COMBINED EXPERIMENTAL AND NUMERICAL APPROACH TO MODEL, DESIGN AND OPTIMIZE THERMAL PROCESSES

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ABSTRACT

This paper focuses on combined experimental and numerical approaches to model thermal processes and obtain accurate results on system behaviour and performance. Interest lies in obtaining repeatable and dependable inputs for choosing appropriate conditions and parameters for enhancing the efficiency and the desired output. These results can also form the basis for system design and optimization. Several fundamental and practical problems are considered and typical results presented to discuss the implications and applications of this methodology. Circumstances where experimental data are used to validate the model, provide greater physical insight and define the boundary conditions, thus allowing the numerical simulation to be carried out, are also presented. Results from a concurrent, or parallel, simulation and experimentation approach are also presented to indicate the usefulness of such a strategy. It is stressed that experimental data are indispensable in obtaining accurate and realistic results for complex practical problems involving thermal transport processes.

Keywords: combined approach, concurrent, experiment, inverse problem, numerical, thermal processes, thermal systems

1 INTRODUCTION

Thermal systems and processes are of interest in a wide range of applications, from manufacturing and transportation to thermal management of electronics, environmental control, and power generation. Because of the complexity of these systems, arising from material property variations, complicated domains, combined transport mechanisms, turbulent flow and other aspects, numerical modeling is needed to study, predict, design and optimize [1–3]. However, in many cases, experimental inputs are essential to completing the modeling effort and a combined experimental–numerical approach is valuable in obtaining accurate and dependable results. Experimental data are critical to the validation of the mathematical and numerical model and to the establishment of the accuracy and predictability of the numerical simulation. This is particularly important for complex transport processes that arise in most practical thermal systems [4].

Experiments are also needed for the determination of material properties that are crucial to any accurate simulation. In many important thermal processes, the boundary conditions are not known or well defined. Numerical determination of the boundary conditions may also be quite involved as is the case in conjugate problems. In such cases, experimental work can be used to provide the appropriate boundary conditions that may be applied for the simulation. An inverse problem must often be solved, using both the experimental data and the numerical model, to obtain the appropriate boundary conditions and solve the problem. Also, there are many problems in which experimentation is particularly suitable over given parametric ranges, while numerical simulation is more appropriate over other regions. For instance, turbulent flow and contact resistance are better treated experimentally than by analysis. Then, a

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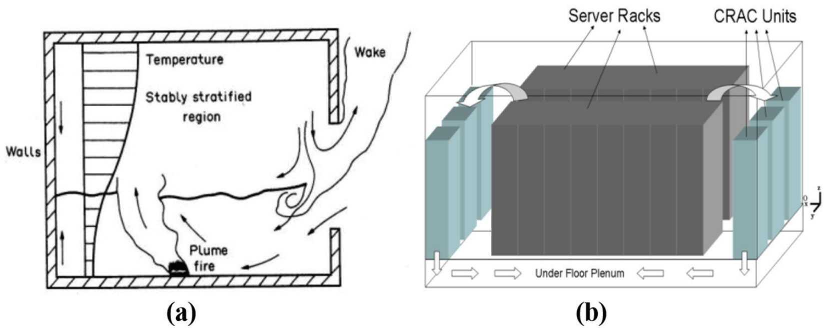


Figure 1. Examples of thermal systems: (a) Room with a fire; (b) Typical data center.

concurrent, parallel, experimental and numerical approach may be used to solve the problem more efficiently and accurately.

Of particular interest in this paper are the following aspects of a combined numerical and experimental approach:

- Validation
- Experimentally obtained boundary conditions
- Solution of inverse problems with experimental inputs
- Use of experimentation in model development
- Concurrent simulation and experimentation

All these are important in obtaining an accurate, efficient and realistic modeling and simulation of thermal processes and systems.

