Casting simulation: How well do reality and virtual casting match? State of the art review

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Over the last ten years or so many man-hours have been dedicated to developing methods for simulating the casting process. The majority of the methods developed have been devised by a combination of computer, mathematics and materials specialists with little or no knowledge of foundries and foundrymen. As a result of this it would appear that although there are many software packages for the foundryman to use there still exist fundamental misunderstandings as to their usefulness and suitability within the foundry.

This paper is an update review and aims to identify how well current software packages are progressing towards their target of predicting casting defects. The relationships between physical phenomena, practical defects and software capability are presented. Some discussion of the use of criterion functions is also presented. Finally issues arising from the post-processing of results are discussed, as the presentation of the results to the layperson in simulation techniques is possibly one of the most important aspects in influencing the adoption of this type of software in the foundry community.

Keywords: simulation software, casting software

Introduction

Since the mid 1980's, software for the numerical simulation of flow and solidification during casting processes has become more accessible to foundries as a result of both software and hardware developments. This has attracted considerable attention from both researchers and farsighted foundry engineers. A recent review of this field describes the massive changes that have taken place over this century with regard to what can be modelled in terms of physical phenomena.[1] There are a large number of packages now commercially available and investment in their development is still growing.[2] Why then is it that only between 10 and 15% of all foundries in the developed world use casting simulation software tools in-house? Modelling of continuous casting processes for both steel and aluminium is now accepted as the norm but, in shape casting, where geometries are more complex and the process physics must deal with transient conditions rather than an equilibrium state, the software has still not been generally introduced.

The foundry industry historically views new technology with scepticism. Many in the industry have been disparaging about this emerging branch of engineering. However, the software developers must take some of the blame for overselling their products. Many promises have been made and sometimes there has been an ''economy with the truth''. There is also the misunderstanding that simulation will give solutions - it doesn't. Casting simulation software at present is still only a tool for use by experts and is not a magic wand.

Range and scales within the foundry industry

Before investigating the reasons why the use of simulation tools has not grown as rapidly as might have been expected, it is necessary to understand what casting process are used and some of the differences there are between them. Table I lists the main casting routes used in foundries and puts some estimates of scales by them. Table 2 lists some typical components and demonstrates the extremes of scale that are exist within these foundry processes.

The extremes of the processes cover about 8 orders of magnitude when talking about mass, about 5 orders of magnitude for filling and solidification times, and about 3 orders of magnitude in minimum length scale. If the modeller wishes to model grain structures in large castings then there is a scale factor of about 5 to 6 orders of magnitude between the geometry of the casting and the physical phenomenon to be modelled.

Even within the same casting, the aspect ratio of the overall size of the component to the thinnest section can be so large that resolution of the geometry during meshing itself becomes a problem computationally for the foundryman as the computing power required, and time-scale for calculation obviate the cost benefits. For example, the IRC at the University of Birmingham has had some experience of castings with an overall space envelope of 1m by 1m by 0.5m with a wall thickness of 2.5 mm. To resolve that sort of geometry with today's meshes requires some 500 million-control volumes. At the IRC it is possible to deal with models containing up to 50 million control volumes in a reasonable time-scale, with a 4 processor machine and 4.5 Gb of RAM. Most foundries could not afford that type of hardware. However hardware costs are falling rapidly and most of the software

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Table I List of most common foundry processes

Process	Range of component mass	Time-scale of process	Material Cast
Sand	100g to 250 tonnes	seconds to days	All metals
Investment	10g to 100 kg	minutes to hours	All metals
Resin Shell	100g 100 kg	minutes to hours	Fe, Cu
Permanent Mould/ Gravity Die	2 kg to 50 kg	minutes	Primarily Al, Zn & Mg, some Cu
Low Pressure Die	5 kg to 25 kg	minutes	Primarily Al & Mg
High Pressure Die	10g to 20 kg	seconds	Al, Mg, Zn
Squeeze Casting	100g to 20 kg	minutes	Al

packages are now being ported onto the PC platform using the Windows NT operating system. A typical configuration might be a Pentium III with a 900MHz chip and between 512Mb - 1GB RAM.

Within each of these main processes there are also subcategories of the process, which can be unique to an individual foundry. With each of the processes much of the physics is also dealing with extremes. For example, in general sand casting, except in very large castings, the velocity of the liquid ranges from 0.1 ms-1 to 5 ms-1. However, in high pressure die casting, the liquid metal velocity is in the range of 40 to 60 ms^{-1}. Similarly the externally applied pressure ranges from 0 in gravity processes to 250 MPa in squeeze casting. It is difficult to imagine therefore, that there is one software code which will be capable of simulating all of the different processes well. It is likely that different models or variations of the same model will be necessary to cover the differences in physics.

Boundary conditions

One of the most difficult aspects of any simulation exercise is the accurate representation of the boundary conditions. When casting simulation was first used in the foundry industry, most of the codes concentrated on the thermal aspects of the problem. At that stage there was neither the software nor hardware available to address the problems of filling and liquid metal flow. Boundary conditions were relatively simple, air temperatures around moulds were assumed to be ambient and even heat transfer coefficients, although not really known for material combinations, could be estimated for different mould/die materials.

