RESEARCH OF STEEL INGOT CASTING AND SOLIDIFICATION USING NUMERICAL MODELLING

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Abstract

Currently, model study is commonly used part of research in field of metallurgical processes. Process of simulation of casting and solidification of steel ingots is no exception. This paper maps possibilities of numerical modelling of casting and solidification of steel ingots, as a part of research of these processes, carried out in Department of Metallurgy an Foundry of Faculty of Metallurgy and Materials Engineering of VŠB-TU Ostrava under the conditions of Regional Materials Science and Technology Center. A few programs and software packages applicable to numerical modelling of ingot casting process are available. These programs provide a wide range of potential results, useful for optimization of ingot casting process and resulting quality of ingots, which are presented in this paper.

Keywords: Steel, ingot casting, numerical modelling, casting and solidification

1. INTRODUCTION

Even though nowadays most of the liquid steel is processed by continuous casting technology, also steel ingots have its irreplaceable function, due to dimensional variability. Continuous casting products are still dimensionally limited, so producers of heavy steel products often rely on the steel ingots. To achieve high-quality final products, it is necessary to come out of semi-finished products with equal quality. During ingot casting process, some external defects such as microporosity and macroporosity, segregation or hot tears and cracks can form, due to incorrect casting conditions, mould design or also due to problematic steel grade. [1,2] To prevent these defects, attention is paid to research and development of the technology of ingot casting. With the advent of computer technology, a new area of research of metallurgical processes, which is numerical modelling, opens. Numerical modelling becomes more and more important thanks to the possibility of simulation of real casting conditions, which is particularly advantageous for high-temperature processes that are too demanding for physical modelling. The process of simulation of casting and solidification of steel ingots is no exception. Mastering of the technology of ingot casting without defects is usually conditional by knowledge of optimal casting conditions. For this purpose, numerical modelling is suitable. Through numerical study, it is possible e.g. optimization of casting speed with respect to steel spattering, adjustment of casting temperature, identification of conditions of defects formation, tracking of segregation distribution etc. This paper is focused on the introduction of possibilities of numerical software used for research and educational purposes at the Department of Metallurgy and Foundry of Faculty of Metallurgy and Materials Science of VŠB-TU Ostrava.

2. PRINCIPLE OF NUMERICAL MODELLING IN SIMULATION SOFTWARE

The principle of numerical modelling is based on a definition of a mathematical model through equations, which describe various physical or chemical phenomena. These phenomena are three-dimensional and vary in time, therefore they are described by systems of differential equations, which is very complicated. For this reason, the investigated domain is cut to subdomains (elements) and relations between these subdomains are described by equations. Depending on the accuracy of computational mesh, a number of equations describing relations between elements, which achieves tens of thousands to millions, increase. Therefore, it is possible to solve these systems of equations only by numerical methods.

Programs for numerical simulations are based on numerical methods, such as Finite Differences Method and Finite Element Method. The principle of Finite Differences Method (FDM) is to cover the investigated domain by a structured computational mesh with the final number of elements and discretization of the domain to the points of the mesh. The partial derivatives in governing equations are replaced by Taylor polynomials (so-called differences) in node points of the mesh, creating the system of algebraic equations, which is solved numerically. The advantage of FDM is its simplicity, which allows implementation of the method to software products. Disadvantages include the necessity of covering geometry by structured mesh (see **Figure 1** left) and thanks to that refinement of the mesh in critical areas makes harder. Also, application of boundary conditions on complicated geometries can be difficult. [3,4,5]

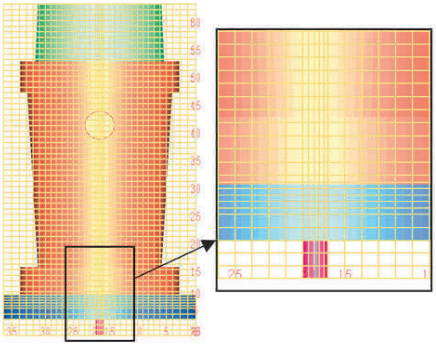

Figure 1 Structured mesh (FDM) [6]

