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Resolving the effects of local convective heat transfer via adjustment of thermo-physical properties in pure heat conduction simulation of Laser Powder Bed Fusion (L-PBF)

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Abstract. Numerical models, especially when validated against experimental findings, are valuable tools that can be used as a cheap and reliable alternative to the expensive and time-consuming experimental investigations. In the current work, a multiphysics model of laser powder bed fusion (L-PBF) has been developed for stainless steel SS 316-L and validated against experimental findings. By configuring the model, the effects of the inverse Marangoni flow on the melt pool morphology and the heat and fluid flow conditions were analysed. It was shown that for high surface tension sensitivities, the total heat flux through the melt pool boundaries increases. The enhanced cooling will lead to a smaller melt pool size with larger depth to width ratio and causes a relatively uniform temperature field, which reduces the role of the conduction heat transfer. Furthermore, a Nusselt number was derived to quantify the role of the Marangoni effect on the convection heat transfer from the melt pool. This expression was used to calculate an effective thermal conductivity required for a modified pure conduction heat transfer calculation. It was shown that, via using a combination of the derived Nusselt number and the concept of the effective thermal conductivity, the average melt pool temperature determined from the modified pure conduction model gets very close to that of the more advanced CFD model.

1. Introduction

L-PBF is a branch of the Metal Additive Manufacturing (MAM) processes, where parts are manufactured layer-by-layer. The L-PBF process has found various functional applications in industries like automotive, energy, aerospace, and medical technology sectors [1], primarily due to its large flexibility in design freedom for manufacturing complex parts.

In L-PBF, tailoring the final microstructure and having a consistent melt track (melt pool profile) is essential for controlling the part quality. A numerical model which is validated against experimental findings can provide deep insights into the effects of the thermo-physical properties on the melt pool profile and its size and at a very low cost. However, by sole use of ex-situ and in-situ experimental analysis, one will miss many details regarding the spatio-temporal variation in the heat and fluid flow conditions. Even with the most advanced online monitoring systems, it is not possible to either determine the correct temperature [2] or fluid velocity at a time resolution even close to those the numerical models can predict. This once more necessitates the implementation of the numerical models as an alternative to the costly and time-consuming experimental investigations.
Computational Fluid Dynamics (CFD) has recently attracted attention for modelling of the L-PBF process, as it can predict the thermo-fluid conditions and the melt pool profiles with a very good accuracy. Depending on their complexity, the CFD models can take different physical phenomena into consideration, such as the surface tension, the thermo-capillary effect, the recoil pressure [3], etc. The author group has recently developed multi-physics models involving the aforementioned phenomena, to predict the lack-of-fusion and keyhole-induced porosities using the same technique [4-5].

Recent studies from the authors have shown that the pure conduction models overestimate temperature and the melt volume, since they neglect the fluid flow [6]. On the other hand, it must be stated that the CFD models are extremely CPU-heavy, as they solve for many more unknown variables such as the velocity components and pressure. This will in turn incur a lot of computational costs on the one who does these calculations. Accordingly, this is not favored by the industries who look for fast-responding models. However, while using the pure conduction heat transfer models, one can get more reliable results at a much lower computational time, if the effective thermal properties are used. By using the fluid dynamics and heat transfer theories, it is possible to determine these effective thermal properties to improve the output from the pure heat conduction models.

In this work we developed a high-fidelity finite volume (FVM) numerical model for the L-PBF process of 316-L stainless steel in the commercial software package, Flow-3D. The predicted melt pool profile is compared with the experimental melt pool micrograph where a very good agreement is achieved. By only keeping thermo-capillarity, the model is modified and then used in a parametric study to investigate the effect of the inverse Marangoni (with positive surface tension sensitivity) flow on the heat and fluid flow conditions inside the melt pool. Furthermore, a Nusselt number is found to quantify the role of convection in the transfer of heat through the melt pool boundaries. This Nusselt number is then used to find the effective thermal conductivity in a modified pure conduction heat transfer model, in order to get more reliable melt pool temperatures.