At present many of the codes address filling as well as the thermal aspects, and some also have the capability to model stress. This immediately raises more issues with regard to boundary conditions. If stress models are used then the heat transfer coefficients change over the time of the simulation as distortion occurs and gaps are produced between the casting and the mould or die. Some software packages consider this while running analyses.[3,4]

The initial boundary conditions for filling can also be extremely complex to set up. During a recent investigation at a UK crankshaft foundry, it was observed that during the semi-mechanical pouring of cast iron crankshafts, the metal stream from the lip poured ladle varied from 20 to 40 mm in diameter, and the distance from the top of the pouring bush ranged from 150 to 250 mm. This led to changes of inlet velocity at the pouring bush from 1.7 ms-1 to 2.2 ms-1 during the pouring of one single mould.[5] During low-pressure die-casting the head of liquid metal changes in the furnace thus affecting the pressure experienced by the metal during filling. Work at the IRC has shown the dramatic effects that this can have on the filling velocities.[6] This is not untypical in foundries. With bottom poured ladles the head height in the ladle will change between the ladle being full and the ladle being empty. Typically, in a steel foundry, this may mean the exit velocity in the ladle nozzle can vary from the beginning, to the end of pouring, by 5 ms-1.[7] It is essential for accurate representation and modelling of the filling of a casting that this change in flux is considered. This can also significantly change the thermal patterns in the casting depending upon the geometry.

Table 2 Extremes of scale in common foundry processes

Components	Process	mass (kg)	filling time (s)	solidification time scale	min. section size (mm)
small electronics components	high pressure	0.01	0.04	seconds	0.1
jewellery, medical, aerospace	Investment	0.1	5	seconds	1
small valve bodies	Sand	5	10	minutes	10
automotive wheels	low pressure (die)	10	60	minutes	5
cylinder heads	permanent mould	10	20	minutes	5
large valve bodies, propellers	sand	10000	200	hours	20
turbine casings	sand	200000	500	days	100

Physics and mathematical solutions

The physical processes that need to be modelled to cover all the shape casting processes are heat transfer; including radiation, convection and conduction; mass transfer (mainly fluid dynamics); phase transformations; including solidification and subsequent solid state changes and stress/strain behaviour. The mathematical models used in software codes must also consider the conservation of mass, momentum and energy.[8]

A wide array of mathematical tools is then applied to the physics in order to solve the physical equations. These come in various guises and combinations of solutions, and include finite difference (FDM) and volume (FVM)[9] methods, finite element methods (FEM),[10] cellular automaton methods (CA)[11] and lately phase field theory.[12] Sometimes there are also combinations of two techniques such as the cellular automaton finite element (CAFE) method proposed by Rappaz and his co-workers.[13]

What does the foundryman want?

The foundryman would like the computer tools to be able to predict or show the following phenomena: hot spots, riser effectiveness, chill effectiveness, insulation effectiveness, solidification direction, macro-solidification shrinkage, surface sink, microporosity, hydrogen porosity, hot tearing, final casting dimensions, casting distortion, residual stress, cold shuts, mould filling time, ingate effectiveness, runner effectiveness, pouring rate, post-pouring temperature distribution, turbulence, mould erosion, cold crack susceptibility, oxide film defects, lustrous carbon defects, bubble entrainment, microstructure, morphology, mechanical properties, grain size, stray grains, freckling and grain orientation. Foundrymen would be delighted if defects such as sand and slag inclusions, finning, veining, scab and buckle could be predicted. Some phenomena in the first list can now be predicted reasonably accurately with a selection of software. On the other hand, some of the above list have to be interpreted or there may be a calibration exercise needed to relate the results to an individual foundry. The second list is rather more difficult as the physics and mechanisms of creation for each of the phenomena are not well understood.

Linking solutions to defects

In order for the simulation software to work it has to link the basic physical equations with numerical solutions using thermophysical data to predict such things as heat flux, thermal contraction, temperature distributions at various times, velocity vectors, density and pressure changes, free surface movement and a variety of other field variables. At present most of these "academic" results then have to be related to defects that the foundryman observes by using criteria functions or other post processing techniques to give visual displays that can indicate where defects are likely to occur or what scale or type of microstructure will be present. The criteria functions are empirically based. As software development improves, the modelling of certain features moves away from requiring the use of criteria functions to the direct modelling of that phenomenon.

Figure 1 attempts to summarise the relationships between materials properties simulation of the casting

