Monte-Carlo based Uncertainty Analysis For CO₂ Laser Microchanneling Model

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Abstract. CO₂ laser microchanneling has emerged as a potential technique for the fabrication of microfluidic devices on PMMA (Poly-methyl-meth-acrylate). PMMA directly vaporizes when subjected to high intensity focused CO₂ laser beam. This process results in clean cut and acceptable surface finish on microchannel walls. Overall, CO₂ laser microchanneling process is cost effective and easy to implement. While fabricating microchannels on PMMA using a CO₂ laser, the maximum depth of the fabricated microchannel is the key feature. There are few analytical models available to predict the maximum depth of the microchannels and cut channel profile on PMMA substrate using a CO₂ laser. These models depend upon the values of thermophysical properties of PMMA and laser beam parameters. There are a number of variants of transparent PMMA available in the market with different values of thermophysical properties. Therefore, for applying such analytical models, the values of these thermophysical properties are required to be known exactly. Although, the values of laser beam parameters are readily available, extensive experiments are required to be conducted to determine the value of thermophysical properties of PMMA. The unavailability of exact values of these property parameters restrict the proper control over the microchannel dimension for given power and scanning speed of the laser beam. In order to have dimensional control over the maximum depth of fabricated microchannels, it is necessary to have an idea of uncertainty associated with the predicted microchannel depth. In this research work, the uncertainty associated with the maximum depth dimension has been determined using Monte Carlo method (MCM). The propagation of uncertainty with different power and scanning speed has been predicted. The relative impact of each thermophysical property has been determined using sensitivity analysis.

Keywords: PMMA, uncertainty, sensitivity, microchanneling, laser

1. Introduction
Polymer based microfluidic devices are used in many applications like flow cells, electrophoresis devices, PCR (polymer chain reaction) devices apart from many other chemical and biological applications. These devices mainly consist of microchannels of different shape and sizes according to their nature of application. Among the several available polymers, PMMA has emerged as a potential alternative for microfluidic device fabrication. The usual advantages of PMMA includes high optical transparency, biocompatibility, lower cost and inertness to many reactive gases and chemicals. When subjected to UV (ultra-violet) lasers and mid IR (infra-red) lasers, they result in cleaner cuts and therefore, can be fabricated easily using laser micromachining systems [1].

PMMA based microfluidic systems can be fabricated using several methods like lithography, embossing, injection molding, micromilling and laser micromachining. However, most of these processes suffer from high input cost, skilled labor requirements, clean room facilities, large time consumption and process complexity. Laser micromachining has come up as a single step processing solution for microchannel fabrication on polymers. Ultrashort lasers (femtosecond and
picosecond), UV lasers and CO\(_2\) lasers have been proved to be specially suitable for fabricating microchannels on PMMA based devices. Though ultrashort lasers and UV lasers remove material by the process of cold ablation with minimum HAZ (Heat affected zone), they inherently suffer from high initial cost and sophisticated beam optics [2].

With the advent of low cost hobbying CO\(_2\) lasers, the cycle time of production of these PMMA based microfluidic devices has been reduced [3]. CO\(_2\) laser has presented itself as a cost effective alternative to costly ultrashort laser systems and UV lasers. Beside being easy to operate and lower maintenance cost, it also possesses simple optics and do not require the clean room facilities. Since the laser ablation method is thermal in nature, the only problem associated with CO\(_2\) laser is heat related defects i.e. melting and resolidification and swelled heat affected zone. However, a number of authors have successfully used the CO\(_2\) laser for microchannel fabrication on PMMA since material removal takes place mostly by direct vaporization rather than involving significant melting and resolidification.