2. Modelling and experiments

2.1. The CFD model

Partial differential equations of balance of mass and linear momentum are solved to find the coupled fields of velocity and pressure. For an incompressible flow we have

\[ \nabla \cdot \bar{V} = 0, \]  
(1)

\[ \rho \left[ \frac{\partial}{\partial t} (\bar{V}) + \bar{V} \cdot \nabla (\bar{V}) \right] = \bar{p} + \bar{P} \left[ \mu \left( \nabla \bar{V} + \nabla \bar{V}^T - \frac{2}{3} \nabla \cdot \bar{V} \right) \right] - \frac{K_C (1-f_i)^2}{C_K + f_i} \nabla \cdot p \beta \Delta T_{ref} \]  
(2)

where \( \bar{V} \) is the fluid velocity vector and \( \bar{p} \) is pressure, respectively in equation (2). \( K_C \) and \( C_K \) are two constants related to Darcy flow, used in order to freeze and free the fluid flow upon solidification and melting. \( \beta \) is the thermal expansion coefficient in equation (2), where the Boussinesq approximation is used, \( f_i \) the liquid fraction function which in this work is assumed to be a linear function of temperature.

The heat transfer equation is solved to find the temperature field

\[ \rho \left[ \frac{\partial}{\partial t} (h) + \bar{V} \cdot \nabla (h) \right] = \bar{P} \left[ k (\nabla T) \right]. \]  
(3)

\( h \) is the fluid enthalpy and \( \rho \) and \( k \) are respectively the bulk density and thermal conductivity. In the L-PBF or welding process, there are three interfacial forces that have a significant impact on the liquid motion.

\[ F_{int} = [P_{recoil} + \sigma(T) \kappa] \bar{n} + \nabla T \cdot \bar{n} (\bar{V} \cdot \bar{n})]. \]  
(4)

\( P_{recoil} \) is the recoil pressure which along with the surface tension force, \( \sigma \kappa \), act normal to the interface, while the Marangoni effect, the second term in equation (5), acts tangential to the interface. \( \gamma \) in equation (4) is the surface tension sensitivity to temperature. Moreover, to track the free surface of the fluid, the VOF method with the split Lagrangian scheme is used. The exposed surface of the metal transfers heat via convection and conduction to the surroundings.
\[-k \frac{\partial T}{\partial n} = h (T - T_{surr}) + \eta (T^4 - T_{surr}^4) + q_{\text{max}} \exp \left( -\frac{2 r_b^2}{r_b^2} \right) + q_{\text{evap}} \]  

Equation (5)

$h$, $\eta$, and $q_{\text{evap}}$ are convective heat transfer coefficient, Stephan Boltzmann constant and the evaporative heat flux expressed in equation (5), respectively. The third term on the right hand side of equation (5) belongs to the laser where $r_b$ is the radius of which the heat flux reaches $e^{-2}$ of its maximum. In this work the heat source is modelled with ray-tracing but with a constant absorptivity.

### 2.2. Experiments and setup

The experiments were performed on an in-house made L-PBF machine developed at Technical University of Denmark (DTU) and with 316-L stainless steel powder [7]. The experimental setup consists of a 250 W single mode fibre laser with a nominal effective beam radius ($r_b$) of 50 µm and 1070 nm wavelength, an F-θ scan lens in addition to an in-house made galvanometer and laser controller to change the scanning velocity. The laser can be used in continuous wave (CW) and pulsed modes up to a frequency of 100 kHz. In the current work, only the continuous mode was utilized. Single track specimens were made on the top of a flat sheet of steel (SS316) with different scanning speeds and input powers where a custom single-layer powder handling unit was used. Then the samples were cut and analysed with light optical microscopy to find the melt pool cross-sectional profile. The scanning speed of the laser in the experiments was set to 210 mm.s\(^{-1}\).

