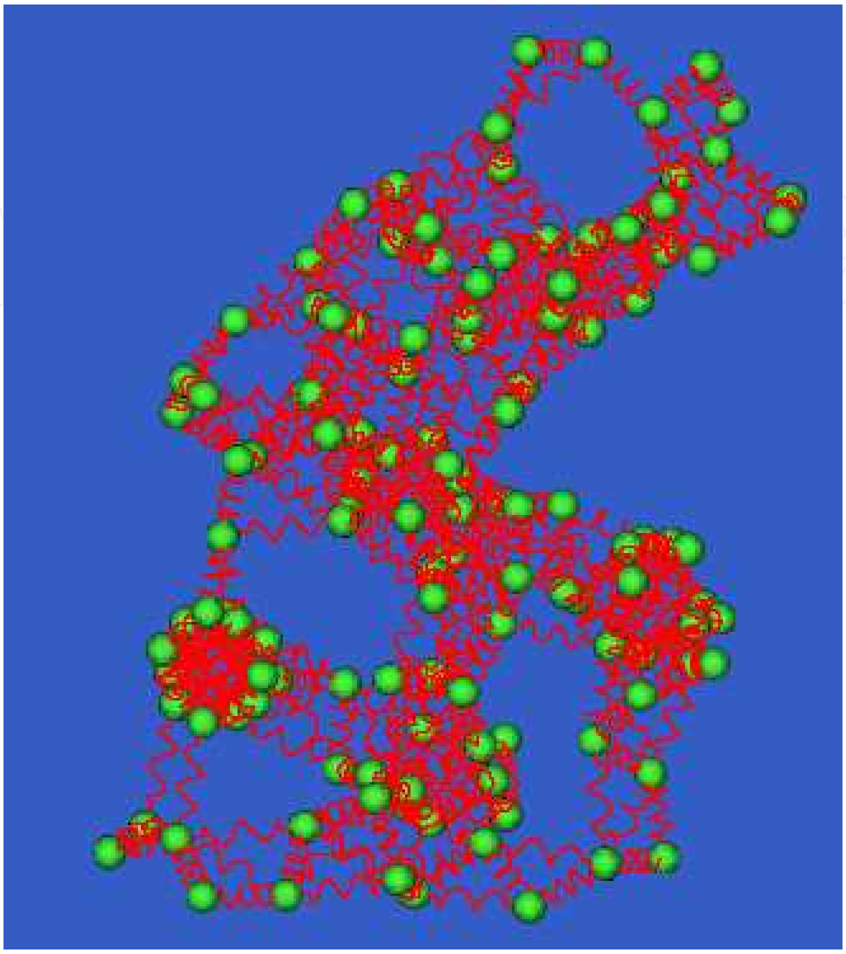

Figure 7. Elastic network model [55]

2.7. Stimulated annealing

"Simulated annealing (SA) is a random-search technique which exploits an analogy between the way in which a metal cools and freezes into a minimum energy crystalline structure (the annealing process) and the search for a minimum in a more general system; it forms the basis of an optimization technique for combinatorial and other problems" [56]. It has attracted significant attention as suitable for optimization problems of large scale, especially ones where a desired global extremum is hidden among many, poorer, local extrema. The method has proved effective in solving problems such as traveling salesman problem in N cities, designing complex integrated circuits, etc. In the latter case it has proved effective in arranging several hundred thousand circuit elements on a tiny silicon substrate in an optimized way so as to avoid/minimize interference among their connecting wires. *"SA's major advantage over other methods is an ability to avoid becoming trapped in local minima. The algorithm employs a random search which not only accepts changes that decrease the objective function (assuming a minimization problem), but also some changes that increase it"* [57].

3. Modeling and simulation of heat transfer — Applications

Modeling and simulation of heat transfer phenomena is the subject matter of various recent studies in many technical and/or engineering applications. It has helped a great deal in operation, achieving enhanced results, increasing efficiency, and optimizing processes. It is one of the basic engineering techniques used in analysis of engineering problems/processes during initial steps/stages of design. This section highlights this significance of heat transfer in various engineering applications via modeling and simulation approach.

3.1. Introduction

Heat transfer analysis has made its distinct position among engineering analyses carried out for any technical/engineering problem/application at first hand. Providing initial data, it paves the way for in-depth analysis and incursion into the problem solving technical intimacies. Its use has gained more importance and popularity especially after the introduction of computer/simulation techniques [2, 3]. Ironically, its use started in complex engineering problems such as determining the heat transfer profile of single crystal turbine blades, determining heat transfer coefficients for material(s) in tube and shells heat exchangers for measuring and enhancing process efficiency [3] and then extended to simpler situation and scenarios.

3.2. Modelling & simulation of heat transfer in process industry

Process industry is one of the major industries that utilise heat transfer and thermodynamic studies to operate and optimize its processes. Equipment such as Heat Exchangers, Boilers, Evaporators, Dryers, Condensers, Ovens, Reboilers, etc., rely and heavily make use of heat transfer studies for their optimum and efficient operation. Several tools such as FLUENT, Modelica, FEMLAB, APROS (Powerful dynamic simulation), BALAS (Conceptual process design), ChemSheet (Process Chemistry), KilnSimu (Rotary Kiln Simulator), etc., are being frequently used to model and simulate the process engineering parameters of different units/unit operations [58].

3.2.1. Boilers

Heat transfer of boilers is extensively studied as it helps immensely in finding the parameters and determining the process efficiency of equipment as well as suggesting its design improvement. Bordbar and Hyppänen [59] explained the use of modeling for problem of radiation heat transfer in a boiler furnace. Temperature and heat flux within the furnace and on the heat surfaces was investigated. They used CFD method for solving velocity field of combusted fuel from the burner using some empirical equations and found that use of CFD on the model developed conforms to measured data and greatly helps in achieving the results.

