

Computer simulation of the solidification process in a three dimensional axisymmetric aluminium casting

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Abstract

The Finite Element Method was used to determine the solidification pattern in a three dimensional axisymmetric aluminium casting. A modified temperature dependent specific heat $C_p(T)$ function was considered to take into account the energy release at the solid-liquid interface. A static triangular mesh was used to simulate the physical domain. An experimental test was run to verify the accuracy of the numerical predictions on an actual Al 99,8% casting, by a careful monitoring of the temperature/time relationships at several points in the solidifying material. In particular, numerical results were compared with experimental ones, both in terms of macrostructure prediction and metallurgical behaviour, obtaining a fairly good agreement.

Riassunto

Simulazione numerica del processo di solidificazione in un getto tridimensionale assialsimmetrico di alluminio.

Nel quadro dello studio numerico dei fenomeni di solidificazione dei getti di alluminio è stato affrontato un caso tridimensionale assialsimmetrico. È stato scelto, a tale scopo, il metodo degli elementi finiti utilizzando elementi triangolari di geometria indipendente dalla temperatura. La transizione di fase è stata simulata attraverso una funzione dipendente dalla temperatura assegnata al calore specifico $C_p(T)$. Un test sperimentale è stato effettuato allo scopo di verificare i risultati numerici, colando un getto in Al 99,8 e campionando l'andamento della temperatura in funzione del tempo in svariati punti del sistema, nel materiale in via di solidificazione.

I risultati numerici posti a confronto con quelli sperimentali, sia in termini macrostrutturali che metallurgici, hanno evidenziato un ottimo accordo.

Introduction

Computer Aided Design (CAD) techniques nowadays represent a useful tool in design practice.

Indeed the use of computer methods can supply important information about the behaviour of complex structures, and now several software packages are available, on large high-speed machines, to solve elastic, elasto-plastic, and dynamic problems of structural analysis.

Many computer codes are also devoted to the solution of related problems, like thermostructural ones, or more advanced items, such as fracture, creep and fatigue, involving highly non-linear material and/or geometrical characteristics.

Also in the field of transport phenomena, such as heat exchange, many numerical methods are commonly used in design and process simulation, both in linear and in non-linear conditions.

More recently, thermal problems involving a phase change, have been faced by using suitable algorithms to simulate the energy release during the solidification (or melting) process. This item has a capital importance in industrial problems such as the Direct Continuous Casting of ingots (D.C.C.) and strip or casting production; D.C.C. has been treated by considering steady-state conditions and solved by the FEM method, with both moving and static mesh techniques. Results have confirmed that numerical methods can well describe complex non-linear problems involving phase transition (1-3).

Their application to mould designing in casting production, as a powerful tool to enhance product quality and reduce production costs, was immediately apparent.

As is well known, mould development is an expensive process requiring quite a lot of guesswork and

experimental examination before obtaining a sound casting, i.e. without macroscopic defects and with proper behaviour. Starting from these considerations, we studied the possibility of simulating, by computer methods, the solidification of an aluminium casting, as an essential step towards achieving automatic designing of the moulds.

In this paper a Finite Element Analysis of a three dimensional axisymmetric aluminium casting is presented, as an example of the real capabilities of the computer method to describe an actual solidification pattern. This kind of analysis was performed with a simple numerical code, "ad hoc" implemented.

An experimental work has been planned to confirm the calculation results; the temperature/time relationships were monitored during thermal transient for a set of points in the bulk of solidifying material, starting from metal pouring up to complete freezing.

Then metallographic inspection in a section of the casting was carried out to compare the microstructure of the material with the numerical predictions. Good agreement between both numerical and experimental results is reported here and discussed.

Mathematical model

The physical phenomena controlling a phase change usually involve a complex relationship between heat flow, solute redistribution, fluid flow, etc.. Numerical modelling is therefore very difficult or, more precisely, an accurate description of a thermal transient, involving phase transitions and related phenomena in a domain characterized by a complex geometry, is quite impracticable.

Nevertheless, in the industrial field, many features of technical topics can be dealt with reasonable accuracy,

with the aid of numerical methods implemented on digital computers, by considering the phenomena mainly driven by a non-linear heat flow, and by appropriately separating the problems. In particular, in the field of casting, a good description of the solidification pattern can be obtained by treating the problem as a non-linear transient heat exchange in the casting-mould assembly, and by incorporating the energy release at the liquid-solid interface in the Heat Capacity function $\rho \cdot C_p(T)$.

