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Rapid Prototyping Simulation: past, present and future

Abstract
The current process of adoption by companies of the new Rapid Prototyping (RP) techniques involve the careful assessment of a number of similar technologies. Each offers various levels of accuracy, mechanical strength, repeatability, speed and model usability. Current technology selection methods involve the assessment of competing claims, the reading of industrial case studies and the production of numerous benchmark models. Even when a technology offering the required technical capabilities is found, the learning curve required to produce useful models and the high costs of implementation may be too much to justify investment. Computer simulation is seen by the authors as one method that could aid this selection process, by providing a low-cost introduction or alternative to RP techniques for assessment, training and research.

The authors provide a broad definition of simulation along with the reasons behind the decision to apply numerical simulation techniques to a given problem. The paper then considers the simulation of one RP technique: stereolithography. We describe the development of this simulation and discuss briefly the computational methodology involved. We then describe the validation of the approach, and the power of the technique. The paper concludes with a brief discussion of future simulation development.

1.0 Introduction

Since its conception in the early 1980's and its subsequent commercialisation in the early 1990's, Rapid prototyping (RP) technology has been successfully adopted by many of the world's large engineering companies. These technologies, which allow complex three-dimensional models to be generated from a computer representation, have been shown to aid in the reduction of product development lead times and costs and in the improvement of product quality. Prototype models, which at one time required the skills and time of craftsmen, are now produced in a fraction of the time, at a fraction of the cost and without the need of a skilled hand, but with the required accuracy and mechanical properties needed of models in today's competitive climate.

There are currently a large number of these RP technologies available on a commercial basis. Each offering "faster model build times", "greater model accuracy", "improved repeatability" and "increased model functionality". Even companies offering machines with the same basic underlying technology, such as stereolithography , possess a bewildering range of process capabilities. It has been claimed that this wide choice tends to confuse the potential investor and, as mistakes can be costly, is currently acting as a barrier to the adoption of RP by smaller companies. Each vendor claims to meet every customers requirements, while offering machines at a wide variety of prices and using a range of model building techniques. Even when a technology offering the required technical capabilities is found, the learning curve required to produce useful models and the high costs of implementation may be too much to justify investment.

The simulation of these techniques on computer is seen as one method which may go some way in addressing these issues. Allowing potential investors and existing users of RP the ability to experiment with the parameters of a particular system prior to making a decision. A complete simulation package may, in the future, lead to a reduction in the time

taken to select a particular technology for a particular application as well as alleviating some of the uncertainty currently associated with RP investment.

This paper will begin with a general discussion of simulation, giving an idea of what a simulation consists of, the reasons for simulation and what problems and trade-offs have to be taken into consideration when developing and using a simulation package. The simulation of one RP technique, stereolithography, will then be discussed. The paper will chart the development of this simulation and will go on to describe briefly the computational methodology involved. The validation and the power of the developed model will then be described and the paper concludes with a brief discussion of future simulation development.

2.0 Simulation

2.1 Definition

A simulation of a system or an organism is the operation of a model or simulator which is a representation of the system or organism. This model is amenable to manipulations which would be impossible, too expensive or impractical to perform on the entity it portrays. The operation of the model can be studied and, from it, properties concerning the behaviour of the actual system or its subsystems can be inferred. [1]

Shubik's definition of simulation (above) although a good 35 years old, is still appropriate for most simulation projects of today. It describes essentially a technique that involves setting up a model of a real situation and then performing experiments on that model. However, with the advent and technological development of the modern digital computer over the last three decades, simulation has tended to be regarded as less of a laboratory-based process of test tubes, Bunsen burners and stopwatches and more of a highly efficient numerical technique, which involves the solution, on computer, of certain types of mathematical and logical models describing the behaviour of a system (or some component thereof) over extended periods of real time. It is this "numerical" simulation, of the stereolithography process, which will be discussed in this paper.

2.2 Goals of numerical simulation

There are a number of reasons why the decision to develop a numerical simulation of a particular system is considered appropriate in any given situation. In most circumstances there is an initial requirement to reduce system costs or time or both, this in turn may require some amount of process improvement or alteration. If however, the system is complex, material costs are high, and down-times are expensive, the need to predict the effect of these improvements and alterations prior to implementing them is made clear. An accurate numerical simulation, presents a way to study the effects of these changes on the operation of a system with a certain degree of accuracy. By making alterations in the mathematical model and observing the effects of these alterations on the simulations behaviour, inferences can be made about the effect such a change may have on the actual system.

A requirement for training and education may also lead to the decision to develop a numerical simulation. When systems are complex and expensive to run or both, a certain amount of training and education must take place "off-machine" to reduce the possibility of any unnecessary wastage of valuable resources and of system damage due to its use by an untrained operator. A simulation can therefore be used as a training device for teaching both students and practitioners the basic theory underlying the system.

The following is a list of other benefits which may be obtained from the development of an accurate numerical simulation of a given system [2].

• Simulation makes it possible to study and experiment with the complex internal interactions of a given system.

• A detailed observation of the system being simulated may lead to a better understanding of the system and to suggestions for improving it, which otherwise would not be obtainable.

• The experience of developing the computer simulation model may be more valuable than the actual simulation itself. The knowledge obtained in designing the simulation study may suggest changes to the system being simulated. The effects of these changes can then be tested via simulation before implementing them on the actual system.

• Simulation of complex systems can yield valuable insight into which variables are more important than others and how these variables interact.

