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Numerical testbed for laser materials processing

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ABSTRACT

Current numerical simulations of laser materials processing usually simplify any process model to a great extent in order to allow for short computation times. This significantly decreases their flexibility and ability to simulate the great variation of today's processes with their subtle but important differences. The simulation presented in this paper can be said to be truly three dimensional as opposed to other reported work that uses symmetric boundary conditions. This enables the investigators to simulate real laser beams. In contrast to the (well-documented) Marangoni flow profile, the authors will show results that do not use the usual simplifying assumptions of flat surfaces. Preliminary output from the simulation deals with the transient coupled velocity and pressure profile and temperature distribution and hence the heat affected zone (HAZ). From this, conclusions can be drawn with regard to improving process efficiency, especially in laser cutting. It will be shown that the traditional perception of equating higher processing speeds with better processing efficiency does not hold in all cases. In fact, the opposite may well hold true. However, to demonstrate this the actual process of producing a part needs to be fully understood. A process may influence the workpiece material properties beneficially when it is performed at reduced speeds (material hardening or softening). The investigators contend that numerical modeling of the above can only be achieved credibly using high performance computing methods.

Keywords: laser materials processing, laser sources, numerical simulation, numerical modeling, fluid flow, Marangoni, free surfaces

1. INTRODUCTION

Laser machine tools have found a secure place for a variety of materials processing techniques such as drilling, cutting, welding, heat-treating and alloying. Their unique capacities can also give rise to novel manufacturing approaches.[1] The application of lasers spans such diverse fields of engineering as welding of parts, heat treatment, surface coating, cutting and drilling and even medical applications like surgical cutting, welding of wounds, modification of tissue and many more. The range of materials to which the laser can be applied to is similarly diverse including ceramics, plastic, metals, biological tissue and wood.

2. NUMERICAL TESTBED - A DEFINITION

Materials processing by the means of lasers is a complex field. The vast amount of literature available concerned with the modeling of laser materials processing highlights the need for unbiased predictive tools. However, Sargent *et al*[2] point out that:

> *"... many projects, while successful in their own narrow areas, never produce general, useful results."*

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This is the main motivation for building a simulation framework which addresses exactly this shortcoming. A testbed has to be versatile and the amount of pre-analysis assumption has to be reduced to the maximum extent possible. With respect to laser materials processing, this holds for the laser source as well as the assumptions made concerning the workpiece. It would be of little use for the practician, who is confronted with a decision to be made about the quality of the laser source to be used in practice, if the numerical model assumed a perfect source. With regard to the model of the workpiece, it would be equally disadvantageous if the experimentalist had to decide *a priori* if the melt flow is of significance or not, or even if the velocities within the melt are above or below a certain threshold value for which the simulation is understood to be valid or not. Obviously, in order to achieve a simulation that addresses these issues, certain simplifications have to be made. The main challenge is to reduce these to an acceptable minimum. In order to fully appreciate the need for a numerical testbed, the main features of laser material processing are outlined as follows.

2.1. Process features

Copley *et al*[3] presented the topography of regions melted by a continuous wave (cw) CO_2 laser beam and developed a theory to explain phenomena due to convective processes related to epitaxial regrowth and surface relief in laser melted regions. At the point of impingement of the laser beam, the temperature increases and, because the temperature coefficient of the surface tension is positive for most materials, the surface tension increases along a line from the impingement point to the edge of the melt pool. Thus any volume element of the surface experiences a net force parallel to the surface causing it to move from the center to the edge of the melt pool. In the case of a moving melt pool the convection pattern becomes unsymmetrical. In Figure 1 the origin of ripples and other topographical features associated with travelling melt pools (such as laser melted regions) is illustrated. Similar effects have been reported by Moore *et al*[4] and the striking resemblance of laser surface melts to welds is pointed out. The most dominant feature is the *chevron pattern* formed by the isolines of temperature and hence the melt pool. Laser surface melts often exhibit a central crest which runs the length of the melt and which is flanked on each side by a trough as shown in Figure 2. The resulting surface roughness due to the ripples is reported to be between 5-15 μm. In laser welding these can easily add up to 0.01 times the width of the weld.[5]