### 3. Results and discussion

#### 3.1. Experimental validation of the multi-physics model

Figure 1(a) shows the 3D view of the temperature contour along with the surface deformation at $t = 6.3$ ms. According to figure 1(a), the peak temperature is about 3500 K which is slightly higher than the boiling temperature for 316-L stainless steel. At this relatively high localized temperature, the recoil pressure is active and overcomes the capillary force, causing a depression at the location of the hotspot, see figure 1(a). Figure 1(b) shows the comparison between the experimental and numerical melt pool profile from the y-z view. Figure 1(c) shows the solid fraction contour along with the velocity vectors from a longitudinal view. According to figure 1(c), in the depression zone, the recoil pressure will drive and pump the liquid material to the back of the melt pool. Right behind the zone of which the recoil pressure is active, the positive Marangoni effect exists which drives the liquid from the hot to the cold part of the melt pool. This effect will act as the second mechanism which drives the material to the cold tail of the melt pool, subsequent to the recoil pressure. At the very back of the melt pool, the liquid metal starts solidifying and as the temperature starts to decrease, the surface tension increases, which will form a hump at the tail of the melt pool, see figure 1(c). In this respect, the hump formation is caused by the movement of the cold liquid metal and its swelling at the back of the melt pool, in addition to the dominant capillary force at the cold tail of the melt pool.

#### 3.2. The inverse Marangoni effect

To be able to investigate the sole effect of the inverse Marangoni flow on the heat transfer from the melt pool boundaries, the recoil pressure and the buoyancy effects are removed from the fluid dynamics part of the developed multi-physics model. Moreover, the heat transfer via radiation and convection to the ambient are removed where in this way, it is guaranteed that all the heat input from the laser goes to the underneath solid domain. In this respect, a parametric study was performed with six different positive surface tension sensitivities ($\gamma$ in equation (4)) in addition to a pure conduction case. The model specification for the parametric study are given in table 1.
Figure 1. (a) The 3D view for the temperature contour at $t=6.3$ ms. (b) Comparison between numerical and experimental melt pool profile. (c) An $x$-$z$ view of the melt pool liquid fraction contour.

Table 1. Model specifications for the parametric study.

<table>
<thead>
<tr>
<th>Case #</th>
<th>Model ID</th>
<th>Power (W)</th>
<th>Speed (m.s$^{-1}$)</th>
<th>$D_b$ (µm)</th>
<th>$\gamma$ (N.m$^{-1}$K$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>conduction</td>
<td></td>
<td></td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>gamma_01</td>
<td>80</td>
<td>500</td>
<td>30</td>
<td>2.5e-5</td>
</tr>
<tr>
<td>3</td>
<td>gamma_02</td>
<td></td>
<td></td>
<td>5.0e-5</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>gamma_03</td>
<td>80</td>
<td>500</td>
<td>30</td>
<td>2.5e-4</td>
</tr>
<tr>
<td>5</td>
<td>gamma_04</td>
<td></td>
<td></td>
<td>5.0e-4</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>gamma_05</td>
<td></td>
<td></td>
<td>7.5e-4</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>gamma_06</td>
<td></td>
<td></td>
<td>1.0e-3</td>
<td></td>
</tr>
</tbody>
</table>

Figure 2. Longitudinal view of the temperature contour along with solid/liquid lines for (a) conduction, (b) gamma_02 and (c) gamma_05 at $t=1.26$ ms. (d), (e) and (f) respectively show the corresponding contours of (a-c), from the top view.

Figure 2 shows the temperature contours and the melt pool boundaries from the longitudinal and top views at $t=1.26$ ms and for chosen cases listed in table 1. One can notice the relatively larger size of the melt pool in the pure conduction case where there is no fluid flow involved. According to figure 2(a) and (d), in the pure conduction case, the hotspot region is larger as compared to the gamma_02 case shown in figure 2(b) and (e). In the pure conduction case, the melt pool will grow equally in width and
depth, see figure 2(a) and (d). However, when the fluid flow is added to the model, the melt pool profile becomes deeper and at the same time smaller in width, see figure 2(c) and (f). It is noted that the higher the $\gamma$, the deeper the melt pool will be. This is in agreement with the experimental findings of Mills et al. [8], who observed a better weld penetration in high-sulphur content steels (with higher $\gamma$), as compared to low-sulphur samples. Details of the melt pool morphology are given in table 2.

