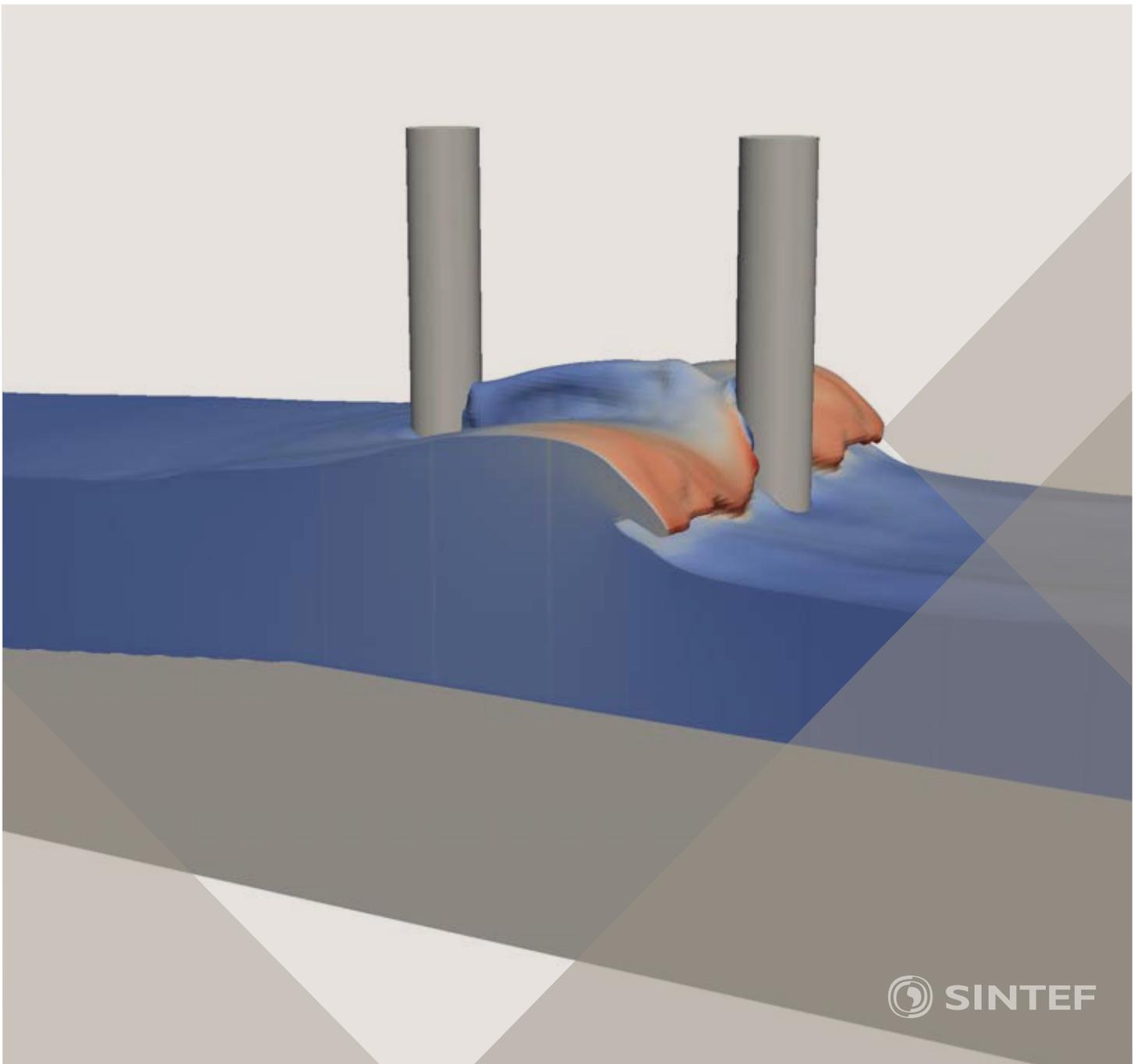


Proceedings of the 12th International Conference on
Computational Fluid Dynamics in the Oil & Gas,
Metallurgical and Process Industries

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

PRAGMATIC MODELLING	9
On pragmatism in industrial modeling. Part III: Application to operational drilling	11
CFD modeling of dynamic emulsion stability	23
Modelling of interaction between turbines and terrain wakes using pragmatic approach	29
FLUIDIZED BED	37
Simulation of chemical looping combustion process in a double looping fluidized bed reactor with cu-based oxygen carriers.....	39
Extremely fast simulations of heat transfer in fluidized beds.....	47
Mass transfer phenomena in fluidized beds with horizontally immersed membranes	53
A Two-Fluid model study of hydrogen production via water gas shift in fluidized bed membrane reactors	63
Effect of lift force on dense gas-fluidized beds of non-spherical particles	71
Experimental and numerical investigation of a bubbling dense gas-solid fluidized bed	81
Direct numerical simulation of the effective drag in gas-liquid-solid systems	89
A Lagrangian-Eulerian hybrid model for the simulation of direct reduction of iron ore in fluidized beds.....	97
High temperature fluidization - influence of inter-particle forces on fluidization behavior	107
Verification of filtered two fluid models for reactive gas-solid flows	115
BIOMECHANICS.....	123
A computational framework involving CFD and data mining tools for analyzing disease in carotid artery	125
Investigating the numerical parameter space for a stenosed patient-specific internal carotid artery model.....	133
Velocity profiles in a 2D model of the left ventricular outflow tract, pathological case study using PIV and CFD modeling.....	139
Oscillatory flow and mass transport in a coronary artery.....	147
Patient specific numerical simulation of flow in the human upper airways for assessing the effect of nasal surgery.....	153
CFD simulations of turbulent flow in the human upper airways	163
OIL & GAS APPLICATIONS	169
Estimation of flow rates and parameters in two-phase stratified and slug flow by an ensemble Kalman filter	171
Direct numerical simulation of proppant transport in a narrow channel for hydraulic fracturing application	179
Multiphase direct numerical simulations (DNS) of oil-water flows through homogeneous porous rocks	185
CFD erosion modelling of blind tees	191
Shape factors inclusion in a one-dimensional, transient two-fluid model for stratified and slug flow simulations in pipes	201
Gas-liquid two-phase flow behavior in terrain-inclined pipelines for wet natural gas transportation	207

