Integrated Computational Materials Engineering and Modelling of Shape Casting Processes – Needs, Benefits, Limitations and Hurdles

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Abstract. In this paper, the industrial needs and potential benefits of ICME for shape castings are described from the point of view of a commercial provider of casting process simulation tools. At the same time, the paper addresses the challenges, limitations, and hurdles regarding the extent to which ICME is or can be adopted on an industrial scale for shape cast components. The discussion is backed by concrete examples illustrating the advantages and limitations of integrating models and simulation in the design chain of cast components, in the design and analysis of the processing route of a casting, as well as over the different length scales through which the structures and corresponding behavior of the cast material are determined. The biggest impact of the ICME approach will only be apparent when the increased accuracy or level of detail provided by the methodology is truly necessary, because it leads to changes in design decisions for the product or manufacturing process.

1. Introduction
In the last several years, Integrated Computational Material Engineering, or ICME, has been a buzz word in the world of materials science and engineering. In its 2008 report [1], the Committee on Integrated Computational Materials Engineering of the National Research Council described ICME as “the integration of materials information, captured in computational tools, with engineering product performance analysis and manufacturing-process simulation.” The NRC’s definition of ICME explicitly addresses the coupling between material – process – performance being captured in computational tools, but what does this mean for modelling of shape casting processes? What are the needs of industry and which benefits can they expect from ICME, what limitation and barriers exist for extending the extent of ICME, and which consequences does or should ICME have for those working in the field of modelling of shape casting processes?

From the authors’ point of view and as shown in figure 1, the concept of ICME for shape castings can be broken down roughly into three different scenarios: integration of materials information across varying scales up to the cast component level; integration of materials information across the various processing steps which lead to a finished shape casting; and integration of materials information from the manufacture of a cast component into the analysis of its performance. Each of these scenarios can be important on its own, and depending on the application and the problem to be solved, two or all three may be required. On the other hand, the problem to be solved also determines the required level of detail and depth of integration within any of the three described scenarios.
In this paper, two examples showing the use of ICME for shape cast components are briefly presented. In the discussion of the examples, the authors attempt to illustrate and discuss the limitations and barriers to a more extensive integration in the sense of ICME. To conclude, the authors summarize what they see as the current barriers and limitations for more extensive use of ICME and contrast these with the perceived industrial needs.

![Figure 1](image-url)

**Figure 1.** Schematic illustrating the principles of ICME for a shape casting process, including three integration scenarios (dotted lines) across length scales, along the manufacturing processes and from manufacturing to performance analysis.

2. **Through process integration over varying length scales.**

Integration over the length scales involved in determining the structures and material behavior of the metal in a shape cast component, including thermodynamics and thermochemistry, can be considered part of ICME. However, it is important to consider that a cast component may undergo a number of processing steps to achieve its final shape and properties, i.e. casting and cooling, heat treatment, machining, etc. In the first example presented here, the modelling of the changes in the microstructure of a heat treated cast iron component to create austempered ductile iron (ADI) are discussed [2].

The focus of the modelling activities was on the optimization of the heat treatment process to obtain the desired ADI structure in a robust and economical way. The project objectives meant that the primary focus was on the changes in microstructure during austenitization, quenching and austempering, which needed to be coupled with a macroscopic consideration of the heat flow during processing. Figure 2 illustrates schematically the methodology used for modelling of microstructural changes during the transformation of ferrite to austenite in a eutectic cell during austenitization. This transformation is modelled as being diffusion-controlled, with local thermodynamic equilibrium assumed at the phase boundaries. Rather than a detailed microscopic description geometrically, a representative eutectic cell was modelled for each macroscopic computational cell.
In addition, a so-called para-equilibrium approach was adopted [2], where the diffusion of all alloying elements other than carbon was neglected and consequently a Fe-C section of the multicomponent phase diagram used. In this case, the para-equilibrium assumption could be justified by previous work [3]. Naturally, it would have been possible to extend this model to a more detailed consideration of multicomponent thermodynamics and diffusion, with corresponding costs in model complexity and computational resources. As the authors state, the criteria for selecting the modelling approach were robustness, availability of data and ease of integration. In this case, the costs of a more detailed microscopic consideration were carefully weighed by the authors against the potential benefits of a more accurate description of the microscopic phenomena on results at the macroscopic level.

