Modelling of Ceramic Particle Motion during Semi-Solid Forming of Aluminium Matrix Composites via CFD-DEM Four-Way Coupling

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Abstract. Today, aluminium matrix composites (AMC) are widely used for the manufacturing of lightweight, yet highly stressed components in automotive, aeronautic and electrical engineering. In order to achieve particle distributions as homogeneous as possible within these component’s volumes and thus ensure optimum component properties, efforts are being made to simulate the manufacturing process prior to production. In this paper, AMC with extremely high particle fractions of more than 25 vol.-% are considered in particular, as their processing still poses significant technological challenges. To model the particle motion in a computational fluid dynamics (CFD) simulation of the semi-solid forming process of this type of materials, a Lagrangian multiphase approach combining CFD and discrete element method (DEM) was used. Here, the DEM allowed all particle-particle interactions to be considered. Thus, different parameters influencing particle agglomeration, particle distribution as well as particle interaction with the cavity can be investigated during a numerical study. More specifically, the influence particle parameters such as cohesion forces and the influence of the forming speed onto the particle distribution in the final component’s volume was analysed. The simulations were performed for a symmetric disc geometry. A forming tool was already available for this geometry, with which components could be manufactured to validate the simulation results. In the end, the study shows that by using four-way CFD-DEM coupling, simulation predictability for the semi-solid forming process of AMC could be significantly improved.

Introduction

Applications of aluminium matrix composites (AMC) combine low component weight with relatively high strength properties and are widely used in automotive, aeronautic and electrical engineering. Thereby, the AMC are categorized according to the reinforcement type into particle reinforced composites, fibre reinforced composites and interpenetrating composites. Due to the comparatively low costs, ceramic particles of SiC or Al2O3 are predominantly used for reinforcing aluminium alloys. These reinforcement particles are quasi zero dimensional and reinforced components exceed the specific material [1] and tribological [2] properties of aluminium alloys depending on the particle loading as well as the particle size.

Generally, AMC are manufactured by casting (e.g. [3]), powder metallurgy (e.g. [4]) or semi-solid routes (e.g. [5]), aiming to produce components with homogenous particle distributions. To guarantee such homogenous distributions, several extensive experimental studies have been carried out in the past resulting in homogenous distributions. Semi-solid routes in particular show a high potential to produce net-shape components with high particle loadings. Therefore different process parameters and their influence on the components need to be determined. Currently, ideal semi-solid process parameters are mainly investigated through experimental studies [6]. Given the high effort of such experimental studies, simulation enables a prediction of the required process parameters as well as a further improvement of the process. However, numerical prediction of the particle distribution depending on the particle motion during the forming process is a challenging task due to contact driven dense flow. In this respect, different numerical approaches have been developed to determine...
the influence of particles onto the flow behaviour. For example, one approach from stir casting modelling focuses on the process parameters of stirring, while modelling aluminium melt with a constant viscosity and ignoring the solid SiC particles (SiC$_p$) in order to determine dead flow zones [7]. Another approach models a disperse flow of aluminium melt and solid SiC$_p$, whereby the melt viscosity changes in dependence on the particle load of the aluminium melt. However, particle-particle interaction is ignored in this approach [8]. A current research project focuses on nano-particle reinforced aluminium alloys produced by low pressure die casting. Here, a Lagrangian multiphase approach without particle-particle interaction is used to model the particle movement during the casting process [3]. In summary, there are several approaches to model the production of AMC. Yet all these approaches have deficits regarding the interaction of the particles with the fluid as well as the interaction of the particles with each other.

Aim of this paper is to model the semi-solid forming process of an AMC with 25 vol-% SiC$_p$ using four-way coupling between the semi-solid aluminium (continuous phase) and the solid SiC$_p$ (dispersed phase), particularly taking the particle-particle interaction into account. Therefore, a new modelling approach combining computational fluid dynamics (CFD) with the discrete element method (DEM) is presented to determine the particle distribution after the process.

