1. Introduction

In SLM, similar to laser welding, if the melting mode is keyhole, due to extremely high energy density, metal vaporizes and plasma is formed. The formation of vapour cavity substantially increases the beam absorption enabling the laser to penetrate deeper resulting in melt pools that are deeper and narrow [1,2]. Also, if the energy density is very high then recovery of the collapsed deep keyhole will not be achieved leading to formation of spherical porosity. The collapse of the cavity can leave voids in the propagation path of the laser beam. Although there are some experimental work reported about the porosity formation with increasing energy density during the SLM process [3], but its formation mechanism is not understood mathematically.

In this paper, a particle scale model is developed using open-source codes LIGGGHTS and OpenFOAM to study the porosity formation due to keyhole collapsing in the SLM process. Discrete element method is used to determine the spatial arrangement of the particles in the powder layer. Thereafter, the volume of fluid approach using the finite volume method is used to identify and track the interface of the powder particles undergoing phase transition. Subsequently, geometrical characteristics of the porosity formation obtained by computational modelling are qualitatively validated with the in-house single track experiments.
2. Numerical modelling and methodology
To understand the interaction of high energy beam with the powder layer and the resulting porosity formation, single track scanning over a powder layer is simulated with the help of a thermo-fluidic powder scale model developed using an integrated discrete element method (DEM) – computational fluid dynamics (CFD) approach. The developed thermo-fluidic powder scale model uses a realistic powder bed for CFD modelling and incorporates the physics of laser irradiation on the powder bed, melt flow due to thermo-capillary force, effect of the recoil pressure and the phase transition (melting, solidification, evaporation and condensation).

2.1. Single layer powder bed Generation
The present work uses a DEM based modelling approach to simulate the powder spreading process. DEM, a Lagrangian based approach, calculates forces acting on granular material from the initial conditions, governing physical laws and contact models. The computational domain considers each particle as an individual entity with its own properties interacting with other particles and boundaries in its vicinity. The motion of each particles is described using Newton’s law of motion for conservation of momentum. In this work, an open source DEM code LIGGGHTS (LAMMPS Improved for General Granular and Granular Heat Transfer Simulations) is being used for powder spreading. Firstly, particle size distribution (PSD) was experimentally measured by performing image analysis on the SEM (scanning electron microscopy) micrographs. Then, a cloud of randomly generated particles with the experimentally measured PSD was generated inside the DEM computational domain and allowed to fall under gravity, after all the powder particles were settled (Fig. 1). Thereafter, using a MATLAB script the particles information of 40 micron thickness was exported to an open source CFD C++ code OpenFOAM (Open field operation and manipulation). The CFD model of thermo-fluidic phenomena, presented in the following, was developed in OpenFOAM.

![Fig. 1. Discrete element method simulation results using open source code LIGGGHTS](image)

2.2. Free Surface Thermo-Fluidic Modelling
Figure 2 shows the computational domain considered for the single track thermo-fluidic simulation. The computational domain consists of an Inconel 718 substrate, an argon inert gas region and a 40 µm thick Inconel 718 powder layer. In the model, transient heat transfer and fluid flow dynamics in the melt pool are considered using the volume of fluid surface tracking method (VOF). The VOF transport equation for interface tracking between two immiscible phases (Inconel 718 and argon gas) is given by [4]
\[ \frac{\partial \gamma}{\partial t} + \nabla \cdot (\gamma \vec{U}) + \nabla \cdot ((1 - \gamma) \gamma \vec{U}_r) = 0 \]  

(1)

where \( \gamma \) is the phase fraction, \( \vec{U} \) is the velocity vector and \( \vec{U}_r \) is the compression velocity.

In the simulation, the thermo-physical properties of the two immiscible phases are calculated using the continuum formulation based on the classical mixture theory. Assuming the flow to be incompressible, laminar and Newtonian, the governing conservation equations for mass, momentum and energy conservation are formulated.