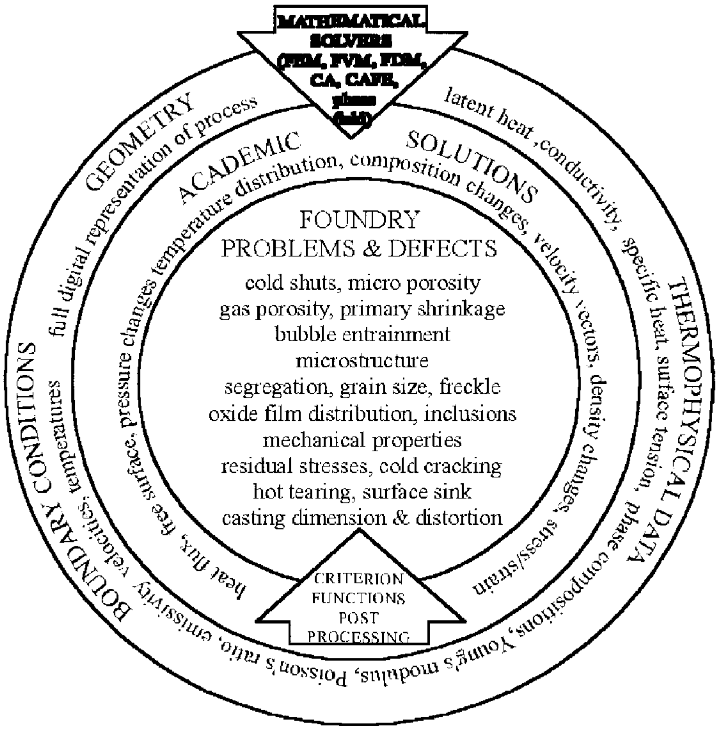


Fig. 1 Schematic showing the relationship between materials data, mathematical models, academic solutions and what the foundryman wants from simulation packages

Table 3 A selection of the process physics not well understood or described in current casting modelling software packages

Feature	Problem	Effect on
Foam Filters [22]	random reticulated foam structure, high tortuosity	surface turbulence, velocities therefore surface oxides
Mould Dilation	distortion & dilation	internal porosity
Mould casting interface separation [23]	stress on solidifying shell combined with internal shrinkage and changes in mould	interface heat transfer coefficient, surface finish
Mould and die coatings	proprietary chemistry. Very thin layer 1 to 100 μm	interface heat transfer coefficient
Metallurgical treatments - grain refinement and modification	number of nuclei, effect on solidification front	grain size & microstructure, alloy feeding and solidification characteristics
In-mould treatment with magnesium ferrosilicon for SG iron	violent chemical reaction	fluid flow, microstructure, dross and oxide inclusions

process and the relationships between academic answers and real defects.

Current limitations and problems still to solve

The current limitations and problems still remaining to be solved fall into a number of areas: those pertaining to process physics, lack of thermophysical data, computational time scales and real defect prediction and representation.

Process physics

It is not apparent to the author that the process physics necessary to describe all aspects of the processes described in Table I are completely understood. A number of those issues still outstanding are pinpointed in Table 3.

Some of these features are modelled in some software packages, for example foam filters, but it is not apparent that the models employed in the simulation actually represent what happens in reality. Research ongoing at the IRC is investigating the flow through filters in order to look at the effect of the material type, temperature and a number of other conditions, which affect the liquid metal flow behaviour.[14] It may be not be possible, or indeed necessary, to model all of the features listed in Table 3 exactly, but they should certainly be considered and their effect on the results estimated before being discarded. For example, for die coatings and mould washes it may just be necessary to obtain good experimental data so that the effect on the heat transfer coefficient can be modelled accurately, however actually modelling the coating as a separate phase is probably not necessary in most circumstances.

Thermophysical Data and Boundary Conditions.

Exothermic materials.

It is common practice within steel and some iron foundries to use exothermic sleeve materials for feeders/risers or ''hot toppings'' which are manufactured from materials that produce a ''thermit'' type reaction when in contact with liquid metal. These proprietary materials put heat back into the riser thus enabling the liquid metal to stay liquid for longer. Only one serious attempt at measuring these properties has been made and the results to date are being kept proprietary for the time being.[15] A number of software packages do have the capability of dealing with these materials provided the thermophysical data are available although there are a number of different ways in which the materials are treated. These are listed in Table 4.

Non-standard alloys

Exotic or proprietary alloys can often cause a problem for the foundryman as there is no universal database of thermophysical data for general access. Data for standard alloys are relatively easy to find. Data for alloys with slight deviations from standard or exotic alloys with low annual production tonnage and potentially with more casting problems do not exist in the public domain and are extremely expensive to produce. There are, however, a number of software packages which can be used to produce calculated thermophysical data from chemical compositions.[16,17]

Mould material properties

Thermophysical data for moulding material properties especially for sand moulds or investment shell moulds is not well documented. Problems arise from the very fact that sand properties will vary from foundry to foundry. Investment shell technology is often unique to a foundry and regarded as a proprietary ''art''. It is difficult to envisage how this issue can be resolved completely in modelling. Some headway is being made in this latter area by use of some simple rule-based techniques in order for foundries to be able to estimate certain thermophysical data.[14] Such tools could be applicable in other situations in the foundry, for example in mould coatings. Work on the modelling of sand core blowing will also contribute to a better understanding of the effect of cores during the casting process.[18]

Table 4 Thermophysical data required and techniques for exothermic materials

Fresh Sleeve (before ignition)	
density, conductivity and specific heat as functions of temperature	standard material properties required for use while the sleeve is heating up
Ignition Phase (elegant approach)	
ignition rate vs. temperature	this considers the rate at which the burn can begin
Ignition Phase (simple approach)	
ignition temperature	temperature at which the complete sleeve starts to burn and release energy
Combustion Phase (elegant approach)	
combustion rate	energy released per second per kg
combustion energy	total amount of energy released
Combustion Phase (simple approach)	
combustion temperature	the sleeve remains at the combustion temperature for the combustion time releasing energy at a fixed rate into the surrounding materials
combustion time	
Burnt Sleeve (after combustion)	
density, conductivity and specific heat as functions of temperature	after combustion many sleeves have poorer insulation properties than before burn so it is essential to consider this stage separately.