NUMERICS, METHODS & CODE DEVELOPMENT	213
Innovative computing for industrially-relevant multiphase flows	215
Development of GPU parallel multiphase flow solver for turbulent slurry flows in cyclone.....	223
Immersed boundary method for the compressible Navier–Stokes equations using high order summation-by-parts difference operators	233
Direct numerical simulation of coupled heat and mass transfer in fluid-solid systems	243
A simulation concept for generic simulation of multi-material flow, using staggered Cartesian grids.....	253
A cartesian cut-cell method, based on formal volume averaging of mass, momentum equations.....	265
SOFT: a framework for semantic interoperability of scientific software	273
 POPULATION BALANCE	 279
Combined multifluid-population balance method for polydisperse multiphase flows	281
A multifluid-PBE model for a slurry bubble column with bubble size dependent velocity, weight fractions and temperature.....	285
CFD simulation of the droplet size distribution of liquid-liquid emulsions in stirred tank reactors	295
Towards a CFD model for boiling flows: validation of QMOM predictions with TOPFLOW experiments	301
Numerical simulations of turbulent liquid-liquid dispersions with quadrature-based moment methods.....	309
Simulation of dispersion of immiscible fluids in a turbulent couette flow	317
Simulation of gas-liquid flows in separators - a Lagrangian approach.....	325
CFD modelling to predict mass transfer in pulsed sieve plate extraction columns	335
 BREAKUP & COALESCENCE	 343
Experimental and numerical study on single droplet breakage in turbulent flow	345
Improved collision modelling for liquid metal droplets in a copper slag cleaning process	355
Modelling of bubble dynamics in slag during its hot stage engineering.....	365
Controlled coalescence with local front reconstruction method	373
 BUBBLY FLOWS	 381
Modelling of fluid dynamics, mass transfer and chemical reaction in bubbly flows	383
Stochastic DSMC model for large scale dense bubbly flows.....	391
On the surfacing mechanism of bubble plumes from subsea gas release.....	399
Bubble generated turbulence in two fluid simulation of bubbly flow	405
 HEAT TRANSFER	 413
CFD-simulation of boiling in a heated pipe including flow pattern transitions using a multi-field concept	415
The pear-shaped fate of an ice melting front	423
Flow dynamics studies for flexible operation of continuous casters (flow flex cc).....	431
An Euler-Euler model for gas-liquid flows in a coil wound heat exchanger.....	441
 NON-NEWTONIAN FLOWS.....	 449
Viscoelastic flow simulations in disordered porous media	451
Tire rubber extrudate swell simulation and verification with experiments	459
Front-tracking simulations of bubbles rising in non-Newtonian fluids.....	469
A 2D sediment bed morphodynamics model for turbulent, non-Newtonian, particle-loaded flows.....	479

METALLURGICAL APPLICATIONS.....	491
Experimental modelling of metallurgical processes	493
State of the art: macroscopic modelling approaches for the description of multiphysics phenomena within the electroslag remelting process	499
LES-VOF simulation of turbulent interfacial flow in the continuous casting mold	507
CFD-DEM modelling of blast furnace tapping	515
Multiphase flow modelling of furnace tapholes	521
Numerical predictions of the shape and size of the raceway zone in a blast furnace.....	531
Modelling and measurements in the aluminium industry - Where are the obstacles?	541
Modelling of chemical reactions in metallurgical processes.....	549
Using CFD analysis to optimise top submerged lance furnace geometries	555
Numerical analysis of the temperature distribution in a martensitic stainless steel strip during hardening.....	565
Validation of a rapid slag viscosity measurement by CFD.....	575
Solidification modeling with user defined function in ANSYS Fluent.....	583
Cleaning of polycyclic aromatic hydrocarbons (PAH) obtained from ferroalloys plant.....	587
Granular flow described by fictitious fluids: a suitable methodology for process simulations	593
A multiscale numerical approach of the dripping slag in the coke bed zone of a pilot scale Si-Mn furnace.....	599
INDUSTRIAL APPLICATIONS	605
Use of CFD as a design tool for a phosphoric acid plant cooling pond	607
Numerical evaluation of co-firing solid recovered fuel with petroleum coke in a cement rotary kiln: Influence of fuel moisture	613
Experimental and CFD investigation of fractal distributor on a novel plate and frame ion-exchanger	621
COMBUSTION	631
CFD modeling of a commercial-size circle-draft biomass gasifier.....	633
Numerical study of coal particle gasification up to Reynolds numbers of 1000.....	641
Modelling combustion of pulverized coal and alternative carbon materials in the blast furnace raceway	647
Combustion chamber scaling for energy recovery from furnace process gas: waste to value	657
PACKED BED.....	665
Comparison of particle-resolved direct numerical simulation and 1D modelling of catalytic reactions in a packed bed	667
Numerical investigation of particle types influence on packed bed adsorber behaviour	675
CFD based study of dense medium drum separation processes	683
A multi-domain 1D particle-reactor model for packed bed reactor applications.....	689
SPECIES TRANSPORT & INTERFACES	699
Modelling and numerical simulation of surface active species transport - reaction in welding processes	701
Multiscale approach to fully resolved boundary layers using adaptive grids.....	709
Implementation, demonstration and validation of a user-defined wall function for direct precipitation fouling in Ansys Fluent.....	717

