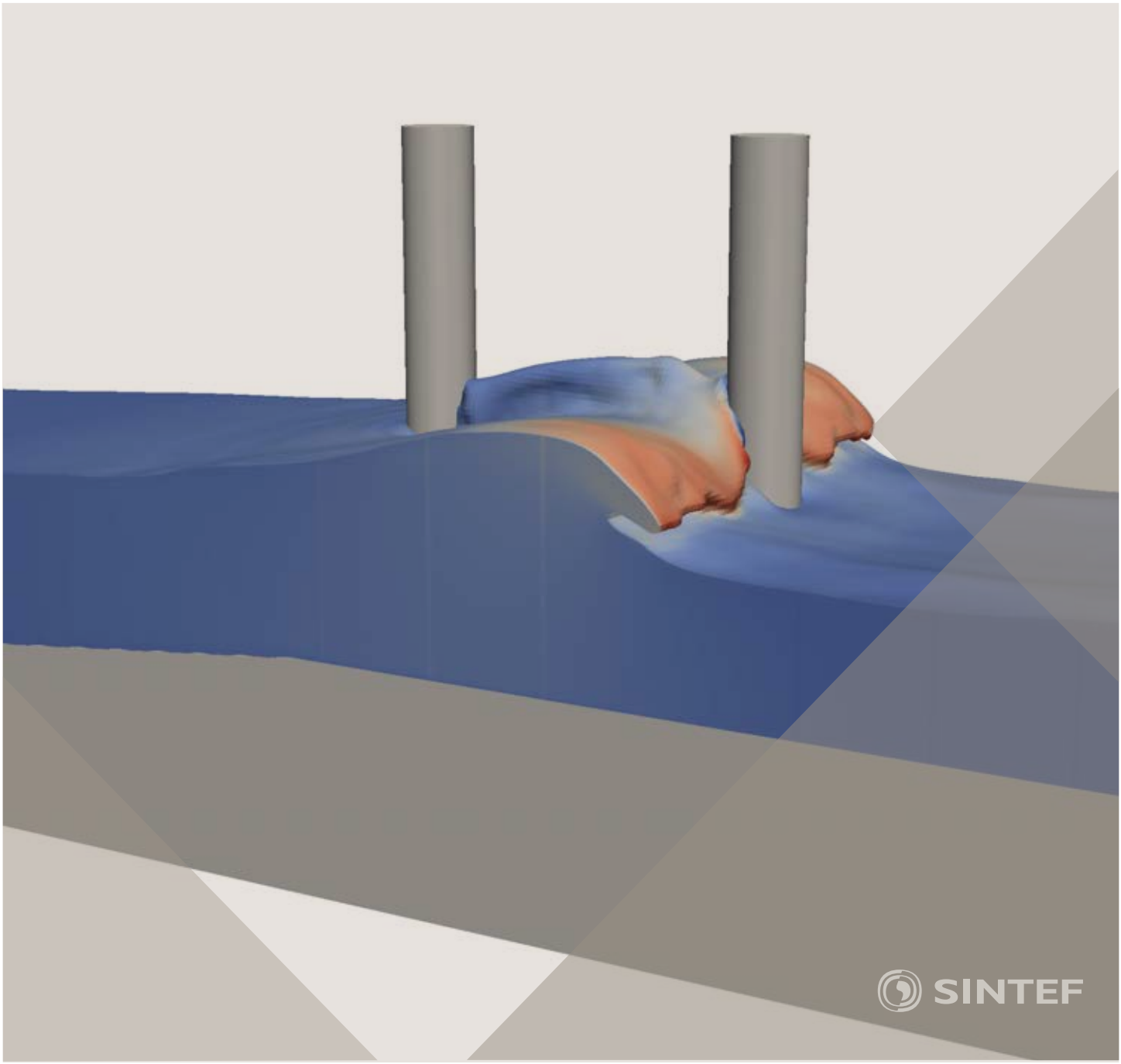
SINTEF
PROCEEDINGS
2

Proceedings of the 12th International Conference on Computational Fluid Dynamics in the Oil & Gas, Metallurgical and Process Industries

