

directChillFoam: an OpenFOAM application for direct-chill casting

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Direct-chill (DC) casting is a semi-continuous casting process that is used for producing aluminium and magnesium alloy billets (D. G. Eskin, 2008). As illustrated in (Figure 1), the process consists of feeding melt (liquid metal) into a mould containing a movable bottom (the ram). The ram is lowered and the billet is pulled downwards by gravity. As the billet exits the mould, its exposed outer surface is chilled with water jets to hasten cooling (hence the term direct-chill).



Figure 1: The direct-chill casting process.

After DC casting, the billets are subject to further energy intensive processing (e.g., extrusion, rolling, forging). If billets contain defects or are of poor quality, they are either rejected or will ultimately result in components of poor quality: this makes DC casting a crucial step in alloy processing. In a push for lower carbon emissions and greater recyclability of metallic components, DC casting is currently the subject of various optimization studies involving the presence of external fields. These studies include:

1. the use of ultrasound (G. I. Eskin & Eskin, 2014; Lebon, Tzanakis, et al., 2019; Lebon, Salloum-Abou-Jaoude, et al., 2019; Subroto et al., 2021; Yamamoto & Komarov, 2021).

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- high-shear melt conditioning with a rotor-stator mixer (Lebon et al., 2018, 2020; Li et al., 2017; Prasada Rao, 2014; Sree Manu et al., 2021; Xia et al., 2013), and
- 3. electromagnetic fields (Hatić et al., 2018).

All these studies benefit from numerical modelling to cut down on the number of experiments that are required to study the process.

State of the field

Direct-chill casting modelling broadly falls into two approaches. One class of solution-multiphase or multiple domain models-uses independent conversation equations for each phase (Ni & Beckermann, 1991). The conservation equations are then coupled using boundary conditions at phase interfaces, thereby requiring these interfaces to be accurately tracked. More recent implementations of these multiple domain models implement grain motion (Heyvaert et al., 2017; Tveito et al., 2018). This approach is computationally expensive for optimization searches.

The other approach is based on the continuum model (Bennon & Incropera, 1987) and can also include the effect of free-floating dendrites (Vreeman et al., 2000). The continuum model avoids the requirement of tracking phase interfaces by implicitly integrating the microscopic description of transport behaviour in a continuum formulation. This approach has been validated with temperature measurements in the sump (Vreeman et al., 2002) and is the starting point for directChillFoam.

Statement of need

directChillFoam is an OpenFOAM (Weller et al., 1998) solver for the computational fluid dynamics (CFD) modelling of the DC casting process. directChillFoam extended OpenFOAM's buoyantPimpleFoam solver to include the following functionalities:

- An improved solidification model that can handle alloys with more than two components and with a liquid fraction-temperature profile that can be entered with an interpolation table. These enable the use of thermophysical properties that can be calculated on the fly by a CALPHAD package (Andersson et al., 2002).
- Switching between mushy and slurry zones in the phase transition region to accurately handle the flow near the solidification front.
- Treatment of the secondary cooling heat transfer boundary condition.
- An energy corrector loop to correctly update the phase fraction while conserving energy, based on the approach of Faden et al. (2018).
- A solute model library to model macrosegregation and a corresponding solver for the solute transport equations.

directChillFoam makes the most of OpenFOAM's modularity and implements each significant functionality within reusable libraries. The power of directChillFoam lies within the ease with which the solver can be extended. For example, directChillFoam has been coupled with a novel acoustic streaming solver (Lebon, 2021) to model acoustic streaming inside a direct-chill casting mould (Lebon, Salloum-Abou-Jaoude, et al., 2019). Such coupling of a newly published complex numerical method would be non-trivial in a commercial CFD software package.

directChillFoam was designed to be used by both academics involved in fundamental casting research and industry practitioners for optimization problems. It has already been used in a number of scientific publications involving melt-conditioned direct-chill (MC-DC) casting (Lebon et al., 2018, 2020) and ultrasonic processing (Lebon, Tzanakis, et al., 2019; Lebon, Salloum-Abou-Jaoude, et al., 2019; Subroto et al., 2021). It has also been presented in introductory modelling doctoral courses that are provided by the Liquid Metal Engineering training centre at Brunel University.



Availability

directChillFoam is available on Github. Documentation is provided for a description of its functionality and included libraries. A tutorial case including code validation using experimental data (Vreeman et al., 2002) is also available.