FREE SURFACE FLOW & WAVES	727
Unresolved CFD-DEM in environmental engineering: submarine slope stability and other applications.....	729
Influence of the upstream cylinder and wave breaking point on the breaking wave forces on the downstream cylinder	735
Recent developments for the computation of the necessary submergence of pump intakes with free surfaces	743
Parallel multiphase flow software for solving the Navier-Stokes equations	752
 PARTICLE METHODS	 759
A numerical approach to model aggregate restructuring in shear flow using DEM in Lattice-Boltzmann simulations	761
Adaptive coarse-graining for large-scale DEM simulations.....	773
Novel efficient hybrid-DEM collision integration scheme.....	779
Implementing the kinetic theory of granular flows into the Lagrangian dense discrete phase model.....	785
Importance of the different fluid forces on particle dispersion in fluid phase resonance mixers	791
Large scale modelling of bubble formation and growth in a supersaturated liquid.....	798
 FUNDAMENTAL FLUID DYNAMICS	 807
Flow past a yawed cylinder of finite length using a fictitious domain method	809
A numerical evaluation of the effect of the electro-magnetic force on bubble flow in aluminium smelting process.....	819
A DNS study of droplet spreading and penetration on a porous medium.....	825
From linear to nonlinear: Transient growth in confined magnetohydrodynamic flows.....	831

MODELLING AND NUMERICAL SIMULATION OF SURFACE ACTIVE SPECIES TRANSPORT - REACTION IN WELDING PROCESSES

Kateryna DOROGAN

Industrial Risk Management Department, EDF R&D, 78401 Chatou Cedex, FRANCE

E-mail: kateryna.dorogan@edf.fr

ABSTRACT

This paper deals with the modelling of steel melting process during TIG welding operations on the nuclear power plants. The issue of the quality assurance of welding operations on some components is of great importance for the nuclear safety management. However, there are many parameters involved in the process which makes the uncertainty of the whole operation important. Moreover, some repair operations make impossible the quality control of the final weld bead. This is the case of one such a weld this study focus on. A way to ensure the quality of such weld beads could be based on the weld pool shape prediction by the numerical simulation. Thus, giving the operating parameters such as arc energy distribution, the flow simulation inside the weld pool could provide the information on the final weld pool dimensions.

The model describing the metal flow during the welding process developed in this work is based on the classical MHD and the enthalpy equations. Yet, the flow in the weld pool is mainly governed by variable surface tension force, the phenomenon known as Marangoni effect. The surface tension variation is in this case highly dependent on the thermal and the surfactant concentration gradients. In order to better evaluate this force, in this work, we present a new formulation of transport-reaction equations for surfactant and relative species in the molten steel. Moreover, this model takes into account species chemical reaction and evaporation. This allows mass fractions and gradients computation at the weld pool surface, and by this mean a better prediction of the surface tension force in case of variable chemical composition. The results of the simulations are compared to experimental data on the weld pool dimensions.

Keywords: Surfactants and interface, CFD, Free surface flow, MHD, Casting and solidification .

NOMENCLATURE

Greek Symbols

β	Thermal expansion coefficient, $[1/K]$
Γ_s	Excess of S concentration in solute, $[kg\cdot mol/m^2]$
γ	Surface tension force, $[N/m]$
γ_m^0	Surface tension of a pure metal at T_f , $[N/m]$
ε	Emissivity of the weld pool surface, $[1]$
η	Yield of the TIG process, $[1]$
λ	Thermal conductivity, $[W/m\cdot K]$
μ	Dynamic viscosity, $[kg/ms]$
μ_0	Vacuum permeability, $[V\cdot s/A\cdot m]$
ρ	Mass density, $[kg/m^3]$

ρ_{ref}	Density of the steel at the liquidus temperature, $[kg/m^3]$
σ	Electrical conductivity, $[Ohm\cdot m]$
σ_{SB}	Stefan-Boltzmann constant, $[W/m^2\cdot K^4]$

Latin Symbols

A	Magnetic potential, $[V\cdot s/m]$
\bar{A}	Thermal surface tension gradient for a pure material, $[N/(m\cdot K)]$
a_s	Sulfur activity, $[1]$
B	Magnetic field, $[T]$
C_p	Specific heat, $[J/K]$
c	Vector of mass concentrations, $[kg/m^3]$
c_s	Sulfur mass concentration, $[kg/m^3]$
D_j^i	Diffusion coefficient of species i in solute j , $[m^2/s]$
D_0^i	Frequency factor for species i , $[m^2/s]$
E	Electric field, $[V]$
F_b	Buoyancy, $[Pa/m]$
f_l	Liquid fraction, $[1]$
g	Gravity, $[m/s^2]$
H	Total enthalpy, $[J]$
ΔH	Heat of adsorption, $[J/(kg\cdot mol)]$
ΔH_s^{Cr}	Partial molar enthalpy of Cr-S interaction, $[J]$
h	Specific enthalpy, $[J/kg]$
\tilde{h}	Convective exchange coefficient, $[W/m^2\cdot K]$
I	Current intensity, $[A]$
j	Current density, $[A/m^2]$
k	Segregation entropy factor, $[1]$
n	Outward normal vector, $[m]$
P_R	Electric potential, $[V]$
p	Pressure, $[Pa]$
Q^i	Activation energy for i -species, $[J/mol]$
R	Gas constant, $[J/mol\cdot K]$
r	Distance from heat source, $[m]$
r_H	Heat source dispersion, $[m]$
r_J	Current source dispersion, $[m]$
S_R^u	Carman-Kozeny term, $[Pa/m]$
T	Temperature, $[K]$
T_f	Melting point, $[K]$
T_l	Liquidus temperature, $[K]$
T_{ref}	Reference temperature, $[K]$
T_s	Solidus temperature, $[K]$
T_0	Ambient temperature, $[K]$
t	time, $[s]$
U	Current tension, $[V]$
u	Fluid velocity, $[m/s]$
v	Welding torch speed, $[m/s]$

\mathbf{x} Space coordinates vector, [m]
 Y_i i-species mass fraction, [1]

Sub/superscripts

Cr Chromium
Fe Iron
Mn Manganese
S Sulfur

INTRODUCTION

This paper is aimed at proposing a new modelling of reacting metal flow formed in the weld pool during Tungsten Inert Gas (TIG) welding operations. Welding being one of the most used repair processes in nuclear engineering, the quality assessment of weld beads appears to be one of the important issues both from nuclear safety and industrial costs points of view. For instance, we are interested in reproducing numerically one such a weld found on French nuclear power plants. This weld appears to be difficult to control and reproduce experimentally due to local variations in chemical composition of welded materials. Moreover, the process make impossible the weld quality control upside down the pieces so that some internal defects could remain unrevealed. Till today, several experimental studies were made in order to understand and reproduce the most critical of those, but these attempts have been mostly unsuccessful.