Earlier, Zeeb [60] used the Monte Carlo method to study the same problem in axisymmetric furnace and got good results. Gómez, Fueyo and Díez, used the same CFD method to solve a model for the calculation of “*shell-side flow and the shell-side, tube-side and tube-wall, thermal fields, and of the shell-tube heat-exchange in convective zone of power station 350 MW boiler. The model allows*

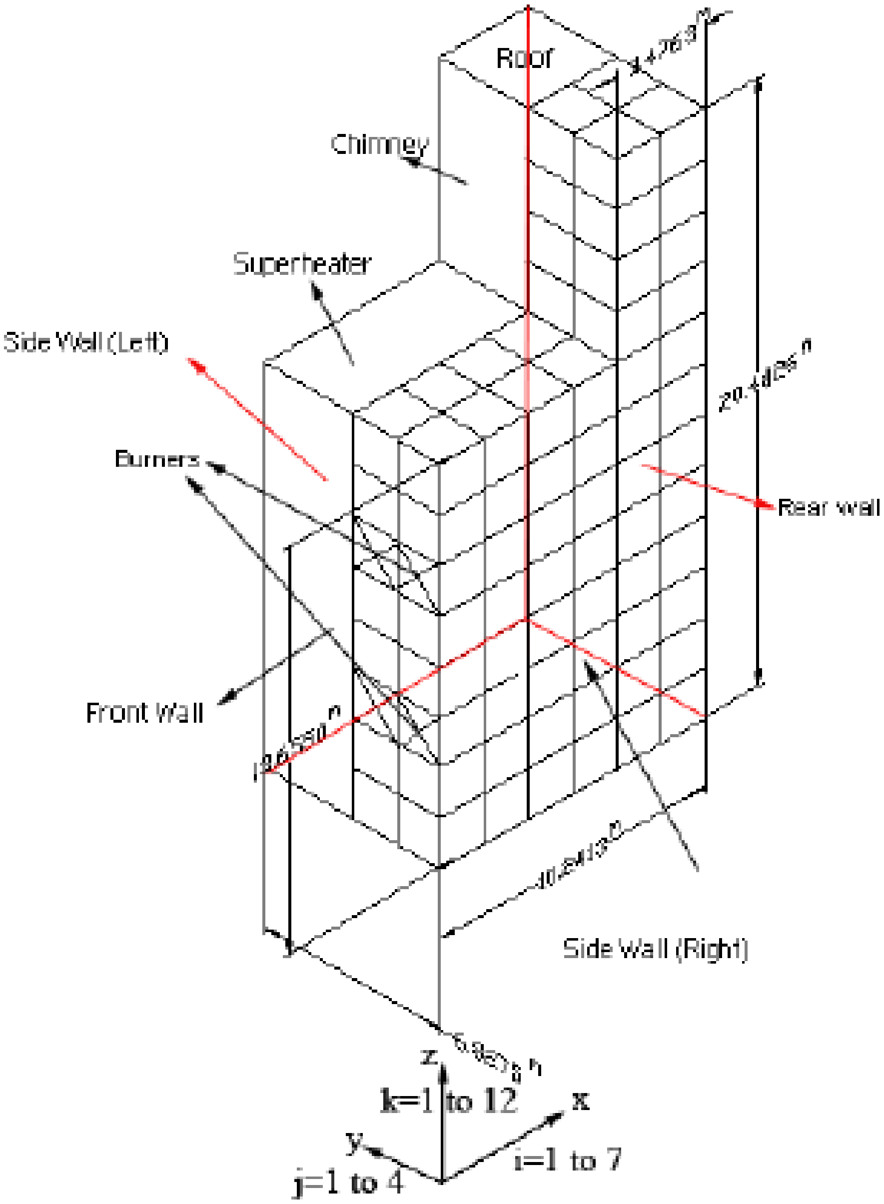

Figure 8. An illustration of our simplified model of the furnace, The names that we used of different parts of the furnace with the volume and surface zones, the position of the burners in the front and rear walls. [59]

for several arbitrarily-interconnected heat-exchanging elements to be simulated in a flexible manner. The model has been validated with the simulations of a real power-station convective zone for different loads, and the agreement between calculated and plant data has been satisfactory" [61]. Sørensen et al. [62] used modeling and simulations to check, measure, optimize, and improve the performance of a fire tube boiler. Model covers effect of flue gas and the water-/steam sides. Various sub-models form final *"overall model for the complete boiler. Sub models have been defined for the furnace, the convection zone (split in 2: a zone submerged in water and a zone covered by steam), a model for the material in the boiler (the steel) and 2 models for resp. the water/steam zone (the boiling)*