Progress in Applied CFD – CFD2017



SINTEF Proceedings

Editors:
Jan Erik Olsen and Stein Tore Johansen

Progress in Applied CFD – CFD2017

Proceedings of the 12th International Conference on Computational Fluid Dynamics in the Oil & Gas, Metallurgical and Process Industries

SINTEF Academic Press

SINTEF Proceedings no 2
Editors: Jan Erik Olsen and Stein Tore Johansen
Progress in Applied CFD – CFD2017
Selected papers from 10th International Conference on Computational Fluid Dynamics in the Oil & Gas, Metallurgical and Process Industries

Key words:
CFD, Flow, Modelling

Cover, illustration: Arun Kamath

ISSN 2387-4295 (online)
ISBN 978-82-536-1544-8 (pdf)

© Copyright SINTEF Academic Press 2017
The material in this publication is covered by the provisions of the Norwegian Copyright Act. Without any special agreement with SINTEF Academic Press, any copying and making available of the material is only allowed to the extent that this is permitted by law or allowed through an agreement with Kopinor, the Reproduction Rights Organisation for Norway. Any use contrary to legislation or an agreement may lead to a liability for damages and confiscation, and may be punished by fines or imprisonment

SINTEF Academic Press
Address: Forskningsveien 3 B
PO Box 124 Blindern
N-0314 OSLO
Tel: +47 73 59 30 00
Fax: +47 22 96 55 08

www.sintef.no/byggforsk
www.sintefbok.no

SINTEF Proceedings
SINTEF Proceedings is a serial publication for peer-reviewed conference proceedings on a variety of scientific topics.
The processes of peer-reviewing of papers published in SINTEF Proceedings are administered by the conference organizers and proceedings editors. Detailed procedures will vary according to custom and practice in each scientific community.

PREFACE

This book contains all manuscripts approved by the reviewers and the organizing committee of the 12th International Conference on Computational Fluid Dynamics in the Oil & Gas, Metallurgical and Process Industries. The conference was hosted by SINTEF in Trondheim in May/June 2017 and is also known as CFD2017 for short. The conference series was initiated by CSIRO and Phil Schwarz in 1997. So far the conference has been alternating between CSIRO in Melbourne and SINTEF in Trondheim. The conferences focuses on the application of CFD in the oil and gas industries, metal production, mineral processing, power generation, chemicals and other process industries. In addition pragmatic modelling concepts and bio-mechanical applications have become an important part of the conference. The papers in this book demonstrate the current progress in applied CFD.

The conference papers undergo a review process involving two experts. Only papers accepted by the reviewers are included in the proceedings. 108 contributions were presented at the conference together with six keynote presentations. A majority of these contributions are presented by their manuscript in this collection (a few were granted to present without an accompanying manuscript).

The organizing committee would like to thank everyone who has helped with review of manuscripts, all those who helped to promote the conference and all authors who have submitted scientific contributions. We are also grateful for the support from the conference sponsors: ANSYS, SFI Metal Production and NanoSim.

Stein Tore Johansen & Jan Erik Olsen

Organizing committee:

Conference chairman: Prof. Stein Tore Johansen
Conference coordinator: Dr. Jan Erik Olsen
Dr. Bernhard Müller
Dr.Sigrid Karstad Dahl
Dr.Shahriar Amini
Dr.Ernst Meese
Dr.Josip Zoric
Dr.Jannike Solsvik
Dr.Peter Witt

Scientific committee:

Stein Tore Johansen, SINTEF/NTNU
Bernhard Müller, NTNU
Phil Schwarz, CSIRO
Akio Tomiyama, Kobe University
Hans Kuipers, Eindhoven University of Technology
Jinghai Li, Chinese Academy of Science
Markus Braun, Ansys
Simon Lo, CD-adapco
Patrick Segers, Universiteit Gent
Jiyuan Tu, RMIT
Jos Derksen, University of Aberdeen
Dmitry Eskin, Schlumberger-Doll Research
Pär Jönsson, KTH
Stefan Pirker, Johannes Kepler University
Josip Zoric, SINTEF