An alternative approach to tackle this problem could be based on the weld pool shape predictions using numerical simulation tools. The model the most widely used to predict the flow pattern in the weld pool is based on the unsteady MHD equations taking into account the Marangoni effect which consists in modelling the surface tension force as a function of temperature and of surfactant concentration on the weld pool surface (Belton, 1976; Heiple and Roper, 1982; Sahoo *et al.*, 1988; McNallan and DebRoy, 1991; Mills *et al.*, 1998; Sampath and Zabaras, 2001).

However, these simulations were only successful in the case of constant chemical composition. In fact, in most practical situations, when two or more different materials are welded, the local variation of the surfactant content causes the modification of the flow characteristics, and an important difference on the weld pool shape may appear. This is for instance the case for sulfur which is known to modify the surface tension of the molten steel. It was found that the surface tension variation with the temperature is non monotonous and highly dependent on the sulfur concentration and its gradient. Moreover, the sulfur concentration in the liquid steel varies with the time and with the temperature since sulfur may create solid inclusions with manganese. Therefore, an accurate evaluation of species mass fractions in the unsteady metal flow is essential for the correct prediction of the surface tension force in these situations.

Thus, this paper presents the new transport-reaction equations of surfactant and relative species in the molten steel together with the MHD and the enthalpy equations describing the flow in the weld pool. It takes into account sulfur and manganese reversible chemical reaction and manganese evaporation.

WELD POOL MODEL DESCRIPTION

Geometry and Mesh

We deal with two fitted steel plates each of size $80 \times 40 \text{ mm}^2$ and of thickness 2 mm put together, thus forming the whole domain of dimensions $80 \text{ mm} \times 80 \text{ mm} \times 2 \text{ mm}$, Fig. 1. In the figure, the red line shows the separation between pieces by the plane $y = 0$.

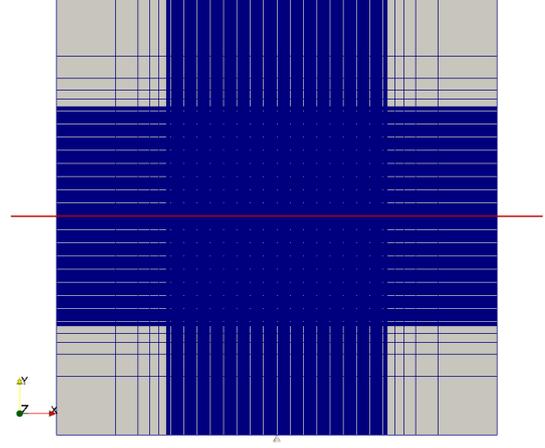


Figure 1: Geometry and mesh of the domain, 2d-cut.

The mesh shown in Fig. 1 is orthogonal and composed of 1.4×10^6 cells with the size of $1.25 \times 10^{-4} \text{ m}$ in the finest central square region of size $40 \times 40 \text{ mm}^2$.

Magnetohydrodynamics equations

The model is a system of incompressible Navier-Stokes and Maxwell equations. For $\mathbf{x} \in \mathbb{R}^3$, $t > 0$ and the state vector $(\mathbf{u}, p, h, P_R, \mathbf{A})^t(\mathbf{x}, t)$ we solve numerically :

Mass continuity equation :

$$\nabla(\rho \mathbf{u}) = 0, \quad (1)$$

Momentum conservation :

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla(\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \mu \Delta \mathbf{u} + \mathbf{j} \times \mathbf{B} + \mathbf{F}_b + \mathbf{S}_R''', \quad (2)$$

Specific enthalpy conservation :

$$\frac{\partial(\rho h)}{\partial t} + \nabla(\rho \mathbf{u} h) = \nabla \left(\frac{\lambda}{C_p} \nabla h \right) + \mathbf{j} \cdot \mathbf{E}, \quad (3)$$

Charge continuity equation :

$$\nabla(\sigma \nabla P_R) = 0, \quad (4)$$

Ampere's circuital law :

$$\Delta \mathbf{A} = -\mu_0 \mathbf{j}, \quad (5)$$

with initial and boundary conditions detailed below. In (1)-(5), \mathbf{u} denotes the fluid velocity, p the total pressure, h the specific enthalpy, P_R the real part of the scalar electric potential and \mathbf{A} the vector magnetic potential. The thermodynamical properties of material are the density ρ , the dynamic viscosity μ , the specific heat C_p , the thermal conductivity λ and the electric conductivity σ , all varying as functions of the temperature (Kim, 1975).

The source terms in the momentum equation (2) correspond to the Laplace forces (expressed via the current density \mathbf{j}

and the magnetic field \mathbf{B}), the buoyancy \mathbf{F}_b and the Carman-Kozeny term describing the velocity relaxation in the porous media during the liquid-solid transition \mathbf{S}_R^u (Kozeny, 1927; Carman, 1956). The buoyancy is expressed using Boussinesq approximation:

$$\mathbf{F}_b = \rho_{ref} [1 - \beta(T)(T - T_{ref})] \mathbf{g}, \quad (6)$$

with β the thermal expansion coefficient, T_{ref} the liquidus temperature of the steel, ρ_{ref} the density of the steel at T_{ref} and \mathbf{g} the gravity. In the enthalpy conservation equation (3), the rhs term $\mathbf{j} \cdot \mathbf{E}$ represents the Joule effect, \mathbf{E} denoting the electric field.

