Computational modelling of heat and mass transfer in solidification and melting processes

General scope

In manufacturing processes such as welding, the workpiece is locally melted under the action of a localised heat source. During the melting and subsequent solidification processes, the molten pool convection plays a key role in the heat and species transport. The knowledge of heat and mass transport in molten pool is important from the perspective of thermo-solutal history of the process concerned, which ultimately determines the final microstructure of the product. As the mechanical properties of a material are highly dependent on the microstructure, the molten pool transport needs to be tuned by changing process parameters in order to obtain required product quality. Traditionally, process parameters for manufacturing processes were chosen based on empirical judgement. However with the advent of advanced techniques and process automation the need for high process efficiency is felt in all sectors of the manufacturing industry. This necessitates a thorough understanding of the physics involved in molten pool transport. Small dimensions, high temperature radiation and opacity limit the scope of experimental studies in molten pools. In these respects a numerical study can potentially provide useful insight into the molten pool transport.

Existing literature on numerical modelling of molten pool transport principally presents laminar flow models. Both experimental and theoretical studies have indicated the onset of turbulence in molten pools under the conditions of high power. For most industrially relevant arc and laser applications the molten pool transport is turbulent in nature. Theoretically, the nature of the transport in molten pool (i.e. whether laminar or turbulent) can be predicted by a stability analysis, but complexities of geometry and flow impose practical restrictions on the achievement of that goal. Even with present computational power it is not possible to carry out DNS or LES of this kind of flows. Therefore, an unsteady Reynolds Averaged Navier Stokes (RANS) simulation has been chosen to study turbulent convection in molten metal pools.

Turbulent heat and mass transfer during melting and solidification processes in manufacturing applications such as welding and laser surface alloying is studied using a suitably modified high Reynolds number k-epsilon model. Numerical simulations of the concerned processes are carried out using this model. The molten pool morphology shows considerable difference compared to the previous numerical studies based on laminar flow models.

Recently, turbulent transport modelling of molten metal pools in laser welding applications has been extended to the modelling of dissimilar metal laser welding of Copper-Nickel couple. A regime diagram also been developed for laser welding applications based on scaling arguments where regions where turbulent transport effects on momentum and heat transfer will be realised are demarcated based on scaling analysis based criteria.

It is planned that in near future LES of laser welding of dissimilar metal will be carried out and the expertise will be extended to model molten pool transport in Electron Beam Welding processes.

Relevance of this work:

This is one of the first research endeavours where turbulent transport in both melting and solidification processes is addressed successfully by using the k-epsilon model. Systematic procedure of scaling analysis of momentum, heat and mass transfer in a typical turbulent molten pool transport is proposed for the first time. With suitable choices of non-dimensional parameters, the governing equations coupled with appropriate boundary conditions are first scaled, and the relative significance of various terms appearing in them are accordingly analyzed. The analysis is then utilized to predict the orders of magnitude of some important quantities, such as the velocity scale at the top surface, velocity boundary layer thickness, temperature rise in the pool, turbulent kinetic energy, and its dissipation rate at the top surface. Using the scaling predictions, the influence of various processing parameters on the system variables can be well recognized, which enables us to obtain a deeper insight into the problem. Moreover, some of the quantities predicted from the scaling analysis can be utilized for an optimized selection of the appropriate grid spacing for full numerical simulation of the process. It is important to recognize that three-dimensional numerical simulations for molten pool transport is expensive but the
scaling analysis provides reasonably accurate results using simple algebraic expressions, which may be used to roughly estimate important quantities such as the maximum temperature in molten pool, and characteristic weld pool penetration. However for more quantitative predictions, a full-blown CFD simulation is required.

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(a) Schematic diagram of continuous laser welding of a Cu-Ni dissimilar couple; (b) Isotherms after 25ms of laser heating at the top surface using turbulence modelling (k-epsilon); (c) Contours of Cu mass fraction after 25ms of laser heating at the top surface using turbulence modelling (k-epsilon); (d) Comparison between laminar and turbulent simulation predictions and the corresponding experimental results for Ni mass fraction distribution along the width of the weld pool in the molten state after 25ms of laser heating and in the solidified state after 7ms of cooling following 25ms of laser heating (The distance in the abscissa is normalised with respect to the pool width). In moving co-ordinate system the co-ordinate of the laser torch is \( x = 4 \text{mm} \), and \( z = 4 \text{mm} \). At time \( t = 0s \ z = 4.0 \text{mm} \) indicates the separation line between Cu and Ni workpieces. The results are shown for a laser power of 3.5kW, laser scanning speed of 8mm/s, laser torch radius of 0.5mm and an absorption efficiency of 12%.**