• Simulation can be used to experiment with new situations about which we have little or no information so as to prepare for what may happen.

• Simulation can serve as a "pre-service test" to try out new policies and decision rules.

• Simulation enables one to study a dynamic systems in either real time, compressed time or expanded time.

• Simulation makes generalists out of specialists. Analysts are forced into an appreciation and understanding of all facets of the system.

2.3 Disadvantages

There are a number of disadvantages that have to be considered before any simulation project is considered. Firstly a simulation can only ever be defined as an abstraction of the real system, and as such can only ever be as accurate as the data and equations attached to it by the developer. Secondly it is generally the case when developing a simulation, that the accuracy of its output when compared to the actual results offered by the system under consideration is directly proportional to the complexity of the mathematical model used in the simulation. Therefore, in order to be useful, a simulation must necessarily embody elements of two conflicting attributes: realism and simplicity.

3.0 Stereolithography simulation.

As previously mentioned, before the development of a numerical simulation of a system is considered, problems (with the system) must be identified which could benefit from such an undertaking. Therefore the initial part of the research project was spent examining the current trends within RP as a whole and identifying the particular issues that seemed to be hindering the widespread adoption of this new technology by smaller companies and its application worldwide. Once identified, we considered the impact of these issues on one particular technology: stereolithography, and to what extent an accurate numerical simulation would help address these issues. The following section presents a brief summary of the findings of that initial research [3].

3.1 Issues

The particular issues, that were discovered to be prevalent within the RP industry could be split into two separate and distinct categories. The first are the issues facing the existing, experienced users of the technology, these are generally related to their pursuit of a more accurate model with a faster build time and the functionality required for the models intended purpose. These people, used to building adequate models, look to new processes, new materials and new technologies to obtain their "ideal" model. However, these new ideas need to be tested beforehand, which means that time must be set aside on the machine for training and experimentation. This can be expensive, delaying the production of other work by tying up machinery that needs a high throughput to be cost effective and using expensive raw materials on a process of trial and error.

The second category are the issues facing the potential investors in RP technology. For these people technology selection and investment justification are the main factors which influence their decision to adopt these new technologies. At this moment there are a wide variety of commercially available RP technologies at a wide variety of prices, each offering similar model build times, model functionality and accuracy. This wide choice leads to the current situation where potential investors have to go through a complex process of technology assessment to ensure the technology selected will cater for their individual modelling needs, and give them the benefits anticipated when the decision to purchase a piece of RP technology was first made. This process involves the careful assessment of

the competing claims of each technology, the reading of industrial case studies, the questioning of existing users and the production and examination of numerous benchmark models. Alongside this process of selection, is a process of investment justification. In his book Automated Fabrication: improving productivity in manufacturing, Marshall Burns emphasised the care needed in the calculation of the total acquisition costs of new RP equipment. The cost of installing capital equipment according to Burns, "is always more than the price tag on the machine" [4]. It is these hidden costs that tend to hinder the adoption of RP techniques by the smaller companies who cannot (due to the short-term financial methods generally used to justify investment), convince senior management of the future benefits of RP.

The aim of the research project is to take a closer look at the simulation of stereolithography, and to develop a platform, (based on other technical research in this area) that will advance the industry closer to the ideal situation where a numerical simulation can used alongside current RP technologies. It is hoped that a simulation will go some way to addressing the issues faced by both categories outlined above. An ideal numerical simulation would provide:

• A better understanding of the curing process.
• Model Evaluation: allowing an evaluation of a number of parameters prior, during and after the build, giving a prediction of the model's accuracy as well as its mechanical properties • Build evaluation: providing an estimation of build times, cure profiles, distortion and shrinkage, as well as giving an indication of the temperatures throughout the vat as polymerization progresses.
• Technology evaluation: when incorporated with other RP simulations, it will aid potential users in their choice of which technology to adopt for each individual modelling application.
• Sensitivity analysis: unlike physical builds, simulations can be performed in a matter of minutes, individual parameter values can be precisely changed and the results investigated, allowing users to optimise the process.
• A platform for the testing of new resins, build styles and process improvements.
• The opportunity to develop a standard set of build parameters and resins for some predetermined model characteristics.
• An educational tool: allowing the training of new RP users "off-machine".

3.2 Model development

Initial work on the development of an accurate simulation focused on the research which has already been completed on modelling the physical and chemical processes in stereolithography. We concluded from these studies that the mathematical modelling could be split into roughly three main areas:

1. modelling of the laser;
2. modelling of the photo-initiated free radical polymerization;
3. modelling of the heat transfer involved in the process.

3.3 Modelling of the laser

Modelling of the laser beam and how its intensity decreases with depth in a vat of resin has over the last five years been the subject of a number of research projects [5] [6]. For instance, in their paper Brulle et al. used the Beer-Lambert Law to suggest an ideal model of laser-induced polymerization, going on to discuss some probable causes for the deviation from this ideal case (Figure 1.0 [5]). A Monte Carlo simulation model was then developed to test the hypothesis stated. These declared that the occurrence of a laser beam with an average Gaussian flux density, but a random space-time evolution, coupled with a polymerizable material which is partially heterogeneous, may lead to the phenomena witnessed experimentally. The initial model takes into account the change of refractive index as the liquid monomer becomes solid polymer and the possible photo-bleaching effect. Their results seem to follow the experimental observations and describe a cure profile which is "torch-like" rather than parabolic. Other work [7], suggests a

