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Effect of Uncertainties in the Simulation and Design of Thermal Systems

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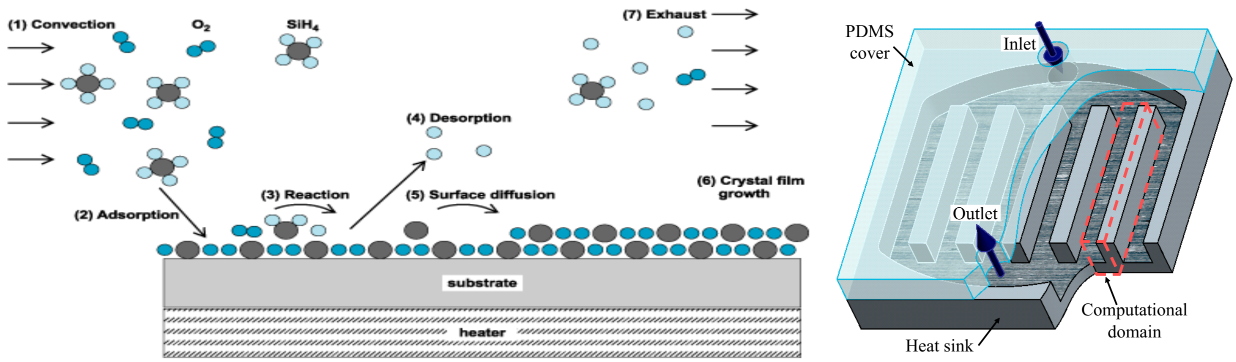
Abstract – In most studies on the simulation, design and optimization of thermal processes and systems, wide ranges of the governing parameters are considered with definite values given to the different parameters. This results in a deterministic simulation, which could then form the basis for deterministic design and optimization of the system. However, uncertainties arise in realistic circumstances due to variations in the operating conditions, errors in material properties, changes in the ambient conditions and variations in the gases and raw materials used in the process. Such uncertainties can have a significant effect on the operation and design of the system. Minor variations in the design variables or operating conditions may lead to system failure and thus impact the reliability of the system or process. Therefore, it is important to include the effect of uncertainties to obtain a reliable and realistic system. In this paper, uncertainties in two thermal systems are considered. The optimal points with and without uncertainties are obtained. For multi-objective optimization, Pareto frontiers, which represent a set of nondominated designs where one objective cannot be improved without detriment to another objective, are determined and compared with those for the deterministic cases. The results demonstrate the importance of uncertainties in system simulation and design. This approach thus provides more reliable and realistic solutions than if the uncertainties are neglected. This basic approach may be extended to the design and operation of other thermal problems and processes.

***Keywords*:** Uncertainties, reliability, optimization, thermal systems, simulation, design

1. Introduction

Modelling and simulation of thermal processes and systems are extensively used for the prediction, control, design and optimization of the process or the system. Typically, different values of the governing parameters like dimensions, materials and geometry, as well as operating conditions like heat input, flow rate, pressure and temperature, are chosen to determine the thermal behaviour of the system. The detailed results on the effect of various parameters are then employed to design and optimize the system or to choose appropriate operating conditions for the desired output or product characteristics. However, in realistic situations, the parameters are not completely known or fixed. Variations and fluctuations may occur, leading to uncertainties. For instance, if the heat flux input in an electronic component is specified at a given value, there may be variations due to fluctuations in the current or the electrical load. Similarly, a given flow rate of the coolant in a cooling system will typically fluctuate around a given mean value. Material properties are generally specified. But there are often uncertainties associated with the chosen values. Essentially all design parameters and operating conditions are subject to uncertainties, which must be considered because the failures of a given thermal system can be dangerous and expensive.

