Distribution of alloying elements in the aluminium casting process

Studiegroep Wiskunde met de Industrie 2008
http://www.math.utwente.nl/swi2008

Controlling the composition of alloy elements is of crucial importance during the casting of aluminium to guarantee sufficient quality of the resulting solidified aluminium blocks. During solidification these alloy elements redistribute around the time-dependent liquid-solid interface. To predict and control this composition, advanced computer simulations are performed. It is necessary to quickly determine the local thermodynamic equilibrium of the alloy elements in the liquid aluminium. However, a direct coupling between the thermodynamic and hydrodynamic software within the simulation is far too time consuming. The Corus challenge is to establish this crucial coupling in an efficient way.

At Corus RD&T aluminium research is carried out for the aluminium company Aleris and for Corus aluminium business units. The research aims at developing new products that are used in aerospace applications, for more environmentally friendly aeroplanes, and in the automotive market, for lighter and stronger cars. The aluminium casting process forms one of the first steps in the aluminium production cycle. In this process liquid aluminium is cast into large solid blocks. The alloy composition determines product properties such as strength, surface quality and dent resistance. During solidification the alloying elements may redistribute in the block. This is caused by the interaction between the solidification process and the local fluid flow. Uneven distribution may lead to unacceptable property variations, leading to an immediate economic loss. Computer simulations are being developed for the prediction of this element distribution. The crucial step for simulations of industrially relevant alloys is that a large number of elements (about 5 or more) can be included in the simulations while maintaining acceptable simulation times. The Corus challenge is to propose solutions to establish this crucial step in an efficient way.

Figure 1(A) shows the aluminium casting process. The aim is to make large slabs or billets of aluminium. The slabs (ingots) are approximately half a meter thick, one and a half meter wide and up to six meters tall, while billets usually have a diameter between 15 and 50 centimetres and a length of up to 6 meters. In casting, the molten aluminium is poured at approximately 680 °C from the top into the mould. The bottom of the mould is initially closed by a block, placed on a lift. After filling, the block drops steadily while the inflow of metal is controlled to maintain a steady level of liquid aluminium inside the mould. At the bottom of the mould water jets spray against the aluminium, thus chilling the molten aluminium. In this way, during a cast of approximately 2 hours a solid ingot is slowly formed.

The casting process is simulated with the finite-element casting model Alsim. This model is being developed by the Norwegian research institute IFE in a joint European collaboration between Corus RD&T and Aleris, the Norwegian research institute Sintef and aluminium companies Hydro and Elkem. The model predicts the fluid flow in the liquid part, computes the solidification (the transition from liquid to solid) and it computes how the metal deforms when cooling down. Figure 1(B) shows a simulation result where the colours indicate how solidification progresses during casting. Currently the model assumes that everywhere in the domain the composition is the same.

Problem formulation. Currently research focuses on expansion of the Alsim model to include the composition during solidification. This step requires that the relation between the local composition of elements i, $C_i(x)$, and temperature $T(x)$ is computed. This relationship is determined by the thermodynamic equilibrium. An example is given in Figure 2. Figure 2(A) gives the binary phase diagram between aluminium (Al) and copper (Cu). The green line in the diagram shows how Al and Cu distribute over the

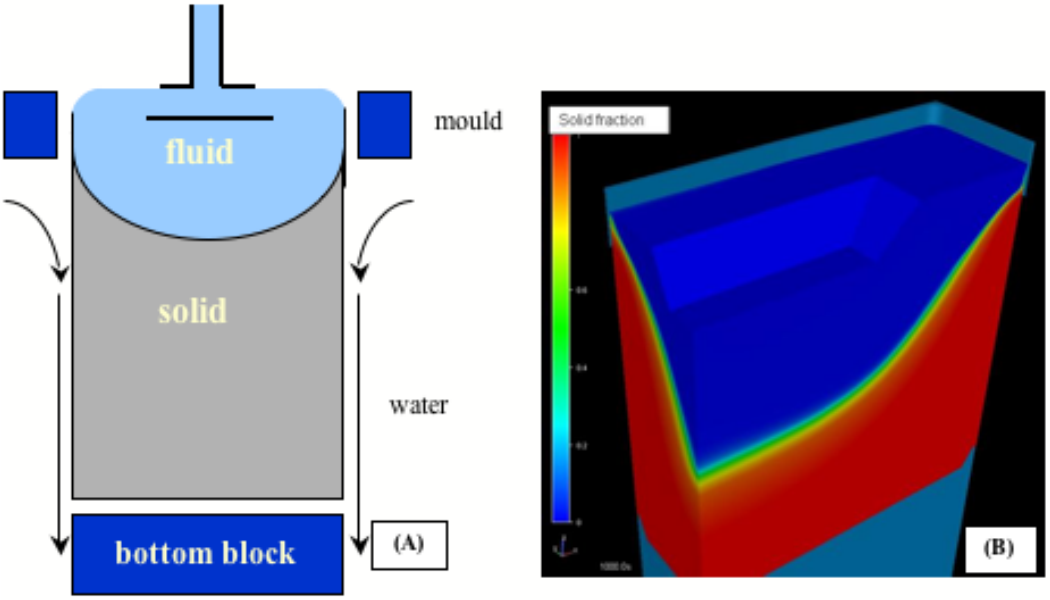

Figure 1: Schematic of the semi-continuous aluminium casting process (A) and Alsim model prediction (B) showing one quarter of an ingot during casting. The colour change shows the transition from liquid (blue) to solid (red) in the casting process.

different phases during solidification of a melt containing 4.5 wt% Cu. Figure 2(B) shows for 4.5 wt% Cu which phases are present at each temperature.