Figure 2. Schematic illustrating a modelling approach for the ferrite to austenite transformation during austenitization heat treatment of ductile iron to form ADI: a) typical ductile iron microstructure with eutectic cell marked in red; b) schematic of the phase distributions in the eutectic cell; c) Fe-C section of the multicomponent phase diagram; d) concentration profiles across the eutectic cell during the transformation (from [2]).

The heat treatment of the component is carried out to modify the microstructure in the cast iron to obtain ADI. This also means that the starting point for a heat treatment simulation of the component needs to consider information about the as-cast microstructure distribution in the casting. In the model of ADI heat treatment, the predicted local graphite nodule count and the ferrite/pearlite fraction distributions were taken from a simulation of the solidification and cooling of the casting and used as the starting point for the heat treatment simulation [2]. As shown in figure 3, different initial nodule count distributions in the casting (exaggerated) lead to greatly varying rates of austenitization and dissolved carbon content in the casting during the austenitization process.

This example clearly illustrates that two of the principles describing ICME are required in the modeling of the ADI manufacturing process: coupling varying length scales (also integrating thermodynamic considerations) and integrating different manufacturing steps. However, the level of detail needed from smaller scales and/or the degree of coupling necessary between length scales is very dependent on the questions to be answered through using modelling and simulation.
3. Integration of process and performance simulation

As can be illustrated by numerous examples, assuming that a casting has uniform, homogenous properties and is free of residual stresses can easily lead to an under- or over-dimensioning of the component, with corresponding penalties in poor performance or addition of unnecessary weight in the design. This means that a consideration of the relationship between material – process – performance can be of critical importance when designing or analyzing (FEM, crash, fatigue life) the design of a cast component [4]. In the example considered here, the influence of the local microstructure in a casting was taken into account in the prediction of the fatigue life of a ductile iron component.

Models integrated in macroscopic casting process simulation for the prediction of the distribution of local microstructures and the corresponding static mechanical properties of ductile iron castings exist for some time [5]. However, the coupling of dynamic mechanical properties (fatigue life) to microstructure for these materials first required extensive experimental effort to determine microstructure dependent S-N curves for the material, illustrated schematically in figure 4 [6].

As shown in the figure, to characterize the relationship between microstructure and fatigue life, samples were prepared from castings with different wall thicknesses and varying process conditions to obtain varying microstructures. The machined samples were then subjected to fatigue testing to determine the corresponding S/N or $\varepsilon/N$ curves. After testing, the samples where characterized (using image analysis) through 22 parameters including the number, shape and size of the graphite nodules and the ferrite/pearlite content. Finally, an extensive variance and regression analysis was used to determine the microstructural parameters which had the largest influence on the fatigue life of the material and to obtain a correlation between these parameters and the fatigue life. In the investigation described here, the local pearlite content was determined to be of primary influence (see figure 4).
Figure 4. Experimental determination of fatigue life for cast iron with varying microstructures: a) sample positions for an experimental casting with different wall thicknesses; b) example of image analysis used to determine microstructural parameters, here graphite nodule size; c) two experimentally determined S-N curves for a compacted graphite iron grade with differing pearlite contents [6].

The description of the durability as a function of pearlite content was coupled to the local microstructures predicted through a casting process simulation and exported for use in the finite-element and durability analysis of a bracket used as a demonstrator component. At the top of figure 5 the predicted fatigue strength of the component and the location of the actual crack initiation in laboratory tests of the component are visualized. The bottom of figure 5 shows that a classical fatigue analysis of the component would predict the start of cracking at a different location than observed. Due to the variations in the predicted pearlite content of the casting, the most highly stressed regions of the bracket have a predicted higher fatigue strength than the regions where crack initiation was observed. The fatigue analysis considering the local material properties more accurately predicted the real crack initiation site (see figure 5).

