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Marangoni driven turbulence in high energy surface melting processes

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ABSTRACT

Experimental observations of high-energy surface melting processes, such as laser welding, have revealed unsteady, often violent, motion of the free surface of the melt pool. Surprisingly, no similar observations have been reported in numerical simulation studies of such flows. Moreover, the published simulation results fail to predict the post-solidification pool shape without adapting non-physical values for input parameters, suggesting the neglect of significant physics in the models employed. The experimentally observed violent flow surface instabilities, scaling analyses for the occurrence of turbulence in Marangoni driven flows, and the fact that in simulations transport coefficients generally have to be increased by an order of magnitude to match experimentally observed pool shapes, suggest the common assumption of laminar flow in the pool may not hold, and that the flow is actually turbulent. Here, we use direct numerical simulations (DNS) to investigate the role of turbulence in laser melting of a steel alloy with surface active elements. Our results reveal the presence of two competing vortices driven by thermocapillary forces towards a local surface tension maximum. The jet away from this location at the free surface, separating the two vortices, is found to be unstable and highly oscillatory, indeed leading to turbulence-like flow in the pool. The resulting additional heat transport, however, is insufficient to account for the observed differences in pool shapes between experiment and simulations.

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1. Introduction

A long-standing question in the modeling of weld pool hydrodynamics is the one of the possible occurrence of turbulence and its influence on heat and momentum transfer. The underlying problem is that no welding model seems to exhibit true predictive capabilities, not even with respect to such a simple overall weld pool property as its post-solidification shape. Rather, all simulations require the adaptation of unphysical input parameters and/or material properties to truthfully reproduce experimental results. For instance, Winkler et al. [1] and Pavlyk and Dilthey [2] tune the heat input characteristics as well as the concentration of surface active species to obtain results matching experiments. More commonly, many authors (e.g. Refs. [2–8]) resort to the modification (i.e. enhancement) of transport coefficients, specifically thermal conductivity and viscosity, to match experimental results. No guideline has been established on how to modify the transport properties and generally they are tuned on an ad-hoc basis without any physical reasoning and a priori dependence on weld pool properties. For example, Pitscheneder et al. [7] enhance the molecular thermal conductivity and dynamic viscosity by a constant factor 7 to match experiments, Anderson et al. [3] increase only the viscosity by a constant factor 30, Mishra et al. [9] increase only the thermal conductivity by a factor 4, De and DebRoy [4] propose an optimization algorithm to determine the best values for thermal conductivity and viscosity with multiplication factors up to 17. Even when uncertainties in boundary conditions, e.g. heat transfer efficiency and energy distribution, are minimal, such as in the conduction-mode (i.e. with negligible vaporization) laser welding experiments conducted by Pitscheneder et al. [7], enhanced transport coefficients are required to match experimental weld shapes, strongly suggesting that the published weld pool models lack the inclusion of significant physics.

Furthermore, previously published computational studies fail to report oscillations and non-axisymmetric flow patterns at the liquid surface, such as have been observed in experiments for

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Nomenclature

A	aspect ratio
c_p	heat capacity
$\frac{D}{Dt}$	material derivative
D_c	characteristic length scale (pool depth)
$\mathbf{F}_{damp}$	momentum sink term due to solidification
g	volume fraction of solid
h_f	latent heat of fusion
k	turbulent kinetic energy
L_c	characteristic length scale (pool radius)
L_K	Kolmogorov length scale
P	laser power
p	pressure
r_q	laser beam radius
S_{latent}	latent heat source term
T	temperature
t	time
t_K	Kolmogorov time scale
T_s, T_l	solidus and liquidus temperature
$\mathbf{u}$	fluid velocity
U_c	characteristic velocity
$\bar{\mathbf{u}}$	mean velocity
u'	velocity fluctuation

Greek symbols

ε	turbulent kinetic energy dissipation rate
η	laser absorptivity
γ	surface tension
λ	thermal conductivity
μ	dynamic viscosity
ν	kinematic viscosity
ω	vorticity
ρ	density

Subscripts

n	normal direction
t	tangential direction

conduction-mode laser and autogeneous gas tungsten arc welds. Kraus [10] observes that “weld pool surface temperature profiles do not reach quasi-steady-state conditions, but rather vary around some time-averaged or mean values”. Zehr [11] reports that “high speed video images of the melt pool seem to reveal substantial oscillations of the free surface as the laser interacts with the workpiece”. Finally, Zhao et al. show highly unstable flow with multiple flow cells using surface particle-image-velocimetry of a gas-tungsten arc-weld [12,13].