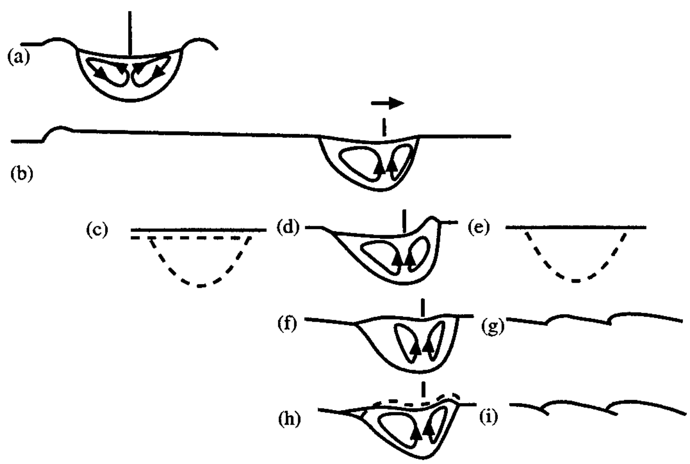


Figure 1. Mechanism of ripple formation: (a) laser translational velocity equals zero; (b) and (d) velocity not equal to zero; projected area of back side of pool (c) less than that at front edge of pool (e); (f) and (g) ripples without back flow; (h) and (i) ripples with back flow[3]

The appearance of humps on the surface of the weld bed is usually referred to as humping phenomena. A sketch of a typical shape of the cross section is shown in Figure 3. The deep depression of the material at the former solid-liquid interface, called undercut, is experimentally found to be associated with the humping phenomenon. In general, these humps occur periodically along the weld bead.[6] The undercut phenomena

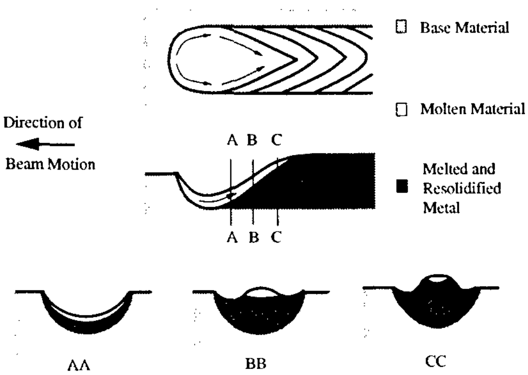


Figure 2. Schematic diagram of the laser surface melting process showing a top view (top), lengthwise cross section (middle), and various transverse cross sections (bottom)[4]

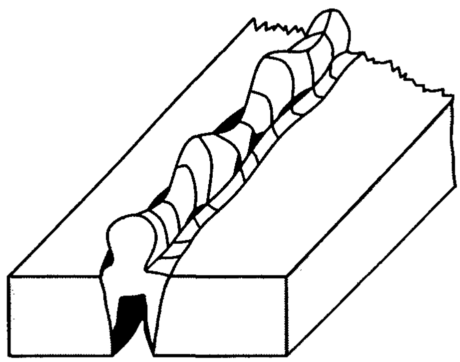


Figure 3: Humping phenomena in laser welding. Sketch of the weld bead based on a microscopic study.[6]

shown in the Figure 3 may lead to stress risers during service life of the manufactured part and is addressed in Atwa *et al.*[7] Additionally these authors point towards problems concerning lack of penetration, root undercut, inclusions and burn-through in the context of premature failure of pipelines.

2.1.1. Laser cutting

Salient features of the laser cutting process are depicted in Figure 4. Process parameters can be adjusted and tuned to provide the quality of cut desired, but this procedure consumes exhaustive amounts of time and effort, without the optimal cutting conditions being found. If a different type of material is to be cut, then this procedure has to be repeated. This has been recognized as a major shortcoming in laser machining set-up.[9] Furthermore the optimum process parameter may well be a transient set of parameters, depending on the path of cut (may be three dimensional), the material (composition) or the cutting condition (cutting speed, sheet thickness, etc.). The effects of melt flow over an edge (refer to Figure 5) have been studied in an extensive manner by Brown and Davis[10] but so far no generic simulation includes these factors.

Regular spaced ripples or "striations" along the cut edge as shown in Figure 6 can be observed during laser cutting. In thin sections these may be clear and regular from the top of the cut edge to the bottom. However, on thicker sections, the striations may be clear towards the top of the edge but are replaced towards the bottom by more random ripples associated with the flow of liquid out of the cut zone.[11] Di Pietro and Yao[9] comment thoroughly on the state of the knowledge concerning the formation of striations:

> *"... the mechanisms affecting the forming of stria are not well understood. Striations will result to some extent due to the non-steady nature of laser cutting. "*