This example clearly shows the potential benefits of the ICME approach to integrate material, process and performance analyses to improve the predictability of performance in the design of a cast component. Note, however, that the development of the necessary material data for the correlation of fatigue behavior to corresponding microstructural characteristics required significant experimental effort. Other factors, such as a weakening of the material through defects (e.g. porosity or nonmetallic inclusions) that almost certainly play a role in the fatigue life of many cast iron components have been completely neglected in this analysis and would require further experimental characterization. This means that the complexity of the real situation has, in this case, only been partially accounted for in the model considerations.

4. Needs, Benefits, Limitations, Barriers to ICME

The previous examples have illustrated the potential benefits of the ICME approach for shape cast components. In industry, especially the demand for lighter and lighter products to achieve reduced energy consumption and emissions means that the design of castings which are economical, durable and fulfill all the in-use requirements will result in increased needs for durable high strength alloys but also for robust designs and production processes. Accurate analysis tools can play an important role is meeting these challenges by shortening development times. The ICME approach in materials development, in casting process layout and in performance analysis provide even more powerful tools to fulfill these needs.

However, there are also inherent limitations in the ICME approach and barriers to its further adaptation, some of which are discussed in the following subsections.
Figure 5. Fatigue life analysis of a ductile iron bracket casting: a) predicted fatigue strength based on the local predicted pearlite content of the microstructure; b) brackets with observed crack initiation sites; c) results of classical fatigue life calculations for the bracket; d) fatigue life prediction considering the local microstructure for the bracket [6].

4.1. Time to Answer – Computational Expense

Not only are the technical demands on cast components growing, there is also a continuous demand to shorten development times. One the one hand, this speaks for the consequent use of the ideas of ICME in design, in order to significantly reduce the number of physical trials required to develop a casting design and the corresponding manufacturing process. On the other hand, this also means that the time available for doing detailed model analyses is limited. Therefore, one barrier to the adaptation of the ICME approach in process or component design are the computational times required e.g. for complex simulations integrating detailed models for different length scales up to the component level. Alone the integration of thermodynamic equilibrium calculations into the simulation of the solidification of an industrial steel grade have been reported to approximately double simulation times, despite simplifications made in the frequency with which the equilibrium calculations were carried out [7].

In many cases, reaching calculation times on the scale of minutes, hours or overnight at the casting level means that the often adopted approaches of e.g. volume-averaging, homogenizing over length scales or making model simplifications (e.g. phase diagram linearization), etc. become a necessity for an effective use of simulation in product or process design. This has been illustrated through the assumption of para-equilibrium e.g. for the ADI heat treatment simulation presented above. It seems obvious that this also means that in many cases it will be difficult to generalize models to be applicable to a wide range of industrially relevant multicomponent, multiphase alloys. Adaptations will always have to be made on a case-by-case basis.

4.2. Lack of Data – Costs of Measurements

The example shown above for the integrated fatigue life prediction of a ductile iron component shows that in many cases extensive (and expensive) experimental investigations are required to develop the necessary material data to allow a complex integration of material models with process and performance simulations. Anyone who has worked in the fields of modelling and simulation will have quickly realized how difficult it typically is to find good, current and reliable data as input to models. These costs can be another barrier for a more extensive adoption of ICME for shape castings.
For complex new materials under development to satisfy future requirements, for example in power generation, aspects of ICME are already being used, see e.g. [8, 9]. Unfortunately, the focus in these modelling and measurement efforts is often on the material’s behavior in use, for example creep strength at increased operating temperatures, but the processing of the materials to manufacture the corresponding components is not considered. In this case, the knowledge and tools are lacking to optimize the processing of the corresponding cast components and correctly predict the solidification behavior and the development of defects in the casting (e.g. creep or other mechanical properties measured up to near-solidus temperatures). This leads to considerably increased costs in manufacturing as well as a slower adoption of the new material in the production of critical components.

One hope for ICME could be that expensive physical experimentation can be replaced by numerical experiments which deliver the same information. Clearly, this can only take place if the corresponding models have been verified and validated to represent the behavior of the real material. Also, the requirements on computational costs for carrying out the numerical calculations must be lower than the actual physical experiments.