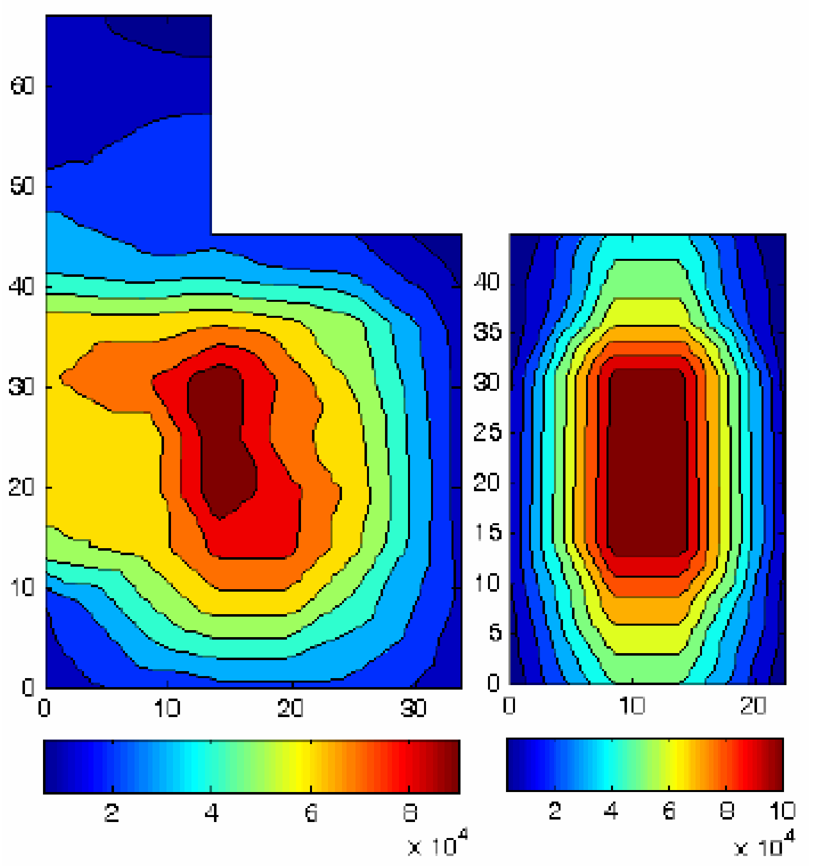

Figure 9. (a) Radiative heat flux distribution on the front wall of the furnace (*Btu / ft²hr*). (b) Radiative heat flux distribution on the side wall of the furnace (*Btu/ ft²hr*). [59]

and the steam. The dynamic model has been developed as a number of Differential-Algebraic-Equation systems (DAE). Subsequently MATLab/Simulink has been applied for carrying out the simulations" [62]. A full-scale experiment was carried out to verify the simulated results and they are found to be in good agreement. In a similar study [63], modeling and simulation was applied for optimizing the dynamic performance of water tube boiler installed on board ship Coral Princess.

In this study, the object function to be optimized takes the weight of the boiler and its dynamic capability into account. *"The dynamic model for simulating boiler performance consists of a model for the flue gas side, a model for the evaporator circuit and a model for the drum. The dynamic model has been developed for the purpose of determining boiler material temperatures and heat transfer from the flue gas side to the water-/steam side in order to simulate the circulation in the evaporator circuit and hereby the water level fluctuations in the drum"* [63]. As in previous study, DAE is used to develop and MATLAB is used to simulate the model. The results are found to be in good agreement with experimental data.

Figure 10. Coral Princess at sea and boiler installed on ship [63]

3.2.2. Heat exchanger

Heat transfer and its modeling and simulation for heat exchangers have been nicely reported in various excellent studies. Dafe., [64] presented the use of FLUENT for CFD codes used to solve problems of heat transfer in plate heat exchangers. The work was carried out to determine the effect of channel geometry and flow conditions on the heat transfer. Two PHE's, one with wave geometry and the other with chevron design were studied. Temperature of the wall was kept constant, water was used as the working fluid, and the mass flow rate varied to study the effect of Reynolds number. Simulated Reynolds number range is 100 – 25, 600.

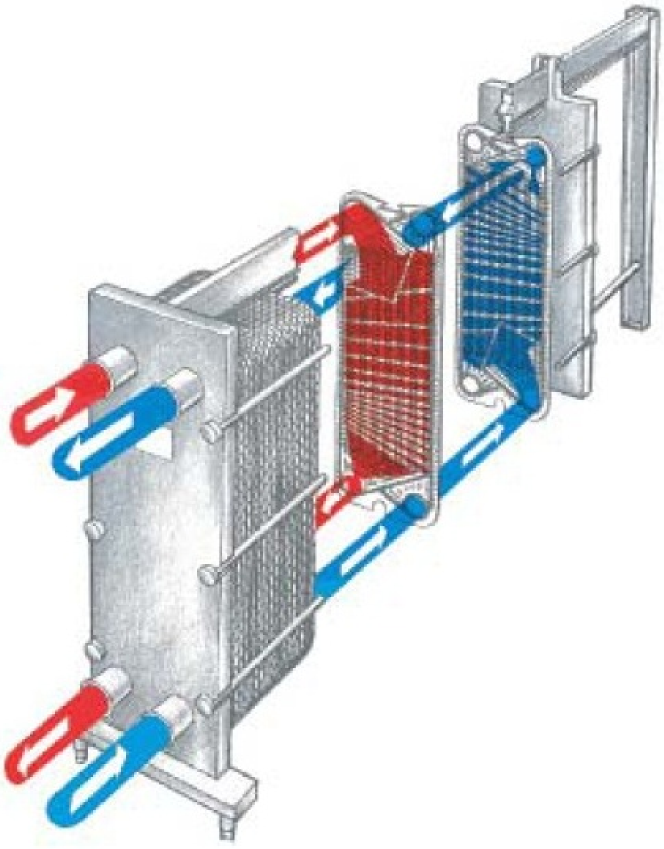

Figure 11. Plate Heat Exchanger [64]

It was efficiently shown that choice of PHE geometry is a strong function of application. Convective design is shown to give better convective properties for low Reynolds number applications while at higher Reynolds numbers chevron design gives better convective properties. Tomas et al., [65] described the use of object-oriented heat exchanger models for simulation of fluid property transitions. The models were written in Modelica. Three models were developed and employed, namely, Model 1: instantaneous property change; Model 2: Ideally mixed volume; Model 3: Transition port delay. Simulations showed that Model 3 is the best for determining computational performance as well as affording flexibility in fluid dispersion modeling. Othman, et al. [66] used CFD as a tool in solving and analyzing problems of heat transfer in shell and tube heat exchanger. Gambit 2.4 was used as tool for simulation. Same experimental parameters at constant mass flow rate of cold water varying with mass flow rate at 0.0151 kg/s, 0.0161 kg/s and 0.0168 kg/s of hot water were used. The CFD model is validated by comparison to the experimental results within 15% error.

