SIMULATION OF THERMAL TRANSPORT PROCESSES TO REDUCE ENVIRONMENTAL IMPACT AND IMPROVE OUTPUT

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ABSTRACT
This paper focuses on thermal transport processes and systems and discusses their modeling, simulation, design and optimization to reduce the effect on the environment, reduce energy consumption and enhance product quality and productivity. These processes are generally quite complex and several challenges are encountered to obtain accurate and reliable results that can be used as the basis for design and optimization. Some major challenges are material properties, model validation, uncertainties in the governing parameters and operating conditions, complex combined transport mechanisms, and multiscale effects. Once accurate simulation results are obtained, these can be used to optimize the process to enhance the output. Reduction in energy and material consumption, as well as the effect on the environment, are of particular concern today. The paper discusses these aspects and presents a few practical systems by way of illustration. For example, working with the changing environment, the energy consumed by the thermal system for the cooling of data centers can be minimized. Similarly, other concerns and approaches are outlined.
Keywords: environmental effects, optimization, simulation, thermal transport, thermal systems.

1 INTRODUCTION

Many engineering systems that are largely based on thermal transport phenomena are encountered in a wide range of applications, such as manufacturing, transportation, energy, environment and cooling of electronic systems, as shown in Fig. 1. The complexity of typical thermal systems makes it necessary to use numerical methods to model and simulate them to understand the underlying basic mechanisms and the system behavior. Experimental results are employed for physical insight and validation. Simulation is also needed to obtain inputs that may then be used to predict, control and design the system. Optimization is needed in most cases for improving the output by enhancing the product quality and the efficiency of the process. It is also valuable in assessing and reducing the energy consumption and minimizing the environmental impact [1, 2].

This paper considers the basic approach to the overall problem and focuses on modeling the transport processes and solving the governing equations numerically with realistic boundary and initial conditions. The results obtained are compared with available analytical, numerical or experimental data to verify and validate the model. It is important to develop an accurate, dependable and physically realistic simulation. The important aspects in simulation and in the design and optimization of the system are discussed. Several practical examples are presented to illustrate the approach. Typical results on practical problems are presented and discussed. Optimization is discussed for appropriate objective functions and for multi-objective optimization that applies in many cases. Of particular interest are the quality of the product, the rate of production, energy consumption and efficiency of the process. The effect of the thermal system on the environment, including the possible effect on climate change, is also considered.

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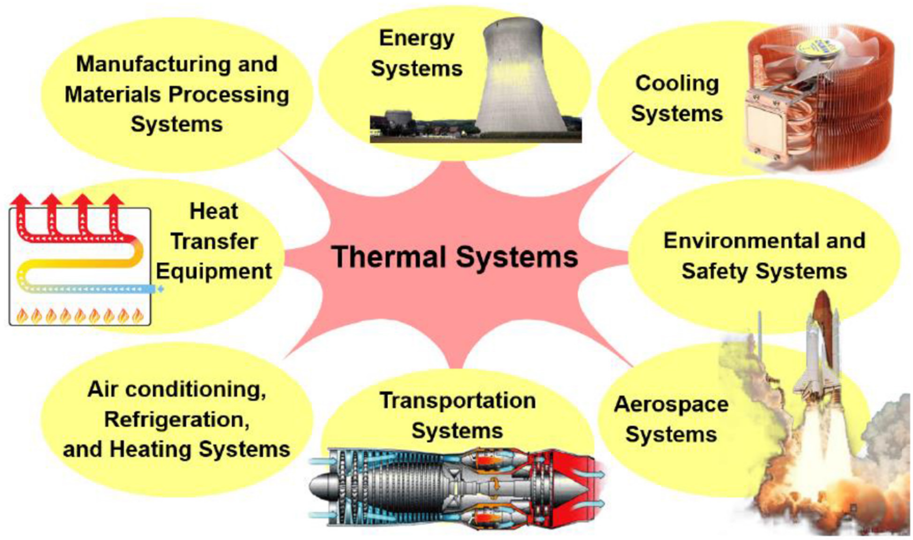

Figure 1: Examples of applications where thermal systems are of particular interest.