The form of equations (4), (5) is based on two assumptions: the fluid is supposed electrically neutral; the electric and magnetic fields are quasi stationary. Using the simplified Ohm's law: $\mathbf{j} = \sigma \mathbf{E}$, the system (1)-(5) is completed by the following relations:

$$\begin{aligned} \mathbf{E} &= -\nabla P_R, \\ \mathbf{B} &= \text{rot } \mathbf{A}. \end{aligned} \quad (7)$$

Initial conditions

We fix the initial difference of the electric potential between the electrodes $U = 11 \text{ V}$ as well as the current intensity $I = 135 \text{ A}$, thus giving the initial values to P_R and \mathbf{A} . At $t = 0$, we consider the workpiece in a solid state at ambient temperature $T_0 = 300 \text{ K}$, and atmospheric pressure, $p_0 = 101325 \text{ Pa}$. Then, the corresponding values of other properties for these values of pressure and temperature are: $\rho_0 = 7500 \text{ kg/m}^3$, $C_{p,0} = 602 \text{ J K}^{-1} \text{ kg}^{-1}$ et $\mathbf{u}_0 = \mathbf{0}$.

Boundary conditions

The boundary conditions will be only detailed for the top (heated) surface of the plates. On the other boundary faces the default wall boundary conditions are fixed. Moreover, in practice there is no mass or momentum flux on these sides since they remain always in solid state.

- *Pressure:* $\partial P / \partial n = 0$.
- *Velocity:* We fix $\mathbf{u} \cdot \mathbf{n} = 0$ and add a flux related to the weld pool surface tension variation, the surface tension $\gamma(\mathbf{c}, T)$ being a function of the temperature T and of the chemical concentration of species composing the steel \mathbf{c} (Belton, 1976):

$$\mu \frac{\partial \mathbf{u}}{\partial n} = f_l \cdot \sum_i \frac{\partial \gamma(\mathbf{c}, T)}{\partial c_i} \cdot \nabla c_i + f_l \cdot \frac{\partial \gamma(\mathbf{c}, T)}{\partial T} \cdot \nabla T. \quad (8)$$

with the liquid fraction f_l , defined as follows:

$$f_l = \begin{cases} 1, & T > T_l, \\ (T - T_s) / (T_l - T_s), & T_s \leq T \leq T_l, \\ 0, & T < T_s. \end{cases} \quad (9)$$

Among several surface active species which may be found in the steel during melting, sulfur is one that may be beforehand quantified since it is introduced in the steel during steel making process. It is also known to modify to a great extent the surface tension of binary Fe-S alloys (Heiple and Roper, 1982).

The most general expression of the surface tension force of the liquid metal containing surface active inclusions

(for instance, sulfur) and varying with temperature is given by (Belton, 1976; Heiple and Roper, 1982; Sahoo *et al.*, 1988):

$$\gamma(c_s, T) = \gamma_m^0 - \tilde{A}(T - T_m) - RT \Gamma_s \ln[1 + Ka_s], \quad [N/m] \quad (10)$$

with

$$K = ke^{-\Delta H/RT}, \quad (11)$$

and with γ_m^0 the surface tension of a pure metal at T_f (with no inclusions), \tilde{A} the opposite of $\partial \gamma(c_s, T) / \partial T$ for a pure material (without surface active inclusions), Γ_s the excess of sulfur concentration in solute, R the gas constant, k the segregation entropy, ΔH the heat of adsorption and a_s the sulfur activity.

Then, considering a more recent work (McNallan and DebRoy, 1991) which takes into account S-Cr interaction in liquid steel, the expression of the surface tension gradients induced by temperature and by sulfur concentration are written in the following form:

$$\begin{aligned} \frac{\partial \gamma(c_s, T)}{\partial T} &= -A - RT \Gamma_s \left[\ln(1 + Ka_s) + \frac{Ka_s}{1 + Ka_s} \frac{\Delta H - \Delta H_s^{\text{Cr}}}{RT} \right], \\ \frac{\partial \gamma(c_s, T)}{\partial c_s} &= -\frac{RTK\Gamma_s}{1 + Ka_s} \end{aligned} \quad (12)$$

with

$$a_s = 10^{e_s^{\text{Cr}} [\text{pct Cr}]} \cdot [\text{pct S}], \quad (13)$$

$$e_s^{\text{Cr}} = -94.2/T + 0.0396 \quad (14)$$

and with ΔH_s^{Cr} the partial molar enthalpy of Cr-S interaction in solute:

$$\Delta H_s^{\text{Cr}} = -94.2R[\text{pct Cr}] \ln 10. \quad (15)$$

Expression (8) describes the phenomenon known as the *Marangoni effect* which consists in the mass transfer along an interface between two fluids due to surface tension gradient. The latter is one of the most important forces acting in the weld pool.

- *Enthalpy:* The enthalpy flux fixed on the top surface is composed of the Gaussian-distributed heat source, radiative and convective heat exchange contributions moving with the torch speed in the x -direction:

$$\frac{\lambda}{C_p} \frac{\partial h}{\partial n} = \frac{\eta UI}{2\pi r_H^2} \exp\left(-\frac{r^2}{2r_H^2}\right) + \varepsilon \sigma_{SB}(T^4 - T_0^4) + h(T - T_0), \quad (16)$$

with r_H the heat source dispersion, I the current intensity, U the current tension, η the yield of the process, $\sigma_{SB} = 5.67 \times 10^{-8} \text{ W m}^{-2} \text{ K}^{-4}$ the Stefan-Boltzmann constant, $\varepsilon = 0.5$ the emissivity of the weld pool surface, $T_0 = 300 \text{ K}$ the ambient temperature and $h = 15 \text{ W m}^{-2} \text{ K}^{-1}$ the convective exchange coefficient.

- *Scalar electric potential and vector magnetic potential:*

$$\begin{aligned} \sigma \frac{\partial P_R}{\partial n} &= \frac{I}{2\pi r_j^2} \exp\left(-\frac{r^2}{2r_j^2}\right), \\ \frac{1}{\mu_0} \frac{\partial \mathbf{A}}{\partial n} &= 0. \end{aligned} \quad (17)$$

For the sake of simplicity, we assume the current source dispersion $r_j = r_H$.