**Table 2. Melt pool size and morphology details for the parametric study.**

<table>
<thead>
<tr>
<th>Case</th>
<th>Length (µm)</th>
<th>Width (µm)</th>
<th>Depth (µm)</th>
<th>D/W ratio</th>
<th>L/W ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>conduction</td>
<td>387.54</td>
<td>107.25</td>
<td>53.62</td>
<td>0.50</td>
<td>3.61</td>
</tr>
<tr>
<td>gamma_01</td>
<td>379.71</td>
<td>96.23</td>
<td>62.03</td>
<td>0.64</td>
<td>3.95</td>
</tr>
<tr>
<td>gamma_02</td>
<td>362.03</td>
<td>89.86</td>
<td>68.99</td>
<td>0.77</td>
<td>4.03</td>
</tr>
<tr>
<td>gamma_03</td>
<td>293.91</td>
<td>68.41</td>
<td>78.26</td>
<td>1.14</td>
<td>4.30</td>
</tr>
<tr>
<td>gamma_04</td>
<td>284.93</td>
<td>62.61</td>
<td>81.74</td>
<td>1.31</td>
<td>4.55</td>
</tr>
<tr>
<td>gamma_05</td>
<td>268.12</td>
<td>57.97</td>
<td>82.03</td>
<td>1.42</td>
<td>4.63</td>
</tr>
<tr>
<td>gamma_06</td>
<td>268.12</td>
<td>53.33</td>
<td>78.26</td>
<td>1.47</td>
<td>5.03</td>
</tr>
</tbody>
</table>

According to both figure 2 and table 2, it was observed that the depth/width and length/width ratio increase with higher Marangoni coefficients. Also it is noted that the melt pool shrinks in size for higher Marangoni coefficients. Interestingly based on figure 2(c) and (f), the mushy zone (the area shown between the red and blue lines) extends to the end and top of the melt pool, for higher fluid flows. This means that the melt pool starts solidifying from the top, even though the top boundary is set to adiabatic. Moreover, one can visually see in figure 2 that the hotspot region, despite getting smaller in size, becomes directed towards the bottom of the melt pool, for higher Marangoni coefficients. Details regarding the calculated average thermal properties of the melt pool are listed in table 3.

**Table 3. Calculated averaged thermal and fluid dynamics related properties belonging to the melt pool.**

<table>
<thead>
<tr>
<th>$\gamma$</th>
<th>$T_{avg,liq}$</th>
<th>$V_{avg}$</th>
<th>$\delta T$</th>
<th>$V_{avg,mag}$</th>
<th>$Ma$</th>
<th>$Ec$</th>
<th>$Pe$</th>
<th>$V_{mush}/V_{melt}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>N.m⁻¹.K⁻¹</td>
<td>m⁻¹</td>
<td>m³</td>
<td>m.s⁻¹</td>
<td>(-)</td>
<td>(-)</td>
<td>(-)</td>
<td>(-)</td>
<td></td>
</tr>
<tr>
<td>2.50E⁻⁰⁵</td>
<td>2151.78</td>
<td>7.523E⁻¹³</td>
<td>71.88</td>
<td>1.55E⁻¹¹</td>
<td>8.17E⁺⁰¹</td>
<td>5.69E⁻⁰⁸</td>
<td>1.92E⁺⁰⁰</td>
<td>0.124</td>
</tr>
<tr>
<td>5.00E⁻⁰⁵</td>
<td>2116.63</td>
<td>7.114E⁻¹³</td>
<td>63.70</td>
<td>2.45E⁻¹¹</td>
<td>1.49E⁺⁰²</td>
<td>1.54E⁻⁰⁷</td>
<td>2.99E⁺⁰⁰</td>
<td>0.139</td>
</tr>
<tr>
<td>2.50E⁻⁰⁴</td>
<td>2037.56</td>
<td>5.236E⁻¹³</td>
<td>43.37</td>
<td>6.46E⁻¹¹</td>
<td>5.52E⁺⁰²</td>
<td>1.32E⁻⁰⁶</td>
<td>7.18E⁺⁰⁰</td>
<td>0.168</td>
</tr>
<tr>
<td>5.00E⁻⁰⁴</td>
<td>2015.50</td>
<td>5.043E⁻¹³</td>
<td>37.59</td>
<td>8.05E⁻¹¹</td>
<td>1.02E⁺⁰³</td>
<td>2.20E⁻⁰⁶</td>
<td>8.85E⁺⁰⁰</td>
<td>0.170</td>
</tr>
<tr>
<td>7.50E⁻⁰⁴</td>
<td>2007.32</td>
<td>4.82E⁻¹³</td>
<td>34.76</td>
<td>9.10E⁻¹¹</td>
<td>1.47E⁺⁰³</td>
<td>2.88E⁻⁰⁶</td>
<td>9.89E⁺⁰⁰</td>
<td>0.170</td>
</tr>
<tr>
<td>1.00E⁻⁰³</td>
<td>1989.97</td>
<td>4.85E⁻¹³</td>
<td>32.09</td>
<td>1.00E⁺⁰⁰</td>
<td>1.85E⁺⁰³</td>
<td>3.70E⁻⁰⁶</td>
<td>1.09E⁺⁰¹</td>
<td>0.173</td>
</tr>
</tbody>
</table>