The techniques that may be used to model the basic transport phenomena and to design and optimize the system are discussed. Though the different objective functions may be combined to yield a single objective function in a few cases, the different criteria generally need to be considered separately. This can be used to generate a Pareto front for dominant solutions from which one objective function can be improved at the expense of the other. Trade-offs, based on the requirements of the problem, can then be employed to achieve the desired optimum [3]. The means to reduce the environmental effect of large thermal systems, such as data centers, are also outlined. The current status and future trends in these important areas are outlined.

2 MODELING AND SIMULATION

The governing equations for thermal processes and systems are based on the usual conservation laws for mass, momentum and energy. A radiative source term arises for non-opaque materials like glass, which emits and absorbs energy as a function of the wavelength. Also, viscous dissipation effects are important for flow of highly viscous materials like polymers and glass due to the large viscosity of the material. The basic equations may be written as [4]:

$$\frac{D\rho}{Dt} + \rho \nabla . \bar{V} = 0 \tag{1}$$

$$\rho \frac{D\bar{V}}{Dt} = \bar{F} + \nabla . \tau \tag{2}$$

$$\rho C_p \frac{DT}{Dt} = \nabla . \left(k \nabla T \right) + \dot{Q} + \beta T \frac{Dp}{Dt} + \mu \Phi \tag{3}$$

where ρ, C_p, k, and β are the density, specific heat at constant pressure, thermal conductivity and coefficient of volumetric expansio n, respectively, $\dot{Q}$ the thermal energy source per unit volume, T the temperature, t the time, p the pressure, and $\bar{F}$ the body force per unit volume. Also, D/Dt is the substantial or particle derivative, given in terms of the local derivatives in the flow. The stress tensor τ can be written in terms of the velocity $\bar{V}$ if the fluid characteristics are known, yielding Navier-Stokes equations for common Newtonian fluids like air and water, which are often employed in cooling of electronic systems.

The viscous dissipation term $\mu\Phi$ represents the irreversible part of the energy transfer due to the shear stress and is important in many practical processes such as polymer extrusion. Governing equations may thus be obtained for different thermal processes and systems. Energy input may be provided by chemical reactions, as is the case in combustion or chemical vapor deposition (CVD) [5]. The coupled equations for the chemical species need to be solved in these cases.

A wide range of numerical methods are available for solving typical governing equations obtained in materials processing, energy systems, cooling of electronic equipment, building fires, gas turbines and so on [6]. However, it is critical to obtain accurate, realistic and dependable results that may form the basis for system design and optimization. To achieve this in practical thermal systems and processes, several challenges are encountered and must be addressed. Some of the main ones are:

1. Material Properties and Characteristics,
2. Verification and Validation,
3. Accurate Imposition of Appropriate Boundary Conditions,
4. Combined Mechanisms,
5. Complex Transport Phenomena,
6. Multiple Scales, and
7. Uncertainty in input data and sensitivity.

A few typical examples are given below to show the outputs from numerical simulation and some of the challenges posed.

3 TYPICAL RESULTS AND DISCUSSION

Typical results for three different examples, representing different areas of thermal systems, are shown here. Figure 2 shows the flow and temperature fields in a channel containing two isolated thermal sources. A vortex generator is placed upstream of the sources to enhance the heat transfer from the sources by generating vortices. The fluid is taken as air, the sources of copper and the channel walls of wood, so that material properties are not a major issue. But, due to conduction in the walls, a conjugate problem has to be solved. A transient solution is needed to investigate the disturbance frequency spectrum and match those due to the vortex generator with those due to the sources. Higher Reynlds number, Re, lead to chaotic behavior. Also, the geometry is generally much more complex in practical systems, requiring three-dimensional solutions. Both experiments and numerical simulations may be employed to obtain the desired results [7].