mathematical representation based purely on the optical analysis of the laser beam path as it travels through the photosensitive resin, calculating the exposure distribution in the resin. Using this model, a solidified profile is determined by a threshold level of exposure.
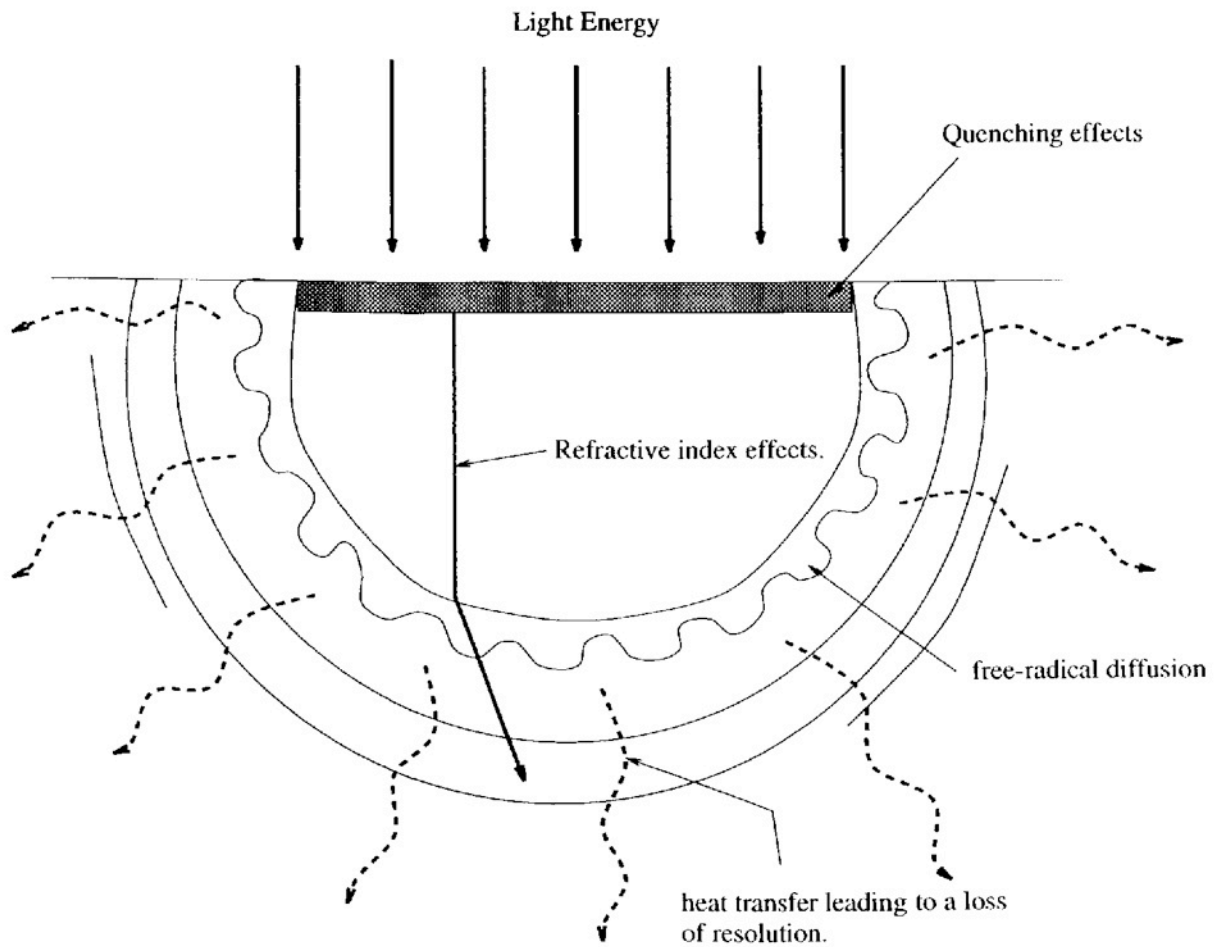

Figure 1: Phenomena associated with photo-reaction [8]

3.4 Modelling of photopolymerization

Modelling of the photopolymerization inherent within stereolithography has its roots firmly in the polymer science of radiation curing. The basic kinetic models proposed by Decker [8] [9] [10], Fouassier [11] [12] [13] and Odian [14] use a set of equations which describe the three steps that make up the laser induced radical chain polymerization process i.e. initiation, propagation and termination (Figure 2).

$$S \xrightarrow{h\nu} R^{\bullet} \longrightarrow RM^{\bullet} \qquad \text{Initiation}$$

$$RM_i^{\bullet} + M \xrightarrow{Kp} RM_{i+1}^{\bullet} \qquad \text{Propagation}$$