3.2.3. Condensers

Heat transfer in condensers is vastly discussed and has been in practice since long for solving efficiency problems and determining process parameters. Various research and industrial studies have explained the use and application of heat transfer via modeling for condensers. Corberan and Melon [67] developed a model to predict the behavior of the finned tube condenser and evaporators that work with R-134a. For simulation of evaporator and condenser, many of the phase change heat transfer coefficient correlations are considered and the most recommended correlations are used. The experimental study to validate the model has been carried out in a small air-conditioning unit with cross-flow air refrigerant type heat exchangers. The model is capable of predicting the heat transfer of an evaporator or condenser with accuracy of ±5% in the studied range. Qureshi et al. [68] developed a mathematical model of evaporative fluid coolers and evaporative condensers to perform a comprehensive design and rating analysis. A fouling model was used to investigate the risk based thermal performance of evaporative heat exchangers. It is solved by Engineering Equation Solver (EES). It showed "*that thermal effectiveness of the evaporative heat exchangers degrades significantly with time indicating that, for a low risk level (pZ0.01), there is about 66.7% decrease in effectiveness for the given fouling model. Furthermore, it is noted that there is about 4.7% increase in outlet process fluid temperature of the evaporative fluid cooler. A parametric study was also performed to evaluate the effect of elevation and mass flow rate ratio on typical performance parameters such as effectiveness for rating calculations*" [68].The model was well validated by experimental results. Acunha Jr et al. [69] further discussed this problem using FLUENT. They studied the air and water behavior inside an evaporative condenser operating with ammonia as the refrigerant fluid. The "*air flow is modeled as a continuous phase using the Eulerian approach while the droplets water flow is modeled as a disperse phase with Lagrangian approach. The coupling between pressure and velocity fields is performed by the SIMPLE algorithm. The pressure, velocity and temperature fields are used to perform qualitative analyses to identify functional aspects of the condenser, while the temperature and the relative humidity evolution contributed to verify the agreement between the results obtained with the numerical model and those presented by equipment manufacturer*" [69]. It was shown that use of deflectors with different angles along the air inlet may attenuate the effects caused by vortex in the entrance region, and hence improve the heat transfer in tubes located immediately above this. Overall results were found to be in good agreement. Lee et al., [70] in a recent study reported the use of modeling and simulation for heat transfer related problems in a simple shell and tube condenser for a longitude baffles for a moderately high temperature heat pump. A simulation method was developed and used to carry out size determination and performance rating of S&T condenser. A good agreement is observed between computed values and experimental data. The deviation (CV) is within 3.16% for size estimation and is within 1.02% for performance rating.

3.2.4. Ovens

Therdthai, et al. [71] used 3D CFD modeling and simulation for the determination of temperature profiles and airflow patterns in continuous oven used for baking process. It was used to predict dynamic responses during continuous baking process. *"According to the simulation results, the heat supply could be reduced whereas the airflow volume should be increased. With this modification, the weight loss of bread was reported to be reduced by 1.4% with an acceptable crust color and a completed baking as indicated by its internal temperature"* [71]. Flick et al. [72] used modeling for determining heat transfer and fluid flow inside pressure cooker. A 3D CFD code was developed and is used to reproduce the experimentally observed trends and some experimentally difficult to characterize phenomena (fluid flow).

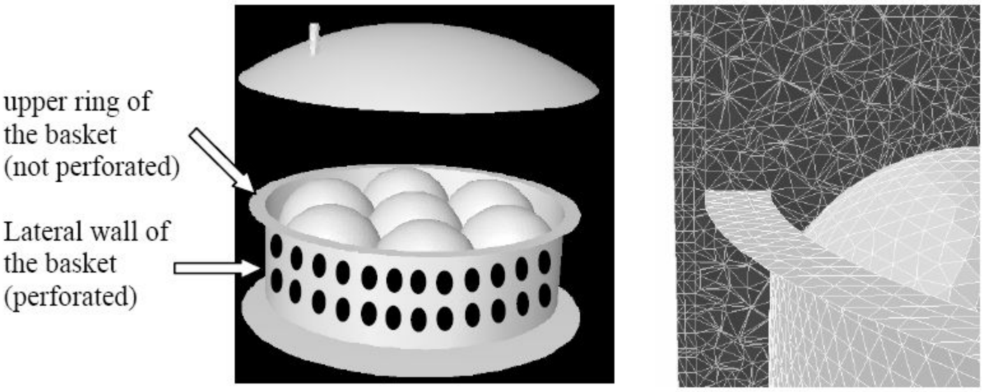

Figure 12. Geometry and mesh of pressure cooker [72]

Further aim of the work is to use numerical simulation for the choice of operating conditions and equipment design which was achieved nicely. Similarly, Sargolzaei et al. [73] applied 1D finite difference and 3D computational fluid dynamic models on the hamburger cooking process. Three different oven temperatures (114, 152, 204°C) and three different pressures (20, 332, 570 pa) were selected and nine experiments were performed. An optimum oven temperature in the range of 114°C to 204°C was proposed. Effect of oven temperature on weight loss is more than pressure. Decreasing oven temperature and increasing cooking time can increase uniformity of temperature distribution in the hamburger, and therefore, microbial safety will increase as well as product quality. The CFD-predicted results were in good agreement with the experimental results than the finite difference (FD) ones. But finite difference model was more economical due to longer time needed for CFD model to simulate (about 1 h). Several other authors used CFD codes for modeling and simulation of heat transfer problems in ovens and found them to be very effective in predicting the results and optimizing process. [74, 75]

3.3. Modeling and simulation of heat transfer in manufacturing industry

Heat transfer studies have also been extensively carried out in manufacturing engineering processes. The models developed, their simulations, and data generated from them have helped immensely in defining process parameters and increasing process efficiencies. Processes such as Casting, Welding, Machining, Powder Metallurgy, Forging, Rolling, Extrusion, Plastics forming have been extensively studied by heat transfer models to improve and optimize their performances. Various commercially available general – purpose and custom built software have been used to perform simulations.