Figure 3 shows the drawing of silica glass in an optical fiber draw furnace. Glass poses major problems with respect to material properties, particularly since its viscosity ν varies exponentially with temperature. A commonly used expression in S.I. units is given in terms of the temperature T and melt temperature T_{melt} is:

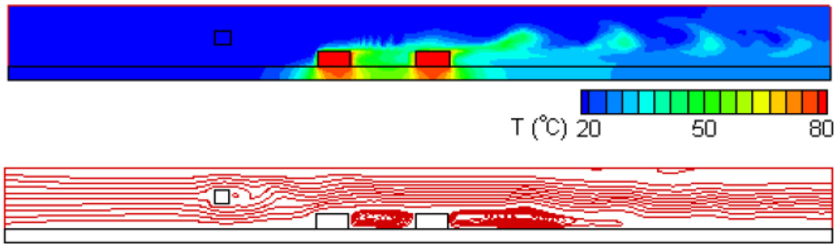

Figure 2: Flow and temperature distributions in a channel with isolated sources and a vortex generator.

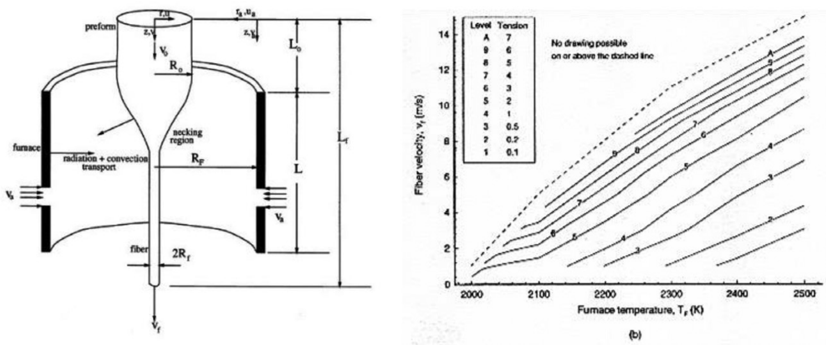

Figure 3: Optical fiber drawn in a furnace and the feasibility region in which the fiber can be successfuly drawn.

$$\nu = 4545.45 \exp\left[32\left(\frac{T_{melt}}{T} - 1\right)\right] \tag{4}$$

All heating modes arise, though radiation is the dominant mode. However, radiation properties vary strongly with composition and temperature and are not easily accessible for glass and other materials involved. If the fiber is drawn at low furnace temperature or at high speed, it would break due to viscous rupture. Figure 3 shows the domain in which the process is feasible. Because of large material property changes and high variation in diameter, going from several centimeters to a 125 µm diameter optical fiber in about 0.3 m, the simulation is complicated and convergence is very slow [8].

Another material processing problem is shown in Fig. 4. This involves the widely used CVD system for fabricating thin films used in electronics, photovoltaics and optical applications [9]. The films are deposited on a chosen heated substrate from reacting gases and surface reactions. The simulation is complicated by the typical large number of intermediate species and reactions that must be included. In many cases, the susceptor is rotating and gases impinge on it, resulting in a 3D problem. Conjugate transport is obviously needed. The film thickness is at the micrometer level, whereas the system is at the macro or engineering scale. Validation is needed and well-controlled experiments are performed to obtain the data for comparison. It is important to have excellent film uniformity and thickness. The end portions,

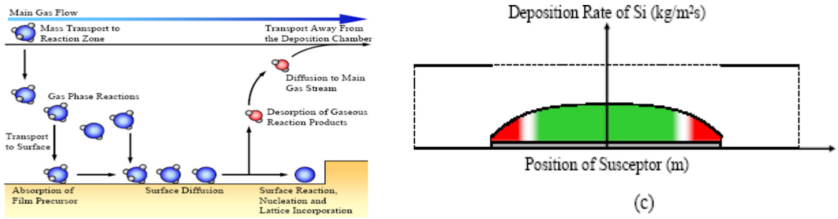

Figure 4: A horizontal CVD reactor for thin film fabrication and a typical result on the deposited film.

shown in red in the simulation, have to be discarded if the thickness is not up to the desired level.