According to table 3, a higher Marangoni effect will lead to a higher average liquid velocity inside the melt pool, as expected. Moreover, the melt pool volume reduces as we increase the Marangoni coefficient $\gamma$, according to table 3. $V_{mush}/V_{melt}$ in table 3 shows the ratio of the mushy zone volume to the total melt pool volume. According to table 3, for $\gamma=1.0e-3$, more than 17% of the melt pool is composed of the mushy zone. At the same time, it was observed that increasing $\gamma$ leads to a decrease in the average liquid temperature inside the melt pool. $\delta T$ is the dimensionless variance of temperature inside the melt pool, in table 3, called the temperature non-uniformity factor, which decreases for higher Marangoni flows. Also the definition of the Peclet number can be helpful to understand the relative importance of convection compared to conduction in heat transfer. Table 3 shows that convection becomes more important with increasing Marangoni effect, as the calculated Peclet number (denoted $Pe$ in table 3) becomes five times bigger for $\gamma=1.0e-3$, compared to $\gamma=2.5e-5$.

Figure 3 shows the velocity magnitude contour along with the velocity vectors in the $x$-$z$ plane and at the centre of the melt pool. According to figure 3(a), the inverse Marangoni effect drives the liquid on the top surface from the cold tail of the melt pool and to the hot centre where the surface tension is higher. This observation is exactly the opposite of the validation case shown in figure 1(c), belonging to a negative surface tension sensitivity which used to drive the liquid from the hot central zone to the cold outer zones. In figure 3(b) and its blow-up it is observed that two circulations are formed on the front and at the back of the laser spot location. However, due to the low liquid volume in the melt pool front, the front circulation is found to be much smaller in size. By increasing the Marangoni coefficient,
it is noted that a strong vertical jet of liquid forms right at the place where these two vortices meet each other see figure 3(c). The mentioned jet of the liquid metal, thus gets heated at the hotspot location and will play the role of a driller which digs in the cold material underneath – resulting in higher depth/width ratios.

Figure 3. The velocity magnitude contours at the x-z cross-section and at the centre of the melt pool for (a) gamma_01, (b) gamma_02, (c) gamma_04 and (d) gamma_06 cases at t=1.26 ms (after reaching the quasi-steady condition).

To have a better understanding regarding the fluid flow and the temperature field inside the melt pool, temperature and x-direction velocity (denoted $u$) fields are plotted against the z-coordinate in figure 4(a) and (b), respectively, at the investigation line A-A which is shown in figure 3(d).

Figure 4. (a) Temperature and (b) $u$-velocity profile along the vertical investigation line A-A (shown in figure 3(d)) for different Marangoni coefficients.