The Finite Element Method (FEM) is currently very popular, thanks to its versatility and ability to describe complicated and extensive problems. A solution of FEM consists of division of computational domain to a finite number of geometrically simple finite elements by triangulation. For each finite element, approximated solution as a linear combination of nodal values and approximation functions is found. Algebraic relations between nodal values of solution for every element are derived and from partial solution, overall solution is assembled. The undisputed advantage of FEM is a possibility of an accurate description of complex geometry also thanks to unstructured mesh (see **Figure 2**), which better fills the entire volume of geometry. Representation of overall solution by functions defined in each element, thanks to that the program can capture local effects such as steep gradients of a tracked variable, is also relatively simple. A certain disadvantage can be a large computational difficulty, which increases with increasing number of elements of computational mesh. [7,8,9]

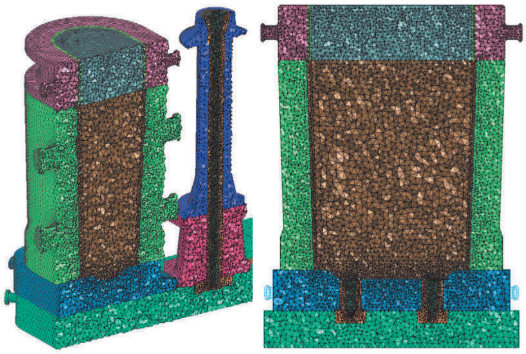

Figure 2 Structured mesh (FEM) [6]

To achieve relevant results, the correct definition of thermodynamic parameters of ingot and mould is necessary. It is equally important to define heat transfer coefficients. Numerical modelling of steel ingot solidification is closely related to heat transfer from the ingot. Especially, during numerical modelling of temperature field and solidification, determination of mechanism and intensity of heat transfer is important.

3. ACHIEVABLE RESULTS

3.1. Filling and solidification

Optimization of ingot casting technology is usually carried out with respect to inner and outer defects formation. Nucleation of these defects can be initiated at the beginning of the casting, therefore, pay sufficient attention to mould filling is important. **Mould filling** is characterized by the laminar and turbulent flow of cast steel. Both laminar and turbulent flow is described by Navier-Stokes equations (1) (one equation for each coordinate x, y, z) together with continuity equation, whose general form is expressed by equation (2). These equations characterize laws of momentum and mass conservation. Depending on the nature of the flow and turbulent model, Navier-Stokes and continuity equations are supplemented by other equations for turbulent quantities (e.g. k and ε or ω). [9,10,11]

$$\frac{\partial v_x}{\partial t} + v_x \frac{\partial v_x}{\partial x} + v_y \frac{\partial v_x}{\partial y} + v_z \frac{\partial v_x}{\partial z} = -\frac{1}{\rho}\frac{\partial p}{\partial x} + \nu\left(\frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2} + \frac{\partial^2 v_x}{\partial z^2}\right) + f_x \tag{1}$$

$$\frac{\partial(\rho.v_x)}{\partial x} + \frac{\partial(\rho.v_y)}{\partial y} + \frac{\partial(\rho.v_z)}{\partial z} = 0 \tag{2}$$

where v is speed (m.s^{-1}), ρ is density (kg.m^{-3}), p is pressure (Pa), ν is kinematic viscosity (m^2.s^{-1}), f is component of external volumetric force (-) and x, y, z are coordinates (-).

Thanks to mould filling simulation, we can track not only the filling process but also the speed field, which is also possible to display by vectors, simultaneously describing flow direction, as can be seen in **Figure 3**. Simulation of mould filling is very useful, especially in initial phases of mould filling, when the spattering of steel can occur due to incorrect casting speed or e.g. mould shape. Filling results are also applied during analysis of casting powder entrainment. On this phenomenon was focused e.g. studies [12,13].

The basis for numerical modelling of processes related to heat transfer is temperature field. **Temperature field** is described by Fourier equation, which can be (as the law of energy conservation) expressed by equation (3). Calculation of other parameters related to the temperature such as temperature field, solid fraction, enthalpy, cooling rate etc. is then based on the temperature field. **Figure 4** demonstrates pictures of temperature field of liquid steel and mould, simultaneously describing the course of mould filling.

$$c\rho \frac{\partial t}{\partial \tau} = \frac{\partial}{\partial x}\left(\lambda \frac{\partial t}{\partial x}\right) + \frac{\partial}{\partial y}\left(\lambda \frac{\partial t}{\partial y}\right) + \frac{\partial}{\partial z}\left(\lambda \frac{\partial t}{\partial z}\right) \tag{3}$$

where c is heat capacity (J.K^{-1}), t is temperature (°C), τ is time (s) and λ is thermal conductivity (W.m^{-1}.K^{-1}).