This paper is focused on the importance and effect of uncertainties on the simulation, design and optimization of thermal systems, i.e., systems in which heat and mass transfer and fluid flow are the dominant considerations. Thermal systems arise in a wide range of practical applications such as manufacturing, thermal management of electronics, power plants, aircraft and rocket engines, heat exchangers and heating/cooling systems. This paper considers two such systems for a study on uncertainties. One is a chemical vapor deposition (CVD) system for the fabrication of thin films and the other is a microchannel cooling system for an electronic chip. These two systems, as sketched in Figure 1, are studied and optimized under uncertainties in operating conditions and design variables. Numerical simulations are carried out to study the resulting heat and mass transfer and flow behaviour. The standard derivations for the variables, which are assumed to follow normal distributions, are taken as 5% or 10% of the mean values. The acceptable probability of failure is chosen as 0.13%, which is the usually accepted level in reliability studies. The basic approach is outlined and typical results on the simulation and design optimization are presented to indicate the effect of uncertainties.



(a) (b)

Fig. 1: (a) Chemical vapor deposition system for the fabrication of thin Silicon films; (b) A microchannel system for thermal management of an electronic component

2. Deterministic Simulation and design

The systems under consideration are modelled and simulated to obtain the resulting heat transfer, flow, temperature distribution and deposition. The basic equations that describe these processes are the usual continuity, momentum force balance and energy equations, that are not given here due to space limitations. These equations are solved numerically for the microchannel flow and heat transfer. For CVD, these equations are the same, but an additional equation for mass transfer in terms of the mass fraction of the species *m* is needed and may be written as

$$\rho \nabla \cdot (\vec{v} m) = \nabla \cdot (\rho D \nabla m) + R \tag{1}$$

where *R* is the production rate of the species. For the fabrication of silicon films, as sketched in Fig. 1 (a), the chemical reaction that provides the solid silicon that deposits on the heated substrate is

$$SiH_4(gas) \rightarrow SiH_4(absorbed) \rightarrow Si(Deposited) + 2H_2 \tag{2}$$

The chemical kinetics of this reaction is given in terms of the partial pressures as

$$K = \frac{K_o p_{SiH4}}{1 + K_1 p_{H2} + K_2 p_{SiH4}} \tag{3}$$

where the p's are the partial pressures of the two species in the reactor, K is the surface reaction rate in mole of Si/m^2s, K_o = A exp (-E/RT), E being the activation energy, and A, K_1, and K_2 are constants which are obtained experimentally [1]. The chemical kinetics for other materials like gallium nitride, silicon carbine and titanium nitride are available in the literature.

Employing these equations, the deposition rate of silicon at various locations on the substate may be determined at different values of the inlet flow rate of precursor gases, susceptor temperature, pressure, and inlet gas concentration. The process is treated as steady, with the time over which the process occurs used to determine the film thickness at any given location. The model is validated by comparisons with experiments [1]. Since the values of the various parameters are specified, this numerical modelling results in a deterministic simulation. The two main objectives are deposition rate and film uniformity, given by the percentage working or acceptable area that meets the given requirements. We can fix one of these and find the optimal conditions for maximizing the other. We can also solve a multi-objective optimization problem to obtain a Pareto front that shows a trade-off between the two.

In a similar way, the microchannel cooling system is considered to obtain the heat transfer, pressure drop, and hot spot temperature. The two main objectives are heat transfer rate and pressure or pumping power. The design parameters are materials, geometry and dimensions, and the operating conditions are heat flux input and flow rate. Again, the problem is solved for various values of these parameters to obtain a deterministic simulation. The simulation results are employed to optimize the system to maximize the heat transfer, minimize the pressure or obtain a Pareto frontier that gives the trade-off between these two objectives.