$$RM_n^{\bullet} + RM_k^{\bullet} \xrightarrow{Kt} RM_{n+k}R \qquad \text{Termination}$$
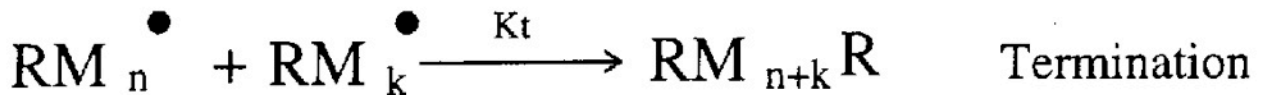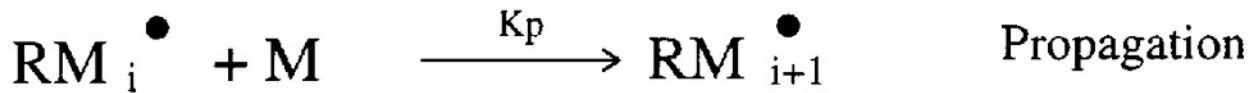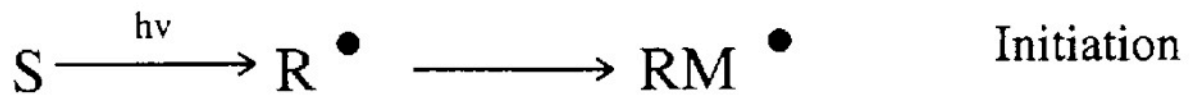
Figure 2: Classical steps in photo-initiated free-radical polymerization [14]
Models based on these equations [15] give a reasonably accurate picture of the polymerization process as it progresses over time; from these equations, values for the rate of initiation and rate of polymerization can be achieved. Early results using these models suggest that they reasonably describe the photochemical processes involved in stereolithography. They show a relatively good correlation with theory and demonstrate (amongst other observations):
• That the percentage conversion of monomer to polymer varies as a function of position and time.
• That this conversion reaches a maximum of approximately 60% as reaction rate becomes diffusion controlled.
• That polymerization produces "bullet shaped" cured profiles.
The problems with these models are:
• The models are only an approximation to the real situation and incorporate some assumptions.
• The theory underlying these models is still a matter of much research.
• The equations do not directly relate to stereolithography and the user is expected to have a certain amount of knowledge of polymer science in order to understand them.
3.5 Modelling of heat transfer
Two strands of research into the modelling of the heat transfer within the process have been discussed in recent years. One is concerned exclusively with the conduction of heat by the resin due to the exothermic polymerization process [16], while the other is also concerned with the modelling of a laser light source that adds heat to the resin, such as a thermal IR laser [17]. Both have been approached in a number of similar ways, each requiring a knowledge of:
• The target's optical and thermal properties during the irradiation.
• The laser beam distribution.
• The dynamics of the irradiation process.
• The processes of phase change in the target material.
Both assume that the material is homogeneous and isotropic and that the thermal properties of the resin do not vary greatly with temperature and are therefore assigned an average value for the temperature range studied. Other heat transfer effects such as forced and free convection have so far been neglected.
4.0 Initial Model
The model we used as the initial basis of the simulation is based upon the two-dimensional, static laser model proposed by Flach et al. The equations that make up this

model describe the physical and chemical changes which occur in a small volume of monomer mixture illuminated by a stationary laser (Figure 3).
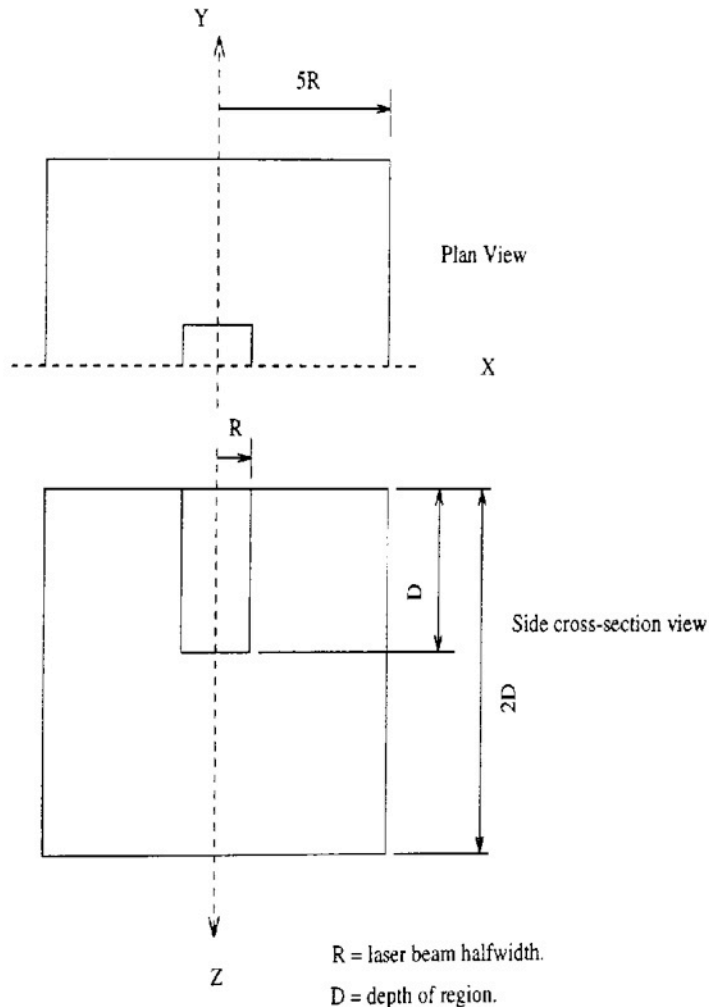

Figure 3: Coordinate system used in initial model.

These equations are solved numerically within a computer program that allows the selection, by the user, of a number of parameters which affect the process. The outputs of the program include spatial and temporal variations in the concentration of monomer and polymer, depletion of the photoinitiator, and the local variations of temperature in and around the region contacted by the laser light [16].