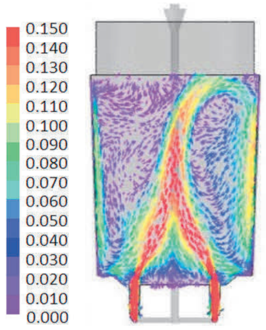

Figure 3 Results of flow field (m.s^{-1}) [6]

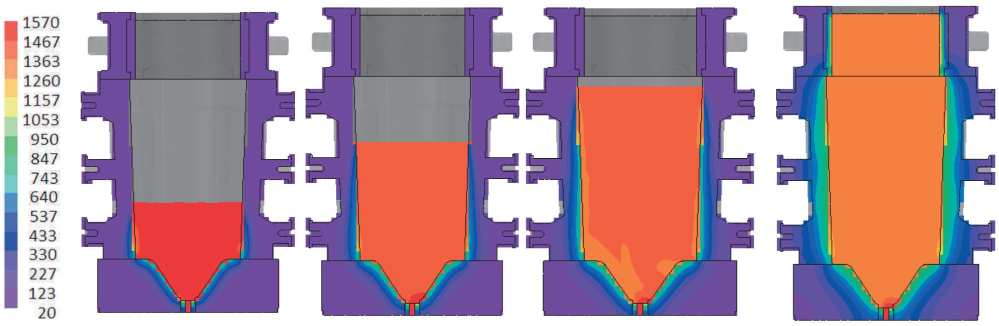

Figure 4 Visualization of mould filling and temperature field (°C) [5]

The process of **solidification**, which is also dependent on many factors, can be evaluated by fraction solid results. An example can be mentioned results of ingot solidification, as can be seen in **Figure 5**. Also, results of heat flux (see **Figure 6**) can be useful to a determination of the intensity of heat transfer.

Simulation of ingot deformities such as **microporosity and macroporosity**, which form during shrinkage of steel, is very popular. Prediction of these defects is solved based on Niyama criterion (4), which expresses the fraction of temperature gradient and cooling rate in a nodal position of mesh during simulation. [2,9,14]

$$Ny = \frac{G}{\sqrt{\dot{T}}} \tag{4}$$

where G is thermal gradient (K.m^{-1}) and $\dot{T}$ is cooling rate (K.s^{-1}).

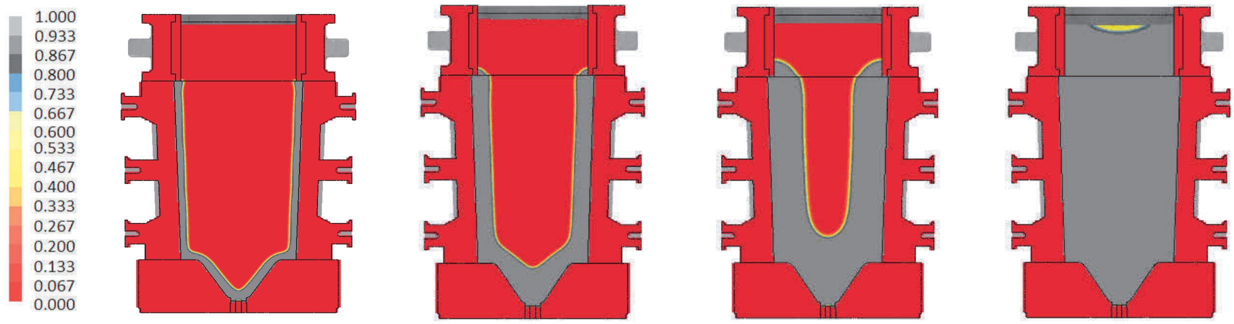

Figure 5 Ingot solidification - fraction solid results (-) [5]