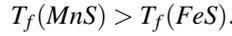
Species transport-reaction equations

Since the surface tension gradients (12) are highly dependent on the sulfur concentration in the weld pool, it is essential to know the sulfur concentration at each time and position in the weld pool. Thus, in this section we detail the transport-reaction equations of the surface-active and related species. For instance, it is well known that Manganese addition is used in steel making processes to capture sulfur particles in order to prevent the steel from hot cracking during manufacturing. In fact, free-state sulfur atoms induce steel liquefaction by forming liquid inclusions with Fe :



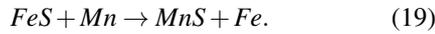
which are characterized by an extremely low melting point: $T_f(FeS) = 1261 K$, thus reducing the melting point of the steel alloy. This may result in hot cracking defects.

To overcome this problem, desulfurization agents such as Manganese (Mn) are added in the steel during melting which allows the liquid inclusions FeS to be replaced by solid inclusions MnS with a higher melting point, $T_f(MnS) = 1893 K$:



Therefore, in the present work, we are interested in modelling the following species-related phenomena:

- The sulfur content in the steel is limited to 0.03% weighted percent, and the Manganese content to 2%.
- **The chemical reaction** between sulfur in solute and Manganese to form MnS takes place during cooling at $T_{reac} = 1853 K$:



Since this reaction takes place at the temperature below the MnS melting point, it results in solid inclusions in liquid steel. These inclusions are created in the region with the appropriate temperature level and especially during the solidification.

- **Manganese evaporation** which takes place at temperatures $T > 2000K$ depending on the saturation pressure and boiling temperature (Pischke, 1994).
- **Diffusion coefficients of species** dependent on the chemical composition of the steel are rather difficult to determine at high temperatures. They are generally expressed as:

$$D_{304L}^i(T) = D_0^i e^{(-Q^i/RT)} \quad [m^2/s], \quad (20)$$

with D_0^i the frequency factor and Q^i activation energy. Following some references (Potard, 1972; Chybanova, 2000), we found the following expressions of these coefficients for sulfur and Manganese:

$$\begin{aligned} D_0^S &= 2.33 \times 10^{-7} m^2/s \quad \text{et} \quad Q^S = 52200 J/mol, \\ D_0^{Mn} &= 3.85 \times 10^{-7} m^2/s \quad \text{et} \quad Q^{Mn} = 69500 J/mol. \end{aligned} \quad (21)$$

- **Thermophoresis (Soret effect)**. Considering Lewis number which gives the rate of the thermal diffusion to the mass diffusion is high enough, $Le(T) \approx 10^2$ as well

as Prandtl number which gives the rate of the momentum diffusivity to the thermal diffusivity, $Pr(T) \approx 0.05$, it seems that the thermophoresis is an important phenomenon to be taken into account. It mainly depends on the thermal gradient referred to the domain size. However, the definition of the thermo diffusion coefficient in the liquid metal seems quite complicated, since most of ten found expressions are based on gas theory and never for high temperature liquid (Talbot *et al.*, 1980; Alam *et al.*, 2009).

In generalized form, the transport-reaction equation of Y_i species (S, Mn) is written :

$$\begin{aligned} \partial_t(\rho Y_i) + \nabla(\rho \mathbf{u} Y_i) - \nabla \cdot \left(\rho \mathbf{D}_{304L}^{Y_i} \nabla Y_i \right) &= \nabla \cdot \left[\left(\mathbf{D}_{th}^{Y_i} \frac{\nabla T}{T} \right) \rho Y_i \right] \\ &- K(T) \rho Y_i Y_j + S_{evap}^{Y_i}, \quad \text{with} \quad K = K_0 e^{(-\frac{E_a}{RT})} \end{aligned} \quad (22)$$

with Y_i the i -species mass fraction, $Y_i \in [0, 1]$, $\mathbf{D}_{304L}^{Y_i}$ the mass diffusion coefficient of the i -species in the alloy (20), $\mathbf{D}_{th}^{Y_i}$ the thermophoretic diffusion coefficient of the i -species, $K(T)$ the rate constant for a bimolecular phase reaction, $S_{evap}^{Y_i}$ evaporation source term involved in Mn equation only. Moreover, we note that the MnS chemical reaction takes place at $T = 1853 K$. Then, the enthalpy equation in (1)-(5) is modified to take into account these contributions: the concentration gradients, the latent heat of evaporation and chemical reaction contribution (though, in this case MnS reaction is isothermal).

Equations (22) together with system (1)-(5), (7) with initial and boundary conditions described in the previous section allow a more physical modelling of the surface tension variations (8) in the case of important thermal and concentration gradients.

RESULTS

The simulations were performed with *Code_Saturne* open source CFD software developed by EDF (Archambeau *et al.*, 2004). It is devoted to unsteady single phase simulations with complex reactive physics, turbulence and scalar transport. It is mainly based on the pressure correction algorithm and uses the finite volume numerical schemes. For more detailed presentation, the reader is referred to the technical documentation available online, <http://code-saturne.org>.

Given the welding parameters :

- the initial difference of the electric potential $U = 11 V$,
- the current intensity $I = 135 A$,
- the welding torch speed $v = 16.3 cm/min$,

as well as the geometry and the mesh described in ‘‘Geometry and Mesh’’ section (Fig. 1) with the cell size of $1.25 \times 10^{-4} m$ and the time step $\Delta t = 10^{-3} s$, we present here some results coming from weld pool simulations of a practical welding operation used as a validation test case. The pieces to be welded include a discontinuity of the chemical composition which corresponds for instance to an initial discontinuity in sulfur content as shown in Fig. 2, 3 with Low sulfur content of 0.0008 wt% (blue) and

High sulfur content of 0.005 wt% (red). In this example, High sulfur material represents the filler metal often used in welding operations to improve the weld pool penetration.