Heat-exchange phenomena are described by the well known "quasi harmonic" equation:

$$\rho \cdot C \frac{\partial T}{\partial t} = \nabla(K \cdot \nabla T) + Q \quad (1)$$

with boundary conditions set as

$$\alpha T + \beta \frac{\partial T}{\partial t} = \gamma \quad (2)$$

where equation parameters can be both temperature and/or time dependent. An analytical solution of the previous equation is, in general, impossible, especially for complex geometries, non-linear materials and, in particular, where an energy release owing to a phase change is involved.

Several numerical solutions of Equation (1) have been proposed, by using the Finite Element Method (FEM), Finite Differences Methods (FDM) or Boundary Elements Method (BEM).

Within the framework of FEM, the solution of Equation (1) has been obtained by several workers (4); the main features of the method consist in the fact that the domain being divided into small subregions (elements), the solution is obtained for a finite number of points (nodes) usually lying on the element boundaries. For each element the temperature field can be calculated on the basis of nodal temperatures by using the appropriate interpolation function:

$$T = [N(x, y, z)] \{T\} \quad (3)$$

where $N(x, y, z)$ is the interpolation function and T the column matrix of nodal temperature.

The discretization process leads to an equation with the form:

$$[T] \{T\} + \frac{\partial}{\partial t} [C] \{T\} + \{F\} = 0 \quad (4)$$

The problem, therefore, can be solved numerically as a system of algebraic equations in the T_i unknown nodal temperatures.

The time dependence of Equation (4) can be faced by considering the problem as a succession of steady states, while the non-linearity feature can be solved by

the usual interactive methods.

Since the behaviour of every element is determined before putting them together to solve the whole problem, the material non-linearity has to be faced, for each element of the domain, by determining the values of the element's thermal conductivity K^e and heat capacity $(\rho \cdot C_p)^e$ on the basis of the temperature dependent $K(T)$ and $(\rho \cdot C_p)(T)$ functions. As recently suggested, this can be done by calculating the "directional" $(K^e)_s$ and $[(\rho \cdot C_p)^e]_s$ material characteristics (5).

$$\left(\frac{1}{K^e} \right)_s = \frac{dw}{dT} / \frac{dT}{ds}; \quad w = \int_{V^e} (1/K) dT \quad (5)$$

$$(\rho C_p^e)_s = \frac{dw'}{dT} / \frac{dT}{ds}; \quad w' = \int_{V^e} (\rho C_p) dT$$

With this method, high temperature gradients can be treated for each element, and the energy release involved in a phase change can be considered by taking into account an appropriate $(\rho \cdot C_p)$ variation near the critical temperature of phase transition, as suggested in (6).

The function $(\rho \cdot C_p)$ is therefore defined by using the enthalpy per unit volume " $e(T)$ ".

$$(\rho \cdot C_p) = \frac{d}{dT} \int_{V^e} e(T) dT \quad (6)$$

Obviously, a finite freezing interval ΔT for phase change has to be considered for the analyzed materials, as pure elements or eutectic alloys, and appropriate mesh and time steps must be chosen to enter the characteristic solidification temperature stops during the numerical computation.