Interface heat transfer coefficients (h)

The interface heat transfer coefficient (h) is probably one of the most "fudged" parts of casting modelling. As the mould material properties are not accurately known, it is not possible to make accurate measurements of interface heat transfer coefficients although some attempts have been made.[19] Often the mould and the interface is treated as one and the same even though there are certain mechanisms occurring which must change the value of h during the casting process. As previously discussed the addition of die coats and mould washes will change h and should be taken into account in a more systematic way than is currently the practice. Often interface heat transfer coefficients are used which enable the user of the software to arrive at the correct defect prediction.

Time-scales

The biggest reduction in time over the last few years has been in the pre-processing stage of computer simulation. This is as a result of the penetration of CAD into engineering and the fact that many more components now originate electronically. E-communication, either by e-mail or ftp (file transfer protocol), has also sped up the data exchange part of the process — time waiting for the postman has been eliminated. The most common feedback heard from foundrymen who use simulation software and from those who have yet to adopt it is that they can "do it" quicker with a pen and paper. Taking into account the fact that with a pen and paper most foundrymen are not going to address all the issues that the software code will, it is still a serious issue. Timescales are reducing and as parallel codes are written and multiprocessor and network computing become commonplace then hardware limitations become less of an obstacle.[20] Benchmark tests by one software supplier indicate that the increase in speed of calculation moving from an SGI Origin 200 of 3 years ago to a well-specified PIII PC running at 800-1000MHz would be of the order of a factor 5 to 6 times.[21] A highly specified single processor PC would currently be expected to give results within 24-48 hours for an "average" job but this is extremely dependant upon the precise geometry and the amount of information that is required from the results. For example a simple solidification on even a complex geometry would run in a matter of a few hours. If the user requires a full filling, stress, venting and solidification analysis the time might be increased by a factor of 10 to 20 times. However when comparing computing time with knowledge or artificial intelligence (AI) based software that learns by experience and rules, those for simulation codes are far longer.

Results from Artificial Intelligence (AI) or heuristic software can be produced in minutes or seconds, numerical simulation software is generally always in the timescale of hours or days. There also seems to be something of a self-limiting rule that ensures that as codes and hardware speed up, more complex problems are addressed which require more CPU time and thus the elapsed time to solve problems remains the same.

The limits in the future in terms of timescales are difficult to predict. It may be that individual foundries will no longer do their own analysis only the pre- and post-processing. Files may be sent to a central server on which CPU time is bought. This is becoming more viable as it can be combined with the rapid transmission of data that is now possible.

Defect representation

The foundryman would like a tool that is capable of showing him graphically what he sees in the casting, i.e. the defect has to be represented graphically in a way that is instantly recognisable as that which he sees in the casting. He does not want to have to interpret coloured contours. Flow simulation should show surface behaviour

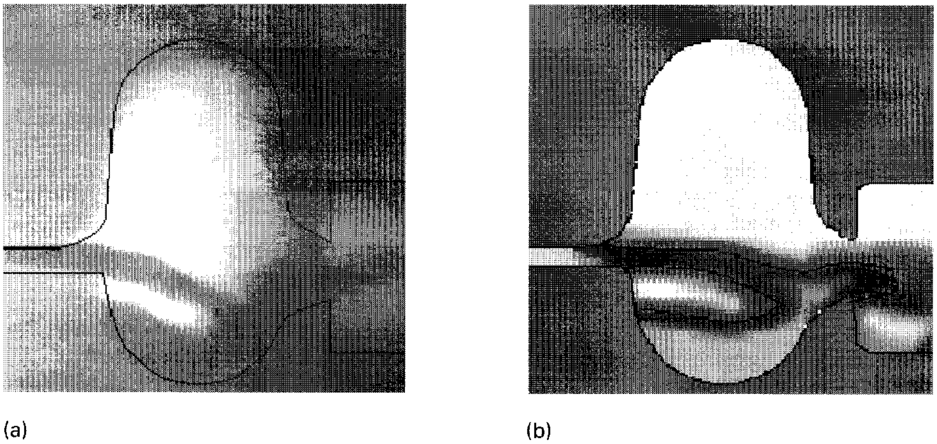


Fig. 2 a) Real time x-ray video capture showing flow of cast iron in a running system. b) Computer simulation of the same running system using Flow-3D, showing the close match between reality and simulation

and if possible indicate where turbulence has occurred. This is not simply recording Reynolds numbers, as it is surface turbulence that has the biggest effect. Porosity and macro-shrinkage should be shown to the quality level that he wishes the casting to be made to.[24] If the porosity is a result of different mechanisms e.g. micro-shrinkage or hydrogen porosity then they should be represented differently. Cold shuts (weld lines) should be shown as lines. Hot tearing should be shown as an absence of material. Bad venting in a die should show the entrapped air at the end of the casting simulation. The probability of oxide films from surface turbulence should be indicated.