3. Results with Uncertainties

Some of the major uncertainties that arise in the CVD process are:

Uncertainties in Operating Conditions

Inlet velocity or flow rate; Susceptor temperature or heat flux input; Inlet mass fractions of reactive gases; Reactor pressure; susceptor rotational speed for impingement-type CVD reactor

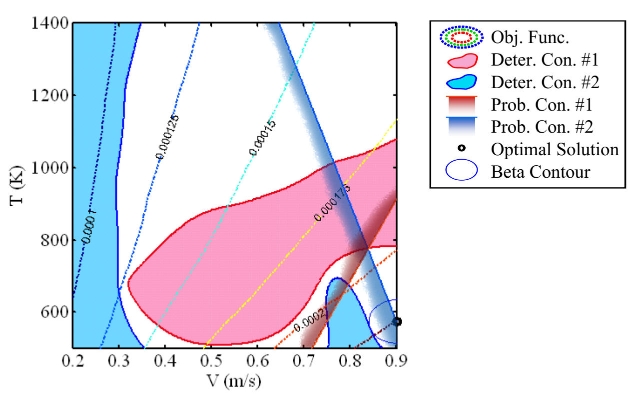
Uncertainties in System Design

Dimensions; Geometry; Inlet configuration; Material and gas properties

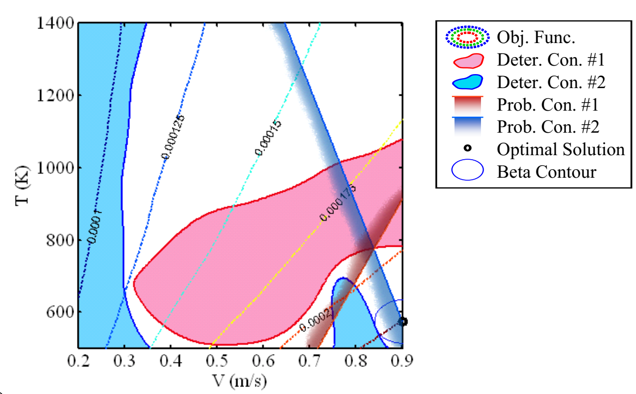
Similarly, uncertainties that arise in the microchannel system are in the flow rate, heat flux input, material properties, ambient conditions and dimensions, though the uncertainty in the last one is usually negligible. The final design or optimal operation of these systems must therefore address the uncertainties in the main design variables and operating conditions. This will ensure a realistic and reliable system, with a low probability of failure.

It is seen that, in practical applications, uncertainties in the design variables or in the operating conditions are unavoidable. Moreover, an optimal design guided by deterministic optimization might not be reliable enough to survive the range of working conditions. An optimization formulation that handles design uncertainty is generally named reliability based design optimization (RBDO) or probabilistic optimization [2]. The two main approaches that may be adopted are the performance measure approach (PMA) that is shown to be more robust compared to the more common reliability index approach (RIA). Details are given in Refs. [3, 4]. Uncertainties have been considered in only a few systems [5, 6] and the overall work done on reliability optimization in thermal systems is minimal.

A systematic strategy of thermal system modelling and optimization including the effects of uncertainties has been presented [7]. Focusing on objectives such as percentage working area (PWA) and mean deposition rate (MDR), the Reliability-Based Design Optimization (RBDO) algorithms are employed, using a modified RIA approach. Probabilistic constraints are established with respect to either normally or non-normally distributed random variables and optimal solutions are obtained subject to the allowable level of failure probability. Figure 2 shows a sample of results for different constraints, with normal distribution of the variables. In the first case, deposition rate is fixed and the percentage working area is maximized. In the second case, the deposition rate is maximized keeping the percentage working area fixed. Deterministic



(a)