CONTENTS

SOLIDIFICATION MODELING WITH USER DEFINED FUNCTION IN ANSYS FLUENT

Moritz EICKHOFF[1]*, Antje RÜCKERT[1], Herbert PFEIFER[1]

[1] RWTH Aachen University, Department for Industrial Furnaces and Heat Engineering, Kopernikusstr. 10, 52074 Aachen, GERMANY

* E-mail: eickhoff@iob.rwth-aachen.de

ABSTRACT

The modelling of solidification processes in combination with fluid flow is one main application of ANSYS Fluent. The solidification is modelled with the enthalpy porosity technique. Therefor the fluid flow is damped like a flow through a porous media of dendrites. In case of materials with large solidification ranges, like the nickel based superalloy 718, the adjustment possibilities of ANSYS Fluent are often not adequate. The program postulates a linear dependency between liquid fraction and temperature. To improve the simulation, the solidification was implemented by a user defined function (UDF). The principal modelling of fluid flow is based on the theory of ANSYS Fluent, but it is now possible to adjust the liquid fraction in fine temperature steps.

Keywords: Rheology, Interphases, Casting and solidification, Process metallurgy, Alloy 718.

NOMENCLATURE

Greek Symbols

ϵ	Turbulent dissipation rate, [-].
λ	Thermal conductivity, [W/(m K)].
μ_D	Dynamic viscosity, [kg/(m s)].
∇	Divergence operator, [-].
ρ	Density, [kg/m³].
τ	Shear stress tensor, [N/m²].

Latin Symbols

A_{mush}	Mushy zone constant, [kg/(m³ s)].
e	Internal energy, [J].
f	Fraction, [-].
F	Force against fluid flow per volume, [N/m³].
g	Gravity, [m/s²].
k	Turbulent kinetic energy, [-].
K	Permeability, [m²].
l	Small number, [-].
p	Pressure, [Pa].
Q_e	volumetric energy source, [J/m³].
S	Momentum sink for turbulence, [kg/(m³ s)].
v	Velocity, [m/s].
t	Time, [s].
T	Temperature, [K].

Sub/superscripts

eff	Effective (molecular + turbulent).
ESR	Electro slag remelting.
ϵ	Turbulent dissipation rate.
k	Turbulent kinetic energy.
liq	Liquidus / liquid.
p	Pulling (movement of the solid).
sol	Solidus.
UDF	User-defined function.
UDM	User-defined memory.
VAR	Vacuum arc remelting.
x	X-direction.
y	Y-direction.
z	Z-direction.

INTRODUCTION

Metallurgical processes are often modeled to obtain details of the inner fluid flow or temperature distribution, due to the difficult observation possibilities with classical measurement methods. The modelling of solidification processes is in focus of research since the 1970s (Erickson, 1975).

One of the common simulation programs ANSYS Fluent uses the enthalpy-porosity approach (ANSYS Inc., Release 14.5, 2012) which was introduced by Poirier (1987). ANSYS Fluent uses the assumption that the liquid fraction is proportional to the temperature in the solidification range. For many standard steels, this assumption will be an appropriate approach. In case of some nickel based superalloys, like alloy 718, the supposition is far-out the real material behavior.

Therefore, user-defined functions implement the solidification to reproduce the real material behavior.

SOLIDIFICATION PHENOMENA

Important for the simulation of solidification processes are the damping of the fluid flow in the mushy region and the solidification enthalpy. The damping is adjustable with the material specific mushy zone constant (Voller et al., 1990) and considers the liquid fraction also.

Figure 1 shows the liquid fraction of an alloy 718 in respect to the temperature in the solidification range calculated by JMatPro. Obviously, the linear approximation made by ANSYS Fluent is not appropriate for this material. After a cooling of 25 % of the temperature range the liquid fraction is not 75 % but only 40 %. Therefore, the

damping of the fluid flow is underestimated by ANSYS Fluent.