Some software packages have some of these things well covered and some examples are shown in Figs. 2 to 9.[25,26,27] A number of packages can now reliably show the behaviour of the free surface of the liquid metal as it fills the mould cavity (Fig. 2a and b).

Most software packages claiming to be for foundry use can now simulate and represent macro-shrinkage and primary pipe accurately providing it is in a standard alloy without the involvement of exothermic foundry consumables (Fig. 3).

When the shrinkage manifests itself as sink, the problem becomes more difficult to predict.[28] The author knows of no package that will combine internal and external ''porosity'' mechanisms and represent both internal micro-porosity and surface sink. One of the earliest packages claimed to be capable of predicting different quality levels in castings of steel alloys (Fig. 4), and anecdotal evidence from the foundry industry appears to support this. With those software packages that deal with filling, cold shuts usually have to be interpreted from isothermal contours. Recent releases of foundry software now enable the prediction of bubbles of air entrapped during filling as a result of poor venting

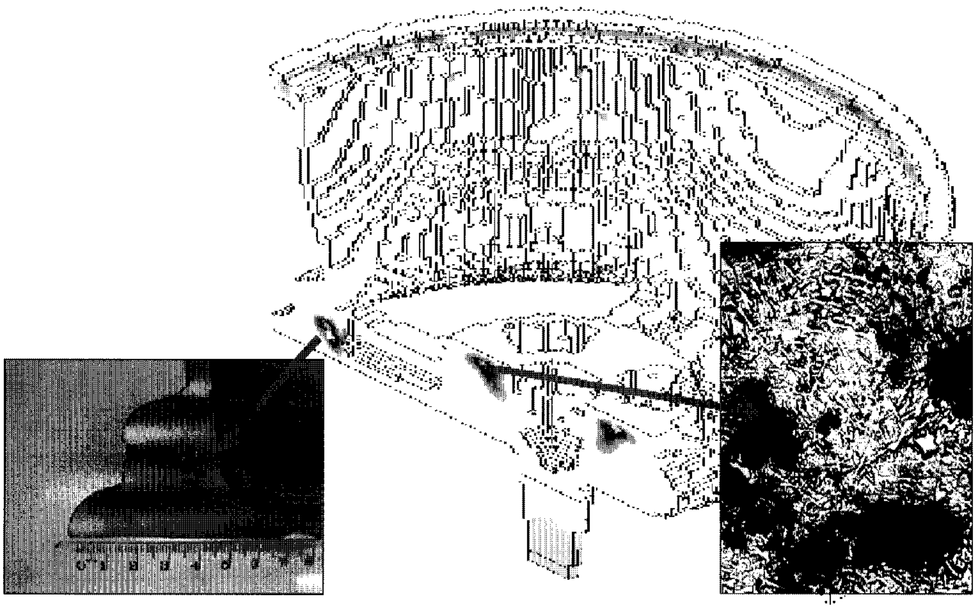


Fig. 3 Prediction of primary shrinkage and microporosity as represented in MAGAMsoft^{TM} and compared with macro- and micro-graphs illustrating accuracy of location and size of the defects

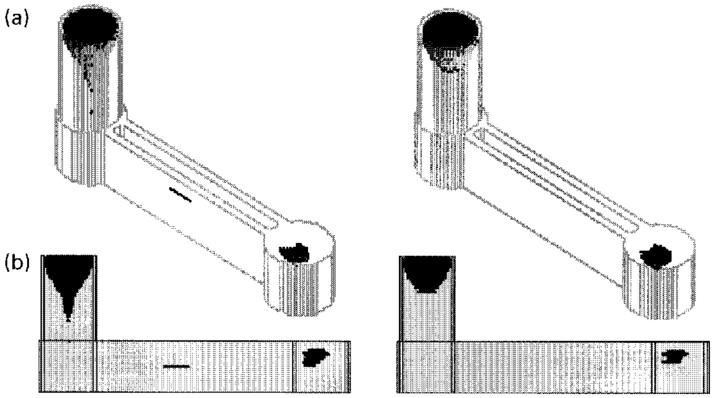


Fig. 4 Simulation results shown in simulated 2D and 3D x-ray representation for two quality levels; a) ASTME 155 equivalent level 1 x-ray quality. b) ASTME 155 equivalent level 4 x-ray quality (SOLSTAR). Note that the shape of the primary pipe is also changed

(Fig. 5). Particle tracking is also now possible thus enabling the distribution and movement of inclusions to be visualised (Fig. 6). Recent developments have been made in interpreting the data generated during simulation in order to try to predict potential areas of oxide films (Fig. 7) and mould erosion during sand casting (Fig. 8). The prediction of stress levels during solidification has been developed by both FEM and FDM codes. The creation of the air gap between casting and mould is shown in Fig. 9 and the prediction of a hot tear in a steel casting is illustrated in Fig. 10.

However there are also some defects which it is unlikely will ever be represented by software in the way they appear. For example slag defects or lustrous carbon defects (Figs. 11 and 12), which require an understanding of the chemistry at the point of generation.