The temperature profile along the z-direction is displayed in figure 4(a) for different Marangoni coefficients. One can see that by choosing a lower Marangoni coefficient, both the peak and the average temperatures increase, based on figure 4(a). It is interesting to note that the temperature is higher at the bottom part of the melt pool, compared to its upper part, for higher Marangoni numbers, see figure 4(a). This means that the return flow belonging to the rear vortex is initially warm, which is driven by the heated downward vertical jet mentioned earlier. This in addition to a lower temperature predicted at the top part of the melt pool, once more underline the rapid cooling in the high-Marangoni cases which will
ultimately cause solidification of the liquid metal from the upper back of the melt pool, which was discussed earlier. Figure 4(b) shows the vertical distribution of the x-direction velocity along the A-A line. It is observed that the peak $u$-velocity increases with increasing Marangoni coefficients, as expected. Moreover, to fulfill the mass conservation, the returning flow is also stronger for the higher Marangoni number cases, see figure 4(b). Moreover, a higher viscous stress is predicted for higher Marangoni numbers, despite a more uniform thermal field.

3.3. The effective thermal conductivity

As the convection and radiation to the ambient are turned off, in the quasi-steady condition, one can divide the total input heat flux into a convective and a conductive part. This can be formulated by

$$q_{\text{tot}}'' = q_{\text{cond}}'' + q_{\text{conv}}'' = k_l \frac{T_{\text{avg,liq}} - T_s}{l_{ch}},$$

where $k_l$ and $h_s$ are the stationary liquid conductivity and the convection heat transfer coefficient from the melt pool to the solid. We assume that the conductive and convective heat fluxes in equation (6), can be found via the average melt pool temperature difference,

$$q_{\text{cond}}'' = k_l \left[ T_{\text{avg,liq}} - T_s \right], \quad (7)$$

$$q_{\text{conv}}'' = h_s \left[ T_{\text{avg,liq}} - T_s \right], \quad (8)$$

where $h_s$ is unknown in equation (8). One can find the solid/liquid heat transfer coefficient by substituting the conductive and convective heat fluxes from equations (7) and (8), into equation (6). We can solve for the unknown heat transfer coefficient via finding the corresponding Nusselt number

$$N_{U} = h_s l_{ch} = \frac{q_{\text{tot}}'' l_{ch}}{k_l T_{\text{avg,liq}} - T_s k_l} = L.$$

When the heat transfer coefficient is determined, one can use the following expression found by Ladani et al. [9] to find the effective thermal conductivity for a pure conduction heat transfer problem

$$k_{\text{eff}}'' = k_l + h_s l_{ch}, \quad (10)$$

where $l_{ch}$ in equations (7-10) is the characteristic length of the melt pool, which is the diameter of a hemisphere which has an equivalent volume to that of the melt pool [6].

Figure 5(a) shows the plot of the calculated Nusselt number as a function of the Marangoni number, both of which are determined from the CFD models belonging to the parametric study.

According to figure 5(a), the Nusselt number increases with the Marangoni number, which underlines the fact that the convective heat transfer is getting stronger. Moreover, figure 5(a) shows the effective thermal conductivity determined from equation (10) and as expected, it increases for higher Marangoni numbers. Figure 5(b) shows the plot of the average melt pool temperature calculated from the effective
conduction model against the one calculated from the CFD model. Accordingly a very good match is observed between the average melt pool temperature calculated from the CFD model and the conduction model using the effective thermal conductivity. As mentioned earlier, the effective thermal conductivity is determined based on the Nusselt number shown in figure 5(a).

4. Conclusion
In this work a multi-physics numerical model was developed for the L-PBF process of 316-L stainless steel and the predicted melt pool profile was validated against the experimental findings. The predicted melt pool profile was in a very good agreement with the experimental micrograph. The multi-physics model was then modified to enable the investigation of the sole effect of inverse Marangoni on the heat and fluid flow conditions inside the melt pool and also its profile, size and morphology. Thus a parametric study was performed to investigate the effect of the inverse Marangoni flow and the results suggest that the melt pool shrinks as the surface tension sensitivity to temperature increases. Furthermore it was found that the temperature inside the melt pool is relatively uniform for higher Marangoni flows. This makes the conduction heat transfer contribution weaker as the temperature gradients become smaller. In addition, a Nusselt number was developed that quantifies the effect of the convection heat transfer through the melt pool boundaries. Moreover, based on the calculated Nusselt number, an effective thermal conductivity was found. Utilizing a combination of the developed Nusselt number and the concept of the effective thermal conductivity, the average melt pool temperature will get very close to the predictions by the more advanced CFD model and at a much lower computational cost.

References