Figure 1 shows two common thermal systems in which experimentation and numerical simulation may be used to provide the inputs for design and for understanding the basic processes involved. The systems shown include a room with a fire, which has a stratified hot upper layer generated in the room due to the fire plume and flow exchange through an opening, and a typical data center, which involves electronic components, racks, servers and cooling arrangements [5]. Because of the various complexities mentioned earlier, an accurate study of the basic processes and of the system in these and other practical problems requires a strong coupling between experimentation and numerical simulation.

2 VALIDATION

An extremely important consideration in the modeling and simulation of thermal processes and systems is that of validation because of the simplifications used to treat various complexities. It is necessary to ensure that the numerical code performs satisfactorily and that the model is an accurate representation of the physical problem [6]. A consideration of the physical behavior of the results obtained is used to ensure that the results and trends are physically reasonable. Comparisons with available analytical and numerical results, particularly benchmark solutions, can then be used for validation of the mathematical and numerical models. Comparisons with experimental results are obviously desirable and it may become necessary to develop an experimental arrangement for providing data for validation. Figure 2 shows the validation of the mathematical and numerical model for the chemical vapor deposition (CVD) system shown.

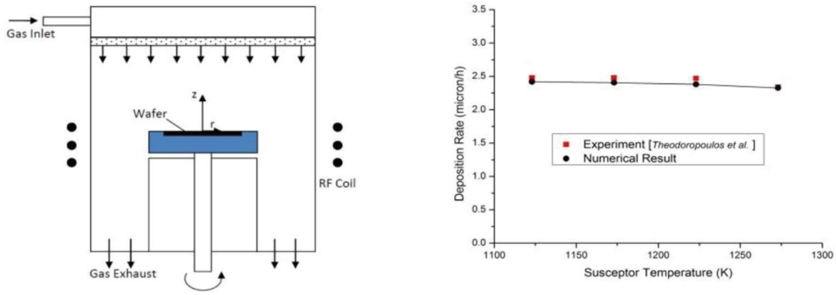


Figure 2. Schematic of a vertical rotating disk reactor along with numerical and experimental results on deposition rate.

The governing equations are the fluid flow and convective heat transfer equations with variable properties, along with chemical reactions and species equations. These may be given as:

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

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

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

where ρ, C_p, k and β are the density, specific heat at constant pressure, thermal conductivity and coefficient of volumetric expansion, $\bar{V}$ the velocity vector, $\dot{Q}$ thermal energy source per unit volume, T the temperature, t the time, p the pressure, and $\bar{F}$ 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 if the fluid characteristics are known, yielding Navier–Stokes equations for common Newtonian fluids like air and water, often employed in cooling of electronic systems.

The species equations and chemical kinetics are given in terms of concentration ω, diffusion coefficient D, rate constant K and partial pressure p by

$$\frac{\partial(\rho u_j \omega_i)}{\partial x_j} = \frac{\partial}{\partial x_j}(\rho D_{ij}\frac{\partial \omega_i}{\partial x_j}) \quad (4)$$

$$K = \frac{K_o p_{SiH4}}{1 + K_1 p_{H2} + K_2 p_{SiH4}} \quad (5)$$

where the last equation is for silicon deposition. Usually, the problem is a very complicated one [7] and involves large number of chemical equations and species for the deposition of materials like gallium nitride, which is case in this example [8]. The figure shows good agreement between experimental and numerical results. Validation thus becomes critical for accurate and dependable results in practical processes and systems.

3 RESULTS AND DISCUSSION

A few results are presented to illustrate the application of combined experimental and numerical simulation to address the various aspects mentioned earlier. Only a brief discussion is given here and additional details may be obtained from the references given.

Experimentally obtained boundary conditions. In this case, the boundary condition is obtained experimentally because of the complicated nature of the analysis needed to determine it. Examples are the shape and dimensions of the dynamic meniscus in surface coating as the material plunges into a liquid [9]. This meniscus is determined experimentally and is then used as an input into the numerical model. Similarly, the temperature distribution at the surface of a CVD susceptor, or wafer, such as in the system shown in Fig. 2, depends on the heat flux, conduction heat transfer, convection at the surface, geometry, etc. It is more accurate and simpler to measure it experimentally, as shown in Fig. 3 for a vertical impinging CVD reactor [10]. With the measured temperature distribution provided as input to the numerical model, the results on flow, thermal field and deposition rate may be obtained for various operating conditions and design parameters. A few results are shown in Fig. 3 to indicate the dependence of deposition rate on inlet velocity and on the inflow concentration of the reactants. Similarly, other results may be obtained and the system can be optimized for high product quality at acceptable deposition rates.