Validation of the mathematical and numerical model is a critical, though often difficult and involved task [10]. In all the examples given above, considerable effort was directed at verification of the numerical scheme and validation of the model. A practical drawtower was available to validate the results for optical fiber drawing. For the other two cases, experimental systems were built to provide data for validation. In several cases, earlier numerical and experimental results may be available in the literature for comparisons with the current results for validation. Once the model has been validated and accurate results have been generated, system design, prediction and optimization may be undertaken.

4 OPTIMIZATION

Optimization of thermal processes and systems is undertaken to enhance the output and reduce the environmental effect. The main objective functions that may be employed for improving the output are:

1. Improved product quality,
2. Increased productivity,
3. Reduced costs, and
4. Efficiency of the process.

Similarly, the objective functions that may be used for reducing the environmental effect are:

1. Reduction in energy consumption,
2. Reduction in material discharges to the environment, and
3. Maximization use of renewable energy sources,

Obviously, several other objective functions can be considered. In many cases, the demands posed by one objective function may go against those of another. In manufacturing, for instance, product quality may often be improved by reducing the production rate. An increase in efficiency, on the other hand, enhances the output and also reduces the environmental effect.

Let us again consider the three systems discussed in the preceding section. For cooling of electronic systems, the heat transfer rate should be maximized so that the compactness of the packaging can be increased. There are many ways to increase the heat transfer rates in the problem sketched in Fig. 2, including increased flow rate, decreased inlet temperature, and geometry variation. However, a critical parameter that must be included is the pressure needed for the flow. We cannot increase the heat transfer arbitrarily, without ensuring that the pressure drop in the channel is acceptable. Figure 5 shows the results of such a multi-objective optimization, considering the two aspects, heat transfer rate and pressure separately to generate a Pareto frontier [11]. The heat transfer is given in terms of Stanton number, which is Nusselt number, Nu, divided by Reynolds number, Re, and Prandtl number, Pr. This Pareto frontier may be used to trade-off between the two objectives to obtain the final design. The results obtained from a composite objective function, F, which involves heat transfer from the two sources, Q_1 and Q_2, as well as the pressure, are shown in Table 1. This objective function is obviously arbitrary and is based on the knowledge about a given system. It is seen that the optimum vortex generator can be obtained for a variety of conditions.

For the optical fiber drawing process, considered earlier, the simulation results from the validated model may be used to optimize the process. The objective function includes thermally induced defect concentration, tension in the fiber and velocity difference across the fiber, all these representing lowering of fiber quality. Thus, the smallest value of this objective function indicates smallest defects, tension, and velocity gap, giving the best fiber quality [12]. Two variables, draw temperature and fiber speed, are considered separately, since these are the dominant parameters and the results shown in Fig. 6 indicate the optimal conditions to obtain the best quality fiber. Similarly, productivity can be considered as another objective function and the process optimized through multi-objective optimization.

Finally, considering the CVD system, discussed earlier, the main aspects of practical interest include film quality and production rate. If the thickness is not uniform or deposition is not satisfactory, the percentage area of the film that may be used in device manufacture is reduced. This percentage working area (PWA) may be taken as the objective function and the inlet velocity V and susceptor temperature T as the two main variables. Figure 7 shows the response surface generated for this problem for Silicon deposition on the basis of simulation