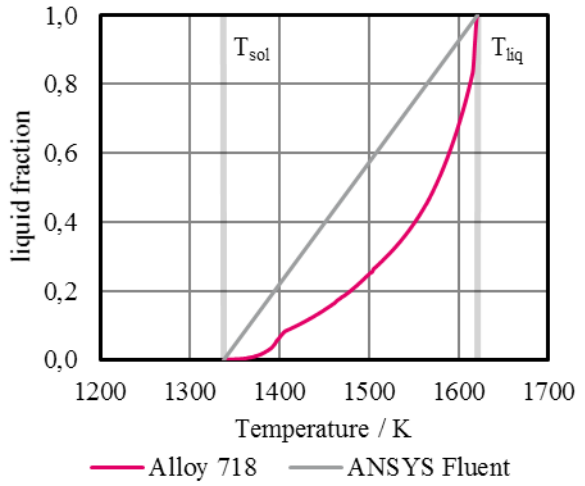


Figure 1: Liquid fraction of alloy 718 (Giesselmann et al., 2015) in comparison to ANSYS Fluent

The deviation of the liquid fraction from alloy 718 results in a nonlinear behavior of the enthalpy in the solidification range, because the solidification enthalpy is dependent on the liquid fraction.
Figure 2 shows the comparison of solidification enthalpies in respect to the temperature in the solidification range. The grey line shows the linear implementation of ANSYS Fluent. Obviously, the change in enthalpy of the mild steel (Koric and Thomas, 2008) is close to the approximation from ANSYS Fluent. Whereas, the red line, representing Alloy 718 (Overfelt et al., 1994), shows a considerably different behavior.

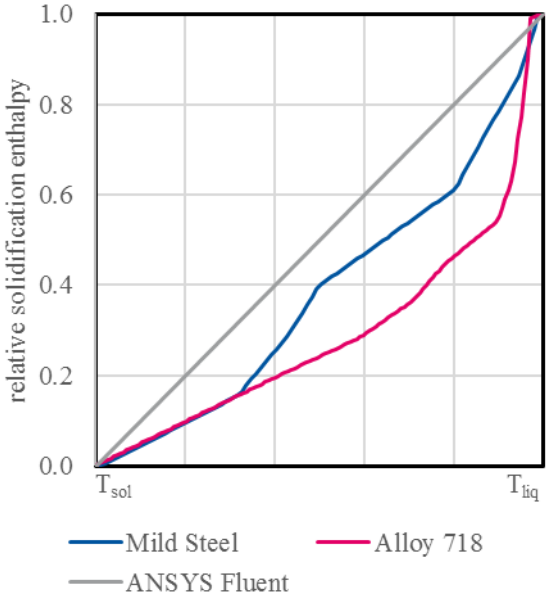


Figure 2: Comparison of solidification enthalpies (Overfelt et al., 1994, Koric and Thomas, 2008)

BUILT-IN SOLIDIFICATION IN ANSYS FLUENT

The solidification module from ANSYS Inc. (Release 14.5, 2012) uses the enthalpy-porosity approach to implement the damping of the fluid flow in the mushy region. Poirier (1987) shows, that the inter dendritic flow follows Darcy's law (Darcy, 1856):

Darcy's law

$$\nabla p = -\frac{\mu_D}{K} \cdot \mathbf{v} \tag{1}$$

Voller and Prakash (1987) implemented the awareness of Poirier (1987) in the fluid flow modeling. Later, a mushy zone constant was introduced to replace the dynamic viscosity μ_D and the unknown permeability K (Voller et al., 1990). The liquid fraction f_{liq} represents the change in permeability, whereas the mushy zone constant A_{mush} implements the different material behavior (2). The small number ε is equal 0.001 to avoid a division by zero (ANSYS Inc., Release 14.5, 2012).

$$\frac{\mu_D}{K} = \frac{(1 - f_{liq})^2}{f_{liq}^3 - l} \cdot A_{mush} \tag{2}$$

The ratio between viscosity and permeability (see formula (2)) is then inserted in the equations (3) and (4) to formulate the force F against the fluid flow v as well as the momentum S against the turbulence quantities Φ.