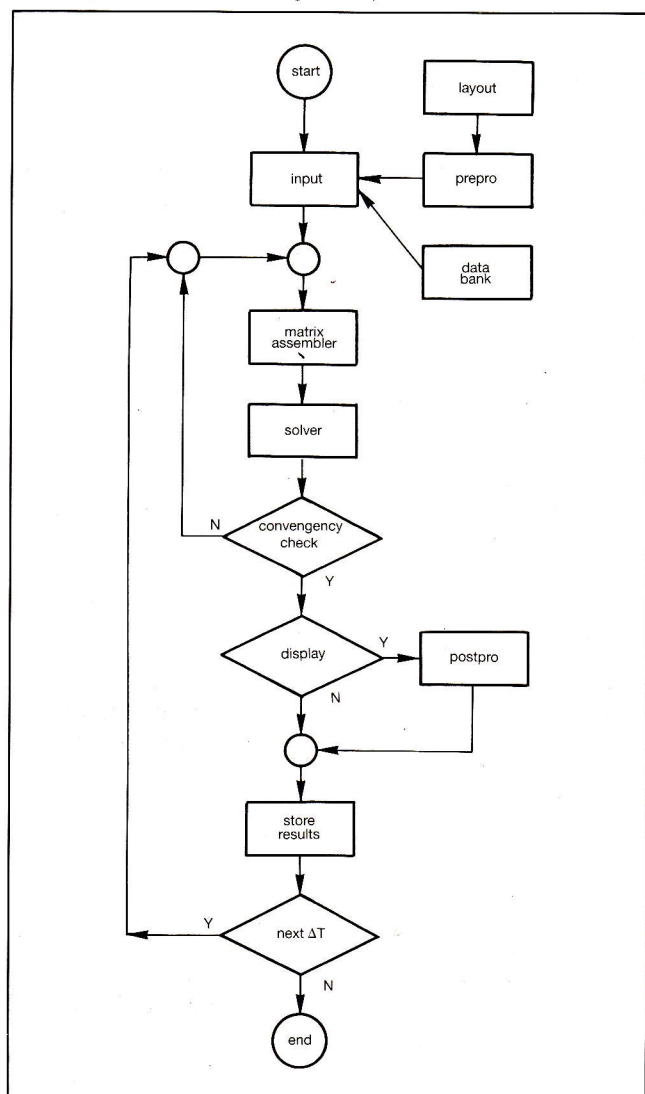
For plane and three-dimensional problems, the simplest types of elements are the linear 3-node triangular and 4-node tetrahedral respectively; in this case, the temperature gradients are single valued. Isoparametric elements, too, can be used with this method and with the same Equations (5), (6); in this case the gradients are calculated at the quadrature points.

Programme characteristics

A computer programme was implemented in FORTRAN IV language on a UNIVAC 1100/70 computer (7), using the previously described Equations. General features of the programme are described by the rough lay-out reported in Fig. 1. Since both plane and axisymmetric three-dimensional and pure three-dimensional problems are allowed by

the programme, a general preprocessing programme performs the mesh of the physical domain on the basis of four-node or eight-node quadrilateral subregions for plane models and eight-node or sixteen-node subregions for pure three-dimensional ones; in the computer programme, three-node triangular and four-node linear tetrahedral elements are now considered. It should be noted that for industrial purposes, the preprocessing programmes are very important to enhance the capabilities of software projects in the CAD technique. As an intermediate step, the structural model can be displayed before elaboration to verify the features of the mesh on a Tektronix CRT. The first section of the calculus programme (the routine INPUT) inputs the data received from the preprocessor, opens the internal files, searches for the material

Fig. 1 - Simplified flow-diagram of the computer program used for the simulation of the solidification in the mould-casting assembly.



characteristics in a data bank and reads boundary and initial conditions in a data file. A following routine (STIFF) assembles the thermal matrix by performing a loop on all elements; the elementary matrices for linear materials are calculated only once.

A solver routine performs the solution of the equation system; two types of capabilities are allowed: an out-of-core solver for large problems and an in-core solver.

A convergence check controls the iterative procedure: non-linear parts of the matrices are renewed until convergence is reached; then the results are stored in a file and/or, eventually, on a tape.

At each time step the results can be processed with the aid of a graphic postprocessor, and displayed on a CRT. The solidification pattern is therefore examinable by a step-by-step procedure and the elaboration can be stopped when an unfavourable situation is detected. In this case the design lay-out must be corrected and the calculations restarted. Two kinds of information arise from the temperature field.

Firstly the position of the solid-liquid interface, with respect to the time step, can be determined; in such a way, shrinkage phenomena can be avoided by proper designing of the casting mould assembly.

It has to be outlined, in fact, that the solid-liquid interface, starting from mould walls, should be driven from feedheads and chills in such a way as to avoid unfed zones, where macro and micro shrinkages can occur.

Secondly, the temperature-time relationships can be calculated for all points of the domain to predict metallurgical behaviour of the solid material as a consequence of the solidification pattern.

Programme capacity is estimated at 90 K for the elaboration section and 70 K for the pre-processing one. The elaboration time can be very long, especially for large three-dimensional problems; the experience of the designer therefore assumes great importance in avoiding expensive computer simulation.

Numerical analysis

As an example of FEM capabilities, a numerical analysis has been planned on a three-dimensional axisymmetric aluminium casting.