4.3. Real Complexity – Production Variability

The essence of the statement “Essentially, all models are wrong, but some are useful” by G.E.P. Box [10] can be used to describe a limitation and potential barrier to further integration of models in the framework of ICME. All models make simplifying assumptions and idealizations in order to make the problem tractable. This means it is extremely important to carefully weigh the benefits of a tighter integration of materials information into a process or performance simulation against the uncertainties introduced by other modelling assumptions – the weakest link in a chain of models or simulations will determine the accuracy of the whole approach. Of course, as scientists and engineers, this is a factor that is always in the minds of those working in the modelling community.

A related factor, which is often forgotten both in the modelling community as well as in the practical use of modelling and process simulation, is that industrial casting processes exhibit variability in production. Even for the high pressure die casting process, which is largely mechanized and automated, variations are observed in casting quality from part to part [11]. Scrap rates in metal casting are seldom one-hundred percent, but typically range from a few to sub-percent levels. From this point of view, a perceived or expected improvement in the accuracy of a model through a higher level of integration in the framework of ICME needs to be critically weighed against the expected “natural” variations in the processing and performance of the component produced.

4.4. Ease of Use – Single Source

There are some efforts to try to define and develop a generic methodology for ICME which would allow a “plug and play” standardized, modular modelling platform that can be adapted to a specific material, manufacturing process chain and product [12]. Although on the surface this idea is attractive, alone the complexity of the different materials to be addressed (plain carbon, low alloy and high alloy steels; grey, ductile, compacted graphite and austempered ductile irons; aluminum, magnesium and copper alloys; etc.) and the need for model homogenization and shortest possible simulation times seems to speak against a generic platform that would allow a “sticking together” of different models.

In addition, it is the authors’ experience that in industry there is a desire to work with as few sources as possible when it comes to modelling and simulation of e.g. the complete manufacturing process of a component. One reason for this is that, despite dedicated interfaces, the transfer of information from one program to another is always connected with additional effort. Another important aspect is that using different tools also means having to deal with different sources or suppliers when questions or problems arise in use. Here, the advantages of using different, coupled tools from different sources needs to significantly outweigh any disadvantages which arise through extra effort required through the interfacing and support of the programs.
4.5. Commercial Interests – Protection of Investments

A final hurdle to a wider use of ICME is that in many cases there are conflicts of commercial interests in the integration of various tools. Clearly, any commercial provider of simulation tools is interested in protecting his market position and the investment he has made in developing his capabilities. Any advantages of an easier integration within ICME will be weighed against the fact that this ease of integration may make a tool interchangeable.

Similarly, if a company using simulation tools finances e.g. extensive measurements or computations to better characterize and understand a material of interest to them, they do so in order to increase their competitive advantage in the market. Understandably, in most cases this company will have a justified interest in protecting the developed information or modelling capabilities and will have very little interest in seeing this information be diffused through open interfaces or databases.

5. Conclusions

In this paper, the authors have tried to illustrate through two different examples that ICME is already being developed and is being used today in the commercial modeling and simulation of shape castings. However, despite the needs and benefits for further development of the approach, there are a number of limitations and barriers to a further adoption of ICME on the commercial level.

No matter whether along design or process chain or over different length scales, the overriding consideration for effective ICME has to be a careful consideration regarding the level of integration needed to ensure that design decisions (component design, process design, material selection) can be made with the required level of confidence. As proposed by Allen et al. [13], the key is not to eliminate uncertainty in design decisions (through a more detailed coupling of models), but rather to leave it where it does not affect the design decisions made. This means that in each case, the trade-offs in the cost of more extensive modelling, computation and integration of tools needs to be balanced against the perceived value of the information or increased accuracy provided. In the design process, this also means that it is important to develop solutions that are robust and insensitive to uncertainties, whether these uncertainties have their source in the models or in inherent production variations [13].

From this point of view, the way in which information is passed from level to level over length scales or along a process or design chain needs to be considered on a case-by-case basis, to find the right level of integration for providing the right information with the necessary accuracy to obtain all of the real and perceived benefits of the ICME approach.

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