3.3.1. Castings

Heat transfer and its modeling and simulation approach have been extensively applied to foundry technology and processes. Determination of time of solidification, prediction of solidification pattern and structure, improvement of gating system, furnace and mold design are the most important areas in which heat transfer has been applied. Sabau et al. [76] presented heat transfer analysis of direct chill (DC) cast process of ingot using boundary conditions. *"Heat transfer phenomena such as (a) direct contact of liquid metal and mold, (b) air gap between mold and ingot surface, (c) water cooling on rolling and end faces of the ingot, (d) ingot contact with the bottom block, and (e) water intrusion between the bottom block and ingot were analyzed. Data on solid fraction and temperature evolution were compared at points located on the end face for the two cases in which heat transfer conditions (a) were assumed to be the same on both ingot faces, and (b) were assumed to be different on the two ingot faces and in the corner. Small differences in solid fraction were observed while temperature distribution showed significant differences when more appropriate heat transfer boundary conditions were used on the end face and corner regions"* [76]. Rafique et al. [77] applied modeling and simulation to the problem of heat transfer during solidification of liquid metal in investment casting mold using C++. A mathematical model was developed using standard transport equations incorporating all heat transfer coefficients to calculate the time for solidification of metal in casting and computer simulation of the model was carried out in C++ to validate the model.

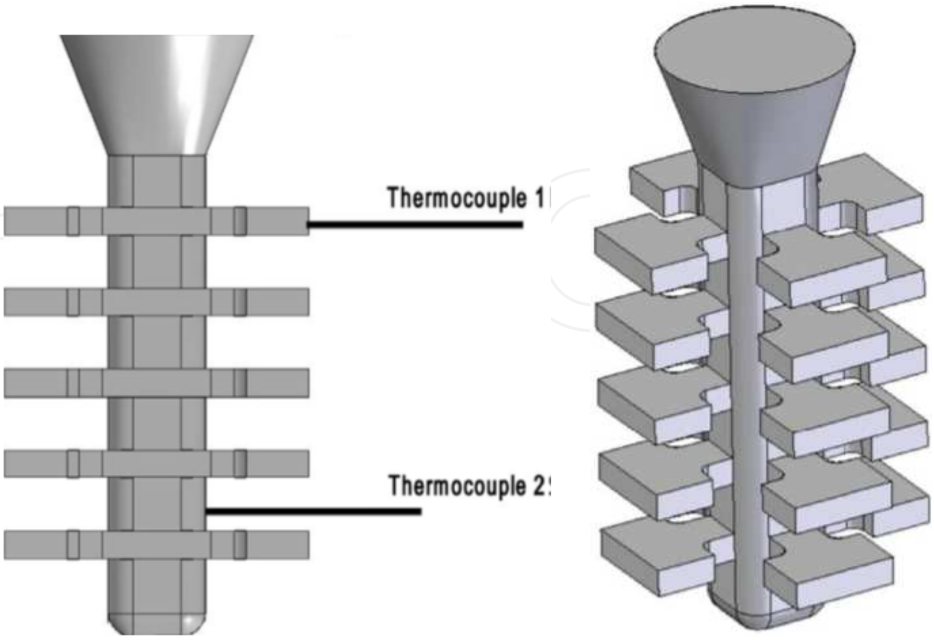

Figure 13. Investment casting tree a) with thermocouples b) schematic [77]

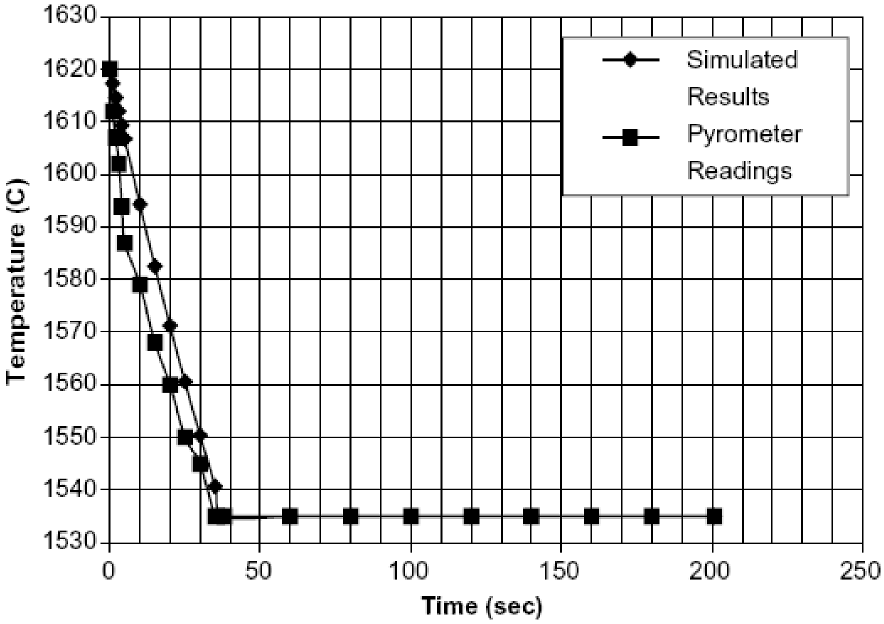

Figure 14. Effect of time on metal temperature (simulated and measured from pyrometer) [77]

The computed results were found in good agreement with experimental data paving the way for process operation, optimization and improvement. Ramírez-López et al. [78] discussed the problem of heat transfer and modeled it using C++ in continuous casting process. "*The algorithms developed to calculate billet temperatures, involve the solutions of the corresponding equations for the heat removal conditions such as radiation, forced convection, and conduction according to the billet position through the CCP. This is done by a simultaneous comparison with the kinematics model. A finite difference method (Crank-Nicholson) is applied to solve the two-dimensional computational array (2D model). Enthalpy (HI, J) and temperature (TI, J) in every node are updated at each step time*" [78]. The results are compared with the surface temperature of three steel casters under different operating conditions and found to be in good agreement. Hardin et al. [79] developed a 3D simulation model for continuous steel slab caster. The temperature predictions are validated using pyrometer data from an operating caster. The stress simulation is based on a visco-plastic constitutive equation for steel, where the semi-solid mush is treated as a compressible porous medium. The stress predictions show regions in the slab where hot tears and cracks are likely to form.