Materials and Method

The numerical investigation on modelling particle motion during semi-solid forming presented in this paper were performed using a symmetric disc geometry (Figure 1). For validation of the simulation results, a forming tool for producing corresponding disc components was available. For the numerical model as well as the experiments a billet with an outer diameter of 65 mm and a height of 80 mm was used to produce disc shaped parts having a height of 15 mm and a diameter of 150 mm. To reduce the amount of particles, the billet was split into an outer billet having a particle loading of 25 vol.-% SiC$_p$ with a diameter greater than 30 mm for both studies (Figure 1a). For the experiments the outer billets were produced using a spray deposition process, while injecting solid SiC$_p$ into an liquid AlSi7Mg0.3 spray. Furthermore, the outer billets were cut out of the spray deposit in a tubular shape and the inner billets of AlSi7Mg0.3 without SiC$_p$ were inserted. For the experimental study as well as the numerical study a tool temperature of 350 °C and a forming speed of 100 mm/s was used in order to produce composites with a gradient particle loading. Initial heating of the billets into the semi-solid state was performed using an induction heating plant from Kuka. During the heating process, a temperature of 580 °C (~ 50 % liquid fraction) was reached within the entire semi-solid billet. For the numerical study a homogenous billet temperature of 580 °C without a temperature gradient was used.

For the numerical study the software tool Star-CCM+ was used, as this program allows to simulate the continuous phase of semi-solid aluminium via volume of fluid (VOF) technique while considering particle-particle interaction of the dispersed phase via DEM. The VOF technique is feasible to model
the free surface of the semi-solid aluminium in a simple and efficient way as introduced by Hirt and Nichols [9]. Cundall and Strack invented the DEM-approach using a soft-sphere model, which allows particle-particle as well as particle-wall interaction using a force-displacement law [10]. Coupling of VOF and DEM is possible due to momentum, mass and energy exchange between both phases using the Euler-Lagrange approach [11].

To simulate the semi-solid aluminium flow, a shear rate and temperature dependent viscosity model based on a modified Quaak model as presented in [12] was used. Therefore, field functions were programmed in order to integrate the material model into the Star CCM+ Software. AlSi7Mg0.3 exhibits a thixotropic material behaviour, which was also implemented through field functions. Using these functions, the rate of shear thinning and shear thickening could be controlled. The used model parameters as well as the validation of the material model for a monolithic AlSi7Mg0.3 without SiCp can be found in [12].

For small particle sizes as well as low particle loadings the influence on the fluid flow is negligible. In this case, so-called one-way coupling can be used. One-way coupling allows to simulate the fluid to influence particle movement while the particle does not affect the fluid flow. However, for higher particle loadings, as considered in this contribution, the influence of particles onto the continuous phase needs to be taken into account via two-way coupling. Here, particles affect the flow of the fluid depending on particle size as well as particle movement, as shown in Figure 2 a). Hereby, different parameters can be chosen in order to specify the fluid-particle interaction. Particle loadings of more than 10 vol-% solid particles exhibit a contact driven behaviour and therefore the particle-particle interaction needs to be taken into account. This method is often referred to as four-way coupling. In the present work this interaction is based on the contact forces of DEM. If two particles collide in a specific direction of incidence a force exchange will occur, due to the soft-sphere modelling the contact is modelled by overlapping those particles depending on the particle momentum. In order to determine the force and momentum exchange, different approaches can be used. In this paper, the Hertz-Mindlin approach was used. During contact loading with the Hertz-Mindlin approach (Figure 2b), the contact forces are split into the normal force $F_n$ and the tangential force $F_t$, which are summarized by a spring-dashpot pair and an additional friction part for the tangential force [13].

![Figure 2: a) Two-way coupling of continuous and dispersed phase and b) contact modelling of DEM based on Star-CCM+ [13]](image)

In terms of the conducted simulations, the following parameters for the fluid solid interaction were chosen. The drag force was modelled by the Schiller-Naumann drag coefficient, which influences the amount of energy exchange between continuous and dispersed phase. Sommerfelds approach was used for the shear lift force and spin lift force in order to model the influences of the flow onto the particle behaviour [14]. Since the main focus of the investigation was on the particle-particle interaction, the fluid-particle coupling parameters listed in table 1 did not change for all simulations.
Contact forces were calculated based on the Hertz-Mindlin approach using the SiC material parameters, in particular the young’s modulus and Poisson’s ratio. As slipping between the particles can occur depending on the direction of incidence, a rolling resistance will be used proportional to the contact force. In order to determine the influence of agglomerations during semi-solid forming, different approaches can be used. Agglomeration can occur depending on different cohesion mechanism as well as form closure during collision between particles. Therefore, a model called “parallel bonds” can be applied in Star CCM+ in order to establish connections between colliding particles. These bonds can subsequently be subjected to different damage models to specify the breakup of particle agglomerates. Given the high numerical expense of the parallel bonds model, another approach to predict agglomeration during forming was used. By specifying a linear cohesion force as a surrogating mechanism for particle agglomeration, particles in contact may bond together. Therefore, an artificial linear cohesion was chosen to model the influence of particle agglomeration onto the forming results.

