On Analytical Concepts of Novel Multi-Resolution Casting Simulations

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Abstract. One of the crucial ingredients of today’s numerical simulation technologies is their cross-scale and cross-platform capabilities for material processes applications. Handling of simultaneous evolution paths at various scales\times (i.e., multi-scaling) during complex material processes where materials microstructure & microchemistry interact with meso and macro events, is one of awkward challenges of computational material engineering. The material phase change and also its thermal energy evolutions are also drastically increasing the complexity of the numerical simulations. The introduction of multi-resolution and multi-scale numerical schemes in recent years and their ground-breaking potentials for computational material science applications have vividly raised the expectations for more resourceful future virtual tools. A crucial point in implementing these novel numerical techniques for simulation of material processes is their flexibility towards the modelling approach (i.e., discrete, continuous...) and also their compatibility with solver-independent platforms. As these multi-resolution\hiphysical techniques should provide some answers to the best ways of designing future high-performance materials along with optimisation of new & existing material processes and also improvement of their life-time performance, a broad & well-structured research work is required. Hence, the proposed multi-resolution framework herein, has been developed based on analytical & numerical techniques built on sound physical and mathematical foundations developed during the last few decades. The combination of recently developed concepts of dynamic\ievolving domains along with cross-scale grid overlapping\interfacing and also sound parallel computing routines have been employed to address the multi-scale challenges of material processes simulations. In the research work herein, analytical and computational aspects of multi-resolution simulation framework for dynamic casting processes (i.e., continuous and semi-continuous casting) are presented and physical\mathematical basis of the analytical-computational solidification and cooling modules are elaborated. Industrial applications of the techniques are also envisaged using parallel-processing and fast computing facilities for full-scale casting applications.

1. Introduction
An efficient numerical simulation tools designed in a way to help industries to solve their problems and to find & optimise the most agile solutions for their material processing technologies is foreseen for today’s fast and competitive industries. With a carefully-designed simulation system, it is possible to automate many aspects of industrial process optimisations in an integrated computerized environment where sophisticated physical \mathematical rules, boundaries, data processes\handling and goal seeking analyses are performed. The research work herein is a part of a general framework which will deliver a numerical simulation tool for implementation of novel and innovative material and process modelling into industrial mainstream procedures for boosting efficiency and competitiveness of market-
oriented products. The multi-resolution & scale-bridging computational framework and its new overlapping and interfacing concepts [1, 2] combine advanced simulation techniques, material models at different length/time scales and modelling methods from diverse scientific disciplines to handle the wide range of material engineering applications.

A series of interactive sub-modules including solidification, cooling and thermal-mechanical routines have formed an integrated computer-based platform which helps engineers to solve challenges in casting technologies. The goal of research work herein is to contribute/respond to some fundamental industrial needs for:

- Optimising and tailoring material processes for increase part quality/performance;
- Improving the confidence/reliance of industrial processes on advanced material modelling and;
- Amplifying the use of computer-based virtual modelling and simulation systems for industries

For the case studies herein, using the analytical-numerical simulation system, the optimisation of industrial casting process under real-world conditions have been conducted. In these case studies, problems of phase changes and thermal energy evolution due to cooling (i.e., air & water cooling) effects have been considered. Moreover, special attention has been devoted to the development of more practical and general solidification and cooling modules. Different sets of in-house experimental casting trials have been used for the verification/calibration of the simulation system. The characteristics of the simulation modules are briefly described herein, where the efficiency of the simulation technique is highlighted. The purpose of this paper is to present a new horizon, which improves the modelling of thermal energy evolution and material solidification during industrial casting processes.

2. Conventional macro-scale casting simulations

The conventional use of fixed Lagrangian, updated Lagrangian and stationary/moving Eulerian techniques for simulation of industrial casting processes have traditionally been popular among engineers and scientists. In the conventional pure Lagrangian and also updated Lagrangian approaches (with adaptive re-meshing), the deformation process of a material body is resembled as a virtual flow where each material element/particle carries its own properties (such as microstructure, temperature, density…). For the simulation of dynamic casting systems where solidified billets are cast in time, as the flow front advances, its properties may change in time. However, the inability of these approaches to follow large deformation/distortions of the computational grid without comprehensive re-meshing [3] is its main deficiency. Alternatively, in the stationary/moving Eulerian approaches, rather than tracking each material element, the evolution of the material flow properties at every point in the numerical grid (i.e., vortices) can be calculated (at sequential time steps). This means that the melt flow properties at a specified location within the grid (i.e., mould) depend on its location and time (advection). In this approach, the conservation of material is satisfied at spatial and time points and the computational mesh is mostly fixed where material moves with respect to the grid. The large deformation/distortions (and melt flow) can be handled with relative ease using convective feature of the method where relative motion of the deforming front in respect to the discretized grid is calculated [3].