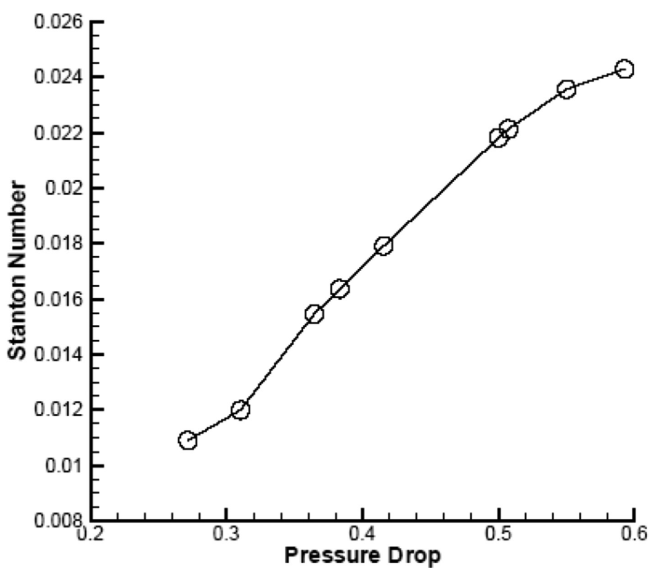

Figure 5: Pareto frontier for the optimization of an electronic system represented by isolated heat sources in a channel.

Table 1: Optimization of a vortex promoter in a channel with two isolated heat sources.

$$F = W_1\overline{Q}_1 + W_2\overline{Q}_2 - W_3\overline{\Delta P}$$

	Geometry	Re*	h_p^*/H
$W_1 = 1,\ W_2 = W_3 = 0$	Hexagonal	5600	0.47
$W_2 = 1,\ W_1 = W_3 = 0$	Circular	5600	0.36
$W_3 = 1,\ W_1 = W_2 = 0$	No vortex promoter		
$W_1 = W_2,\ W_3 = 0$	Hexagonal	5600	0.47
$W_1 = W_2 = W_3$	Square	5600	0.16
$W_1 = W_2 = 2 \times W_3$	Circular	5600	0.47
$W_1 = W_2 = 3 \times W_3$	Hexagonal	5600	0.47
$W_1 = W_2 = W_3/2$	No vortex promoter		
$W_1 = W_2 = W_3/3$	No vortex promoter		

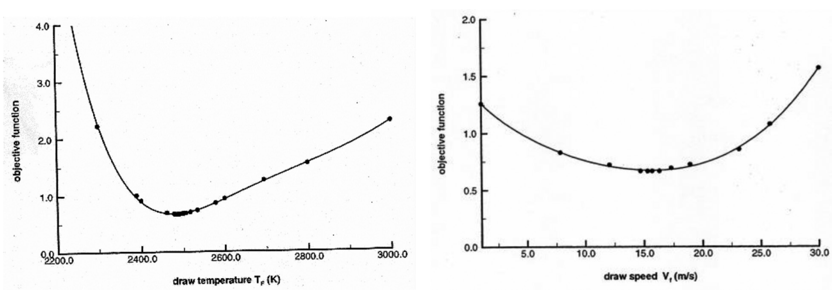

Figure 6: Optimization of the optical fiber drawing process in terms of main operating parameters; draw temperature and fiber speed.