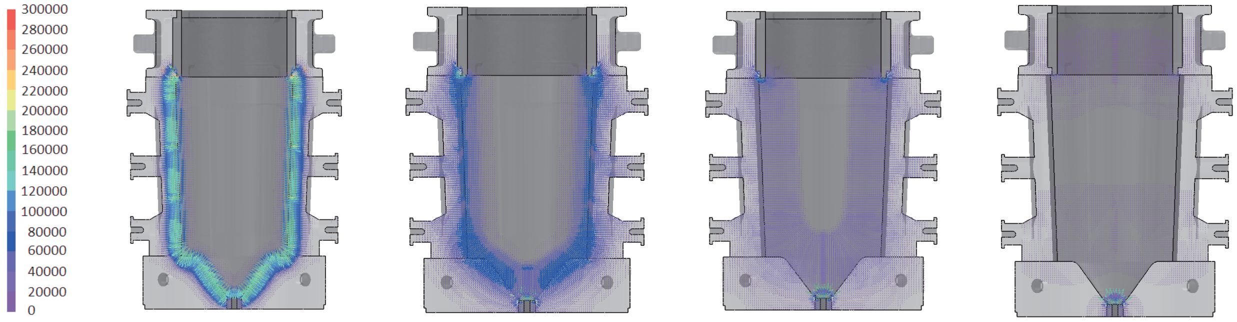

Figure 6 Visualization of heat flux results (W.m^{-2}) [5]

This issue has been recently dealt by authors [5,6,15]. Results of prediction of internal porosity of ingot through Niyama criterion is shown in **Figure 7**. Very important is influence of computational mesh density on quality of internal porosity results (see **Figure 7**). As can be seen, porosity changes its shape and size in dependence on mesh density. On a very coarse mesh, the porosity may not be noticeable. Different shapes of shrinkage cavity at different density of mesh, are also visible. If some part of an element of the mesh contains shrinkage cavity, the software fill by shrinkage cavity the whole element, which affects the resulting shape and size of visualized shrinkage cavity. This example demonstrates the importance of computational mesh in procedure of numerical modelling.

3.2. Prediction of macrosegregation

With regard to segregated elements effect on steel properties, prediction of macrosegregation is very helpful tool of optimization of ingot quality. Thanks to its possibilities, the software provides a computation of **macrosegregation** based on chemical composition and thermodynamic properties of steel for a range of alloying elements such as C, P, S, Mn, Si, Cu, Ni etc. The software works with the equation of liquid species conservation (5) and solid species conservation (6). [9] Results of macrosegregation of phosphorus in 40 t ingot are illustrated in **Figure 7**. [16] Computation of segregation uses temperature field at the end of mould filling and is focused only on liquid fraction contained in mould. As it has been found out by authors of study [12,16], if the computation of segregation

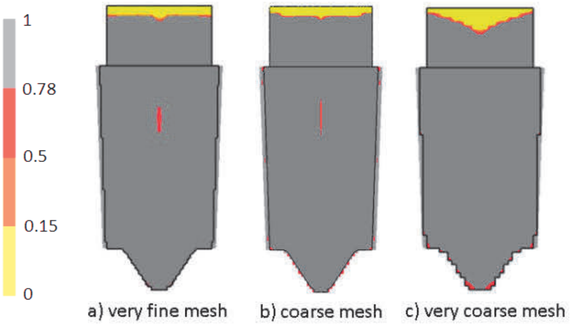

Figure 7 Visualization of internal porosity in ingot, dependent on size of mesh elements and mesh density [5]

is divided into two phases (separate computation of filling, separate computation of solidification based on exported filling results) and if the thin solid crust on the interface between mould and ingot is created, the program is not able to determine content of element in solid fraction. This phenomenon is confirmed by results of segregation of P, which can be seen in **Figure 8**, where zero content of P in the region of solid crust is visible. Therefore, it is appropriate to calculate filling and solidification as one coherent simulation, where the development of macrosegregation is captured in initial stages of solidification (i.e. from the moment of solid crust emergence).

$$f_l\rho_l\frac{\partial c_l^m}{\partial t}+f_l\rho_l v_l.\nabla c_l^m=\nabla.(f_l\rho_l D_l^m\nabla c_l^m)+(c_l^m-c_{sl}^m)\frac{\partial}{\partial t}(\rho_s f_s)+\frac{S\rho_s D_s^m}{l}(c_s^m-c_{sl}^m) \quad (5)$$

$$f_s\rho_s\frac{\partial c_s^m}{\partial t}=(c_s^m-c_s^m)\left[\frac{\partial}{\partial t}(\rho_s f_s)+\frac{S\rho_s D_s^m}{l}\right] \quad (6)$$

where c is concentration, m is species, l is diffusion length, S is interfacial area concentration, D is diffusivity, s and l represent liquid and solid interface.