Table 1: Used particle models and SiC material data

| Particle-Model          | Parameter                  | Value                      |
|-------------------------|----------------------------|----------------------------|
| Drag Force              | Drag Coefficient           | Schiller-Naumann           |
| Shear Lift Force        | Shear Lift Coefficient Method | Sommerfeld                |
| Spin Lift Force         | Particle Lift Coefficient Method | Sommerfeld                |

**Particle-Particle-Interaction**

| Hertz Mindlin           | -                          | -                          |
| Rolling Resistance      | Rolling Resistance Method  | Force Proportional         |
| Linear Cohesion         | Work of Cohesion           | 0; 1 N/m                   |

**Particle-Wall-Interaction**

| Hertz Mindlin           | -                          | -                          |
| Rolling Resistance      | Rolling Resistance Method  | Force Proportional         |

**SiC material data**

E-Module: E = 400 GPa  
Density: ρ = 3210 kg/m³  
Poisson’s ratio ν = 0.33

For discretization of the model a polyhedral mesh with a base size of 2 mm and a particle size of 0.7 mm was used to reduce large computing times caused due to the huge number of particles. For the experimental billets, particles with a size distribution around 53 – 70 µm (F220) were used. This equals particles ten times smaller than in the simulations. In order to further reduce computing times, a reduction of E-Module is assumed. Therefore, reference simulations with the materials E-Module of 400 GPa compared to a simulated E-Module of 4 GPa and 100 MPa were performed, showing no significant influence of the E-Module onto the particle distribution. As a result, the E-Module was reduced to 100 MPa in the simulations. The time step in the implicit unsteady solver for the continuum simulation was optimized by the adaptive time stepping feature in Star CCM+.

To improve modelling of AMC, a comparison between a state-of-the-art Lagrange approach without particle-particle interaction, the DEM approach and the experimental results is made. Afterwards the influence of cohesion and forming speed is modelled. The results of these investigations to the modelled particle distributions are discussed in the following.

Results of the Experimental Study Compared to the Numerical Results

The components produced in the real experiments were air cooled and visually checked after forming. Here, a complete form filling without defects could be observed for all components. A comparison between the particle distributions of the side view is shown in Figure 3. Here, the zones with light grey indicate areas without SiCp, while the darker areas are aluminium with SiCp inside. For the DEM approach, the infiltration depth of the aluminium alloy into the reinforced alloy is predicted correctly, while showing differences in the width. The differences in the width may occur because of the
simplification in temperature distribution of the billet. Inductive heating is used in order to heat the billets, resulting in a small temperature gradient between the outside and inside of the billet as well as a lower SiCₚ temperature. Hereby, the initially constant temperature throughout the part in the simulation results in a lower viscosity of the billet. Thus, particles are more likely dragged in the fluid. In the purple area, the lower edge is predicted correctly by the DEM approach, while form filling in the upper edge is predicted incorrectly. At the end of the forming process segregation effects can occur due to temperature exchange between the tools and the billet. At the beginning of the simulation due to the higher temperature a segregation effect might not be reached. Another reason for the different predictions of the particle distribution in the edges of the part can be found in the handling of particle interactions. The observed form filling in the upper and lower edges in the DEM approach is heavily dictated by particle collisions and the particles effect on the continuous phase. Particles frequently change their trajectory as they are pushed against the walls. Size reduction of the DEM particles would deliver a better spatial discretization at the cost of computation time and might minimize this effect. The Lagrangian approach ignores such collisions and therefore particles cannot change their trajectory because of particle-particle interaction. For the high particle load of 25 vol.- % this results in numerous overlapping particles, which are considered parasitic. Since the particles in the simulation are ten times bigger than in reality a microsection comparison between different zones in the components are not yet affective. To summarize this section, an improvement can be made through the DEM approach in predicting the particle movement during forming. In order to further improve the predictability of particle distributions the possibilities of the new approach will be presented in the next section. For future manufacturing of AMC components with semi-solid forming, the influence of process parameters should be simulated in order to determine the optimized process parameters regarding particle distribution. Therefore, a comparison of the particle distribution over the disc’s volume is used.