The basic concepts of discretization in space and time to define simpler subspaces (i.e., cells) with exact/approximate solutions have also been employed in almost all of the existing numerical solvers. Different types of the meshing/gridding methods which discretise the virtual domain into small individual cells/nodes have been developed over past seventy years [3]. The technology which is able to discretize a wide variety of complex geometries, adapt into large deformation of the numerical domain (i.e., adaptive re-meshing) and cope with non-conformal aspects of multi-domain grids has already been mobilised. There have also been various attempts to introduce innovative discretization techniques for dynamic systems with evolution in time [4] and interfacing technology for moving grids (i.e., continuous casting). Most of these techniques have been developed for numerical simulation of complex geometrical systems based on the solution technique (i.e., discrete, continuous…), accuracy, CPU time and complexities. Although, the fixed Lagrangian grid has extensively been used for domain discretization in solidified part of the billet [4], its application for melt part of the domain with its internal microstructure evolutions is limited.
3. Novel evolving casting simulations
To improve the simulation technique for continuous and semi-continuous casting process a novel dynamic mesh technique has already been developed [4]. In the dynamic mesh approach, the generation of the billet is modelled using new subdomains/zones which are generated & joined at specific time points to resemble the extension of the billet. These newly generated zones are overlapping/attached to the main domain at discrete time points where comprehensive mapping procedures (including grid overlapping, nodal condensation, propagation interface…) are applied to re-assemble the domain to handle the new material (i.e., melt material) and energy input. The added dynamic subdomains/zones can be stationary or moving depending on requirement of the numerical model for the industrial process. As the numerical solution is performed on a full parallel-processing machine, multiple instances of the same solver (or alternatively different solvers) can independently be employed for the main domain and its attached/overlapping zones. The generated subdomains (which can be at different length/time scales) would gradually integrated into the main domain (and become a part of main domain) as the phases within the subdomains/zones come to the end (i.e., microstructure, solidification…). Figure 1 shows a casting simulation case study (3D quarter model) using dynamic mesh technique. More comprehensive discussion about the dynamic meshing and finite zoning techniques can be found in [1, 2, 4].

Figure 1. Dynamic meshing technique for continuous casting process (symmetric quarter model)

One of the challenges for the simulation of continuous casting processes is that the location and the shape of the solidification interface are dynamic (time-dependent). During the simulation time these boundaries evolve and may have translational and rotational movements. These moving boundaries can be taken into account using multiple mesh resolutions (overlapping grids) within the simulation domain using some hybrid/mixed techniques [2].

4. Solidification: enhanced analytical-numerical approach
The concept of numerical simulation of material processes and in particular casting processes has already attracted many interests among scientists, material engineers and industries. One of the challenging aspects of numerical simulations for casting applications is the change of phases and solidification phenomena during the process. The solidification phenomena during casting process can be modelled at different levels of scales and sophistication. For macro scale simulations, there are different approaches for defining the phase transition. This section highlights a brief description of the analytical-numerical technique which has been developed herein to enhance the accuracy and efficiency of solidification numerical modelling.

Most popular scheme for the industrial macro-scale solidification modelling is the application of the Scheil-Gulliver equation [5, 6] where a global non-equilibrium approach is formulated for solute redistribution during solidification (no solute would diffuse back into the solid in the standard form). The solid fraction is defined by melt flow, solidus and liquidus temperatures as well as the partition coefficient. The Scheil-Gulliver equation in its simple and standard form can be written as [5, 6];

\[
\begin{align*}
C_L &= C_0 f_1^{k-1} \\
C_S &= k C_0 (1 - f_S)^{k-1}
\end{align*}
\]

(1)