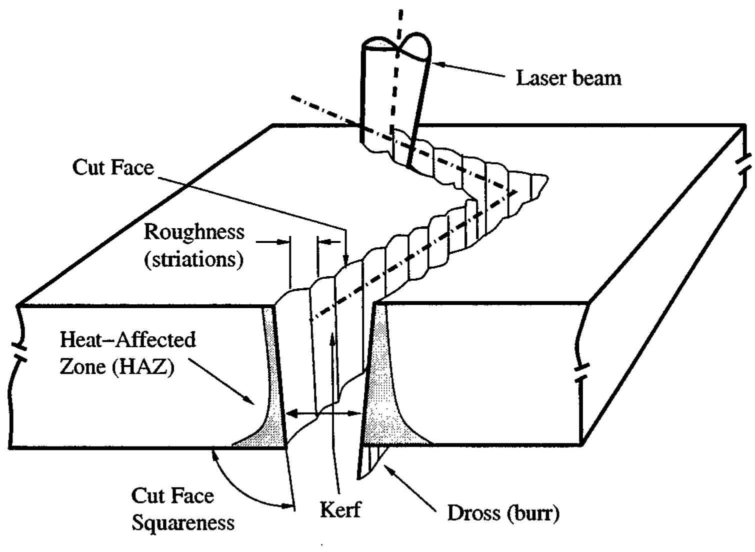


Figure 4: Factors in Laser Cutting[8]

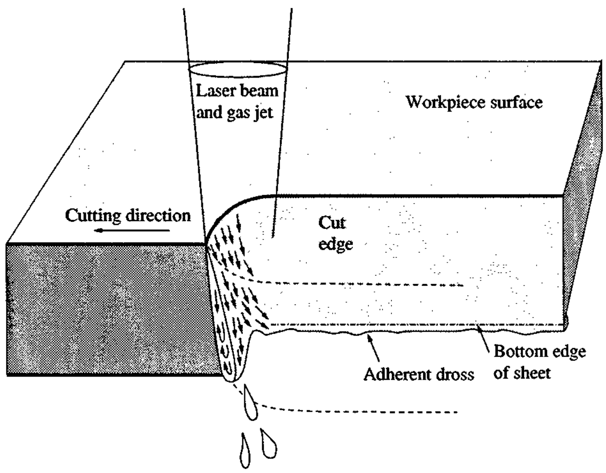
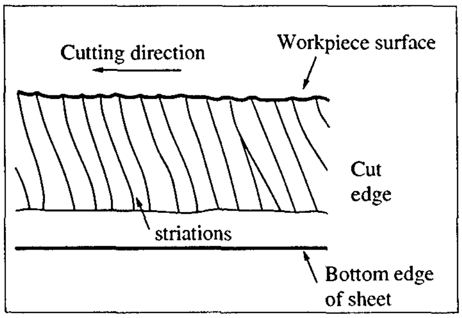


Figure 5. A schematic of the cut zone. The high surface tension of the melt and its adhesion to the workpiece results in dross adhering to the lower edge of the cut.[11]

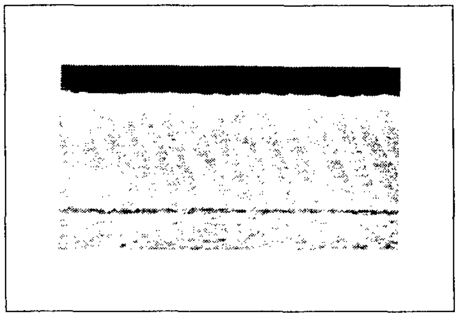
A similar scatter of theories and the limited predictive capabilities of current simulations prevails in context with other features in laser materials processing such as humping, rippling and dross formation.

The ambiguity in process parameters becomes obvious in the following example reported by Klocke *et al.*[12] For a 3 mm thick sheet PRMMC (particle reinforced metal matrix composites) - such as SiC-Al with 20% SiC, a cutting speed of 600 mm/min can be achieved. Increasing the laser power or decreasing the cutting speed can increase the cut width. When cutting pure aluminum a smaller width of cut is achieved. The dross for pure aluminum with similar cutting parameters is shorter and the cut face squareness is larger with a reduced cutting speed. Usually the surface roughness is reduced by increasing the cutting speed or laser power. The reverse is true for pure aluminum. A relationship between HAZ and dross has been reported.

Laser cutting of ceramics is still a problem due to their low thermal shock resistance. Sometimes the cutting performance with ceramics is increased when the focal spot is above the material surface. This results in a wider cut and the shield gas can be used more effectively for melt removal. For 10mm thick ZrO_2 an optimum focal



(a) Schematic



(b) Micrograph[11]

Figure 6: Striations in laser cutting

spot position is 5mm above the surface, and cutting speeds of up to 500 mm/min in cw mode are reported.[12] When cutting Al_2O_3 an optimum speed of 50 mm/min has been reported[12] and attributed to the smaller amount of melt generated. An occurrence of macroscopic crevice formation was observed due to the high brittleness of the material. Improvement was reported when using a Nd:YAG as supposed to a CO_2 laser. Cutting without cracking was achieved, and this was attributed to the smaller focal spot and higher intensity. All the prevoius examples highlight the need for a versatile and precise simulation.