One of the most important feature of microchannel is depth at its center. In any fabrication process controlling of depth dimension is essentially required which varies according to nature of application of microfluidic devices. There are few analytical models available for predicting the microchannel depth and cut channel profile for CO\(_2\) laser ablated PMMA. All of these models are primarily based on conservation of energy principle. All of these models also state that maximum depth of the CO\(_2\) laser etched PMMA microchannels is dependent upon the values of thermophysical properties (enthalpy, beam absorptivity and material density) and laser beam parameters (beam diameter, power and scanning speed). Though the laser beam parameters are generally constant for particular type of laser, the values of thermophysical parameters of PMMA are quite variable. In fact, the values of these thermophysical properties can significantly differ and largely depends on way of manufacturing [3]. In the condition of unavailability of exact values of these thermophysical properties, the final output depth may differ considerably from the predicted result. An improper control over the depth dimension can cause major obstacle towards utility of CO\(_2\) laser as a fabrication tool despite all other advantages.

Uncertainty analysis deals with the uncertainties in the value of input parameters to be propagated through calculations, in order to determine the uncertainty in the output parameters. Uncertainty analysis, when applied in initial planning phase can save time, money and embarrassment to the experimentalist [4]. In other terms, it basically states the reliability of the given model for predicting certain output. The propagation of uncertainty with different input variables can be quantified which helps in determining the acceptable limit of the predicting model in such cases. Monte-Carlo method is one of the most acceptable and reliable technique to determine the uncertainty of the parameters. Monte-Carlo simulation is an iterative technique for investigating the physical systems utilizing stochastic techniques. It basically determines the tolerances of output parameters on both sides.

In this work, sensitivity analysis has been applied and influence of each parameter has been discussed. The influence of their associated uncertainty on the total uncertainty has also been detailed. The application of sensitivity analysis for different manufacturing and design processes is not new. Sensitivity analysis has been an important statistical analyzing tool and has been used by various authors for different processes viz. laser welding [5], submerged arc welding [6] and laser micro-drilling [7] etc. Uncertainty for a laser tissue interaction model for predicting temperature and thermal dose was carried out by Jain et al. utilizing Monte-Carlo simulation [8]. They also determined the sensitivity of different input parameters. However, uncertainty analysis has not yet been carried out on laser microchanneling process. Such an analysis will help in applying depth prediction model in case of CO\(_2\) laser ablation since the uncertainty may exceed beyond acceptable limit if proper input variables are not used.
2. CO$_2$ laser ablation mechanism and energy based models

PMMA is a thermoplastic amorphous material. The thermal conductivity of PMMA is very low which results in high thermal diffusion time. Due to high thermal diffusion time, the heat remains accumulated in a local space for longer period of time. CO$_2$ laser ablation is a kind of pure thermal ablation in which material removal takes place due to localized heating, melting and vaporization. The energy gets stored locally as soon as it is deposited on the surface. PMMA (C$_5$O$_2$H$_8$)$_n$ decomposes into monomers, carbon dioxides, carbon monoxide and water. These byproducts are perfectly volatile in nature and results in formation of plumes around the microchannel. The cut microchannels are clean and ready to be usable for many microfluidic devices without any post-processing. Microchannels are an integral part of many microfluidic devices. CO$_2$ laser direct writing of microchannels is an utmost simple process involving laser system and substrate material (figure 1 (a)). For any microchanneling process, width, depth and heat affected zone (HAZ) or softened zone are three main output processes (figure 1 (b)).

There are few analytical models available for CO$_2$ laser etched microchannel depth prediction. These models are based on conservation of energy principle. Yuan and Das [9] have developed a model for depth prediction of microchannels for smaller depths (22 $\mu$m to 130 $\mu$m). According to Yuan and Das, the depth profile is given as:

\[ z = \frac{\alpha}{\rho \times H_v} \sqrt{\frac{1}{\pi w^2}} \frac{P}{U} e^{\frac{y^2}{y_{th}^2}} \]  

(1)

where $z$ is the laser etched channel’s depth, $\alpha$= absorptivity of the material for CO$_2$ laser wavelength, $\rho$ = density of the material, $H_v$ = enthalpy of vaporization, $P$ = average laser power, $w$ = original beam spot radius, $U$= scanning speed, $y_{th}$= threshold beam radius and $y$ is the distance from the center of the microchannel in width direction.