Where \( C_L, C_S \) and \( C_0 \) are liquid, solid and initial compositions and \( f_1, f_S \) and \( k \) are solid & liquid mass fractions and coefficient \( k = \frac{C_L}{C_S} \) (which can be determined from phase diagram), respectively. The formulation is valid for local equilibrium state between the solid and liquid at interface, and moderate to low cooling rates. Different numerical methodologies have been developed [4] to handle the phase change phenomena within numerical domains, namely; conduction-based, conduction-convection based
and enthalpy-based methods. The enthalpy-based scheme is to use the enthalpy concept where enthalpy (which is a thermodynamic quantity defining the total heat energy of a system) can be combined with other numerical features to account for change of phase during solidification. In the mainstream industrial software tools, the enthalpy method is generally combined with Volume of Fluid (VOF) and domain porosity features (to damp the fluid momentum when it turns into solid). Although VOF has been developed and used extensively to treat problems in fluid dynamics with liquid–gas interfaces but it has been extended to solidification problems in material science [7]. For the VOF technique within the mold, the surface tension forces are implemented in the momentum equation (as a source term) using technique introduced in [8]. The domain porosity would also enable the smooth change of phase from liquid to solid by damping the momentum equation using momentum sink terms. The introduction of momentum sink terms in the energy equation might introduce more numerical challenges since the convergence of the system become more difficult. Consider the mass continuity and momentum equation for the melt flow inside the mold as [3];

\[ \nabla \cdot \mathbf{U} = 0, \quad \frac{\partial (\rho \mathbf{U})}{\partial t} + \nabla \cdot (\rho \mathbf{U} \otimes \mathbf{U}) = -\nabla p + \nabla \cdot (\mu \nabla \mathbf{U}) \quad (2) \]

A momentum sink term is traditionally introduced into melt momentum equation (for temperatures between liquidus and solidus) to damp the melt velocity to zero due to solidification phenomena. A practical approach for momentum damping can be defined using the Kozeny, Carman approach and its modification by Blake [9]. Let’s assume the equation for fluid flow in resistive media as;

\[ \frac{\Delta p}{L} = \alpha \left( \frac{1-k_{f}}{k_{s}} \right) \left( \frac{\nu_{s}}{d} \right) \quad (3) \]

Where \( \frac{\Delta p}{L} \), \( k_{f}, \mu, d \) and \( \nu \) are pressure gradient, domain porosity (liquid volume fraction), melt viscosity, primary channel width and melt superficial velocity. Variables \( \alpha, \beta \) can be defined for material processes during solidification based on the alloy and process properties. Two different types of momentum sink terms can be defined for the melt solidification, namely: viscous and quadratic terms. The basic viscous sink term for fluid flow in a porous media can be defined as [10];

\[ L_{v} = \frac{\mu}{K} U \quad (4) \]

Where \( K \) is the permeability of the resistive domain. Voller et al. has modified [11] the fluid viscous loss model and the permeability of the domain as;

\[ L_{q} = -\frac{\mu}{K} (u - u_{s}) \quad (5) \]

Where \( u_{s} \) is the solidified slab speed (can be assumed as casting speed) and \( K \) is permeability which can be calculated based on the resistance against the melt flow inside the dendrite channels during solidification. Ignoring the re-melting and the solute concentration effects (temperature exchange at interface…), Gu et al. [12] has proposed the following equation for the permeability:

\[ K = C \frac{f_{l}^{2}}{f_{s}} \lambda_{s}^{2} \quad (6) \]

Where \( f_{l}, f_{s} \) and \( \lambda_{s} \) are volume fractions of liquid and solid phases (at the solidification front) and primary dendrite arm spacing. The constant \( C \) can be assumed as \( C=6\times10^{-4} \) [12]. The secondary arm spacing and its resistance effect have not been explicitly defined in the equation (5). The broader equation for estimation of permeability have been derived by the author using the combination of physical and analytical approach as [13];

\[ C_{LV} = C \cdot \lambda^{2} \left( \frac{1-f(T)}{f(T)} \right)^{\alpha} \quad f(T) = C_{1} \cdot \left( 1 - \left( \frac{T-T_{L}}{\Delta T} \right) \right)^{\gamma} \quad \Delta T = T_{L} - T_{S} \quad (7) \]