3. MODELING STRATEGY

This paper will not provide a detailed discussion of the physical/mathematical modeling strategies used by the authors. The underlying physical model and its mathematical modeling will be published elsewhere. Here the authors wish to focus on the main principle, rather than the implementation. From the definition of a numerical testbed given above, two main features are immediately apparent. The model has to be three-dimensional in the spatial discretization, and the flow of the molten material must be included in the model. The first feature is due to the fact that a symmetry assumption would a) infer a perfect source and b) reduce the applicability to straight lines, which in practice represent only a fraction of the work to be performed. The fluid flow is important, because we can only discard it sensibly if the simulation clearly shows that it is of no significance. Doing so beforehand involves a sound complex physical reasoning which is extremely difficult, especially as today the scientific community as a whole is not in agreement on the explanation of certain phenomena as dross, stria and ripples. From studying the literature available it becomes obvious that modeling the physics involved is extremely complex and indeed justifies a separate numerical analysis. For example Chen *et al*[13] modeled oxidation effects in laser cutting, the assist gas flow in a kerf was studied by Vicanek *et al*[14] and Kar *et al*[15] developed a gas-dynamical model in order to describe the the plasma formation, velocity and particle size distributions in the plasma during laser ablation. On their own though, as mentioned before, the published work does not contribute significantly towards a comprehensive simulation of the process itself. Rather, it has to be incorporated on a phenomenological basis into a numerical testbed. This will be done in this paper and in future work. The main strategy is depicted in Figure 7 and shall be outlined below in the example of the incorporation of the stagnation pressure of a shield (or shroud) gas into the current testbed.

A unique set of unrestricted parameters is input to the numerical testbed. No restrictions that would result from previous assumptions in the model itself (e.g. neglecting the fluid flow) are present in the testbed. Certain phenomena can, at present, only be incorporated on a knowledge basis. This means that the explicit treatment in terms of discrete differential equations would increase the computational effort beyond current capabilities. Rather, these phenomena are studied beforehand parametrically, and by identifying the respective parameters during the simulation in the testbed, the output knowledge of prior simulations can be retrieved. In other words, for the example of the shroud gas stagnation pressure, a large quantity of simulations of the stagnation pressure field would be performed beforehand on varying surface profiles. For certain surface profiles

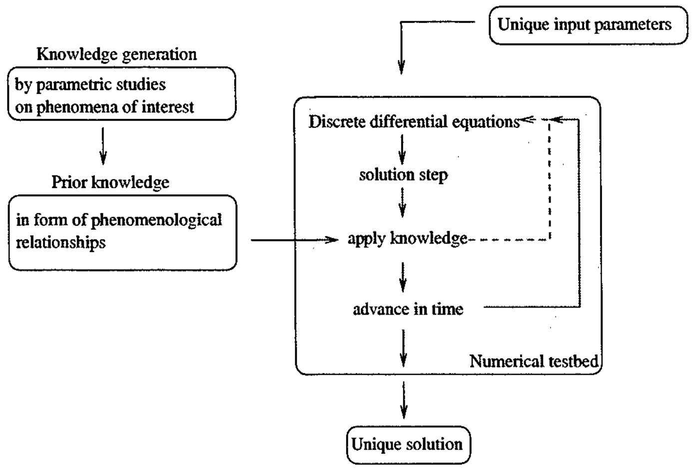


Figure 7: Strategy for the numerical testbed

the stagnation pressure distribution will be close to the analytically exact solution of the Navier-Stokes equation for a stagnation flow targeting a flat plate. Hence this can be utillised as "knowledge". If this is not the case, characteristic parameters of the surface will be extracted and the pressure distribution will then be reconstructed from the parameterized solution of the shroud gas simulation and subsequently incorporated into the testbed at that time step. For the subsequent time step, a new set of parameters will be identified and a new gas flow profile profile retrieved.