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References

- Andersson, J. O., Helander, T., Höglund, L., Shi, P., & Sundman, B. (2002). Thermo-Calc & DICTRA, computational tools for materials science. *Calphad: Computer Coupling of Phase Diagrams and Thermochemistry*, 26(2). https://doi.org/10.1016/S0364-5916(02)00037-8
- Bennon, W. D., & Incropera, F. P. (1987). A continuum model for momentum, heat and species transport in binary solid-liquid phase change systems—i. Model formulation. *International Journal of Heat and Mass Transfer*, 30(10), 2161–2170. https://doi.org/10. 1016/0017-9310(87)90094-9
- Eskin, D. G. (2008). *Physical Metallurgy of Direct Chill Casting of Aluminum Alloys* (pp. 1–303). CRC Press. https://doi.org/10.1201/9781420062823
- Eskin, G. I., & Eskin, D. G. (2014). Ultrasonic Treatment of Light Alloy Melts, Second Edition. CRC Press. https://doi.org/10.1201/b17270
- Faden, M., König-Haagen, A., Höhlein, S., & Brüggemann, D. (2018). An implicit algorithm for melting and settling of phase change material inside macrocapsules. *International Journal* of Heat and Mass Transfer, 117, 757–767. https://doi.org/10.1016/j.ijheatmasstransfer. 2017.10.033
- Hatić, V., Mavrič, B., Košnik, N., & Šarler, B. (2018). Simulation of direct chill casting under the influence of a low-frequency electromagnetic field. *Applied Mathematical Modelling*, 54, 170–188. https://doi.org/10.1016/j.apm.2017.09.034
- Heyvaert, L., Bedel, M., Založnik, M., & Combeau, H. (2017). Modeling of the coupling of microstructure and macrosegregation in a direct chill cast Al-Cu billet. *Metallurgical and Materials Transactions A*, 48(10), 4713–4734. https://doi.org/10.1007/s11661-017-4238-z
- Lebon, B. (2021). acousticStreamingFoam: An acoustic streaming solver. In *GitHub repository*. GitHub. https://github.com/blebon/acousticStreamingFoam
- Lebon, B., Li, H. T., Patel, J. B., Assadi, H., & Fan, Z. (2020). Numerical modelling of melt-conditioned direct-chill casting. *Applied Mathematical Modelling*, 77, 1310–1330. https://doi.org/10.1016/j.apm.2019.08.032
- Lebon, B., Li, H.-T., Patel, J. B., Assadi, H., & Fan, Z. (2018). Numerical modelling of melt conditioned direct-chill (MC-DC) casting of AZ31 magnesium alloy. *Magnesium 2018*, 100–106.
- Lebon, B., Salloum-Abou-Jaoude, G., Eskin, D., Tzanakis, I., Pericleous, K., & Jarry, P. (2019). Numerical modelling of acoustic streaming during the ultrasonic melt treatment of direct-chill (DC) casting. *Ultrasonics Sonochemistry*, 54, 171–182. https://doi.org/10. 1016/j.ultsonch.2019.02.002



- Lebon, B., Tzanakis, I., Pericleous, K., & Eskin, D. (2019). Numerical modelling of the ultrasonic treatment of aluminium melts: An overview of recent advances. *Materials*, 12(19), 3262. https://doi.org/10.3390/ma12193262
- Li, H. T., Zhao, P., Yang, R., Patel, J. B., Chen, X., & Fan, Z. (2017). Grain refinement and improvement of solidification defects in direct-chill cast billets of A4032 alloy by melt conditioning. *Metallurgical and Materials Transactions B: Process Metallurgy and Materials Processing Science*, 48(5), 2481–2492. https://doi.org/10.1007/s11663-017-1016-7
- Ni, J., & Beckermann, C. (1991). A volume-averaged two-phase model for transport phenomena during solidification. *Metallurgical Transactions B*, 22(3), 349–361. https://doi.org/10. 1007/BF02651234
- Prasada Rao, A. K. (2014). Understanding the evolution of the microstructure in meltconditioned direct-chill cast Al alloys. *Materials and Manufacturing Processes*, 29(7), 848–852. https://doi.org/10.1080/10426914.2014.921698
- Sree Manu, K. M., Barekar, N. S., Lazaro-Nebreda, J., Patel, J. B., & Fan, Z. (2021). In-situ microstructural control of A6082 alloy to modify second phase particles by melt conditioned direct chill (MC-DC) casting process – A novel approach. *Journal of Materials Processing Technology*, 295, 117170. https://doi.org/10.1016/j.jmatprotec.2021.117170
- Subroto, T., Lebon, B., Eskin, D. G., Skalicky, I., Roberts, D., Tzanakis, I., & Pericleous, K. (2021). Numerical modelling and experimental validation of the effect of ultrasonic melt treatment in a direct-chill cast AA6008 alloy billet. *Journal of Materials Research and Technology*, 12, 1582–1596. https://doi.org/10.1016/j.jmrt.2021.03.061
- Tveito, K. O., Pakanati, A., M'Hamdi, M., Combeau, H., & Založnik, M. (2018). A simplified three-phase model of equiaxed solidification for the prediction of microstructure and macrosegregation in castings. *Metallurgical and Materials Transactions A*, 49(7), 2778–2794. https://doi.org/10.1007/s11661-018-4632-1
- Vreeman, C. J., Krane, M. J. M., & Incropera, F. P. (2000). The effect of free-floating dendrites and convection on macrosegregation in direct chill cast aluminum alloys: Part i: Model development. International Journal of Heat and Mass Transfer, 43(5), 677–686. https://doi.org/10.1016/S0017-9310(99)00174-X
- Vreeman, C. J., Schloz, J. D., & Krane, M. J. M. (2002). Direct chill casting of aluminum alloys: Modeling and experiments on industrial scale ingots . *Journal of Heat Transfer*, 124(5), 947–953. https://doi.org/10.1115/1.1482089
- Weller, H. G., Tabor, G., Jasak, H., & Fureby, C. (1998). A tensorial approach to computational continuum mechanics using object-oriented techniques. *Computers in Physics*, 12(6), 620–631. https://doi.org/10.1063/1.168744
- Xia, M. X., Prasada Rao, A. K., & Fan, Z. (2013). Solidification mechanisms in melt conditioned direct chill (MC-DC) cast AZ31 billets. *Materials Science Forum*, 765, 291–295. https://doi.org/10.4028/www.scientific.net/MSF.765.291
- Yamamoto, T., & Komarov, S. V. (2021). Influence of ultrasound irradiation on transient solidification characteristics in DC casting process: Numerical simulation and experimental verification. *Journal of Materials Processing Technology*, 294, 117116. https://doi.org/10. 1016/j.jmatprotec.2021.117116