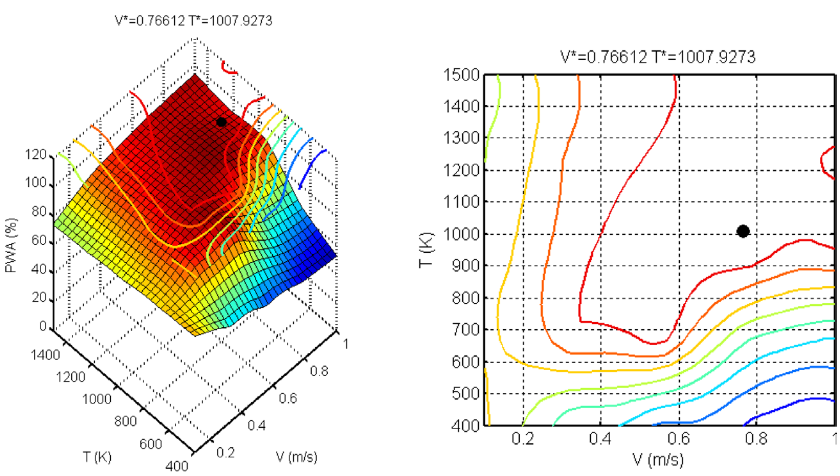

Figure 7: Response surface and optimal point to achieve maximum percentage working area in a typical CVD reactor for depositing Silicon.

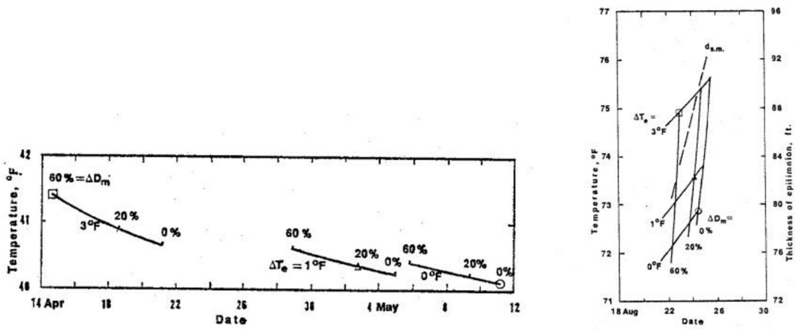

Figure 8: Effect of thermal discharges to a lake on its temperature cycle and temperatures at the onset of summer stratification and summer maximum.

results and the optimum point, which is also shown on a two-dimensional plot. Other objective functions have also been considered. In such complex processes, uncertainties arise in the design parameters and operating conditions. These are important and must be included to obtain the final, realistic, optimal design [13].

5 ENVIRONMENTAL CONSIDERATIONS

Optimization of thermal systems and processes with respect to efficiency and productivity also lead to a reduction in the environmental effects. However, there are several aspects that need to be treated directly to reduce the environmental impact. One of these is the discharge of thermal energy and material into the environment. The water from the condensers of a power plant are often cooled by discharge into and intake from a natural lake or pond [14, 15]. The flow causes enhanced mixing, as well heat input into the lake. The overall effect is to alter the annual thermal cycle of the lake and raise the temperatures to lose the additional energy. Figure 8 shows the effect on the temperatures and on the onset of summer stratification and the location of the summer maximum. The results are shown for no discharge and for up to three 1000 MW power plants discharging into a fairly large lake in north America. The temperatures rise by a few degrees and the thermal cycle is shifted by several days. These effects, though seemingly modest, accumulate over the years and serve to destroy organic life in the lake and thus are unacceptable.

Data centers are another important and interesting thermal system, since the cooling often requires a considerable amount of energy, very much like power plants [16]. Modeling and numerical simulation can be used to obtain the flow and temperature fields, as shown in Fig. 9. These can be used to pinpoint hot spots and areas of low heat transfer, so that the system may be designed to meet the stringent temperature constraints of electronic systems.

However, another interesting consideration arises with respect to the effect of the environment on the thermal energy needed for cooling. Since several data centers are often available for a given enterprise, spread out over the country or the world, one could vary the load, depending on the environmental conditions to minimize the power consumption [17]. Thus, colder regions may be effectively employed in the summer and warmer in the winter without the extensive use of the power consuming chillers to cool the data center. The load could be kept low to cool the system with the use of a simple fan. At larger loads, the chiller will be needed, as demonstrated in Fig. 10. The load and location of the data center can thus be