Since the model describes a real physical process a number of assumptions had to be made to simplify its development. These are [16] [2] [5]:

• The photopolymer resin obeys the Beer-Lambert law of exponential absorption.
• The laser irradiance distribution is Gaussian.
• The flow of material due to convection or diffusion in any direction is negligible.
• There are no light scattering, diffraction, refraction or reflection effects.
• The chemical reaction occurs only in the cuboid region of width 2R and depth D.
• The conduction of heat occurs over a cuboid region of width 10R and depth 2D.
• The heat generated is due to heat of polymerization only.
• The heat loss from the surface of the vat is negligible.

• All physical and thermodynamic properties are independent of degree of conversion and temperature (i.e. constant).
• A square root dependence of the rate of polymerization on the light intensity is assumed to continue throughout polymerization. This stems from the assumption of steady-state production of all radical species and that the termination step is purely bi-molecular.
• The evolution of the polymerization zone is unaffected by volume shrinkage.
• The evolution of polymerization is unaffected by oxygen inhibition.

The model consists of four partial differential equations (PDEs), one governing the rate of change of light intensity with respect to depth two of which govern the radical-chain polymerization which occurs in the region, and one of which governs the heat transfer in the resin due to the exothermic reaction [3].

5.0 Early Results
Early results from the model were in relatively good agreement with Flach et al. and showed a good correlation with the theory [14] [8] [9] [10] [11].
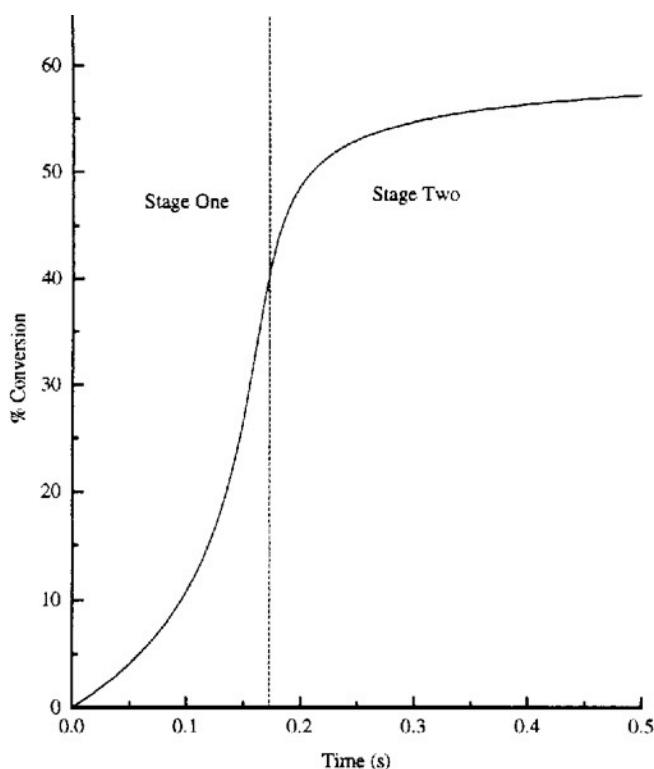
Figure 4: Graph showing degree of conversion with respect to time.
Figure 4 shows a graph of degree of conversion with respect to time. Two stages of the polymerization process can clearly be seen. In stage one the chain reaction develops rapidly up to about 40% conversion. This is followed by a progressive slowing down (stage 2) which is attributed to the increasing viscosity of the polymer system reducing the mobility of the reactive sites and the decreasing probability of an encounter between the polymer radicals with the reactive double bonds. Actual polymerization profiles recorded by real time infra-red (RTIR) spectroscopy would produce similar results but would have an initial induction period, due to the presence of atmospheric oxygen which is known to strongly inhibit the polymerization by reacting with the initiating radicals as well as with the growing polymer radicals [9].
Figures 6 and 7 (see end of paper) show the concentration of photoinitiator with respect to time. Figure 6 shows the change in photoinitiator concentration at the axis of the region (r = 0) with varying depth and Figure 7 shows radially the change in photoinitiator

concentration on the surface of the resin (z = 0). Both graphs clearly show the steady decrease of photoinitiator concentration as the polymerization progresses; this is in agreement with the theory. The photoinitiator plays a key role in light-induced polymerization in that it produces the free radicals with time which, by reacting with the monomer, initiate the chain process.

Figures 8 and 9 show how the monomer concentration changes with depth and radial position. The graphs show that, as expected, monomer concentration decreases with time throughout the region, until it reaches a minimum value of 1.30 mol l -1. This value corresponds with the values obtained for percentage conversion.

Figures 10 and 11 gives some idea of the flexibility of the model. These graphs show percentage conversion and temperature with respect to time, with varying values of quantum yield for photoinitiation (f). This value is a measure of the efficiency of the initiation process, i.e. 0.1 in our model equated to 1 radical pair that is able to initiate chain propagation is produced for every 10 photons absorbed. Results show that the higher f value results in a higher polymerization rate due to the faster production of free radicals and therefore a higher rate of heat generation.

Figures 14, 15, 16, 17 and 18 are contour plots showing the temperature distribution throughout the region over the time step calculated. Preliminary results are promising with temperature increasing rapidly due to the exothermic reaction to a maximum temperature of 68°C and heat being dissipated slowly throughout the region. Temperature rises to a maximum at the layer surface but decreases rapidly with depth, because polymerization is incomplete and inhomogeneous, since the light is, in principle exponentially absorbed. The results also show that heat transfer is greatest in the radial direction; this phenomena is unexpected and is currently under investigation.