The governing energy conservation equation is given by

\[ \frac{\partial (\rho C_p T)}{\partial t} + \nabla \cdot (\rho \vec{U} C_p T) = \nabla \cdot (k \nabla T) + S_{\text{Latent}} + Q_{\text{Losses}} + Q_{\text{Laser}} \]  

(2)

The source term \( S_{\text{Latent}} \) in Eq. 2 accounts for the evolution of the latent heat during phase change. The source term \( Q_{\text{Losses}} \) in Eq. 2 represents evaporation heat loss, radiation heat loss and convective heat loss due to the flowing argon gas. It is defined as

\[ Q_{\text{Losses}} = (q''_{\text{evaporation}} + q''_{\text{radiation}} + q''_{\text{conv}}) |\nabla \gamma| \frac{2 \rho C_{\text{peff}}}{\rho_{\text{metal}} C_{\text{metal}} + \rho_{\text{gas}} C_{\text{gas}}} \]  

(3)

The evaporative heat loss is the product of the latent heat of vaporization \( L_v \) and the vaporized mass flow rate \( \dot{m}_v \).

\[ q''_{\text{evaporation}} = -L_v \dot{m}_v \]  

(4)

The vaporized mass flow rate of the escaping vapour \( \dot{m}_v \) [5] is given by:

\[ \dot{m}_v = (1 - \beta) \frac{M P_v}{\sqrt{2 \pi M R T}} \]  

(5)

where \( M \) is the molar mass, \( R \) is the ideal gas constant and \( P_v \) is the recoil vapor pressure which is given by

\[ P_v = 0.54 P_0 \exp \left[ \frac{L_v M (T - T_v)}{R T T_v} \right] \]  

(6)

where \( P_0 \) is the atmospheric pressure, \( L_v \) is the latent heat of vaporization and \( T_v \) is the vaporization temperature. \( \beta \) in Eq. 5 is the retro diffusion coefficient and it represents the extent of condensation of escaping vapour. In this study, \( \beta = 0.18 \) was assumed.

The source term \( Q_{\text{Laser}} \) in Eq. 2 accounts for heating by the moving laser beam. The energy input from the laser beam is approximated by a Gaussian distribution and is defined as
\[
Q_{\text{Laser}} = \frac{2\eta P}{\pi R_{\text{spot}}^2} \exp \left[ -2 \frac{(x-x_i - vt)^2 + (z-z_i)^2}{R_{\text{spot}}^2} \right] f_{\text{top}} |\nabla \gamma| \frac{2\rho C_{\text{peff}}}{\rho_{\text{metal}} C_{\text{metal}} + \rho_{\text{gas}} C_{\text{gas}}} \tag{7}
\]

where \(\eta\) is the absorption coefficient, \(v\) is the laser traversal velocity, \((x_i, z_i)\) denotes the beginning point of the laser melting and \(f_{\text{top}}\) is the unit function representing the top portion of the powder particle where heat flux is applied.

The momentum conservation equation is given by
\[
\frac{\partial (\rho \vec{U})}{\partial t} + \vec{V} \cdot \nabla (\rho \vec{U}) = -\nabla p + \vec{V} \cdot \left( \mu \left( \nabla \vec{U} + (\nabla \vec{U})^T \right) \right) + \vec{F}_N + \vec{F}_D + \vec{F}_S \tag{8}
\]

The buoyant force due to the natural convection is implemented in the current model with the help of a source term \(\vec{F}_N\) in Eq. (8) which is given as
\[
\vec{F}_N = \rho_l \vec{g} \beta_T (T - T_{\text{ref}}) \tag{9}
\]

where \(\rho_l, \beta_T\) and \(T_{\text{ref}}\) are the liquid metal density, thermal expansion coefficient and reference temperature, respectively. The source term \(\vec{F}_D\) appearing in Eq. (8) is defined in Eq. (10). It aids to smoothly bring down the velocity of the fluid at the liquid-solid interface and makes the fluid velocity in the un-melted solid zone as zero.

\[
\vec{F}_D = \frac{\left(1 - f_{\text{liquid,metal}}\right)^2}{f_{\text{liquid,metal}}} \frac{\gamma^2}{\gamma + b} \vec{C} \vec{U} \tag{10}
\]

The constant \(C\) in Eq. (10) represents mushy zone constant and a value of 160,000 kg m\(^{-3}\) s\(^{-1}\) is considered in the current model [6]. The term \(b\) is another constant having a small value (~10\(^{-6}\)) and is used to prevent division by zero when the liquid fraction \((f_{\text{liquid,metal}})\) becomes zero.

The source term \(\vec{F}_S\) in Eq. 8 term represents the forces which are acting at the interface and is given by
\[
\vec{F}_S = \left\{ \sigma \hat{n} + \frac{d\sigma}{dT} \left[ T \hat{n} \right] - \hat{n} \left( \frac{\nabla \rho}{|\nabla \rho|} \right) \right\} |\nabla \gamma| \frac{2\rho}{\rho_m + \rho_g} \tag{11}
\]

where \(\sigma\) is the surface tension coefficient, \(\kappa = -\left( \nabla \cdot \hat{n} \right)\) is the mean curvature of free surface, \(\hat{n} = \nabla \rho / |\nabla \rho|\) is the interface normal unit vector and \(d\sigma /dT\) is the temperature coefficient of surface tension.