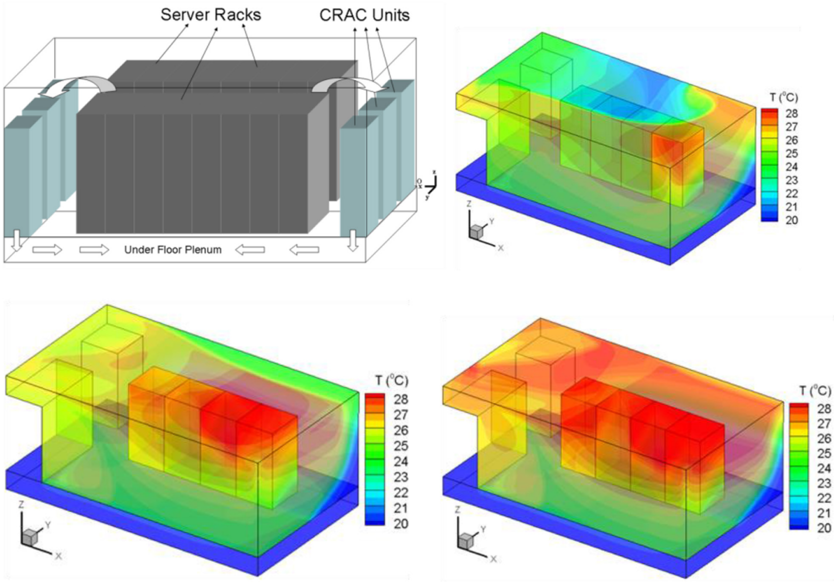

Figure 9: Calculated flow and temperature fields in a typical data center.

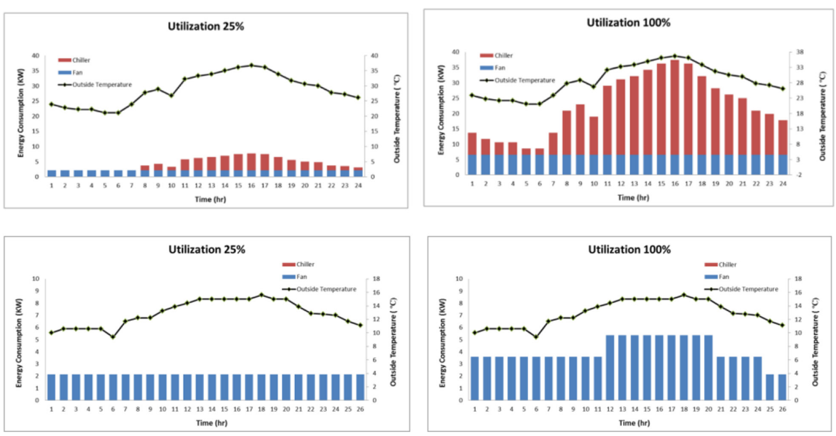

Figure 10: Effect of environmental conditions and load on power consumption for cooling of data centers. Top: Princeton, NJ, in August and Bottom: Seattle, WA, in January. The red portion represents the power consumed by chillers.

optimized to minimize the power consumption and substantially reduce the effect on the environment. In fact, the environmental conditions are effectively used to reduce the thermal input needed.

6 CONCLUDING REMARKS

Thermal processes and systems are of interest in a wide range of applications, from transportation and energy to manufacturing, heating/cooling, safety and environmental problems. The mathematical modeling and numerical simulation musty address several challenges, such as accurate property data, validation, complex domains, combined mechanisms, and multiple scales to obtain accurate, realistic and dependable results for design, prediction, control and optimization. It is also critical to optimize the systems to enhance the output in terms of product quality, efficiency and effectiveness, while reducing the impact on the environment. This paper outlines the basic approaches that may be adopted and presents several important examples to demonstrate the need for such optimization. It also presents the current and future trends and needs in this area.

REFERENCES

[1] Jaluria, Y., *Design and Optimization of Thermal Systems,* 2 edn., CRC Press: Boca Raton, FL, 2008.