3.3.2. Welding

The application of heat transfer phenomena on welding and joining processes have been studied to check, determine and ascertain its effect on welding process, weld design, determination of weld structure and effect of process control parameters on weld formation. Hu et al. [80] described heat and mass transfer during gas metal arc welding using a unified comprehensive model. Based on this, a thorough investigation of the plasma arc characteristics during the gas metal arc welding process was conducted incorporating all parameters such as interactive coupling between arc plasma; melting of the electrode; droplet formation, detachment, transfer, and impingement onto the work piece; and weld pool dynamics. The assumed Gaussian distributions of the arc pressure, current and heat flux at the weld pool surface in the traditional models were shown not to be representative of the real distributions in the welding process. In the second part of this study [81], the transient melt-flow velocity and temperature distributions in the droplet and in the weld pool were calculated. They simulated the crater formation in weld pool as well as the solidification process in the electrode and in the weld pool after the current were turned off. The predicted droplet flight trajectory is in good agreement with published data. Takemori et. al. [82] studied the numerical simulation of the heat transfer on the compressor during the welding process. It is used to determinate housing and internal components temperatures of the compressor during the sealing welding. A lumped parameter model was used to study various welding variables initially. After that, the best welding process was analyzed in detail using a numerical solution of a 3D transient model. All the monitored temperatures during the simulation were found very close to the temperatures measured experimentally, thus validating the model. Daha, et al. [83] discussed the problem of heat transfer in keyhole plasma arc welding of dissimilar steel joints (2205 – A36) using 3D heat transfer and fluid flow model. An adaptive heat source is proposed as a heat source model for performing a non-linear transient thermal analysis. Temperature profiles and solidified weld pool geometry are presented for three different welding heat input. The reversed bugle shape parameters are proposed to successfully explain the observations. The model was also applied to keyhole plasma welding of 6.8 mm thick similar 2205 duplex stainless steel joint for validation. The simulation results were found in good agreement with independently obtained experimental data.

3.3.3. Machining

Machining processes have been studied by heat transfer methods and their use has increased lately with the introduction of modeling and simulation techniques. Their use has made easier the defining process, determining its parameters, driving its efficiency and optimization. Processes such as facing, turning, milling, shaping, grouching, honing have been modeled to investigate effect of process itself, material, lubricant, etc. as a function of heat transfer process. Åkerström [84] discussed the problem of heat transfer associated with thermo-mechanical forming of thin boron steel sheets into ultra-high strength components via modeling and simulation. The objective is to predict the shape accuracy, thickness distribution, and hardness distribution of the final component with high accuracy. Method based on multiple overlapping continuous cooling and compression experiments (MOCCCT) in combination with inverse modeling (mechanical response) and a model based on combined nucleation and growth rate equations (austenite decomposition) was developed and used. FE – code LS – DYNA was used for simulating these models. The results were compared for forming force, thickness distribution, hardness distribution, and shape accuracy/springback with experimental values and found to be in good agreement. Iqbal et al [85] discussed the problem of interface heat transfer coefficient for finite element modeling of high-speed machining. They used an improved heat transfer coefficient for heat generation and frictional contact, derived from an experimental setup, consisting of an uncoated cemented carbide pin rubbing against a steel workpiece while the latter was rotated at speeds similar to the cutting tests. This "pin-on disc" set-up had temperature and force monitoring equipment attached to it for measurements. Results show that the estimated interface heat transfer coefficient decreases at low rubbing speeds and then becomes approximately constant for high rubbing speeds. At these low rubbing speeds, the estimated values show a dependence on temperature. Interface heat transfer coefficient for a range of rubbing speeds of the dry sliding process is produced from modeling and simulation results and found to be in good agreement with experimental values. In a similar study [86], they used and developed a Lagrangian finite element code DEFORM 2D for studying same phenomena and found it to be useful. Ma et al. [87] discussed and applied FE analysis on thermal characteristics of Lathe Motorized Spindle. The structure feature of the spindle was introduced defining two major internal heat sources of motorized spindle with the aim to calculate the heat transfer coefficients of the major components of the lathe spindle. *"A 2D temperature field model has been developed with finite element method. Based on it, the temperature field and temperature rises of the spindle have been simulated and the reasonability of temperature distribution of the spindle unit has also been discussed. The results yielded reference for evaluating the thermal behavior of the high speed NC motorized spindle and proved to be effective practically"*. [87]

3.3.4. Forming processes

Forming processes, in general, such as rolling, forging, extrusion have been vastly studied by heat transfer methods and their modeling and simulation. This comprises the main area of heat transfer application in metal forming industry and processes related to it. These studies have revealed in great detail the discrepancies (defect formation and its causes, energy inefficiency, etc.) in processes and helped increase their efficiency and optimization. Behrens [88] discussed the modeling and simulation of friction and heat transfer models in hot forging processes. Two representative forging tests were carried out; the forming load and surface temperature distribution were recorded incorporating effects such as prevailing normal stress and shear yield stress of the workpiece material, the temperature and surface roughness of the tool and workpiece as well as the relative sliding velocity. By means of these data, the models were appropriately extended and adjusted using the software FORGE ®.