Where \( C, C_{1} \) are constant coefficients, \( \lambda \) is the primary dendrite arm spacing and \( \alpha, \beta, \gamma \) are power coefficients which can be calibrated for the alloy processes (for Aluminum alloys \( \alpha = 3, \beta = 2 \) and \( \gamma = 1 \)). Coefficients \( C \) and \( C_{1} \) can be assumed as \( C = 0.0006 \) (similar to Gu et. al) and \( C_{1} \) can be assumed between 1 & 1.2. A more detailed version of the simplified loss term can also be developed [13] using primary & secondary dendrite arm spacing and melt isolation phenomena. Similarly, based on physical concepts of energy damping and a mathematical formulation of melt flow kinetic energy, a quadratic sink term can also be derived as [13].
\[ C_{LQ} = \begin{cases} C \beta \left( 1 - \frac{T - T_E}{T_E - T_S} \right)^{2}, & T_E < T < T_L \quad \alpha = 1 \\ \beta + C \left( 1 - \beta \right) \left( 1 - \frac{T - T_L}{T_E - T_S} \right)^{2}, & T_S < T < T_E \quad \alpha = 2 \end{cases} \] (8)

Where \( T_E \) is a temperature which denotes the starting point for dendrites bridging phase during solidification. For aluminum alloys, the simple assumption can be that \( T_E = \frac{T_L - T_S}{2} \) and \( \beta = \gamma \left( \frac{T_E - T_S}{T_L - T_S} \right) \)

where \( \gamma \) is a coefficient which depends on the material microstructure evolution during solidification (when growth and progression of dendrites starts to create significant resistance against the melt flow near the interface). For Aluminum alloys where equiaxed grain growth are perceived, it can be assumed that \( \gamma = 0.6 \). The coefficient \( C \) can be calculated and calibrated from the total momentum of the melt within the mold prior to the solidification phenomena. More comprehensive discussions about these mathematical derivations of momentum sink terms can be found in [13].

5. Enhanced analytical HTC calculation

Numerical modelling of cooling processes (i.e., water spray, air cooling…) is one of the most challenging part of the casting simulations. Many thermal evolution studies have been carried out in last two decades to develop an estimation technique for the dynamic Heat Transfer Coefficient (HTC) on the cast billet surface. These works are considering different water boiling regimes (nucleate, unstable and stable filming regimes) and also Leidenfrost effects. The variation of HTC against the billet surface temperature can be divided into four distinctive zones, namely: below water saturation temperature, between water saturation and Critical Heat Flux (CHF) temperature (nucleate boiling regime), from CHF temperature to Leidenfrost temperature (unstable boiling regime) and finally above Leidenfrost temperature (film boiling regime). In the work herein, the analytical HTC calculation developed by the author [14] has been implemented using in-house coding. Figure 2 shows the variation of the HTC with respect to cast billet surface temperature (i.e., at the impinging point) using analytical formulation for different water boiling regimes. More comprehensive discussions about the mathematical derivation of HTC functions can be found in [14].

![Figure 2. Variation of HTC with billet surface temperature using analytical calculations (T_{Le}, T_B, \mu_w, H_f, \gamma, C_P, \rho_w, K_w, \rho_v, Q, L_B, \gamma, \kappa, n_v, T_{CHF})](image)

6. Industrial-scale casting simulation

The development of new numerical framework for industrial casting simulation has motivated the comprehensive sets of parallel simulation & experimental studies herein. The thermal-fluid CFD simulation for mold filling solidification and evolving thermal-mechanical simulation [13] for stress-strain states have been carried out for simulation case studies. The most challenging parts of thermal-fluid CFD applications for the industrial casting processes are the numerical solidification and
cooling simulations. The numerical-analytical aspects of solidification and cooling has briefly been described in previous sections where the change of phase from fluid to mushy and solid state under the thermal gradient caused by cooling process have been modelled. In the research work herein, new porosity functions derived for the momentum sink terms have been implemented and coded in-house. The cooling effects of water spray cooling during casting process and its solidification phenomena has also been implemented using an in-house code which includes the newly developed HTC functions for different water boiling regimes.

Two sets of casting trials which have been carried out for verification and measurement purposes, namely, horizontal and vertical direct chill casting procedures. These continuous and semi-continuous casting trials are performed in-house at semi-industrial scale where round and rectangular aluminium billets were cast using air & water spray cooling. Figure 3 shows the horizontal direct chill casting trails in which a round cross section billet were cast. The parallel numerical simulations trials have also been carried out to examine and calibrate the parameters for the derived mathematical models for solidification and HTC calculations.

Figure 3. Horizontal semi-industrial direct chill casting process and its numerical 3D half model

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