Figures 19, 20, 21 and 22 are contour plots showing the percentage of monomer converted to polymer over the entire region. These show conversion reaching a maximum of 60%. If we assume that gelation occurs at approximately 20% conversion we see that the centre of the irradiated area requires less than 0.1 sec to be polymerized; plotting the contour at this conversion gives an indication of the cured profile, which as expected, has a parabolic shape. The maximum conversion reached also agrees with theory which states that the radical chain polymerization is never complete; there is always some unreacted monomer inside the polymer.

5.1 New Developments

Although the early results were encouraging, further developments were needed to ensure the mathematical model was as close an approximation to the real process of stereolithography as possible. This meant we had to begin to address some of the assumptions made in the initial model. This section briefly describes two of these developments and some of the results obtained so far.

5.2 Dark reaction model

As reported by Flach et al. [20] the equation which describes the rate of change of monomer concentration with time used in the initial model assumes that polymerization stops when the light source is turned off. This is found to be an incorrect assumption as polymerization proceeds for a length of time afterwards. It was necessary therefore to modify the model to accommodate this "dark reaction" by the introduction of a an intermediate species, which are formed during the "light period" and are then consumed during the "dark period" [20].

5.3 Initiator efficiency model

Initiator efficiency (f) is defined as the fraction of the radicals produced upon decomposition of the initiator that actually initiate propagating chains. Initial model results were based upon the assumption that initiator efficiency was a constant value of 0.1 throughout the polymerization reaction, this is was found not to be the case in reality. As the viscosity of the reaction medium increases, the diffusive displacement of the radicals

away from each other becomes difficult and radicals tend to react with one another rather than with monomer molecules to initiate propagating chains. This reduction in the diffusive displacement causes a change in the initiator efficiency until it reaches a limiting value of zero. An initial attempt was made to incorporate this effect into the model by using a model suggested by Batch et al [22]. This model assumes that initiator efficiency follows the behaviour outlined in Figure 5. Initial results (Figures 12 and 13) using this model shows that varying the initiator efficiency as polymerization progresses leads to a lower final conversion of around 45% and a peak temperature of 90°C. The innacuracies in the results of this model, shown in both figures are due to limitations in the computational method used. This is currently being addressed.
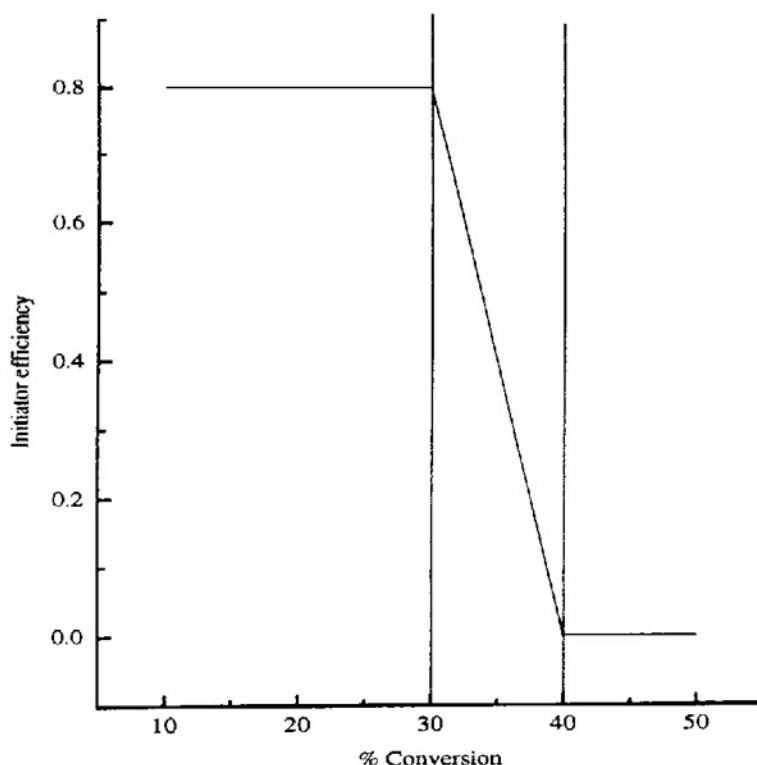
Figure 5: Graph showing initiator efficiency with respect to percentage conversion of monomer.

6.0 Discussions

The model presented in this paper contains the key elements of the photo-chemistry and thermal variations which are required to understand the stereolithography process. The results are not yet fully validated but they are in qualitative agreement with polymer theory and the work by Flach et al. Moreover, points of quantitative agreement have been identified, which is encouraging. Initial attempts have also been made to develop the model further these have produced some interesting results which must be fully investigated before any comparisons with the actual stereolithography process can be made.

7.0 Conclusions

There are a number of outstanding issues which inhibit the widespread adoption of RP technology. These are related to the accuracy, repeatability and ease of use of the various processes. A numerical simulation will help to resolve several of these issues and we have presented a model of the curing process which forms the basis of a full simulator of stereolithography. Preliminary results are in reasonable agreement with theory and

experimental results, but some further investigation and development is needed to enable the model to be a useful tool for stereolithography research.

8.0 Future Work

The main thrust of this initial work was to develop the basis and framework of a stereolithography simulation and to briefly discuss the initial model which, when developed, will become the basis of this simulation. Future developments are planned which will improve the accuracy of the simulation results and improve the usability of the simulator. This will include:

• Cure profile determination [16] The observation of cure profiles is one of the easiest ways to validate the simulation results, real cure depths and line-widths can be measured against modelled. The observation of cure profiles will include not only single strings but also cured layers.