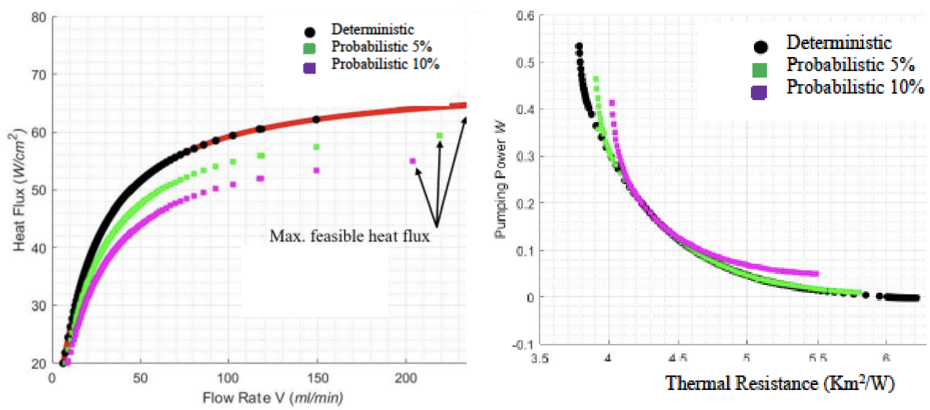


(b)

Fig. 2. (a) Maximizing PWA with fixed MDR; (b) Maximizing PWA with fixed MDR, with uncertainties in variables.

constraints are given on the root mean square and kurtosis of the film thickness, thus quantifying its quality. Probabilistic constraints are shown. The failure is brought down to less than 0.13%, which is the accepted level in RBDO. Due to the uncertainties, the optimal point moves from that obtained from the deterministic design to satisfy this condition. Without uncertainties, the failure rate was over 40% in both the cases shown in the figure and, by including uncertainties, a more realistic and practical optimal design is obtained. Further details are given in [7] and other references on reliability-based design are also given in this paper. This aspect has only recently been incorporated in the design and optimization of thermal systems.

A similar study is carried out on the microchannel cooling system, using the PMA approach for the reliability-based design. Figure 3 shows some typical results obtained. Figure 3 (a) shows the heat flux that can be removed with different levels of uncertainties in the flow rate. The points shown in the different curves refer to Pareto frontiers. The maximum heat flux that can be removed with a given constraint on the pressure input is shown for 3 different levels of normally distributed uncertainties. Figure 3 (b) shows the corresponding Pareto fronts, indicating the trade-off between the heat removed and the pressure needed. Using these results, a reliable and robust design or operating condition can be obtained so that the failure is less than 0.13%.



(a) (b)

Fig. 3: (a) Heat flux removed as a function of flow rate; (b) Pareto frontiers at different uncertainties in the flow rate.

4. Conclusions

This paper focuses on uncertainties that arise in essentially all practical thermal processes and systems due to fluctuations in the operating conditions, variations in properties and changes in the design parameters. Two important thermal systems are considered and the approach to obtain a reliability-based design optimization to address the uncertainties is outlined. The resulting design has an acceptable level of failure and thus provides a realistic and reliable design. The importance of uncertainties and the need to include their effect on design and optimization are presented and discussed.

References

[1] Y. Jaluria, *Advanced Materials Processing and Manufacturing.* Cham, Switzerland: Springer, 2018.

[2] Agarwal, N. and N. R. Aluru, “A domain adaptive stochastic collocation approach for analysis of MEMS under uncertainties,” *J. Comput. Physics*, vol. 228, pp. 7662-7688, 2009.

[3] Tu, J., K. K. Choi and Y. H. Park, “A new study on reliability-based design optimization,” *J. Mech. Design*, vol. 121, pp. 557-564, 1999.

[4] P. George, J. Meng, and Y. Jaluria, “Optimization of the chemical vapor deposition process for gallium nitride, in *Proc. Int. Heat Transfer Conf.,* Kyoto, Japan, pp 10-15, 2014.

[5] B.D. Youn and K. K. Choi, “Selecting probabilistic approaches for reliability-based design optimization,” *AIAA journal*, vol. 42, pp. 124-131, 2004.

[6] S.K. Sarangi, K. K. Bodla, S. V. Garimella and J. Y. Murthy, “Manifold microchannel heat sink design using optimization under uncertainty,” *Int. J. Heat Mass Transfer*, vol. 69, pp. 92-105, 2014.
[7] P.T. Lin, H.C. Gea and Y. Jaluria, Y., “Systematic strategy for modelling and optimization of thermal systems with design uncertainties, *Frontiers Heat Mass Transfer*, Vol. 1, pp. 013003-1-20, 2010.