Romoli et al. [10], assumed the channel etched profile to be triangular for determining the maximum channel depth. The maximum channel depth was derived as:

\[ z = \frac{k\alpha}{\rho \times w} \frac{P}{U} - \frac{kQ_{th}}{\rho w^2} \]  

(2)

where $k$ is a constant related to the chemical bond energy of the polymer and $Q_{th}$ is threshold energy.

Prakash and Kumar [11] also developed an analytical model based on law of conservation of energy. The convection and radiation losses from the surface were ignored in this modeling.
Table 1. Input parameters.

| Parameters           | symbol | units       | parameter identification | values with uncertainty              |
|----------------------|--------|-------------|--------------------------|--------------------------------------|
| laser Power          | P      | Watt (W)    | constant                 | to be decided                         |
| scanning speed       | U      | mm/sec      | constant                 | to be decided                         |
| absorptivity         | α      | -           | variable                 | 0.92 [10], 0.95 [11]                  |
| density              | ρ      | Kg/m$^3$    | variable                 | 1070 [11], 1185 [13], 1190 [14], 1200 [15], 16 [16] |
| Enthalpy of          | $H_v$  | KJ/Kg       | variable                 | 2280 [16], 2150, 2035 [17], 2231 [11], 2757 [18] |
| vaporization         |        |             |                          |                                      |

The CO$_2$ laser beam was assumed to be perfect Gaussian in nature and circular in shape. The developed model’s predicted result were found to be close to actual microchannel depth for channels with wide depth variations (145 $\mu$m to 562 $\mu$m). According to Prakash and Kumar, maximum depth of the channel is given as:

$$z = \frac{\alpha}{\rho \times H_v} \sqrt{\frac{2}{\pi w^2}} P U$$  \hspace{1cm} (3)

Since this model was found to be covering wider ranges of depth dimension, it is used in this work for uncertainty and sensitivity analysis.

3. Uncertainty analysis

Uncertainty analysis determines the range representing the uncertainty in an output parameter due to noises associated with the input parameter values. Each output parameter depends upon many input parameters and the uncertainty in exact value of these variable input parameters finally leads to uncertainty in prediction of output parameters. The input parameters can be categorized into constant parameters and variable parameters. The value of constant parameters do not change with material. On the other hand, the values of variable parameters vary with different types of PMMA. In this research work, the uncertainties in input parameters were determined based on the published research. The input parameters and their associated noises are shown in table 1.

Laser power (Watt) and scanning speed (mm/s) are the most standard parameters in any laser machining operation. The depth of laser micromachined channel is directly dependent on both these parameters. In order to have microchannel dimensions in permissible range (in microns), the numerical values of laser power was taken as 1, 1.5 and 2 Watts as used by Prakash and Kumar [11] for uncertainty calculations. The scanning speed was varied at six different levels i.e. 10, 12, 14, 16, 18 and 20 mm/s for each power level selected. The values of scanning speed were chosen so as to ensure the output parameter value within the permissible limit of microchannels. Some of these values were taken from Prakash and Kumar [11]. The absorptivity of CO$_2$ laser beam for different grades of transparent PMMA do not vary much. Most of the available literature used either 0.92 or 0.95 as the beam absorptivity. The material density also varies (from 1070 Kg/m$^3$ to 1200 Kg/m$^3$) with different grades and types of PMMA. Enthalpy of vaporization varies from 2000 KJ/Kg to 2757 KJ/Kg as shown in table 1. All the variables were assumed to follow normal distribution.
3.1. Monte-Carlo method

Monte Carlo method (MCM) is a powerful simulation based technique for ascertaining uncertainty propagation. MCM is very commonly used to investigate and examine the physical and mathematical systems utilizing stochastic techniques. MCM is an iterative approach and is based on random number generation using computer program. For the problems involving uncertainty variations, Monte-Carlo approaches are known to be precise and accurate. In this method each variable is assigned some error within the estimated uncertainty in the variable. This error is chosen randomly based on the uncertainty distribution. MCM can be explained using the flow diagram as shown in figure 2.