The lay-out of the casting-mould assembly is shown in Fig. 2.

In spite of the apparently simple shape, the solidification pattern is very interesting, since two quite different situations can be outlined and analyzed at the same time.

The first one corresponds to the cylindrical part, where a slow solidification process is expected (the temperature gradients at the solid-liquid interface take a direction perpendicular to the mould walls during the

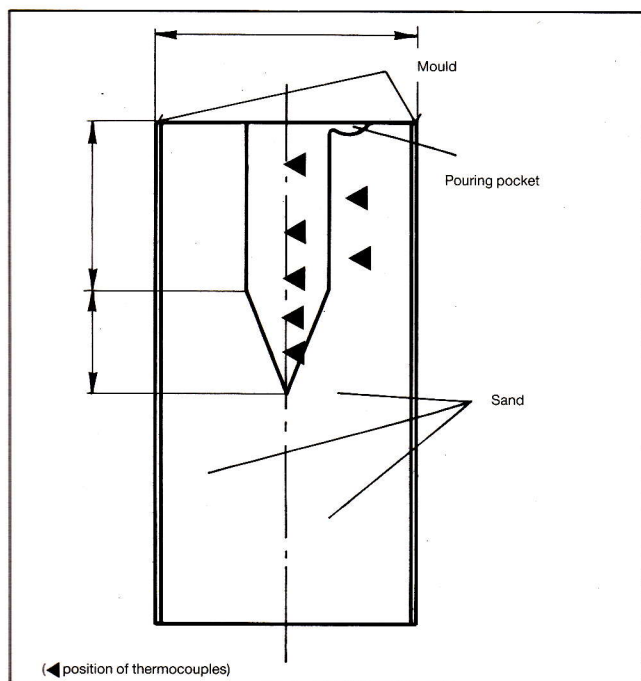


Fig. 2 - Design of the experimental mould used to perform the temperature sampling; Cr-Al (type K) thermocouples positioned in the mould cavity along the symmetry axis have been used to detect the temperature/time relationships during the thermal transient.

transient, without changing in direction), while the second refers to the conical part characterized by a faster solidification process (the temperature gradients, in this case too, start perpendicularly to the walls, but they change direction during the transient, to become almost parallel to the symmetry axis).

Fig. 3 shows the F.E. model used to perform the calculations. A triangular mesh, consisting of 814 linear triangular elements, simulates the casting, while 524 elements are used to describe the mould.

Material characteristics used in the calculations are reported in Table 1; a linear behaviour for foundry sand was assumed. Initial conditions of 750°C for liquid metal (pouring temperature) and 30°C for the mould, have been set.

Since pure aluminium 99.9% was used, a finite freezing

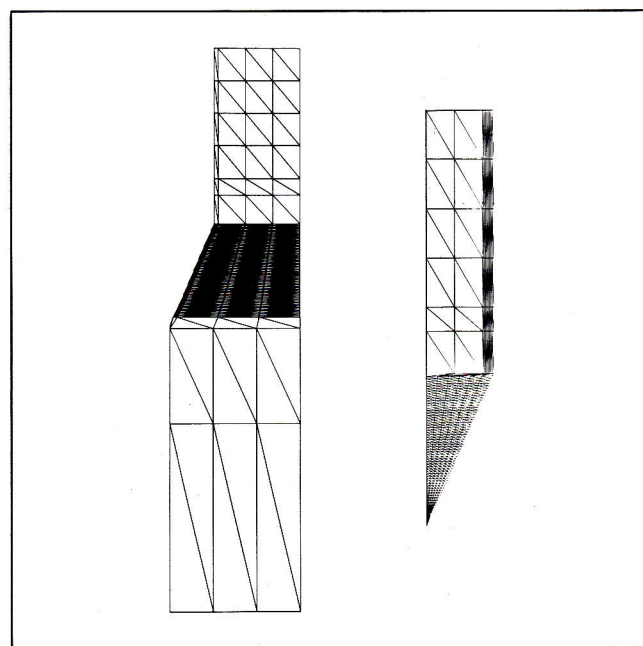


Fig. 3 - Structural mesh adopted to describe the mould-casting assembly; 814 linear triangular elements simulate the solidifying metal while 524 elements of the same kind have been used for the sand mould. As can be seen the conical part of the casting has been better defined by a more refined mesh.

range of $\pm 0.5^\circ\text{C}$ around the critical melting temperature (660°C) was considered. Starting from the initial conditions just described, a step-by-step iterative elaboration was performed, using time intervals of variable length ranging from 1.0 s for the early stages of solidification, to 5 s for the later ones.