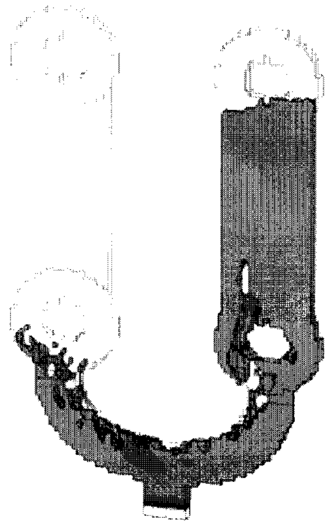


Fig. 5 Entrapped gas during die-casting as represented by MAGMAsoft^{TM} using the "venting" option

Conclusion

During the last three years the penetration into the foundry industry of casting simulation software has rapidly increased although the proportion of foundries in the West with software is still less than 25%. Foundrymen are gradually beginning to "believe" in the concept of casting simulation as they realise that it is a tool to help them perform their job better, not a threat to their job. The influence of casting simulation on foundry practices is increasing as there is a growing realisation that only controlled processes can be modelled.

The software packages and hardware have improved so that results are obtained more quickly and can solve a wider range of problems. Work on developing software for the prediction of microstructure and porosity is ongoing, and will become part of standard software packages in the near future.[13,29, 30] Work on understanding boundary conditions and improving thermophysical data input continues and will continue to have a significant influence on the accuracy of the results obtained by simulation.

Simulation is moving into other areas of the foundry process than metal casting. Work on injection of waxes and de-waxing for investment casting is being carried out with the associated work on the development of flow models and measurement of thermophysical data.[14] Core blowing is also being modelled and used successfully to save money.[18]

Numerical optimisation techniques are also being developed in order to move away from the concept of casting simulation as a tool to change it to an "intelligent" tool.[31] It is possible that the use of artificial intelligence (AI) or use of rules developed by numerical simulation could deliver the very fast response times that industry is still demanding.

One of the biggest issues that remains, and will continue to cause problems, is the representation of results. Software packages are only as good as the way in which they transfer their results across to the user and if that representation is difficult to understand then the software will not succeed as well as one that does. This is

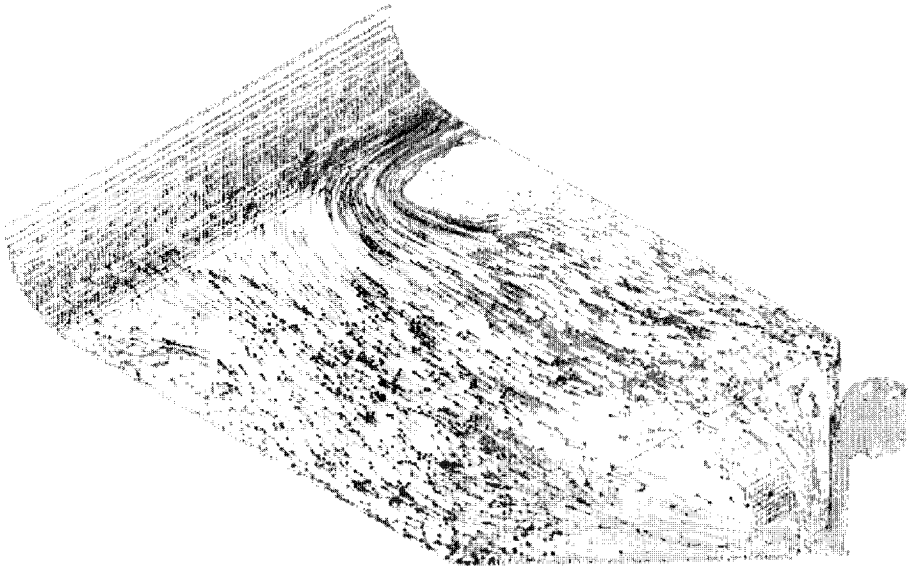


Fig. 6 Particle tracking enables the interpretation of where inclusions might be washed to during the casting process as well as indications of bulk filling history, the development of dead zones and eddies