The first term is the surface tension force acting normally to the interface, the second term is the force due to Marangoni convection acting tangentially at the interface and the third term is the recoil pressure exerted by the metal vapour on the top surface of the molten pool.

For thermo-fluidic CFD simulation, an element size of 4 \(\mu\)m provides mesh independent and computationally. To make sure the solution is stable, self-adaptive time step based on the Courant–Friedrichs–Lewy (CFL) condition was used. For each time step, volume fraction advection, continuity, momentum, and energy transport equations were solved. The material properties of IN718 used in this simulation is taken from Ref. 7.

### 3. Results and discussion

Single track scanning over a powder layer has been simulated for two scanning velocity \((v = 0.5 \text{ m/s and } v = 0.7 \text{ m/s})\) keeping power \((P = 100 \text{ W})\) to be the same. Fig. 3 shows the top view of the deposited single tracks at 1175 \(\mu\)s for \(v = 0.5 \text{ m/s}\). In the figure the substrate, the unmelted powder layer, and a penetrated melt pool caused by recoil pressure can be clearly seen. Due to heating by the laser beam the powder layer melts and forms a bulk melt. Once the laser beam traverses forward the bulk melt re-solidified in to bulk solid.

Figure 4 shows maps of temperature field along a cross section of the computational domain for the scanning velocity of \(v = 0.7 \text{ m/s and } v = 0.5 \text{ m/s}\) illustrating the elongated melt pool (melting and solidification). It can be clearly seen for the both cases that due to recoil pressure, a topologically
A depressed cavity starts to form. As the temperature exceeds the boiling point, recoil pressure starts to act and due to melt displacement from the centre of the melt pool, a bulge is formed. As the laser beam moves forward, the melt pool size increases and finally it reaches a quasi-steady state. It can be seen that substantial melting of the substrate has taken place. The melting in the substrate is crucial in determining surface morphology and metallurgical bonding of the solidified powder layer with the substrate. As the laser beam moves away, molten metal starts filling the depressed region.

![Solidified track and Molten pool boundary](image)

**Fig. 3.** Top view of the deposited single tracks at 1175 μs (P = 100 W, v = 0.5 ms⁻¹).

The filling of molten metal causes recovery of the topologically depressed region. If the depressed region is substantially deep, it may collapse with gas entrapped within it. As shown in Fig. 4, porosity-free single track deposition is achieved for the case of v= 0.7 m/s. But if the energy density is further increased (v= 0.5 m/s) then recovery of the collapsed deep keyhole will not be achieved leading to formation of spherical porosity. The collapse of the cavity leaves voids in the propagation path of the laser beam. Therefore, high energy density is not preferable as they will lead to porosity.

In order to qualitatively validate the simulation results and to obtain understanding of the porosity formation, single tracks were deposited by varying the scanning velocity. The tracks were deposited on a 40 μm thick Inconel 718 powder placed on a 1 mm thick Inconel 718.

Figure 5 shows the top view and longitudinal cross-section of the deposited single tracks at v= 0.5 m/s. Clearly, as observed in simulation (Fig. 4), for the case of v= 0.5 m/s spherical porosity forms along the laser traversal direction.
Fig. 4. Simulation results showing the temperature field (longitudinal cross-sectional view), (a) $v = 0.7 \text{ ms}^{-1}$ and (b) $v = 0.5 \text{ ms}^{-1}$.

Fig. 5. Longitudinal cross section of an Inconel 718 single track with porosity formed at the bottom of solidified molten track ($P = 100 \text{ W}, v = 0.5 \text{ ms}^{-1}$).
4. Conclusion
A three-dimensional open-source DEM – CFD simulation incorporating the physics of melting mode transition, melt flow dynamics and the physical phenomena (convection, melting, evaporation and solidification) has been developed. For focused laser beam, keyhole mode of melting occurs where both thermo-capillary force and recoil pressure play a dominant role resulting in a narrow and deeper melt pool. In keyhole mode of melting, if the depressed region is substantially deep then it collapse leading to spherical porosity formation. The collapse of the cavity can leave voids in the propagation path of the laser beam. Therefore, deep keyhole is not preferable as they will lead to porosity, but if stable keyhole is formed then better mechanical and microstructural properties is achieved.

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