Solution of inverse problems with experimental inputs. There are circumstances where experiment data can be obtained over only a limited region because of access, time or other limitations. In such cases, numerical modeling and experimentation may be used together to solve an inverse problem in order to define and quantify the boundary conditions and then proceed to the numerical simulation of the complete problem [11,12]. An example of this

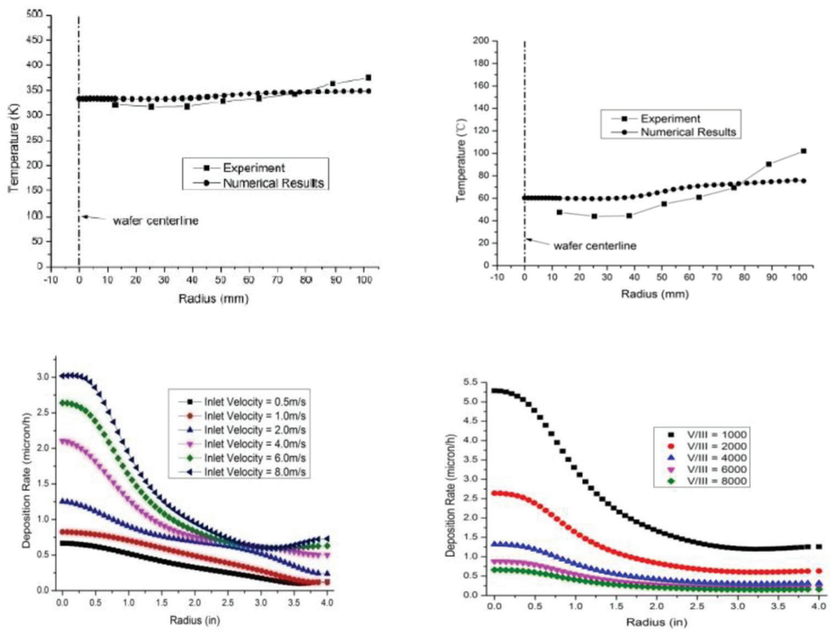


Figure 3. Measured susceptor temperature with no flow and no rotation (top left) and with 1 m/s inlet flow with rotation at 60 rpm (top right), along with calculated results on deposition rate at 600 rpm.

problem is given in Fig. 4, which shows a heated jet in cross-flow. If limited data taken downstream can be used to determine the location and conditions at the inlet, it would allow the determination of, for example, a polluting source as well as the impact on the environment.

The temperature data obtained downstream in the flow is used to solve the inverse problem to determine the inlet velocity and temperature of the jet. Figure 4(b) shows the improvement