A MATLAB program was created to run MC simulations and uncertainties were calculated at different laser power and scanning speed. Monte-Carlo method is an essential tool for determining the uncertainty propagation. For a precise mathematical model, Monte-Carlo method can be used to simulate the process as many times as required with variable randomness. Total 10,000 iterations were made for each simulation run. Independent random numbers were generated based on normal distribution for normally varying variables.

4. Sensitivity Analysis

In any experiment, it is very important to determine what are the more sensitive parameters that influence the outcome of the experiment. Sensitivity analysis indicates which variable requires more attention than other parameters and which are less important. The variance based sensitivity index is a model-free approach to determine the relative sensitivity of the input variables within a given space. According to this, the first order sensitivity index is given as [19]:

\[ S_{ix} = \frac{\partial r}{\partial x} \cdot \frac{\sigma_x}{\sigma_r} \]  

(4)
Where, r and x are output and input variables respectively and \( \sigma \) represents standard deviation. Sensitivity index is a dimensionless parameter. Larger is the sensitivity index, larger the sensitivity of the parameter towards output variable.

5. Result and discussion

The uncertainty propagation plot was generated using Monte Carlo method while assuming the input variables with normal distribution i.e. larger probability of lying around a central point. The propagation plot is shown in figure 3 (a), 4 (a), and 5 (a) for 1 W, 1.5 W and 2 W of laser power respectively. The propagation was visualized with varying scanning speed at six different levels (10, 12, 14, 16, 18 and 20 mm/s). In all three figures it was observed that physical contours of uncertainty decreases with increase in scanning speed. This is obvious since a decrease in scanning speed ultimately results in larger energy deposition resulting in larger maximum depth. The larger maximum depth involves larger uncertainty with it. The largest contour of uncertainty was observed in figure 5 with 2 W power and 10 mm/s scanning speed. This is also the power and scanning speed setting for maximum energy deposition within available range of parameters.

The histograms for maximum depth at different power and scanning speed settings have been shown in figure 3 (b), 4 (b), and 5 (b). The histograms clearly show that the average maximum depth was distributed over a wide range of scanning speeds in all three cases. Absolute uncertainty and percentage uncertainty were quantified using MCM and has been detailed in table.
2. The largest absolute uncertainty was found to be $\pm 46.85 \, \mu \text{m}$ at 2 Watt power and 10 mm/s of scanning speed. The minimum absolute uncertainty was $\pm 11.59 \, \mu \text{m}$ at 1 Watt power and 20 mm/s of scanning speed. Although, the absolute uncertainty varies with different power and scanning speeds, the percentage uncertainty dwells around 10% in all the cases. The percentage uncertainty was calculated using equation 5.

$$\text{Percentage uncertainty} = \frac{\text{Absolute uncertainty}}{\text{Maximum depth}} \times 100 \%$$

First order sensitivity index were calculated using equation 4 for each maximum depth value (table 3). Sensitivity index of enthalpy of vaporization was largest followed by density and absorptivity respectively. This is due to largest uncertainty associated with enthalpy of vaporization. The sensitivity index of absorptivity and density are quite small compared to enthalpy of vaporization in all the parameter settings. This is because the uncertainty in absorptivity and density are very small for all types of transparent PMMA for CO$_2$ laser machining. Also, since the material removal in microchannel fabrication scales to small weight loss, the density effect is small. Laser power and scanning speed can also be combined into one parameter as energy deposition. This ratio affects the laser microchanneling process as one parameter irrespective of different power and scanning speed values.