The application of the extended models allows for a more accurate description of the interaction at the contact interface and delivers more realistic results. Rabbah et al. [89] explained the use of modeling and simulation of heat transfer along a cold rolling system. *"They used a semi analytical solution for the work roll subjected to predict transient thermal profiles of work rolls with multiple cooling / heating zones. It was derived from the heat balance equation using the finite difference method and Runge-Kutta method. Numerical simulations are based on both recursive calculation methods and iterative methods"* [89]. The model suggested is used for the numerical simulations in rolling using the work roll temperature distribution within a very short computing time. The thermal profile development depends primarily on the cooling water flow. Thus, the cooling conditions (fluid temperature) and the corresponding heat transfer coefficients are very important in the model adjustment process. The objective of the study was the development of a control law to reduce to the maximum the deformations of both the strip and the work rolls which was simulated efficiently. Parvizian et al. [90] discussed the modeling and

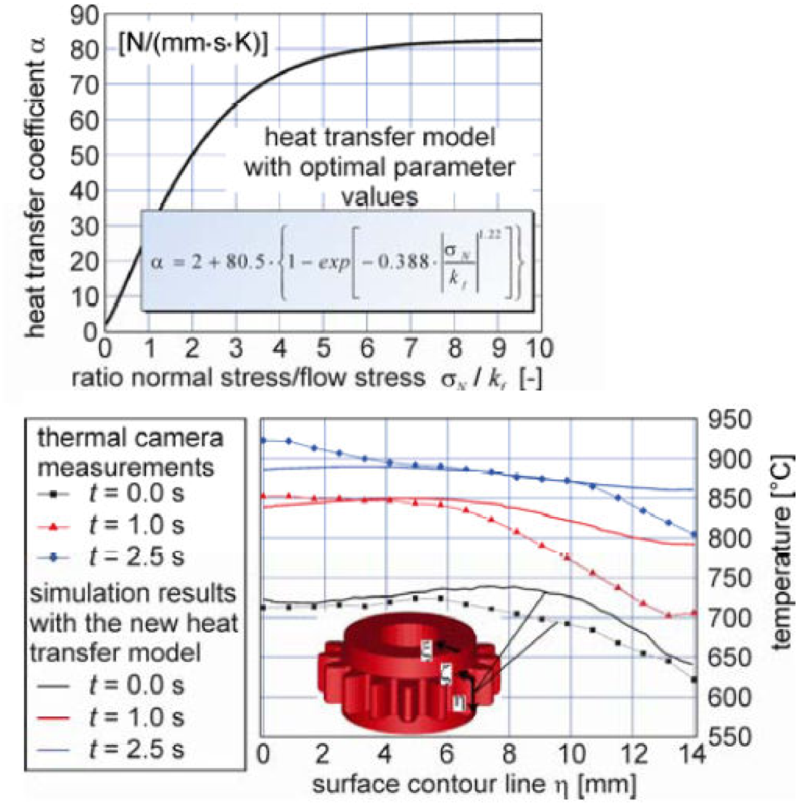

Figure 15. Finite element results based on the developed method [88]

simulation of aluminum alloys during extrusion, cooling and further forming processes. Individual steps are combined into multi-stage processes in order to optimize the production process as a whole. *"A number of aspects of the structural simulation as well as that of extrusion as a thermomechanical process are considered. These aspects include contact and adaptive mesh refinement, heat transfer inside the billet, heat transfer between the workpiece and the container, frictional dissipation, mechanical energy and surface radiation"* [90]. Commercial finite-element program ABAQUS and an external remeshing software incorporate the effects of python scripting and mesh refinement respectively. The achieved results were in good agreement.

3.4. Modeling and simulation of heat transfer in defense applications

Application of heat transfer phenomena in defense applications such as determination of efficiency of engines, their design and material design, performance, and selection; determination of heat transfer profiles of guns, barrels and shells; design and selection of suitable high-performance materials (composite structures and their design), etc., has been a major field of study. Many excellent studies explain in detail the application of heat transfer principles and their simulation approaches as applied to defense applications. Wu et al. [91] explained the phenomena of heat transfer in a 155 mm compound gun barrel cooled by midwall cooling channels. *"Finite element analysis (FEA) method was employed to validate the results obtained by theoretical analyses. The present study showed: (1) natural air cooling is ineffective for transferring the heat out of the barrel because the combined convection and radiation heat transfer coefficient is relatively small; (2) forced midwall cooling has great heat extraction capability and is able to keep the chamber temperature below the cook-off temperature by increasing the heat transfer coefficient; (3) an optimal flow rate should be selected to balance the cooling efficiency and the pressure loss"* [91]. A similar study conducted by Mishra et al. described an accurate modeling of gun barrel temperature variation over time to assess wear and the number of shot fires needed to reach cook-off. *"Using lumped parameter methods, an internal ballistics code was developed to compute heat transfer to the gun barrel for given ammunition parameters. Subsequently the finite element method was employed to model gun barrel temperature history (temperature variation over time). Simulations were performed for a burst of nine shots and the results were found to match satisfactorily to the corresponding experimental measurements"* [92]. An important and unique advantage of the developed scheme is that it easily couples internal ballistics simulations with the finite element methods and also accurately calculates gun barrel temperature history and wear calculations. Sutar et al. explained unsteady heat transfer in externally heated Magnesio Thermic reduction reactor. *"Simulations were carried out using Anupravha, a computational fluid dynamics (CFD) and heat transfer solver to study the temperature profiles inside the reactor including its lining. The results are studied for both preheating and reaction stage which gives an idea about the reaction temperature and molten mass inside the reactor proving present study's significance for correct design of reactor thereby preventing nuclear radiation to the surroundings"* [93]. Numerous other studies review the use of modeling and simulation techniques for heat transfer analysis in military, defense as well as strategic applications [63, 76, 94 – 96].