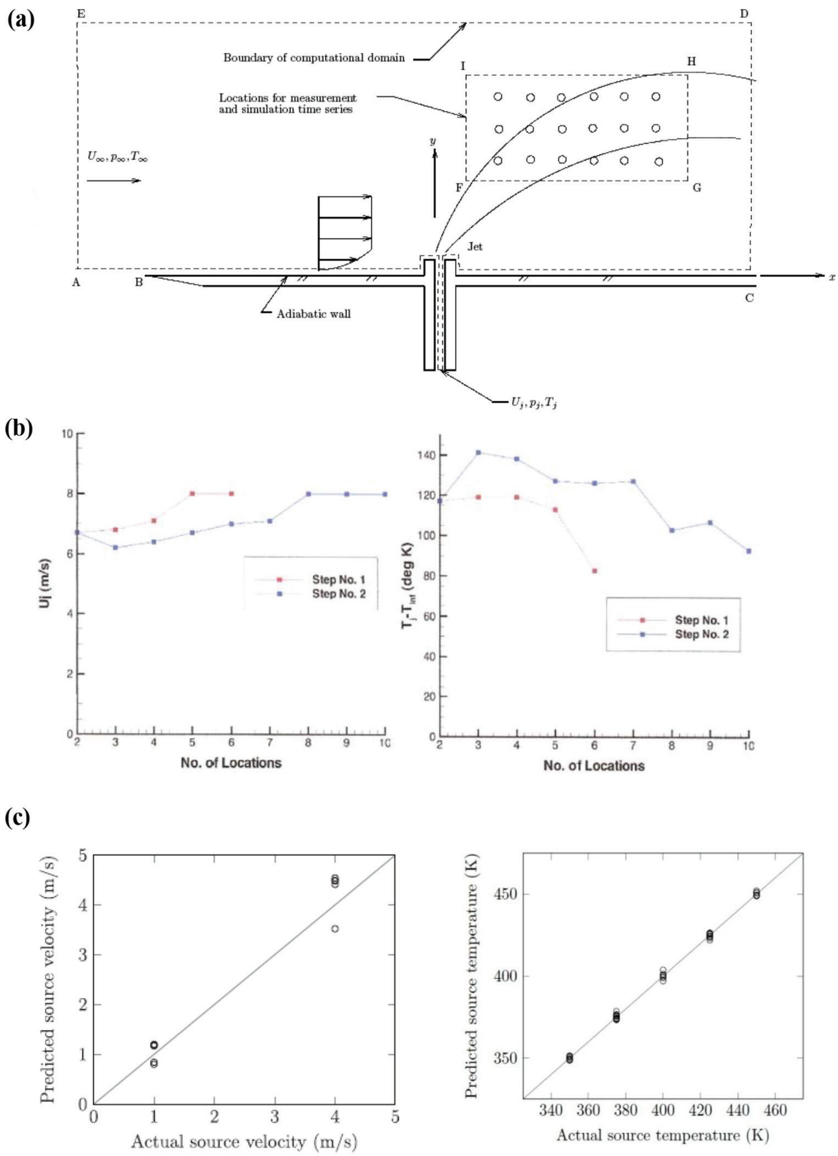


Figure 4. Inverse problem to determine jet inlet temperature and velocity from experimental data taken downstream. (a) Flow configuration; (b) Using experimental data to determine inlet conditions; (c) Accuracy of prediction.

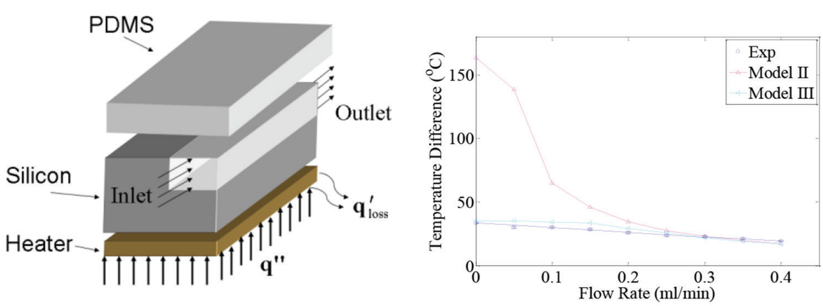
in the determination as more data points are used. Step 1 refers to only one unknown, with the other variable known, and step 2 refers to the case of both velocity and temperature as unknown. Figure 4(c) shows a comparison between actual values and predicted ones from the inverse solution. A good agreement is seen. This approach was also used for finite heat sources in a channel and for determining the temperature distribution at the wall of a furnace [13].