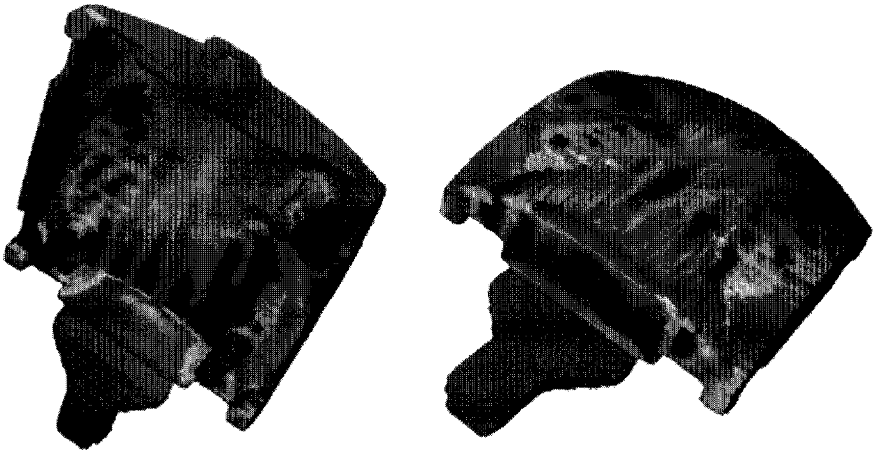
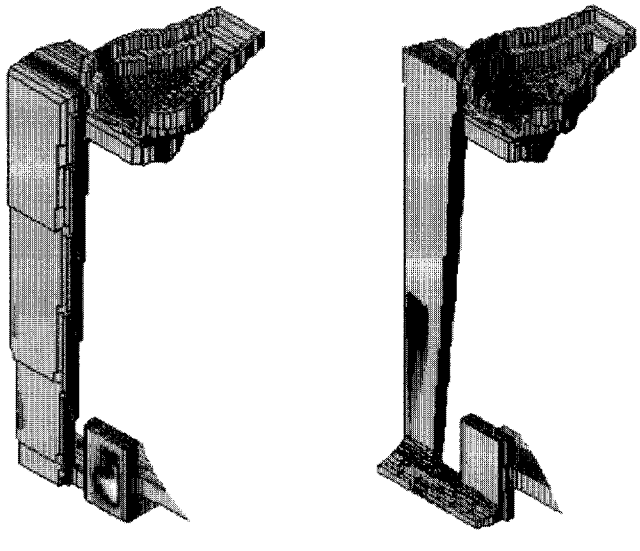
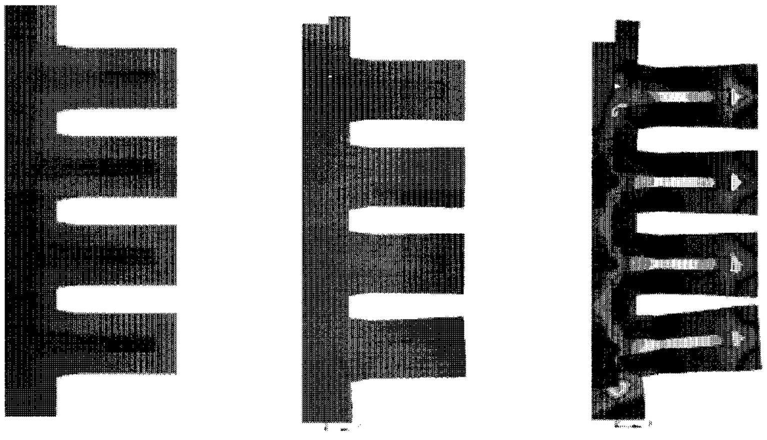


Fig. 7 High-pressure die-casting of a Zinc alloy. The darker areas show the regions of the casting that are more susceptible to the creation of oxide films from turbulence. (Flow-3D^{TM})



(a) high erosion (b) reduced erosion

Fig. 8 Prediction of susceptibility to mould erosion using the MAGMAsoft criterion function



(a) liquid metal in shell (b) start of solidification (c) room temperature

Fig. 9 Gap creation between mould wall and casting, and stress development during investment casting (ProCAST^{TM})