• Determination of temperature effects on model build.

• A moving laser light source [16]. The development of the model will allow either a two-dimensional stationary laser light source or a three-dimensional moving one to be used as the basis for the simulation.

• A Thermal IR laser model.

• An animation capability. Results from the simulation need to be interpreted rapidly, and with relative ease. The addition of an animation capability will allow the user to view and analyse results.

• A non-vertical laser beam model to accommodate angle of incidence.

• A non-Gaussian laser model. Nearly all current models make an assumption that the laser beam intensity distribution is Gaussian.In reality this is far from the case, as a pure Gaussian mode implies the use of expensive control apparatus.

• The determination of resin working curves [16].

• Incorporating the effects of Refractive index changes on cured profiles.

9.0 Acknowledgements

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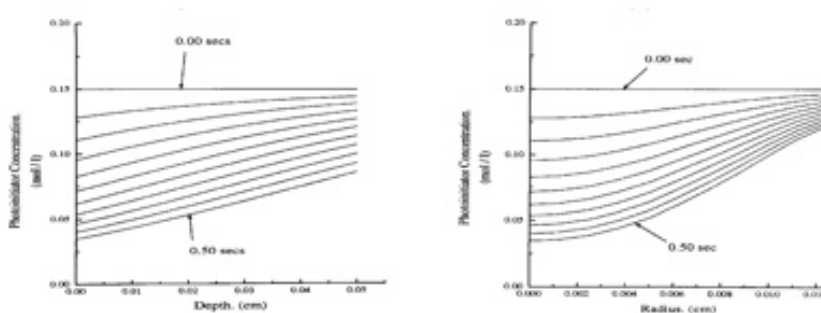
Figures 6 and 7: Showing the concentration of photoinitiator with respect to time, at r = 0 (Figure 6) and z = 0 (Figure 7) at equal time intervals.
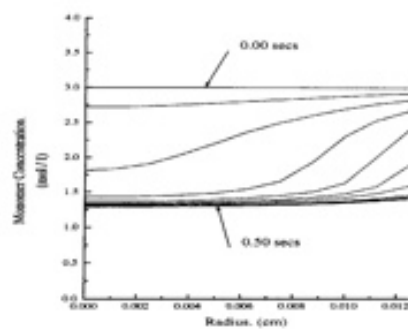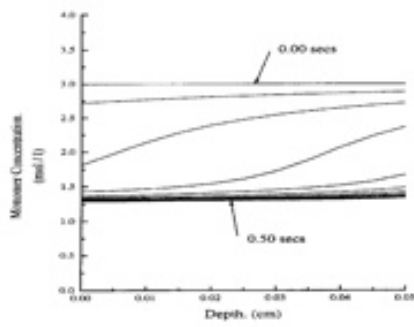
Figures 8 and 9: Showing the concentration of monomer with respect to time, at r = 0 (Figure 8) and z = 0 (Figure 9) at equal time intervals.
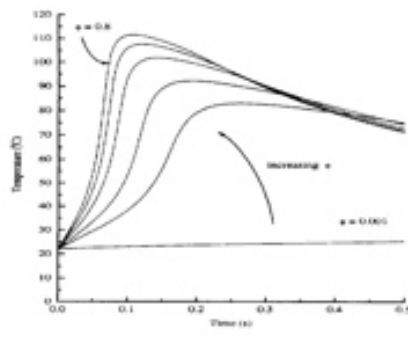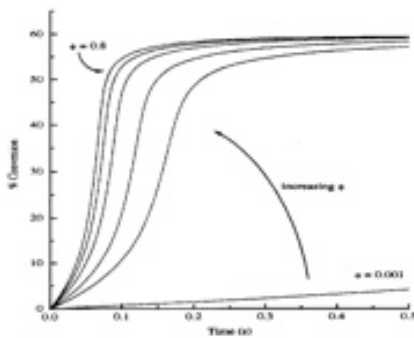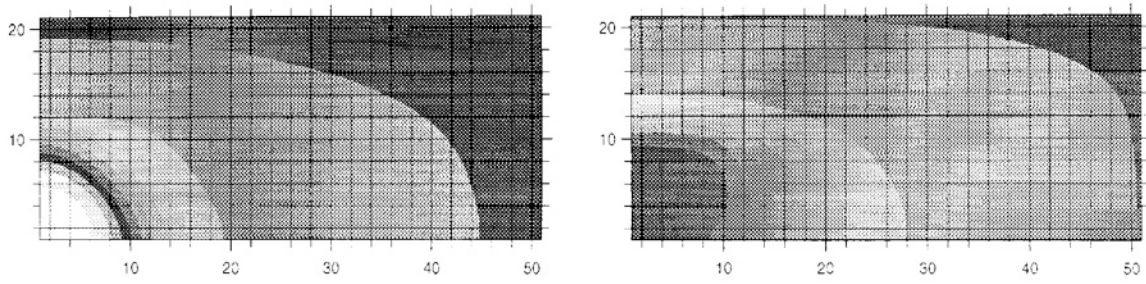