Both the temperature field and the temperature-time relationships for a selected set of nodal points lying on the symmetry axis, were analyzed at each time step, using a post-processing programme. The calculations were stopped when solidification of the conical part of the casting was completed, while the cylindrical one was characterized by a very slow freezing rate. The total elaboration time was 8 min.

Fig. 4 shows the pattern of the solidification isotherm of 660°C for a set of time steps. In addition, a typical

TABLE 1 - Material characteristics used in simulation.

Material	K (cal/°C cm s)	Cp (cal/°C g)	ρ (g/cm ³)	e (cal/g)
Al 99,8	K (T) (+)	Cp (T) (+)	2.7 (+)	95 (+)
Sand	0.0016 (+++)	0.217 (+++)	1.8 (++)	—

(+) Handbook of Chemistry and Physics - 56th Edition - CRC Press (1975-76)

(++) Experimental

(+++) J.R. Simonson - An Introduction to Engineering Heat Transfer. Mc Graw-Hill, London (1967)

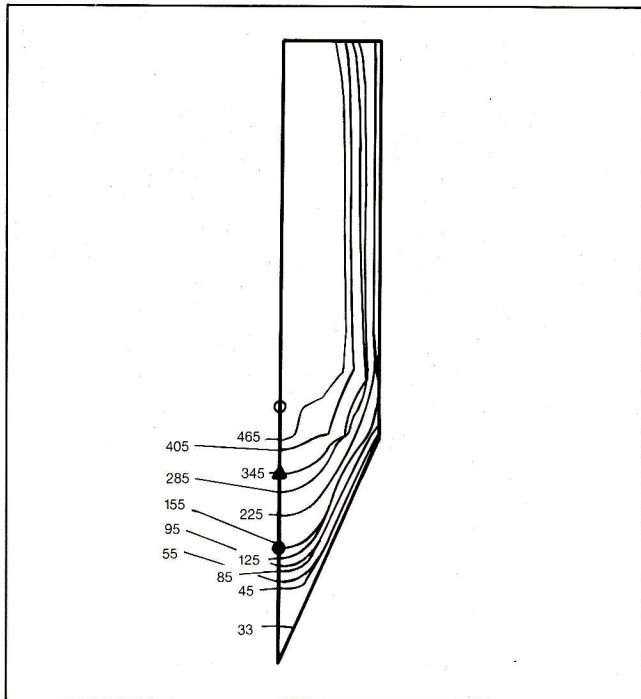


Fig. 4 - Pattern of the liquids isotherms at 660°C during the thermal transient; after 250 s the lower part of the casting is completely solidified while a large part of the remaining is liquid. The cylindrical part slowly solidifies, and here the solidus surface is parallel to the mould walls.

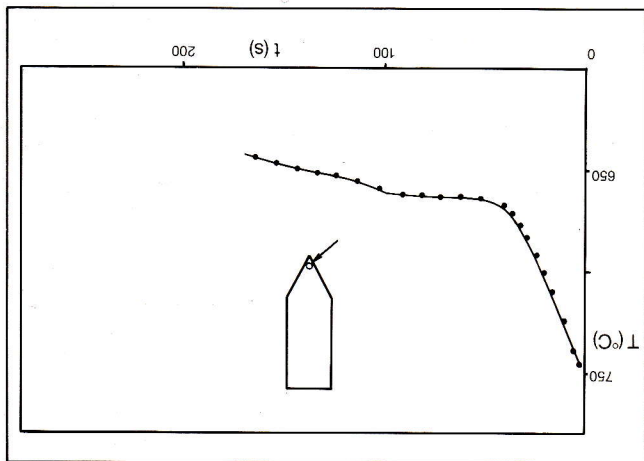


Fig. 5 - Typical temperature/time relationship calculated in a point of the symmetry axis in the lower part of the casting. The curve shows the typical trend of the solidification: a continuous decrease from 750° (pouring temperature) to the critic liquidus temperature (660°C); a temperature stop corresponding to the energy release during the transitions from the liquidus state to the solidus one; and finally a slower decrease of temperature, with respect to the early stage of the transient.

temperature/time relationship calculated at a point of the conical part, lying on the symmetry axis, is shown in Fig. 5.