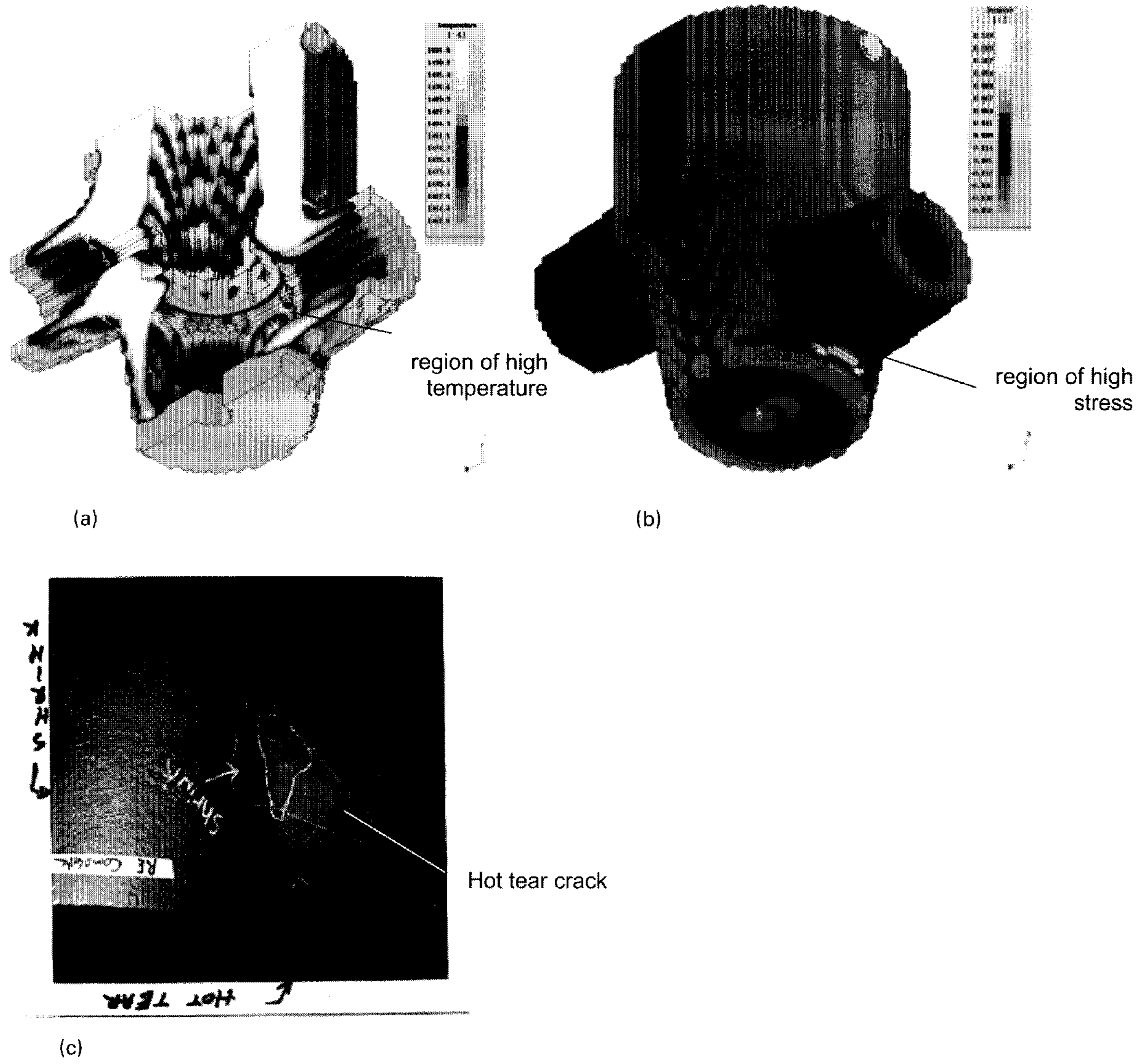


Fig. 10 Representation of hot tearing in the MAGMAsoft^{TM} code. a) shows the isotherms on solidification b) shows the surface stress concentrations (lighter area) and c) is a photo of the casting surface itself

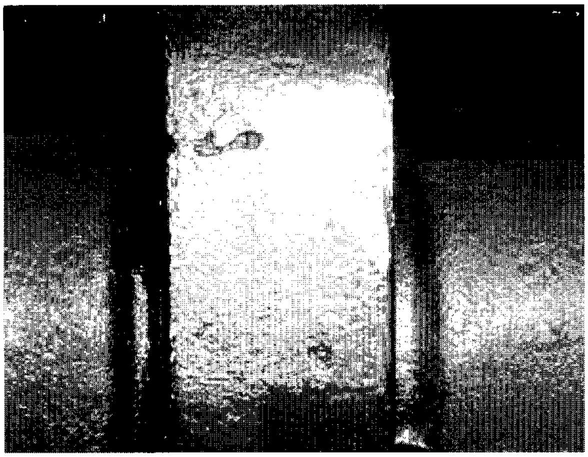


Fig. 11 Slag or sand defects on the surface of a chilled grey iron casting

becoming increasingly important with the new breed of computer literate young engineers for whom virtual reality is not just a concept.

Taking these factors into consideration it would appear that at the present time no single piece of software completely satisfies the requirements of the foundry industry. It is also unlikely that any single numerical technique will be able to cope with the range of problems. For practical reasons, mainly timescales, it is hybrid software packages that are likely to be most successful, combining experiential data with a numerical analysis and optimisation approach.

Simulation is helping the foundryman ask questions about his own process, process control and working practices. Maybe it is this that puts foundrymen off using simulation software as much as it could be used because they rather the like the mystique of the their process! Simulation is not the magic wand that foundrymen are looking for, but it is probably the most powerful tool that has been introduced into their industry in the last fifteen years. Its implementation is becoming easier as the software engineers consider the needs of the foundryman. However, there are still many areas of simulation that need improving, and in order to do that well the academics developing the techniques have to understand better the fast moving nature of the foundry process and the practical nature of most foundrymen.

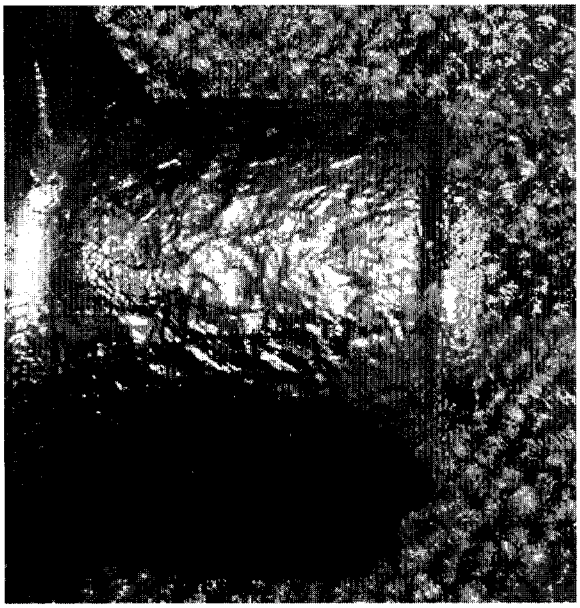


Fig. 12 Lustrous carbon defect on the surface of a grey iron casting produced using a resin shell mould

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