Figures 10 and 11: Showing the degree of conversion and temperature at r = 0, z = 0 with increasing Quantum Yield (f).
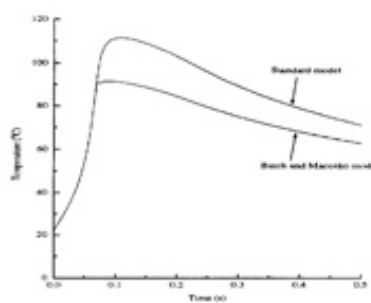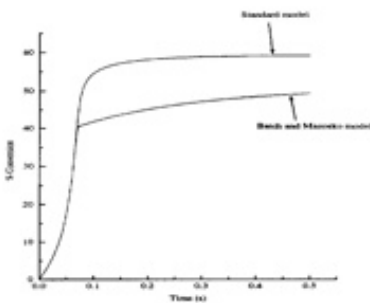
Figures 12 and 13: Showing the degree of conversion and temperature with respect to time at r = 0, z = 0 for Batch and Macosko varying initiator efficiency model.
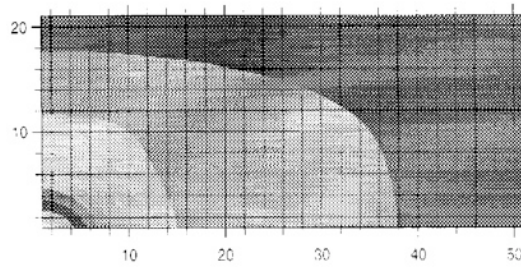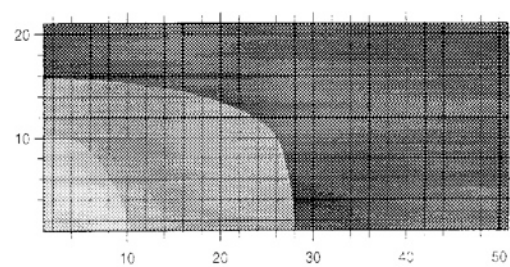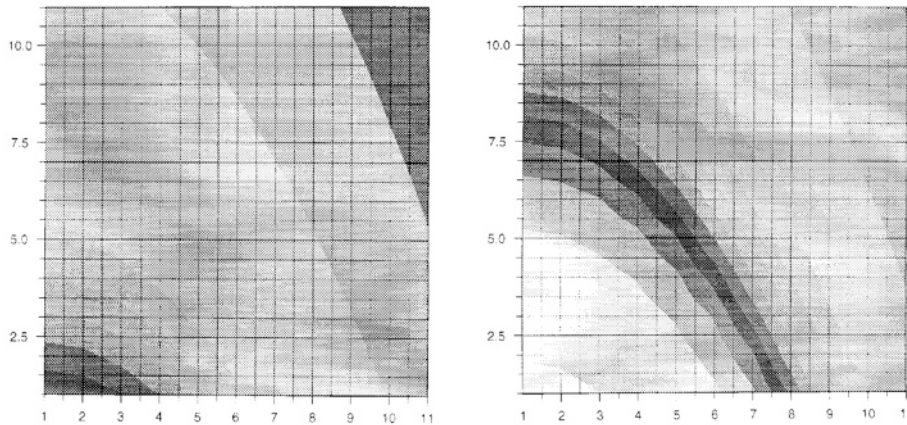

Figures 14 and 15: Contour Plots showing temperature throughout region at t = 0.1s and t = 0.15s.
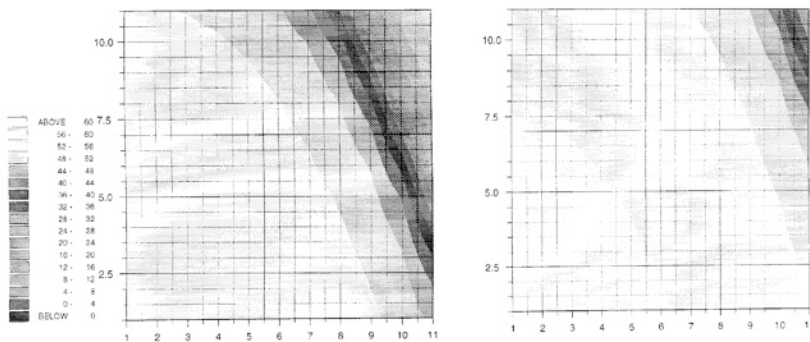
Figures 16 and 17: Contour Plots showing temperature throughout region t = 0.18s and t = 0.30s.
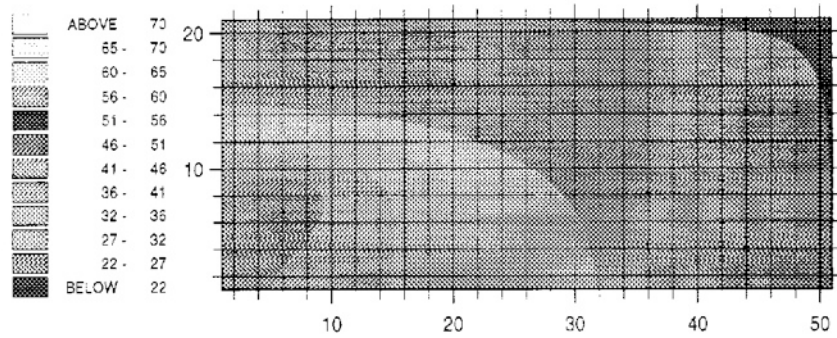
Figures 18: Contour Plot showing temperature throughout region at t = 0.45s.

Figures 19 and 20: Contour Plots showing percentage monomer conversion throughout the region at t = 0.1s and t = 0.15s.

Figures 21 and 22: Contour Plots showing percentage monomer conversion throughout the region at t = 0.30s and t = 0.45s

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