$$\mathbf{F} = \frac{(1 - f_{liq})^2}{f_{liq}^3 - \epsilon} \cdot A_{mush} \cdot (\mathbf{v} - \mathbf{v_p}) \tag{3}$$

$$S = \frac{\boldsymbol{(1 - f_{liq})^2}}{\boldsymbol{f_{liq}^3 - \epsilon}} \cdot \boldsymbol{A_{mush}} \cdot \Phi \tag{4}$$

The necessary turbulence quantities depend on the used turbulence model. Equation (4) is equal for all quantities like turbulent dissipation rate ε, turbulent kinetic energy k, specific dissipation ω and so on (ANSYS Inc., Release 14.5, 2012).
To show the implementation of the formula above, the momentum equation of the solver (5) is given below. The damping force F of the fluid flow (Equation (4)) is inserted in the last term.

$$\frac{\partial}{\partial t}(\rho \cdot \boldsymbol{v}) + \nabla \cdot (\rho \cdot \boldsymbol{v} \cdot \boldsymbol{v}) = -\nabla p + \nabla \cdot (\boldsymbol{\tau}) + \rho \cdot \boldsymbol{g} + \boldsymbol{F} \tag{5}$$

As mentioned in the previous chapter, the solidification enthalpy is distributed linear over the temperature range of solidification and implemented as source term S_m in the energy equation (6).

$$\frac{\partial}{\partial t}(\rho \cdot e) + \nabla \cdot \big(\boldsymbol{v} \cdot (\rho \cdot e + p)\big) = \nabla \cdot \big(\lambda_{eff} \cdot \nabla T + \boldsymbol{\tau_{eff}} \cdot \boldsymbol{v}\big) + Q_e \tag{6}$$

USER-DEFINED SOLIDIFICATION MODEL

To reconstruct the real material behavior of alloy 718 an in-house developed solidification model based on UDFs is used for several process models, like electro slag remelting (ESR) and vacuum arc remelting (VAR).

Approach

The aim of the modified solidification model is to implement the nonlinear behavior of the liquid fraction in respect to the temperature. The curve progression can be received for example from a Scheil-Gulliver approach like in Figure 1 or other calculation programs for thermophysical data.
The idea was to reconstruct the solidification model of ANSYS Fluent by user-defined functions. Therefore, the main equations ((3) and (4)) for the damping are also used.
The solidification enthalpy is included in the heat capacity of the material.

Implementation

The implementation of the modified solidification model is based on a DEFINE_ADJUST function for the liquid fraction and several DEFINE_SOURCE functions for the damping. A modified heat capacity includes the change in enthalpy.
The liquid fraction should be adjusted very detailed to represent the real fluid flow. Therefore, liquid fraction and solidification enthalpy out of the thermophysical database are divided in 1 K steps.

Damping of the fluid flow

A DEFINE_ADJUST UDF loops over all the cells in the fluid regions to get the temperature of the cells. A look-up function searches the corresponding liquid fraction for these temperatures out of the tabulated liquid fractions. The liquid fraction is saved in a user-defined memory (UDM) for post processing.
Analog to the calculation procedure in ANSYS Fluent the ratio between viscosity and permeability is calculated with equation (2) and saved in another UDM. This ratio is the damping term of velocities and turbulence quantities (see equation (3) and (4)).
The damping force and momentum values are calculated in several DEFINE_SOURCE UDFs. One UDF for each velocity direction and the turbulence quantities, typical turbulent dissipation rate ε and turbulent kinetic energy k. The source value is the negative product of the damping term with the velocity or turbulence value (See equations (7) to (11)). If a pull velocity v_p moves the solid region, it has to be subtracted from the fluid velocity, here in the x direction:

$$F_x = -\frac{\left(1-f_{liq}\right)^2}{f_{liq}^3+\epsilon}\cdot A_{mush}\cdot\left(\mathrm{v_x}-\mathrm{v_p}\right) \qquad (7)$$

$$F_y = -\frac{\left(1-f_{liq}\right)^2}{f_{liq}^3+\epsilon}\cdot A_{mush}\cdot v_y \qquad (8)$$