Figure 3: a) Manufactured disc (90°) and b) side view of the disc in comparison to the simulation results

Result and Discussion of the Numerical Study

In order to compare the particle distribution in the simulated discs’ volumes, four zones were compared. Thereby, the disc was sliced into four parts of 3.75 mm height to determine zones with supposedly inhomogeneous particle distributions from a top view. In Figure 3, the state-of-the-art Lagrange approach is shown in comparison to the VOF-DEM approach presented in this paper. Two-way coupling with the continuous phase as well as particle interaction show an influence on the resulting particle distribution. Differences are observed, especially in the centre of the component (Zones 2 & 3), which can be attributed to the lack of particle interactions in the Lagrangian simulation.
Particles that collide are not deflected and thus do not change their movement. Zone 1 and 4 show a particle distribution starting from the initial diameter of the outer billet for both simulations. Due to the heat transfer from the billet into both punch and cavity a higher viscosity and therefore lower fluid velocity is reached, which shortens the travelled distance of particles in those zones. Particle distribution in the side view shows a nearly symmetrical homogenous infiltration depth for the Lagrangian approach. Only the outer edges show zones without particles. However, the particle distribution from the DEM approach is sharper in the middle and not symmetrical in the side view. Additionally, more particles can be observed in the upper half of the disc (Zone 1 & 2) compared to Zone 3 & 4. Additionally, a better form filling with particles in the edges is observed. The Lagrangian approach allows particles to overlap without the particles influencing each other. Thus, agglomerations are not built with this approach. In contrast, DEM is feasible of modelling agglomeration build ups as well as break ups during forming.

![Image: Particle distribution of the Langragian approach (left) vs DEM approach (right) only particles visualized](image)

Four-way coupling is very challenging in terms of computing time. An increase in forming speed by 61.5 % and therefore reduction in process time, reduces the needed time for simulation by 35 %. The influence of cohesion as well as forming speed are simulated using a forming speed of 260 mm/s. Agglomeration of SiCₚ should be avoided in order to improve mechanical properties of produced AMCs. Therefore, a cohesion force given by the work of cohesion was used to visualize the influence of agglomeration on the flow results as well as the particle distribution (Figure 5 (left)). The simulations with cohesion forces show local zones without any SiCₚ, which would reduce the improved properties of an AMC structure. Compared to the simulation without cohesion in Figure 5 (right) the simulation exhibits a different flow behaviour resulting in a different interpenetration depth in the side view. Flow behaviour with cohesion is influenced by artificial attracting forces resulting in a shorter infiltration depth of the non-reinforced aluminium alloy. Particles attracting each other are less influenced by the continuous flow of the semi-solid aluminium resulting in a change from the point of the deepest infiltration in zone 2 without cohesion to zone 3. Due to the unknown amount of artificial cohesion force currently no significant agglomerations of SiCₚ can be found at the end of the simulation, while the cohesion force still influences the flow behaviour significantly.
So far, all comparisons refer to simulation parameters, which aim to demonstrate the general possibilities of the new modelling approach. Currently, experimental studies at the Institute for Metal Forming Technology (IFU) were only used for analysing the influence of process parameters onto the particle distribution. Forming speed as a process parameter is known to significantly improve the forming results during semi-solid forming [12]. Therefore, forming speed is varied with two different speeds (260 mm/s, 100 mm/s) as shown in Figure 4 and 5 (right). Here, a significant influence of forming speed on the particle distribution is proven. For lower forming speeds more inhomogeneous zones as well as defects can be found due to the longer temperature exchange with the tools. Since the viscosity of semi-solid AlSi7Mg0.3 is temperature and strain rate dependant, a higher forming speed also decreases the viscosity, which results in an overall higher flow speed especially in the upper half of the billet. Due to the higher flow speed the particles are dragged further in zone 2 and show the point of the deepest infiltration depth in this zone in contrast to zone 3 in the simulation with the slower forming speed. Therefore, a higher forming speed results in a particle distribution mostly below the symmetry line in the side view due to the initially higher shear rate at the contact zone with the punch.

Conclusion

In this paper a new modelling approach for a semi-solid manufacturing process of AMC was presented in order to improve particle distribution prediction. Therefore, four-way coupling was used, considering fluid-particle interaction via the Euler-Lagrangian multiphase approach using VOF and DEM. In order to examine the behaviour of different process parameters, simulation is a cheap and time efficient way in contrast to experimental studies. In this paper, two forming speeds were used, in order to show the influence of process parameters onto the particle distribution. Here, process parameters influence the particle distribution in a significant way. A higher forming speed caused a shift towards the top side of the disc, as well as a lack of particles/form filling on the outer diameter. In future research discs with different process parameters will be manufactured, in order to validate the influence of process parameters compared to the simulated particle distributions. Agglomerations
of SiCp in the manufacturing process needs to be avoided. Predicting such agglomerations with simulation is key to further improve manufacturing of AMC. Therefore, a possibility in the four-way coupling is to use cohesion forces between particles in contact, resulting in agglomerations depending on the used cohesion force. The particle movement as well as the final distribution can be influenced through cohesion, showing a different form filling and interface in the simulated disc. In future work a specific cohesion force for the SiCp needs to be determined in order to correctly predict agglomerations.