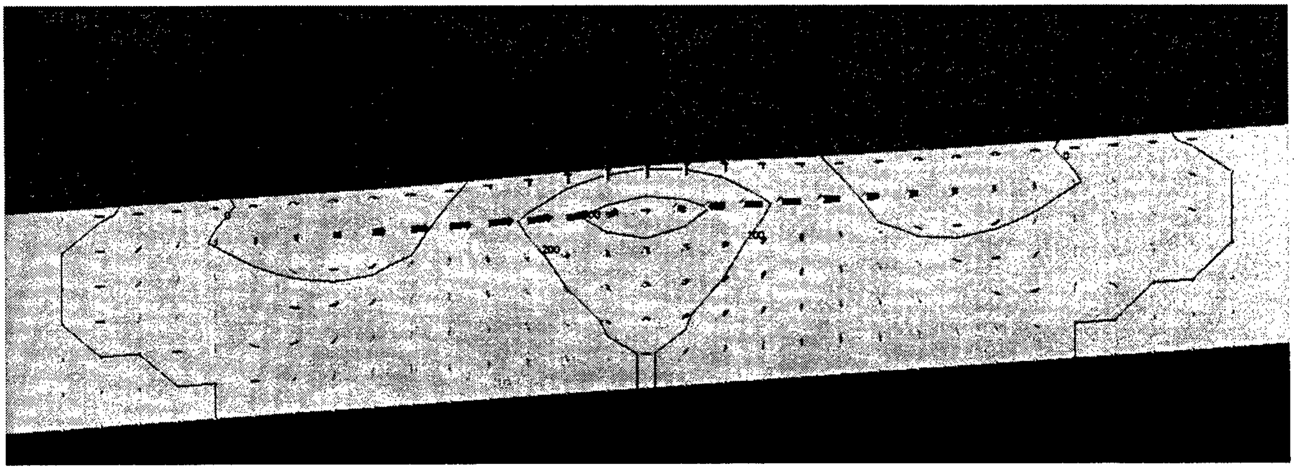
4. ROAD-MAP

The time frame for the development for the numerical testbed is set for three years. In this paper the authors have presented the work and results of the first year. During that year, a model has been developed for the solution of the incompressible Navier-Stokes equations with free surfaces, surface pressure due to the curvature of the surface and Marangoni surface tension driven flow with energy balance. Preliminary results from this work are presented. In the forthcoming year, the model will be extended significantly. Knowledge based modules will be incorporated to allow for shield (shroud) gas pressures, evaporation at the surface and melt outflow will be incorporated and hence the cutting process will be captured. This has to go along with full parallelization of the code, since for a realistic simulation the discretization needs a significant increase in density of discrete points. During the third year, the incorporation of knowledge modules is expected to continue, with application to case studies.

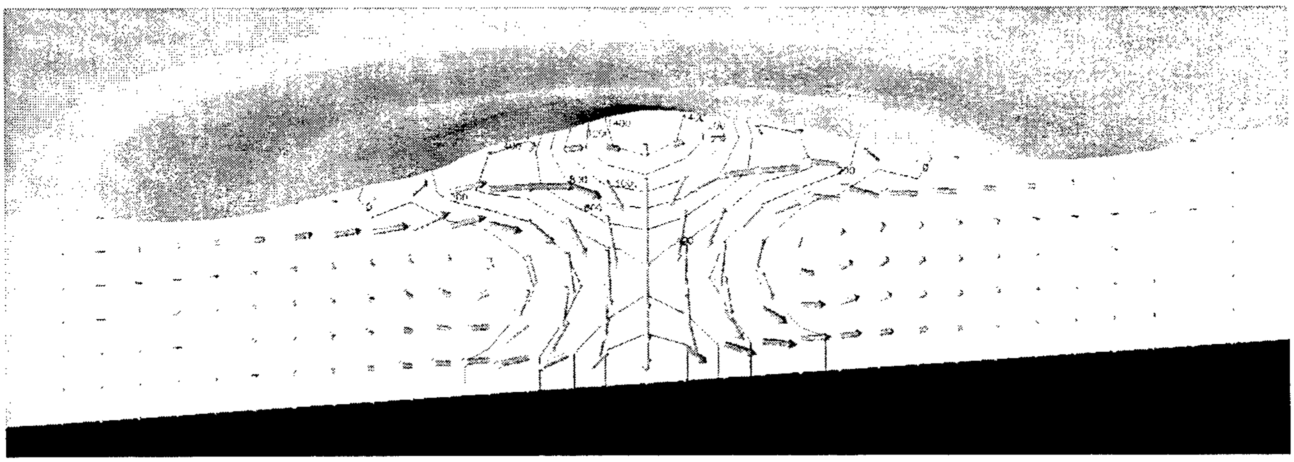
4.1. Preliminary results

The preliminary results from this simulation are concerned with computing the dynamic behaviour of a weld pool subject to Marangoni surface driven flow. In Figures 8 and 9 a time sequence simulation is shown. Initially the surface is flat, evolving through a set of dynamic oscillations during time. Isolines of pressure in the melt pool are plotted and the velocities are indicated by their respective vectors, with the magnitude of velocity represented by their length. The trace of the height of the central point of the free surface is plotted over time in Figure 10.