$$F_z = -\frac{\left(1-f_{liq}\right)^2}{f_{liq}^3+\epsilon}\cdot A_{mush}\cdot v_z \qquad (9)$$

$$S_k = -\frac{\left(1-f_{liq}\right)^2}{f_{liq}^3+\epsilon}\cdot A_{mush}\cdot k \qquad (10)$$

$$S_\epsilon = -\frac{\left(1-f_{liq}\right)^2}{f_{liq}^3+\epsilon}\cdot A_{mush}\cdot \epsilon \qquad (11)$$

The five source terms have to be included for the corresponding values in the ANSYS Fluent interface. The program implements the source terms in the momentum equation (5) as well as the turbulence model.

Solidification enthalpy

To implement the nonlinear behavior of the solidification enthalpy (see Figure 2) the enthalpy is included in the heat capacity of the material (see Figure 3). Therefore, it is not necessary to modify the energy equation (6) of the solver.

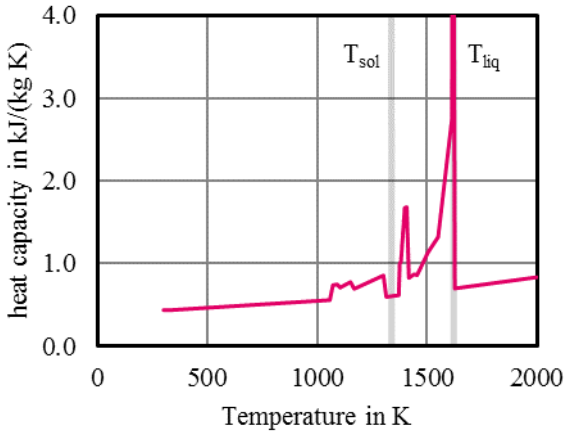


Figure 3: Heat capacity of alloy 718 including the solidification enthalpy (Giesselmann, 2014)

Obviously, most of the solidification enthalpy is needed or set free near to the liquidus temperature. This refers to the steep slope of the liquidus fraction in this area (compare Figure 1).
Another possibility to implement the enthalpy of solidification would be a DEFINE_SOURCE UDF. The advantage of the presented solution is the reversible character of the heat capacity. Because some parts of the simulated region maybe melt on again, the solution with source term would be more elaborate. Whereas the heat capacity offers directly the possibility for change of sign in the temperature derivation.

COMPARISON OF THE MODELS

To compare the built-in solidification of ANSYS Fluent with the UDF based solidification model a test case was set up. Figure 4 and Figure 5 show the flow of hot metal through a cooled pipe. The left face is a velocity inlet of hot liquid metal. The top wall is at constant temperature, which is lower than the solidus temperature. At the right side, the boundary is an outflow. The contour plot visualizes the liquid fraction from one (white) to zero (black). The black line symbolizes the position of 1 % solid fraction. The vectors and their lengths show the velocity.
In Figure 4 the solidification model of ANSYS Fluent was used. Therefore, the liquid fraction increases uniformly over the whole solidification range.

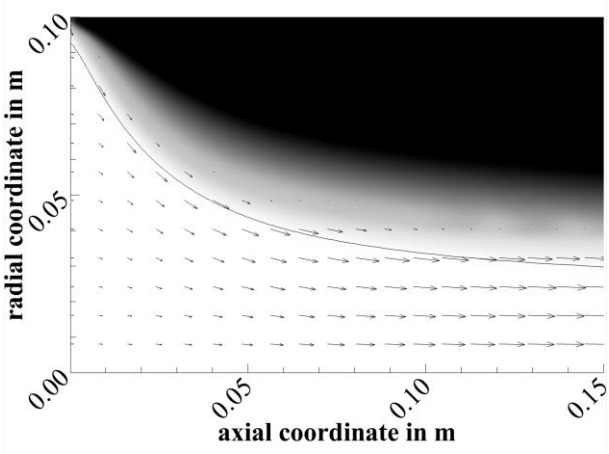


Figure 4: Test case: Built-in Fluent solidification model

Figure 5 shows the same test case simulation as Figure 4 with the UDF based solidification model. Obviously, the shape of the solidified area is slightly different, but more interesting is the case that there is sharp edge in the middle of the gray scale. Therefore, the fluid flow is damped at this position abruptly.