A few hypotheses as to how to account for lacking physics, and thus improve the prediction of weld pool models, have been proposed and tested by other authors. One identified deficiency is the common comparison of post-solidification weld pool shapes with numerical simulation results not including the solidification stage. Ehlen et al. [14] and Saldi et al. [15] have determined that the weld pool shape can significantly change during this last stage of a welding process. Unfortunately, while the inclusion of the solidification stage can improve the predictions in some situations, it still does not ensure predictive capabilities [15].

Another possible source of error may be attributed to the often neglected motion of the liquid–gas interface. Simulations conducted by Ha and Kim [16] based on Pitscheneder's laser welding experiments [7] however show a very limited influence of a deformable free surface on the weld pool shape. The same conclusion has been made by Zehr [11] based on 3D simulations of conduction-mode laser welding.

Winkler et al. [1] have proposed the lack of surface chemistry and surface mass transfer processes in published models, resulting in a homogeneous distribution of surface active elements such as sulfur in the pool and at its surface, as potential source of the discrepancy. The group was able to improve their predictions using a mass transport model for a surface active element [17], and even more so when taking into account the effect of multiple surfactants [18].[1] However, even though their results using a laminar flow assumption are promising, they do conclude that there is a need to address the question of turbulent flow in weld pools. This conclusion is reinforced by the previously mentioned experimental observations of flow instabilities which are not seen in the simulations by Winkler et al. even when including the effects of surfactant redistribution.

Although sometimes done without explicit justification (e.g. He et al. [20], Roy et al. [21]), the hypothesized occurrence of turbulence has been a natural reasoning for many authors (e.g. Anderson et al. [3], Choo and Szekely [22]) to justify increasing transport coefficients, which given turbulent flow would occur naturally due to turbulent diffusion. A few authors have attempted to replace the tuning of transport properties by the use of turbulence models such as RANS [23–36] or LES [37]. While this leads to improved agreement with experiments (as does any increase of transport coefficients), the use of particularly RANS turbulence models developed for aerodynamics in complexly shaped, Marangoni driven weld pool flows with a free surface and non-smooth solid–liquid interface, is questionable. In fact, Pavlyk and Dilthey [2] conclude their numerical study of a gas-tungsten-arc weld with the statement “that neither an increase of the transport coefficients by a constant factor nor an application of the k-ε model improved the correspondence between the predicted and actual weld pool shapes”, and support further investigation of the role of turbulence in such flows.

To analyze the possible role of turbulence, Chakraborty and Chakraborty [38] have presented a scaling analysis for high energy surface melting processes such as the laser welding process of interest here. The analysis allows the estimation of the flow regime based on three dimensionless numbers: *(i)* the melt pool depth-to-radius aspect ratio $A = D/L$, *(ii)* the Prandtl number Pr and *(iii)* a dimensionless number N inversely proportional to the Marangoni number Ma, $N = (\mu/(\rho|\partial\gamma/\partial T|\eta P/(\mu\pi\lambda)))^{1/3}$

For the Pitscheneder experiment (see Table 1 for material properties) at a welding power of 5200 W and a sulfur concentration of 150 ppm, the values of those dimensionless numbers are $A \approx 1.5$, $Pr = 0.178$ and $N \approx 0.01$. According to the analysis by Chakraborty and Chakraborty [38], the onset of turbulence is expected for $2A^{2/3}N^{-2} \geq \mathscr{O}(Re_{crit})$, where Re_{crit} is estimated from experiments to be around 600 [38,39]. Turbulent thermal diffusion is predicted to exceed molecular thermal diffusion when

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[1] It should be noted that Winkler et al. use a value for the standard heat of absorption in disagreement with the commonly used value [19], which may have lead to fortuitous improvement of the results due to a resulting altered surface tension temperature dependency $d\gamma/dT$.

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