3.5. Modeling and simulation of heat transfer in energy applications

Heat transfer via modeling and simulation has been rigorously applied in energy applications (energy generation and production methods) for process identification, operation, improvement and optimization. It has been applied in all areas of energy methods (source tapping, method determination and generation of power from source, conversion of power to energy and its distribution, etc.) and all field of energy generation and production (thermal, hydral, wind, geothermal, solar, fuel cell, nuclear, etc.) and has generated excellent results coupled with capital saving. Schimon et al. [97] modeled and simulated different components of power plant and associated heat transfer phenomena using Modelica. The heat transfer for the heat exchanger component was modeled by calculating the heat transfer coefficient in dependency on the flow velocity of the medium in the pipes. Dymola (a Modelica based tool) was used to perform simulations. The models were realized with time domain differential equations and algebraic equations. Bandyopadhyay [98] presented modeling and simulation of heat transfer phenomena in solar thermal power plants. Models developed were based on the fundamental conservation algebraic equations along with phenomenological laws and simple representative equipment characteristics whose simulations were carried out. Different detailed equipment characteristics including thermal stresses, time variations of components etc. were incorporated in the developed models and then were simulated for control and optimization. Ramousse et al. [99] presented a fuel cell model that takes into account heat transfer in MEA and bipolar plates along with gas diffusion in the porous electrodes, water diffusion, and electro-osmotic transport through the polymeric membrane. Heat and mass transfer phenomena in the cell are combined with *"coupled charge and mass transfers in the electrodes, considered porous to construct the model. The results show that thermal gradients in the MEA could lead to thermal stresses at high current densities. The feeding gas temperature influence on the cell temperature is also important"* [99] and shown to bear significance on overall cell performance. Yuan et. al [100] extended the use of modeling and simulation to similar problems in PEMFC and SOFC. They further used modeling and simulation and predicted convective heat transfer and pressure drop in flow ducts of fuel and the oxidant.

3.6. Modeling and simulation of heat transfer in miscellaneous applications

Apart from the above branches, heat transfer and its modeling and simulation is also applied in various other fields of engineering and technology such as electronics, environmental engineering, biomaterials and biomedical engineering, etc., to take advantage of process modeling, operation, and optimization. Guérin et al. [101] used finite volume approach to model and simulate the heat transfers between the different environmental elements to synthesize realistic winter sceneries. They simulated snow fall over the ground, as well as the conductive, convective, and radiative thermal transfers according to the variations of air and dew point temperatures, the amount of snow, cloud cover, and day-night cycles.

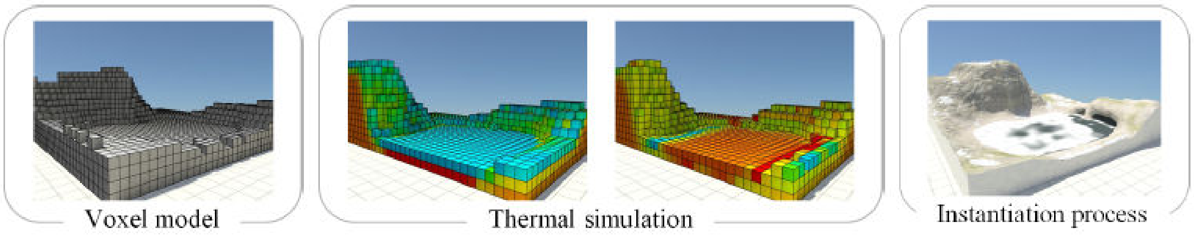

Figure 16. Synthetic overview of winter scenery generation process (high altitude partially frozen lake) [101]

The model also takes into account the phase changes such as snow melting into water or water freezing into ice and yielded good results and inferences. Lakatoš et. al. (2006) [102] used FEMLAB to simulate heat transfer and electromagnetic fields for the development of protected microcomputer prototypes. Heat field was extended and simulated from heat sources inside a monitor case along with electromagnetic fields in electronic systems. The temperature dependence on time was interpreted along with value of steady temperature. Elwassif et. al. developed and used a bio heat transfer model for getting information on the thermal effects of DBS using finite element models to investigate the magnitude and spatial distribution of DBS-induced temperature changes. "*The parameters investigated include stimulation waveform, lead selection, brain tissue electrical and thermal conductivities, blood perfusion, metabolic heat generation during the stimulation and lead thermal conductivity/heat dissipation through the electrode.*" [103]. It was shown that depending on stimulation/tissue parameters, temperature of surrounding tissue is increased by to 0.8°C in clinical DBS protocols.

4. Conclusions

Heat transfer studies comprise an important part of engineering analysis for any system ranging from automotive to process to energy applications. These are first hand analyses in any engineering problem/application related directly and/or indirectly with heat. Lately, modeling and simulation techniques and use of high-speed computers have greatly facilitated the thermal and heat transfer related analysis. More and more models are being developed, tested and used to ease out the calculations involved in the process also yielding direct results and even predicting future trends and auxiliary data. The present chapter deal with and explained in detail this field of engineering in a rational and practical way. Modeling and simulation of heat transfer phenomena as developed and applied is presented in various engineering applications. New and novel processes (investment casting, numerical machining, fuel cell technologies etc.) have also been discussed. The chapter draws attention to the use of modeling and simulation techniques and use of simulation packages (C++, MATLAB ® SIMULINK ®, Modelica, FLUENT, SolidCAST, COMSOL Packages, etc.) for solving heat transfer related problems of conventional and advanced processes, at the same time encouraging the reader to develop his/her own models for specific engineering problem/application.

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