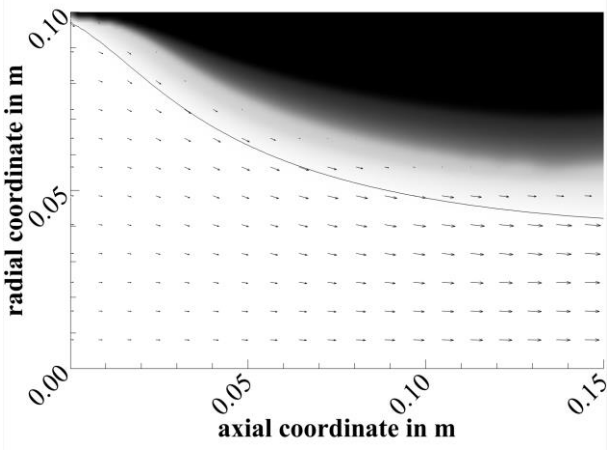


Figure 5: Test case: UDF solidification model

The comparison of the two test cases show the similarity of the models as well as the decisive differences. Whereas the flow in first case is damped smoothly, the damping with the UDF based model is more abrupt.

CONCLUSION

A modified solidification model for ANSYS Fluent was introduced. It offers the possibility to reproduce the real material behavior in context of liquid fraction in respect to temperature. Which is important for the damping of the fluid flow in the mushy region as well as the distribution of the solidification enthalpy over temperature.

The solidification model of ANSYS Fluent was modified and calculated in a user-defined function to adjust the liquid fraction concerning the cell temperature properly. The damping of the motion values is then implemented by source terms for velocities and turbulence quantities.
The solidification enthalpy is included in the heat capacity of the material. Therefore, the enthalpy can be fitted very detailed.
A test case shows the similarities and differences of the two models. The modified solidification implements a more abrupt damping of the fluid flow.
The modified solidification model is able to replicate the material behavior more detailed than the built-in solidification module of ANSYS Fluent.

REFERENCES

ANSYS INC., (Release 14.5, 2012), "ANSYS® Academic Research Help System".

DARCY, H.P.G., (1856), "Dètermination des lois d'ècoulement de l'eau à travers le sable".

ERICKSON, W.C., (1975), "Use of a general-purpose heat-transfer code for casting simulation", United States.

GIESSELMANN, N., (2014), "Numerische Untersuchungen des Elektroschlacke-Umschmelzprozesses für Alloy 718", Dissertation, Aachen, RWTH Aachen University, Fakultät für Georessourcen und Materialtechnik, 140.

GIESSELMANN, N., et al., (2015), "Coupling of Multiple Numerical Models to Simulate Electroslag Remelting Process for Alloy 718", *ISIJ International*, **55**, 1408-1415.

KORIC, S. and THOMAS, B.G., (2008), "Thermo-mechanical models of steel solidification based on two elastic visco-plastic constitutive laws", *Journal of Materials Processing Technology*, **197**, 408-418.

OVERFELT, R.A., et al., (1994), "Porosity in cast equiaxed alloy 718", *International Symposium on Superalloys 718, 625, 706 and Various Derivatives*, Pittsburgh, 189-200.

POIRIER, D., (1987), "Permeability for flow of interdendritic liquid in columnar-dendritic alloys", *Metallurgical and Materials Transactions B*, **18**, 245-255.

VOLLER, V.R., et al., (1990), "Modelling the mushy region in a binary alloy", *Applied Mathematical Modelling*, **14**, 320-326.

VOLLER, V.R. and PRAKASH, C., (1987), "A fixed grid numerical modelling methodology for convection-diffusion mushy region phase-change problems", *International Journal of Heat and Mass Transfer*, **30**, 1709-1719.