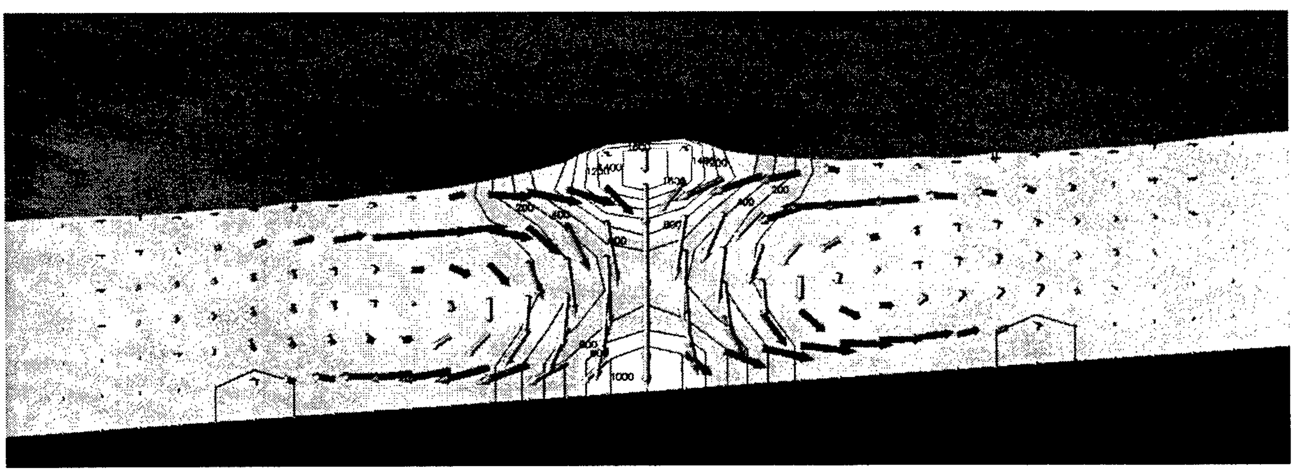
The time step of the simulation is 0.5×10^{-4}s and hence the time interval between the first and second maxima is $(333 - 135) \times \Delta t \approx 0.01s$. This leads to a frequency of about 100 Hz. As this is a solution to a very coarsely discretised general problem, the results can certainly only be interpreted in a qualitative manner. It shows clearly the complex interplay of different physical forcing and oscillation phenomena.