[2] Bejan, A., Tsatsaronis, G. & Moran, M., *Thermal Design and Optimization*, John Wiley & Sons: New York, 1996.

[3] Deb, K., *Multi-Objective Optimization Using Evolutionary Algorithms*, John Wiley & Sons: New York NY, 2002.

[4] Jaluria, Y., Thermal processing of materials: From basic research to engineering. *ASME Journal of Heat Transfer*, 125(6), pp. 957–979, 2003.
http://dx.doi.org/10.1115/1.1621889

[5] Mahajan, R.L., Transport phenomena in chemical vapor deposition systems. *Advances in Heat Transfer*, **28**, pp. 339–425, 1996.
http://dx.doi.org/10.1016/S0065-2717(08)70143-6

[6] Minkowycz, W.J., Sparrow, E.M. & Murthy, J. (eds), *Handbook of Numerical Heat Transfer*, John Wiley & Sons: New York, 2006.

[7] Icoz, T. & Jaluria, Y., Design of cooling systems for electronic equipment using both experimental and numerical inputs. *ASME Journal of Electronic. Packaging*, **126**(4), pp. 465–471, 2004.
http://dx.doi.org/10.1115/1.1827262

[8] Paek, U.C., Free drawing and polymer coating of silica glass optical fibers. *Journal of Heat Transfer*, **121**(4), pp. 774–788, 1999.
http://dx.doi.org/10.1115/1.2826066

[9] Eversteyn, F.C, Severin, P.J.W., Brekel, C.H.J. & Peek, H.L., A stagnant layer model for the epitaxial growth of silicon from silane in a horizontal reactor. *Journal of Electrochemical Society*, **117**(7), pp. 925–931, 1970.
http://dx.doi.org/10.1149/1.2407685

[10] Roache, P.J., *Verification and Validation in Computational Science and Engineering*, Hermosa Publishers: Albuquerque, New Mexico, 1998.

[11] Zhao, H., Icoz, T., Jaluria, Y. & Knight, D., Application of data driven design optimization methodology to a multi-objective design optimization problem. *Journal of Engineering Design*, **18**(4), pp. 343–359, 2007.
http://dx.doi.org/10.1080/09544820601010981

[12] Cheng, X. & Jaluria, Y., Optimization of a thermal manufacturing process: drawing of optical fiber. *International Journal of Heat and Mass Transfer*, **48**(17), pp. 3560–3573, 2005.
http://dx.doi.org/10.1016/j.ijheatmasstransfer.2005.03.012

[13] Lin, P.T., Gea, H.C. & Jaluria, Y., Systematic strategy for modeling and optimization of thermal systems with design uncertainties. *Frontiers in Heat Mass Transfer*, **1**(1), p. 013003, 2010.
http://dx.doi.org/10.5098/hmt.v1.1.3003

[14] Moore, F.K. & Jaluria, Y., Thermal effects of power plants on lakes. *Journal of Heat Transfer*, **94**(2), pp. 163–168, 1972.
http://dx.doi.org/10.1115/1.3449888

[15] Kirillin, G., Shatwell, T. & Kasprzak, P., Consequences of thermal pollution from a nuclear plant on lake temperature and mixing regime. *Journal of Hydrology*, **496**, pp. 47–56, 2013.
http://dx.doi.org/10.1016/j.jhydrol.2013.05.023

[16] Joshi, Y. & Kumar, P. (eds), *Energy Efficient Thermal Management of Data Centers*, Springer: New York, 2012.
http://dx.doi.org/10.1007/978-1-4419-7124-1

[17] Le, K., Zhang, J., Meng, J., Bianchini, R., Jaluria, Y. & Nguyen, T.D., Reducing electricity cost through virtual machine placement in high performance computing clouds, SC11. *Proceedings of 2011 International Conference for High Performance Computing, Networking, Storage and Analysis. ACM) Conference*, Seattle, WA, USA, 2011.