Use of experimentation in model development. This is a particularly important application of the combined experiment and simulation approach. It is frequently used in practical thermal systems for developing a valid, accurate and physically realistic model. Figure 5 shows an example of this approach by considering a microchannel flow for heat removal from an electronic chip. The experimental system is sketched in Fig. 5(a), indicating a heater and a silicon block containing the microchannel. Several models were considered for simulating the thermal processes involved [14]. These included microchannel flow with imposed boundary conditions, microchannel with the heater and the entire system. The last two are referred to as Model II and III, respectively. The experimental results were compared with the numerical results, as shown in Fig. 5(b). At high flow rates, both the models gave results which were very close. But, at low flow rates, Model II did not perform satisfactorily, indicating the need to model the entire system, as given by Model III. Similarly, in other applications, such as casting, models may be developed, going from simple models to fairly elaborate models, and the experimental data may be used to choose the appropriate model [15].

Another example is shown in Fig. 6, where the comparison between experimental and computed results, for two different heat input conditions in the system sketched in Fig. 6(a), are used to choose the appropriate boundary condition as adiabatic and thus develop a more realistic model for the system shown.

Concurrent simulation and experimentation. In the solution of practical thermal convection problems, it is often found that numerical simulation is particularly suitable over a certain domain, whereas experimentation is more appropriate and accurate over other domains. Then, the two could be used *concurrently* or in parallel to obtain a more efficient approach to solving the problem.

Conventional engineering design and optimization are based on sequential use of computer simulation and experiment, with the experiments generally being used for validation or for providing selective inputs, as discussed earlier. However, the conventional methods fail to use



(a) (b)

Figure 5. Sketch of a microchannel flow system for heat removal from an electronic chip and the experimental-numerical results on the temperature.

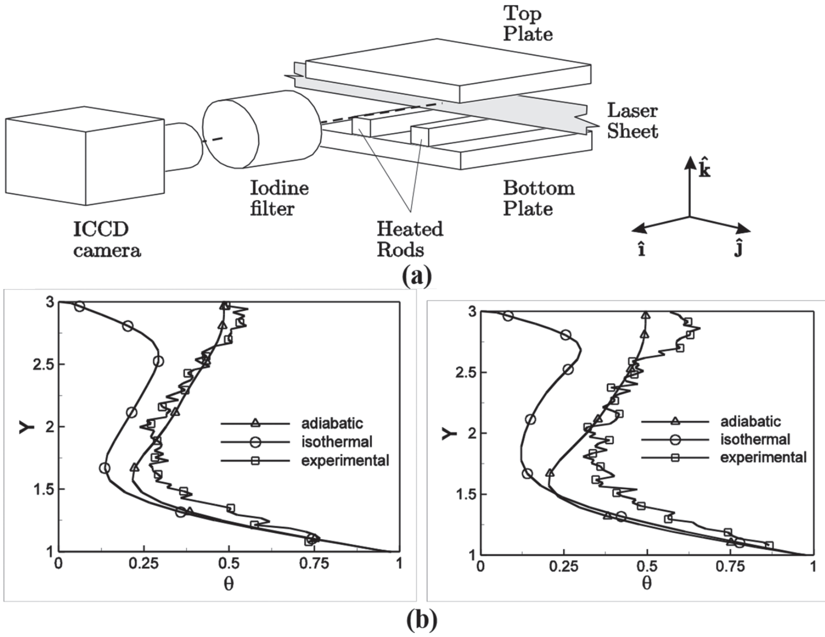
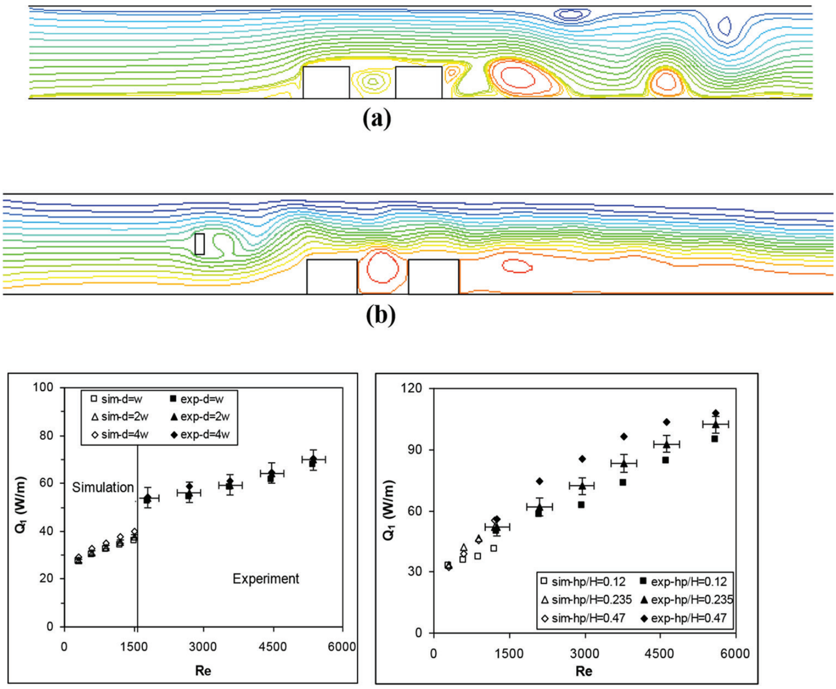