As expected, the lower part of the casting exhibits a

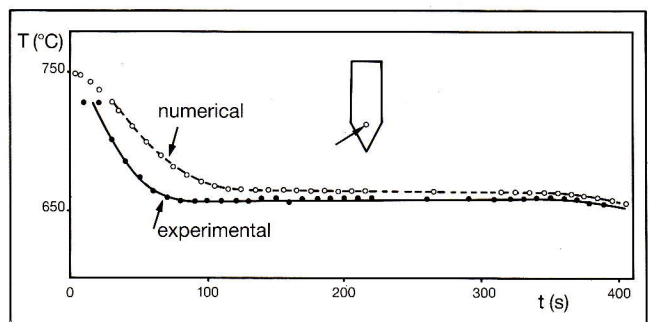
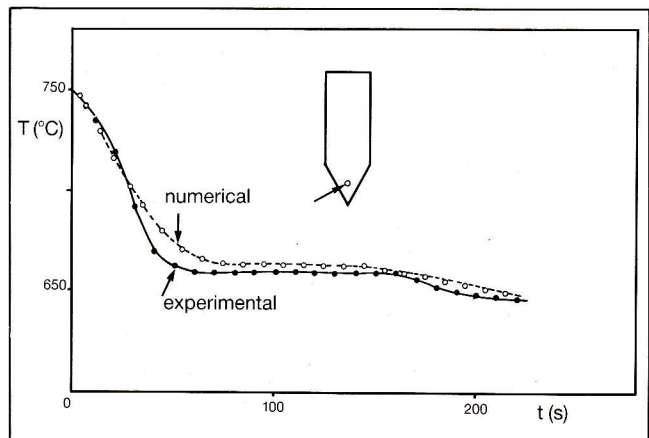
more rapid solidification process than the upper one. In fact, after 250 s a large part of the cone appears completely solidified, while the cylindrical part is practically still in the liquid state.

From this solidification pattern, some microstructure behaviour can be predicted: small grains should be present in the conical zone, characterized by a fast solidification process, large columnar grains in the cylindrical zone, and medium size grains in the intermediate part. In addition, a large shrinkage in the center of the cylindrical part of the casting is to be expected.

Experimental casting test

An Al 99,8% casting has been produced by employing the same boundary conditions used in the numerical analysis. The temperature field was monitored, as a function of time, starting from metal pouring and using Cr-Al thermocouples positioned along the symmetry axis; after complete freezing, the casting was cut along a symmetry plane, surface machined and etched to reveal the macrostructure.

Fig. 6 - Comparison between experimental and numerical results in two points of the symmetry axis; as can be seen, the programme can properly describe the time dependence of the temperature in points characterized by very different temperature/time relationships. In fact the first curve describes a slower transient ≈ 150 s; the other one a transient ≈ 400 s.



Two typical T-t curves are reported in Fig. 6 and compared with the calculated ones (curves refer to zones characterized by very different solidification rates).

Clearly, the experimental points compare well with the calculated ones. Some differences appear in the early stage of the slower transient, probably due to the convective exchanges immediately after metal pouring, not taken into account in the numerical code.

The macrostructure of a section of the casting is shown in Fig. 7; this picture completely confirms the results of numerical analysis.

In fact, large columnar grains appear in the cylindrical part, formed during the slow thermal transient. In this part, the solid-liquid interface moves parallel to the mould walls, and the thermal gradients have the same direction during the solidification process, as well predicted by the calculations.

On the other hand, grains more reduced in size can be detected in the conical part as a consequence of the higher solidification rate. In this zone the temperature gradients change continuously, in direction and modulus, with respect to the previous part.

Finally, a large shrinkage appears in the middle of the casting owing to the large volume reduction during transition from the liquid to the solid phase.

Conclusion

Mould designing represents one of the most important and critical operations in the casting industry. For complex products, several experimental tests are generally performed before obtaining useful results. Nevertheless, even if the validity of the design is always strictly dependent on manual skill, any further improvement in the quality and reduction of the cost, absolutely needs an automatic method for a preliminary inspection of the project.

With this aim, we studied numerical methods (for an application to computers) useful to simulate the solidification process of the casting.