In comparison to the experimental results a few weaknesses in the current model are shown, both the state-of-the-art as well as the new modelling approach show differences in predicted particle distribution. In the simulations a homogenous temperature distribution of 580 °C was used. Due to the inductive heating process a temperature gradient exists in the billet, which should be considered in future work. Another parameter is the particle size of 0.7 mm, which is ten times bigger than the actual particle size. In future work, more computing power will be used in order to reduce computing time as well as particle size to further improve the model. However, aim of the paper was to prove the feasibility of the new modelling approach combining VOF with DEM, in order to improve predictability of particle distributions in simulations of semi-solid manufacturing of AMC, which could be proven.

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References

[1] A. B. Pandey, "Metallic Matrices", in ASM Handbook Vol. 21: Composites, ASM International, 2001, pp. 150–159.
[2] M. K. Gupta, L. Ranakoti and P. K. Rakesh, "Effects of Reinforcement on tribological behaviour of Aluminium Matrix Composites", in Automotive Tribology, K. K. Jitendra, B. Shantanu, K. P. Vinay, and K. Vikram, Eds. Springer, 2019, pp. 131–143.
[3] G. Zheng, J. Jakumeit, T. Pabel, C. Kneissl and L. Magagnin, "Computational Simulation of Nanoparticle Distributions in Metal Matrix Composite Casting Processes", Miner. Met. Mater. Ser., vol. 6, pp. 171–179, 2021.
[4] D. Yilong, T. Fei and Y. Kun, "Effect of SiCp particle size and anneal on properties of Al/SiC composites prepared by powder liquid -phase sintering", 16th Int. Conf. Electron. Packag. Technol. ICEPT 2015, pp. 347–353, 2015.
[5] L. Schomer, C. Seyboldt and M. Liewald, "Semi-Solid Metal Forming - A Process for Manufacturing Composite and Hybrid Materials", Defect Diffus. Forum, vol. 381, pp. 47–51, 2017.
[6] A. Storz, T. Schubert, T. Weissgärber, C. Seyboldt and K. R. Riedmüller, "Efficient Processing of Metal-Matrix-Composites by Combining Direct Pressure Sintering and Subsequent Thixoforging", Mater. Sci. Forum, vol. 825–826, pp. 167–175, 2015.
[7] H. Su, W. Gao, H. Zhang, H. Liu, J. Lu and Z. Lu, "Optimization of stirring parameters through numerical simulation for the preparation of aluminum matrix composite by stir casting process", J. Manuf. Sci. Eng. Trans. ASME, vol. 132, no. 6, pp. 061007-1-061007–7, 2010.
[8] Z. Yang et al., "Experimental and simulation research on the influence of stirring parameters on the distribution of particles in cast SiCp/A356 composites", J. Eng., vol. 2017, no. Article ID 9413060, p. 11 pages, 2017.
[9] C. W. Hirt and B. D. Nichols, "Volume of fluid (VOF) method for the dynamics of free boundaries", J. Comput. Phys., vol. 39, no. 1, pp. 201–225, 1981.
[10] P. A. Cundall and O. D. L. Strack, "A discrete numerical model for granular assemblies", Géotechnique, vol. 29, no. 1, pp. 47–65, 1979.
[11] M. Sommerfeld and S. Lain, "2.6 Euler–Lagrange Methods", in Multiphase Flow Handbook, 2nd ed., J. D. Michaelides, E.E., Crowe, C.T., & Schwarzkopf, Ed. CRC Press, 2016, pp. 202–241.

[12] M. Liewald and K. R. Riedmüller, "A new one-phase material model for the numerical prediction of critical material flow conditions in thixoforging processes", CIRP Ann., vol. 68, no. 1, pp. 293–296, 2019.

[13] SIEMENS, "CFD program Simcenter STAR-CCM+ documentation", Simcenter, Available: https://docs.sw.siemens.com/documentation/external/PL20210730658209000/en-US/userManual/starccmp_userguide_html/, 2021, [Accessed: 26. Nov. 2021].

[14] M. Sommerfeld, "Theoretical and Experimental Modelling of Particulate Flows", in Technical Report Lecture Series 2000-06, 2000, pp. 19–24.