3.3. Prediction of risk of hot tearing and cracking sensitivity

During solidification and cooling of steel ingot, stresses due to anisotropy of mechanical properties can occur. In the worst case, these stresses can lead to violation of integrity of ingot and degradation of its quality. To elimination of defects formed due to internal stresses (hot tearing, cracks), tools able to predict critical areas are applicable. For this purpose, Hot Cracking Sensitivity (HCS) computation, which is described in more detail in literature [9,17], is usable. Authors of study [17] developed a criterion for steel, which can be expressed by equation (7). The higher the value of the HCS, the more sensitive the material to crack.

$$HCS=\frac{1}{\dot{\varepsilon}^{max}} \quad (7)$$

where $\dot{\varepsilon}^{max}$ is maximum strain rate sustainable by the mushy zone (s^{-1}).

To **hot tearing** prediction, Hot Tearing Indicator, which is a part of software, is useful. This tool computes hot tearing sensitivity of steel in temperature range over solidus temperature. As an example, results obtained during research of technology of slab ingot casting by authors [16] (see **Figure 9** left), can be used. The higher value of Hot Tearing Indicator, the higher sensitivity to hot tearing. [8] Nucleation and growth of cracks are support by plastic deformation of steel, same as porosity presence. Prediction of **cracking** of ingots provides the Cracking Indicator. This tool is used to the computation of cracks, formed after the finish of solidification of ingot and is based on stress computation coupled with porosity computation. [9] Visualization of Cracking results is shown in **Figure 9** right. Just like Hot Tearing Indicator, the higher value of Cracking, the more sensitive the material is to crack.

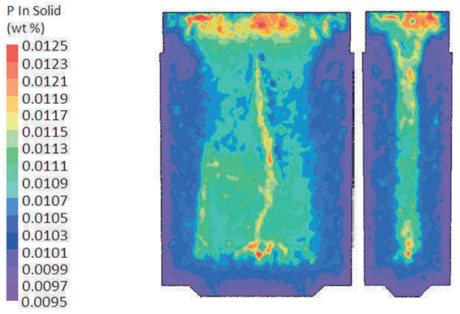

Figure 8 Visualization of macrosegregation [16]

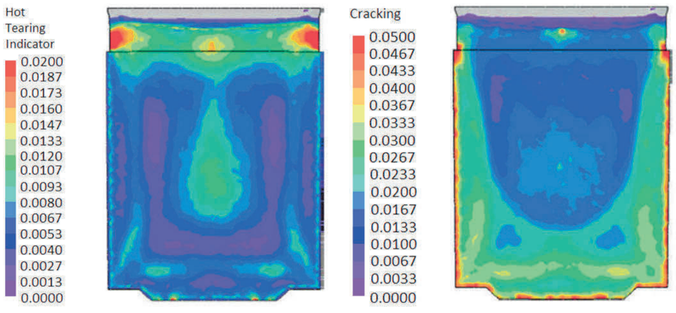

Figure 9 Results of Hot Tearing Indicator (left) and Cracking (right) [16]

4. CONCLUSIONS

Steel ingots are sensitive to the formation of the defects, which can lead to quality degradation. Thus, prediction of these defects is very important part of research of ingot casting technology. In this respect, numerical modelling is a very useful tool, which provides identification of conditions of defects formation and on that basis casting conditions or mould design can be appropriately adjusted. Currently, there are many programs intended for numerical modelling. These programs can numerically investigate the entire process of ingot casting and help to avoid financial losses associated with ingot quality degradation due to defects creation. From the numerical analysis of casting and solidification of steel ingot, it was found out that:

- Numerous numerical methods are used for simulations of ingot casting technology, including the Finite Element Method and the Finite Differences Method.
- The phenomenon involved in process of ingot casting and solidification are based on governing equations. These equations are during numerical modelling solved by numerical methods.
- To obtain relevant results, not only the correct setting of the numerical model but also the definition of thermodynamic parameters of steel and materials of casting assembly, are important.
- In the process of numerical modelling, it is of particular importance the computational mesh whose quality can greatly influence the extent of predicted defects.