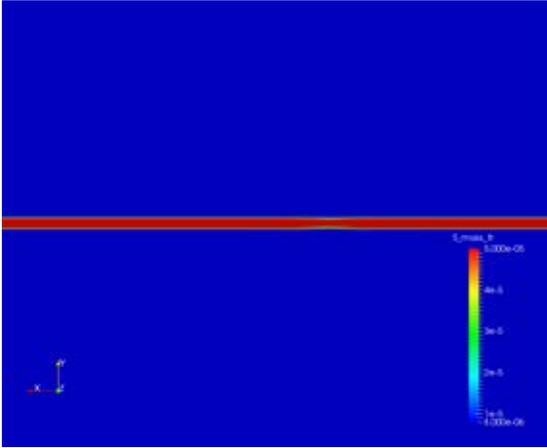


Figure 2: The sulfur mass fraction presenting a discontinuity (the filler metal) at $t = 0$ s, top surface view, $z = 0.002$.



Figure 3: The sulfur mass fraction presenting a discontinuity (the filler metal) at $t = 0$ s, $x = 0$ cut.

The results presented in Fig.4 - Fig.9 show the velocity, pressure, temperature and surface tension gradient wrt the temperature approximations as well as the spatial distribution of the sulfur mass fraction in the weld pool at the stationary state. We can see that the negative values of the surface tension gradient wrt the temperature imply the outward fluid velocities on the top surface which result in more spreading weld pool.

We've also performed a sensitivity analysis of the results on the mean sulfur content in the weld pool. It appeared that the external weld pool width is decreasing with a growing sulfur concentration and that at the same time, the internal width is increasing for the sulfur content above 0.006 wt%. This is a quite relevant conclusion which reflects the correct treatment of the surface tension variation with sulfur content. In fact, the surface tension force on the weld pool surface is known to decrease with an increasing sulfur concentration. Moreover, the surface tension gradient wrt the temperature changes the sign when the sulfur concentration exceeds 0.005 wt%. Thus, the flow direction in the weld pool turns opposite : we expect to have a more penetrating weld pool for high sulfur concentration versus a more spreading one for low sulfur content (Heiple and Roper, 1982; McNallan and DebRoy, 1991).

Then, Figures 10 and 11 show the final weld pool shape in a stationary state whose dimensions (external and internal widths) are highly dependent on the initial sulfur content. We compare these dimensions with the experimental data provided by operating company for a welding operation performed in the same operating conditions. We note that

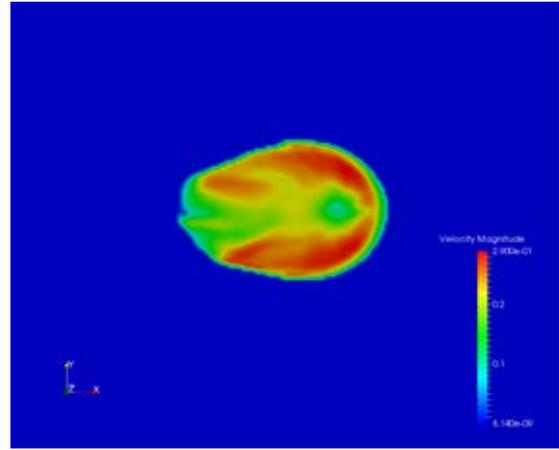


Figure 4: The fluid velocity in the stationary regime, top surface view with $z = 0.002$.

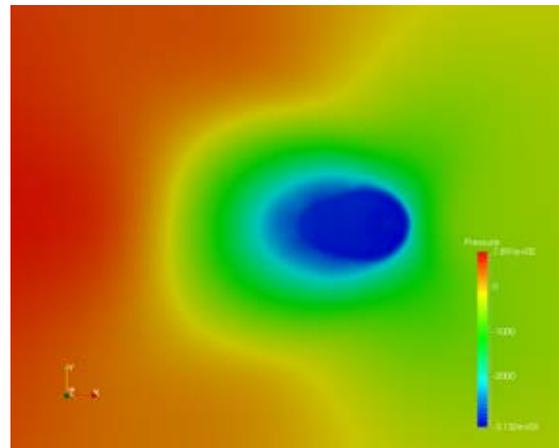


Figure 5: The pressure approximation in the stationary regime, top surface view with $z = 0.002$.

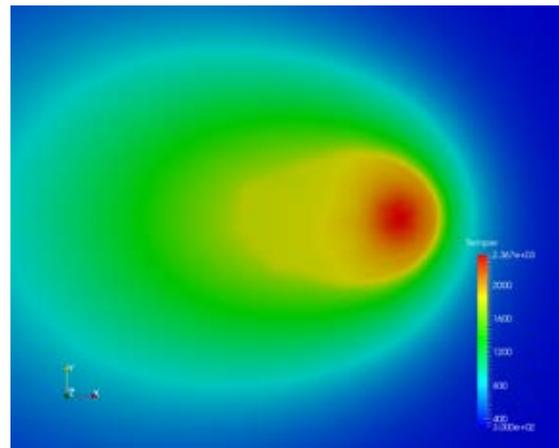


Figure 6: The temperature approximation in the stationary regime, top surface view with $z = 0.002$.

the data on the weld pool dimensions obtained in this case are in quite good agreement (Table1).

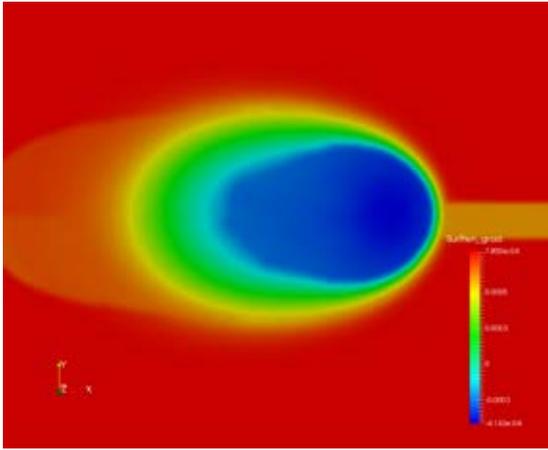


Figure 7: The surface tension gradient induced by temperature in the stationary regime, top surface view with $z = 0.002$.