(a) 1 $\times \Delta$ t

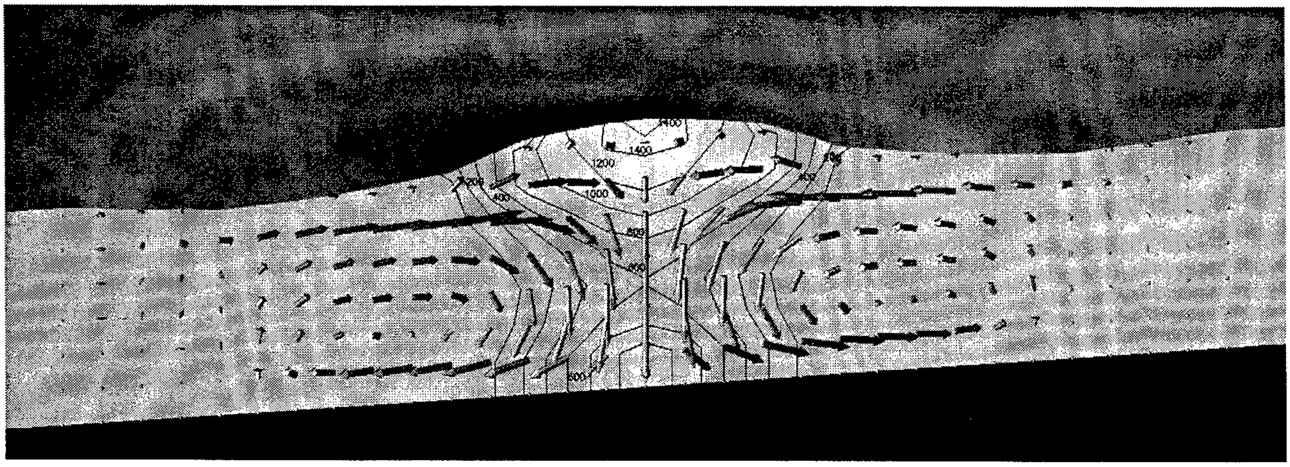


(b) 100 $\times \Delta$ t

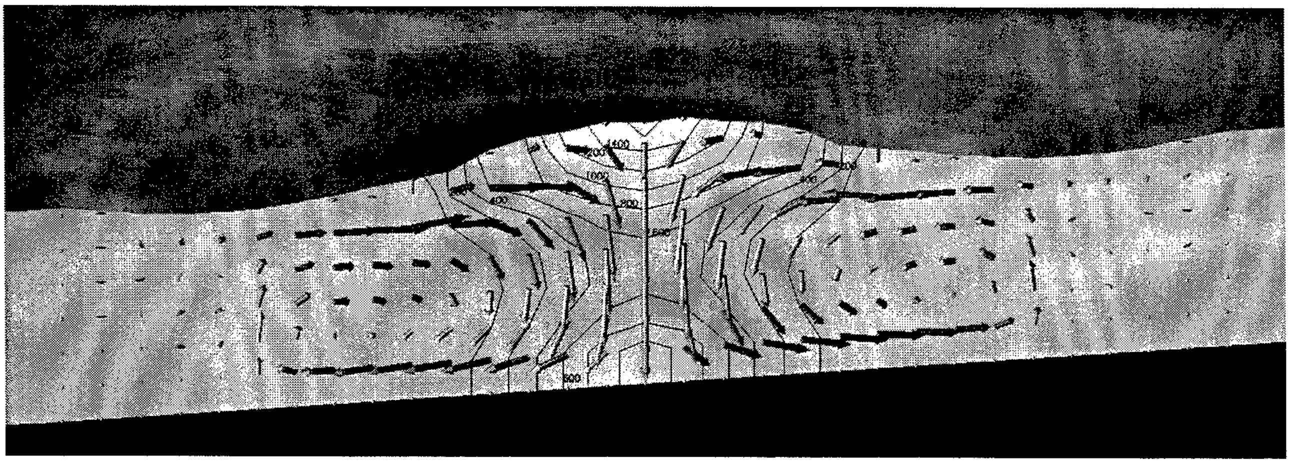


(c) 200 $\times \Delta$ t

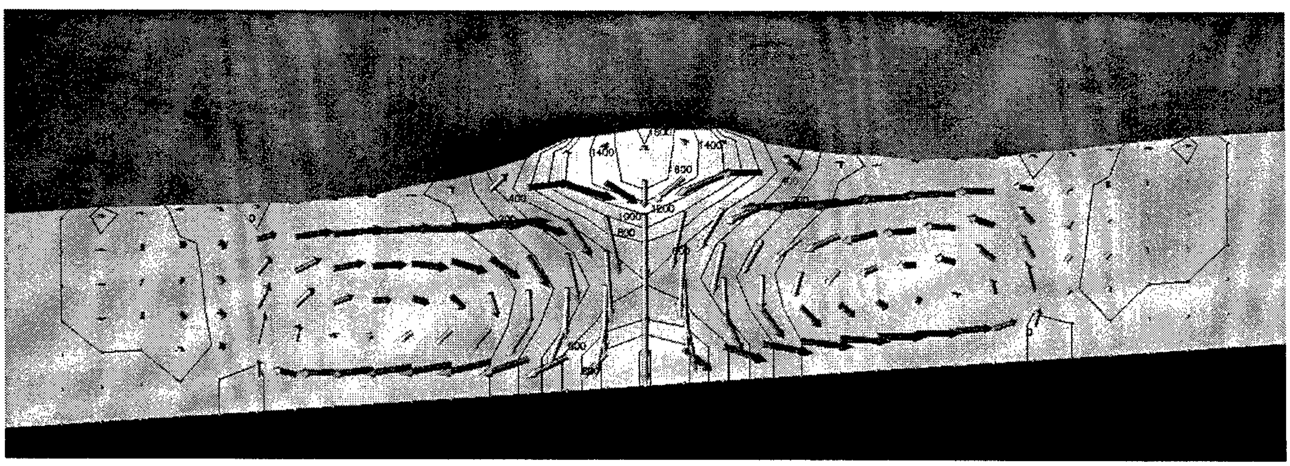
Figure 8: Time sequence of surface, pressure and velocity distribution