6. Conclusion

The property parameters of transparent PMMA are generally not readily available and one has to spend time and energy in its determination. However, the values of these properties lie within a certain range. The range of variation of these property values were identified from various available literature. The uncertainty associated with maximum depth prediction due to noises associated with input parameter values were assessed in this work. The maximum uncertainty was found to dwell around 10% which implies that in case of unavailability of correct values of input property parameters, the value of maximum depth may deviate to maximum 10% of predicted values. The histograms of maximum depth at different power and speed settings showed that the value varied uniformly between minimum and maximum scanning speeds. Absolute uncertainty was found to increase with increase in laser power and decrease with increase in scanning speed. It can be concluded that absolute uncertainty increases with increase in maximum depth value. The relative importance of input parameters towards uncertainty in output was examined using first order sensitivity index. The enthalpy of vaporization was found to be highly sensitive parameter compared to absorptivity and density. Based on this fact, it can be stated that noise in enthalpy of vaporization acts as the major factor responsible for overall
Table 2. Uncertainty in maximum depth.

| Power (W) | Scanning speed (mm/s) | Maximum depth (µm) | Absolute uncertainty (µm) | Percentage uncertainty (%) |
|-----------|-----------------------|--------------------|---------------------------|---------------------------|
| 1         | 10                    | 232.24             | 23.294                    | 9.986                     |
|           | 12                    | 193.53             | 19.3755                   | 9.968                     |
|           | 14                    | 165.89             | 16.6534                   | 9.995                     |
|           | 16                    | 145.15             | 14.4497                   | 9.911                     |
|           | 18                    | 129.02             | 12.8765                   | 9.936                     |
|           | 20                    | 116.12             | 11.5986                   | 9.945                     |
| 1.5       | 10                    | 348.36             | 34.9267                   | 9.982                     |
|           | 12                    | 290.30             | 29.1964                   | 10.013                    |
|           | 14                    | 248.83             | 25.0857                   | 10.037                    |
|           | 16                    | 217.72             | 21.833                    | 9.984                     |
|           | 18                    | 193.53             | 19.3251                   | 9.942                     |
|           | 20                    | 174.18             | 17.4284                   | 9.962                     |
| 2         | 10                    | 464.48             | 46.8588                   | 10.044                    |
|           | 12                    | 387.07             | 38.8462                   | 9.992                     |
|           | 14                    | 331.77             | 32.8725                   | 9.865                     |
|           | 16                    | 290.30             | 29.1007                   | 9.980                     |
|           | 18                    | 258.04             | 25.9151                   | 9.999                     |
|           | 20                    | 232.24             | 23.2784                   | 9.979                     |

Table 3. Sensitivity indexes of input variables.

| Power (W) | Scanning speed (mm/s) | Sensitivity index of α | Sensitivity index of ρ | Sensitivity index of H_v |
|-----------|-----------------------|------------------------|------------------------|--------------------------|
| 1         | 10                    | 0.09187                | 0.325904               | 5.71736                  |
|           | 12                    | 0.09167                | 0.328914               | 5.77392                  |
|           | 14                    | 0.09209                | 0.324386               | 5.69799                  |
|           | 16                    | 0.09275                | 0.329742               | 5.75608                  |
|           | 18                    | 0.09273                | 0.327746               | 5.74097                  |
|           | 20                    | 0.09148                | 0.325861               | 5.76178                  |
| 1.5       | 10                    | 0.09177                | 0.329964               | 5.73224                  |
|           | 12                    | 0.09152                | 0.330290               | 5.75370                  |
|           | 14                    | 0.09324                | 0.330106               | 5.78502                  |
|           | 16                    | 0.09135                | 0.323869               | 5.72811                  |
|           | 18                    | 0.09192                | 0.326219               | 5.74481                  |
|           | 20                    | 0.09252                | 0.326472               | 5.73244                  |
| 2         | 10                    | 0.09177                | 0.331513               | 5.77414                  |
|           | 12                    | 0.09152                | 0.326502               | 5.76369                  |
|           | 14                    | 0.09324                | 0.328735               | 5.77999                  |
|           | 16                    | 0.09241                | 0.327101               | 5.75724                  |
|           | 18                    | 0.09299                | 0.327971               | 5.79654                  |
|           | 20                    | 0.09252                | 0.325887               | 5.72482                  |
model uncertainty. Though, the input variables considered are limited, many more values may be acquired to make this model more fruitful.

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