Figure 6. An experimental system for heat removal from two isolated heat sources that approximate electronic devices and comparison between experimental and numerical results to determine the correct boundary condition.

the advantages of using experiment and simulation concurrently in real time. Numerical simulation can easily accommodate changes in geometry, dimensions and material, whereas experiments can more conveniently study variations in the operating conditions such as flow rate, imposed pressure and heat input. Also, laminar and stable flows can be simulated conveniently and accurately, whereas transitional and turbulent flows are often more accurately investigated experimentally. By using concurrent numerical simulation and experimentation, the entire domain of interest can be studied for system design and optimization efficiently and accurately. This is the main motivation for this approach.

A simple physical system, consisting of multiple isolated heat sources, which approximate electronic components, located in a horizontal channel in a two-dimensional configuration, with or without a vortex generator to enhance heat transfer, is considered. Figure 7(a) and (b) shows the computed streamlines in the two cases. Numerical and experimental methods are used concurrently to study a wide range of design variables and operating conditions. The temperature and velocity distributions, the heat removal rates and pressure drop are calculated for laminar flows, as well as the beginning of oscillatory flow. Experiments are used for translational and turbulent flows. The first part of the simulation results deals with the determination of the critical flow conditions up to which numerical simulation can be used satisfactorily.

Figure 7(c) and (d) shows the results for a wide range of conditions with and without a vortex generator, respectively. The heat transfer from the first heat source facing the incoming flow is plotted against the Reynolds number Re based on channel height. The results at small values of Re, up to transition, are based on laminar flow calculations, whereas the results at



(c) (d)

Figure 7. Concurrent experimentation and numerical simulation. (a) Computed streamlines for isolated heat sources in a channel; (b) Computed streamlines for isolated heat sources in a channel with a vortex generator; (c) and (d) Numerical and experimental results on heat transfer from the first source for (a) and (b).

larger Re are experimental ones shown with error bars. First, validation of the model is easily established. The results, which cover a wide range of Re and other parameters, are obtained efficiently by selectively using simulation and experimentation. Then the results are used for design and optimization of the system to maximize the heat transfer while keeping the pressure head within acceptable limits [16–18].

4 CONCLUSIONS

Experimentation is needed in various thermal processes and systems in order to provide the inputs needed for accurately defining the boundary conditions, simplifying the modeling and obtaining results over regions where simulation is inaccurate, inconvenient or inefficient. In addition, experimental data are needed for the validation of the models used. This paper presents various circumstances where the numerical simulation may be efficiently combined with experimentation, and indeed driven by experimental data, to obtain accurate, valid and realistic numerical predictions. Several examples of such problems are given and the difficulties with specifying the boundary conditions as well as with simulating the entire domain for design and optimization are outlined. Approaches for using experimental data driven simulation in such cases are discussed and results are presented for some simple and complex problems. It is shown that such approaches are critical to an accurate numerical simulation in many cases of practical interest.

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