In more detail, we wanted to obtain:

- a) a complete knowledge for the movement of the solid-liquid interfaces in the casting without feeding systems, only successively inserted to avoid feeding defects and properly to drive the solidification process;
- b) the time-temperature relationships in the whole bulk of the casting, the microstructural behaviour strongly depending on this parameter.

In this paper we applied such methods within the framework of the finite element method to a three-dimensional axisymmetric aluminium casting, obtaining a complete description of both solid/liquid interface movement and T-t curves.

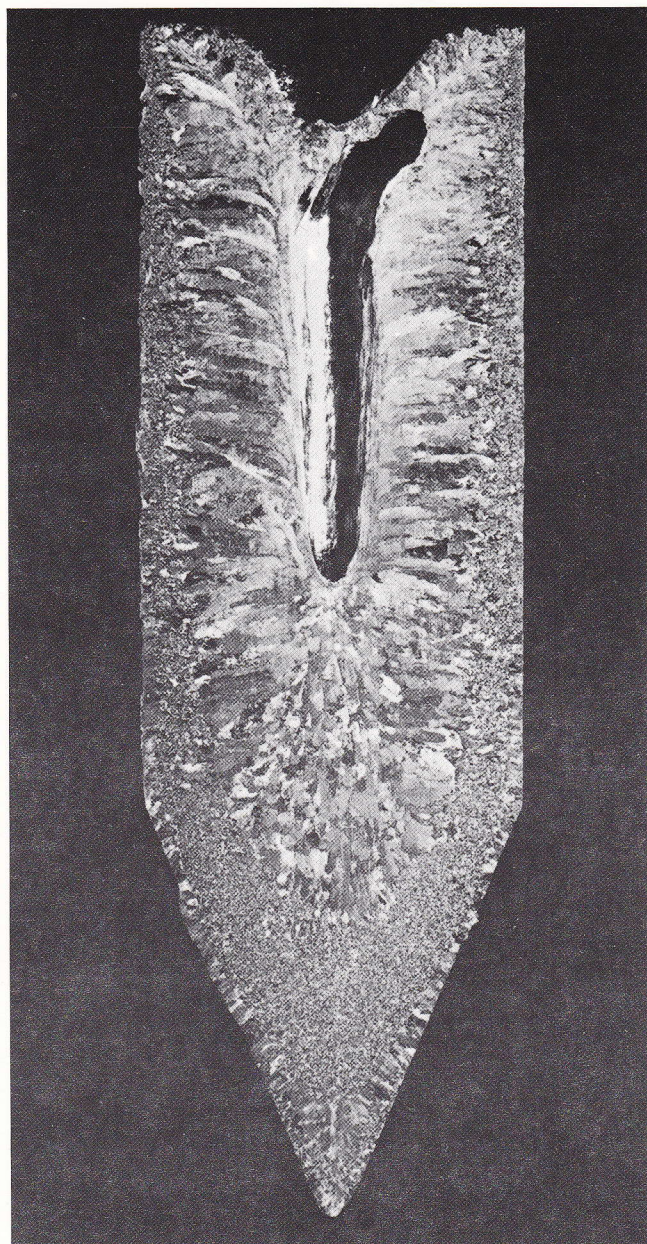


Fig. 7 - Macrostructure of a section of the Aluminium 99.8% casting as obtained after complete freezing (three-acid etching).

This simulated pattern has been well confirmed by experimental work carried out using the same boundary conditions.

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REFERENCES

- (1) Weckman, D.C., et al. *Z. Metall.* **70** (1979), 750-757.
- (2) Weckman, D.C., and P. Niessen. *Met. Trans. B*, **13B** (1982), 593-602.
- (3) Clyne, T.W., *Mat. Sci. Engng.* **65** (1984), 111-124.
- (4) Zienkiewicz, O.C. *The Finite Element Method in Engineering Science*. Mc Graw Hill, London, 1971.
- (5) Lemmon, E.C. In R.W. Lewis, K. Morgan, and O.C. Zienkiewicz (Eds.), *Numerical Methods in Heat Transfer*. John Wiley & Sons, Chichester, 1981.
- (6) Comini, G., et al. *Int. J. Num. Meth. Engng.* **8** (1979), 613-624.
- (7) Abis, S. *Modello simulativo per transienti termici comprendenti transizioni di fase – Codice programmatico HEATR-TRASPH (caso non lineare)*. ISML Technical Report n. 83/26 393.