Numerical modelling of the technology of steel ingot casting can be divided into the simulation of:

- filling and solidification of the ingot;
- macroporosity and microporosity formation in the ingot;
- macrosegregation formation;
- hot tearing and cracking sensitivity.

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REFERENCES

[1] CHVOJKA, J. *Vady ingotů*. Praha: SNTL - Nakladatelství technické literatury, 1968, p. 254

[2] ŠMRHA, L. *Tuhnutí a krystalizace ocelových ingotů*. Praha: SNTL - Nakladatelství technické literatury, 1983. p.305

[3] MARŠÍK, F. *Termodynamika kontinua*. Praha: Academia, 1999. p. 323. ISBN 80-200-0758-X

[4] MARŠÍK, F. *Numerické metody mechaniky kontinua*. Praha, Akademie věd ČR, 1990, 295 s.

[5] KLUS, P. *Studium plnění a tuhnutí ocelového ingotu pomocí numerické simulace v prostředí software QuickCAST*. Ostrava: VŠB-TU Ostrava, 2017, p. 121

[6] TKADLEČKOVÁ, M., MICHALEK, K., GRYC, K., SOCHA, L., JONŠTA, P., SATERNUS, M., PIEPRZYCA, J. and MERDER, T. Research and Development of the Solidification of Slab Steel Ingot from Special Tool Steels. In *ARCHIVES OF METALLURGY AND MATERIALS*. 2017, vol. 62, iss. 3, pp. 1453-1485. DOI: 10.1515/amm-2017-0225

[7] REDDY, J. N. *An introduction to the finite element method*. 3rd ed. New York: McGraw-Hill Higher Education, 2006. p. 766. ISBN 0-07-246685-5.

[8] SMITH, I. M., GRIFFITHS, D. V. and MARGETTS, L. Programming the finite element method. 5th ed. Chichester: Wiley, 2014. p. 664. ISBN 978-1-119-97334-8.

[9] ProCAST User Guide 2016 - macrosegregation in ProCAST. JGU, ESI US R&D, Columbia, Maryland.

[10] LAUNDER, B. E. and SPALDING, D. B. The Numerical Computation of Turbulent Flows. In *COMPUTER METHODS IN APPLIED MECHANICS AND ENGINEERING*. 1974, vol. 3. pp. 269-289

[11] SPURK, J. H. and AKSEL, N. *Fluid mechanics*. 2nd ed. Berlin: Springer, 2008. ISBN 978-3-540-73536-6.

[12] TKADLEČKOVÁ, M., MACHOVČÁK, P., GRYC, K., MICHALEK, K., SOCHA, L. and KLUS, P. Numerical modelling of macrosegregation in heavy steel ingot. In *ARCHIVES OF METALLURGY AND MATERIALS*. 2013. vol.58, iss. 1**,** pp. 171-177. DOI: 10.2478/v10172-012-0169-2

[13] POLA, A., GELFI, M. and LA VECCHIA, G. M. Comprehensive Numerical Simulation of Filling and Solidification of Steel Ingots. In *MATERIALS*. 2016. vol. 9, iss 9. DOI: 10.3390/ma9090769

[14] QuikCAST 2010, Reference Manual. 2010 ESI Group.

[15] REIDLER, M., MICHELIC, S. and BERNHARD, C. Numerical Simulation and Experimental Validation of the Formation of Shrinkage Cavity During Solidification of Steel. In *METAL 2016: 25TH ANNIVERSARY INTERNATIONAL CONFERENCE ON METALLURGY AND MATERIALS*. Ostrava: TANGER, 2016, pp. 97-103

[16] TKADLEČKOVÁ, M., MICHALEK, K., MACHOVČÁK, P., KOVÁČ, M. and SOCHA, L. Study of Casting and Solidification of Slab Steel Ingot from Tool Steel Using Numerical Modelling. In *ARCHIVES OF METALLURGY AND MATERIALS*. 2015. vol. 60, iss. 4, pp. 2879-2885. DOI: 10.1515/amm-2015-0460

[17] DREZET, J. M., GREMAUD, M., GRAF, R. and GÄUMANN, M. A new hot tearing criterion for steel. In *4th European Continuous Casting Conference*, Birmingham, 2002, pp. 755-763.