In simulations of the casting process that include the effect of composition, the thermodynamic equilibrium needs to be determined each time step in a large number of grid cells. Commercial software is available that computes the thermodynamic equilibrium via a minimization of the Gibbs free energy, but this is a computationally time consuming step. A direct coupling between the database and the casting simulation, as illustrated in Figure 3(A), is thus not acceptable.

Mathematical Challenge. An alloy is determined by its overall composition. During casting local variations of up to 10% or more may occur. One can see therefore that there is no need to recalculate the equilibrium each time step at each grid cell of the casting simulation, since the concentration and temperature range in which the alloying elements vary is limited. The question is rather, how the solidification path in the computations can be constructed in a computationally efficient manner. For this challenge several points need to be kept in mind:

- The solidification region used in the simulation represents a limited area in a multi-dimensional space. The example in Figure 2 shows the complexity of a relatively simple case of two elements. The industrially relevant case where more elements are used, the complexity rapidly increases, since each additional element increases the dimensionality of the problem. The question is how this space can be manipulated such that a lower-dimensional space becomes available for the numerical simulation.

- Figure 2 also shows that thermodynamic equilibrium data contains highly irregular features such as discrete transition points (e.g. a eutectic point) and large variations in the regions in which phase equilibria appear (e.g. some phases appear only over a range of 5 °C while others are present over several hundred degrees Celsius). It is important that methods are proposed that warrant that all relevant phases are included and that a control of the computational accuracy can be warranted.

- Despite the complexity, the number of phases that appear is limited and usually known a priori. This knowledge may be used to apply data reduction to the system. The question is *if* and *how* this knowledge can be used.

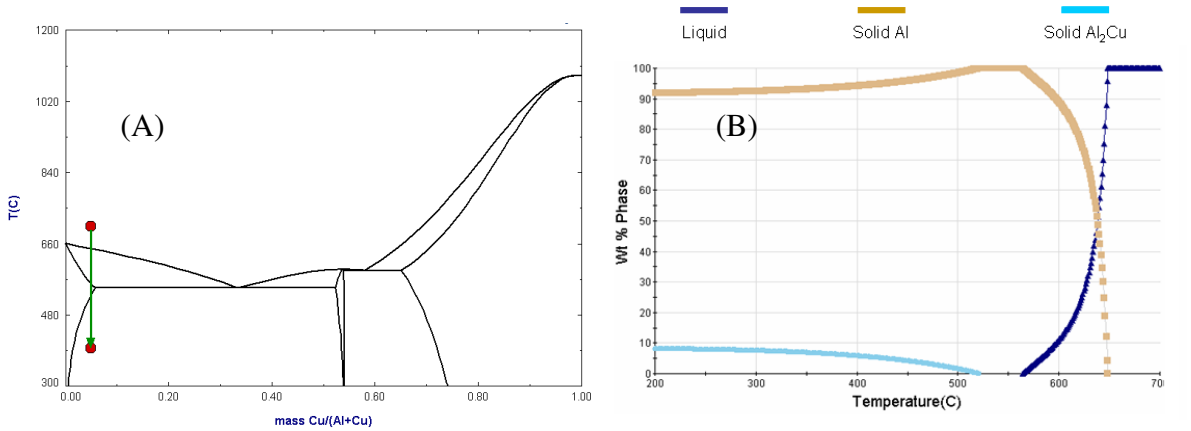

Figure 2: Solidification and phase formation during cooling of an Al-Cu mixture. The phase diagram (A) gives the relation between phases, composition and temperature. (B) shows the phase formation during solidification of Al with 4.5 wt% Cu, also indicated by the green line in (A).

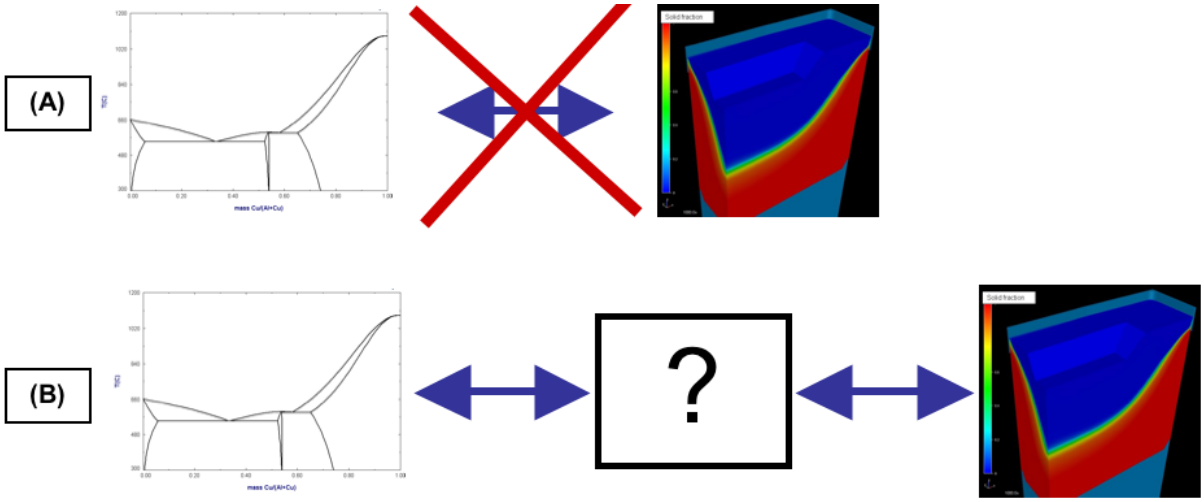

Figure 3: The Corus challenge: Composition needs to be included in casting modelling. (A) Direct coupling between thermodynamic software and the simulation is too time consuming. (B) The challenge is to propose efficient coupling step(s) between the simulations and the thermodynamic database.