(a) 300 $\times\Delta$ t



(b) 400 $\times\Delta$ t



(c) 500 $\times\Delta$ t

Figure 9: Time sequence of surface, pressure and velocity distribution

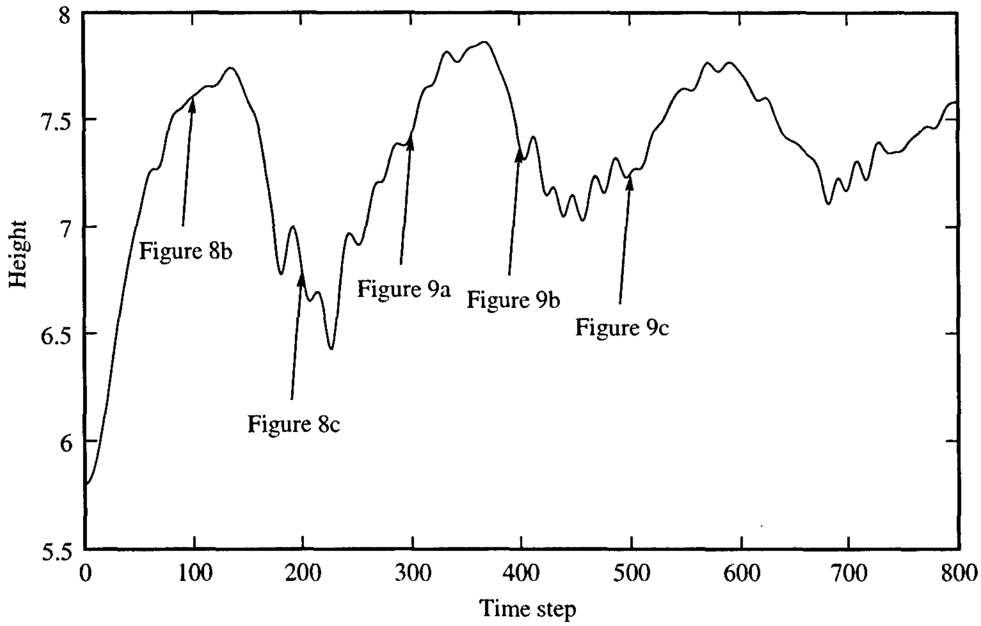


Figure 10: Time sequence of the evolution of the height of the central point of the free surface

Initially the flow is confined to the volume immediately underneath the surface, with the velocities aiming towards the center of the weld pool surface. In consequence a stagnation pressure builds up. Since initially less energy is required to lift the surface, rather than to initiate a recirculation flow field, the surface moves upward. The build-up of liquid in the center is counteracted by gravity and surface tension. This leads to a build-up of recirculation that eventually reduces the surface height in the center. Since this is a dynamic process, several oscillations are observed before a steady state profile is assumed.

5. DERIVATION OF SECONDARY INFORMATION FROM A NUMERICAL TESTBED

The authors believe that the full scale testbed will provide significant findings for the practician. With respect to the laser cutting process, this could involve the precise prediction of the heat affected zone. Most simulations available to date are not capable of capturing the extent of the HAZ at the outflow edge (shown in Figure 11), since the fluid flow is often neglected.

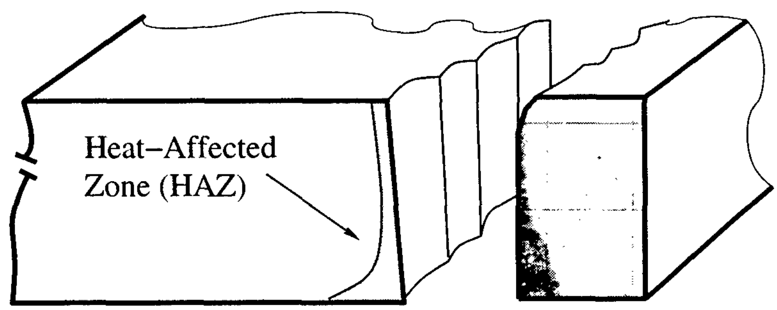


Figure 11. Schematic and micrograph of the HAZ when cutting a ceramic tile. The microstructural change in the HAZ is clearly visible due to its darker shading.

Predicting the size and cooling rate of the HAZ is of major importance since this can impact on the mechanical properties of the finished product, when phase transformations due to the temperature distribution are considered (e.g. tempering, hardening). Hence reduced cutting speeds (as opposed to the optimum speed, usually defined as being the speed associated with best quality results) may enhance properties of the workpiece in the proximity of the cut. Predicting dross distribution has a direct benefit during part manufacture, since the build up of dross usually requires further processing steps to remove it, with associated quality issues.

6. CONCLUSION

The authors are optimistic that the final result will be a versatile tool for the applied scientist and engineer. It is expected that the numerical testbed can be used in a diverse manner, ranging from evaluation of the applicability of certain simplified simulations to gaining insight into ripple, stria and dross formation with a predictive capability with respect to the HAZ. The authors contend that, in order to achieve these aims, a significant computational resource is needed, and this may not always be justified. With regard to usability on the shopfloor, this is a serious limitation. As experience shows, though, computational resources are getting more and more accessible at significantly less cost, and hence the investigators envisage that this will ultimately broaden the use of this tool at the shopfloor as well.

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