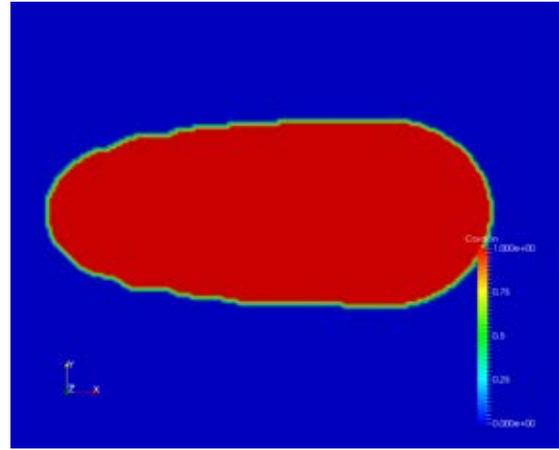


Figure 10: Final weld bead shape, top surface view with $z = 0.002$.

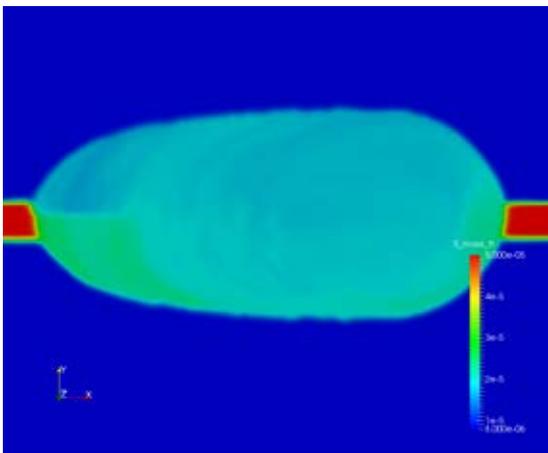


Figure 8: The sulfur mass fraction in the stationary regime, top surface view with $z = 0.002$.



Figure 11: Final weld bead shape, $x = 0.005$ cut.

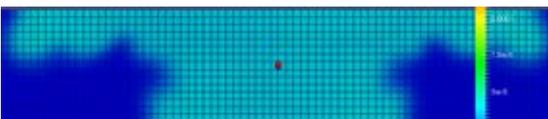


Figure 9: The sulfur mass fraction in the stationary regime, $x = 0.005$ cut.

Table 1: Comparison of weld pool dimensions

	Simulation	Measurement
External width (mm)	8.4	8.2
Internal width (mm)	4.26	4.5

CONCLUSION

Based on a practical case of a welding operation, we have introduced in this paper a new transport - reaction equations for surface active and related species which are involved in the surface tension modelling when studying welding and metal melting processes. This modelling is new and offers a tool for the unsteady quantification of the sulfur content in the molten steel all along the welding operation and the solidification. It takes into account sulfur and manganese chemical reaction, temperature dependent mass diffusion, manganese evaporation and thermophoresis. Moreover, the surface ten-

sion law accounts for sulfur and chromium interaction, which influences the sulfur surface activity. Some sensitivity analysis has also been made to study the global effect of the sulfur content on the weld pool dimensions. The numerical results obtained with these simulations are in good agreement with the experimental data, the conclusion which allows to validate both the modelling and the numerical approach for the present case.

REFERENCES

- ALAM, M., RAHMAN, M. and SATTAR, M. (2009). "Transient magnetohydrodynamic free convective heat and mass transfer flow with thermophoresis past a radiate inclined permeable plate in the presence of variable chemical reaction and temperature dependent viscosity". *Nonlinear Analysis: Modelling and Control*, **14(1)**, 3–20.
- ARCHAMBEAU, F., MECHITOUA, N. and SAKIZ, M. (2004). "Code_saturne: a finite volume code for the computation of turbulent incompressible flows". *Int. J. Finite Volumes*, **1**, 1–62.
- BELTON, G. (1976). *Metall.Trans. B*, **7B**, 35–42.
- CARMAN, P. (1956). *Flow of gases through porous media*. Butterworths, London ed.
- CHYBANOVA, L. (2000). *Proprietes physico-chimiques des metaux liquides contenant des sulfures et des oxydes et la cinetique des echanges a la limite avec les materiaux de construction*. Ph.D. thesis, Oural Technical University.
- HEIPLE, C. and ROPER, R. (1982). "Mechanism for minor element effect on gta fusion zone geometry". *Weld. J.*, **61(4)**.
- KIM, C.S. (1975). "Thermophysical properties of stainless steels". *Argonne National Laboratory*.
- KOZENY, J. (1927). "Ueber kapillare leitung des wassers im boden". *Sitzungsber Akad. Wiss., Wien*, **136(2a)**, 271–306.
- MCNALLAN, M. and DEBROY, T. (1991). "Effect of temperature and composition on surface tension in fe-ni-cr

alloys containing sulfur". *Metallurgical Transactions*, **22B**, 551–560.

MILLS, K., KEENE, B., BROOKS, R. and SHIRALI, A. (1998). "Marangoni effects in welding". *Phil. Trans. R. Soc. Lond.*, **356**, 911–925.

POTARD, C. (1972). *Contribution a l'etude de la diffusion dans les alliages liquides ternaires. Application a la solidification*. Ph.D. thesis, Grenoble.

SAHOO, P., DEBROY, T. and MCNALLAN, M.J. (1988). "Surface tension of binary metals - surface active solute systems under conditions relevant to welding metallurgy". *Metallurgical Transactions*, **19B(483)**.

SAMPATH, R. and ZABARAS, N. (2001). "Numerical study of convection in the directional solidification of a binary alloy driven by the combined action of buoyancy, surface tension, and electromagnetic forces". *Journal of Computational Physics*, **168**, 384–411.

TALBOT, L., CHENG, R., SCHEFER, A. and WILLS, D. (1980). "Thermophoresis of particles in a heated boundary layer". *J. Fluid Mech.*, **101**, 737–758.