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Direct numerical simulation of melt–gas hydrodynamic interactions during the early stage of atomisation of liquid intermetallic

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ABSTRACT

The dynamic interactions between Raney Ni–Al intermetallic melt and argon gas at the start of atomisation, near the nozzle of close-coupled gas atomiser, for the first time, are numerically investigated using a front-tracking formulation. Some key geometric parameters of a real device are used in the model in order to simulate the real atomiser. In the model predictions of gas/melt movement, the gas jets cause melt stream pinch off and force the melt stream to wet the melt nozzle tip. Meanwhile, the melt flow has a strong influence on the evolution of gas recirculation via significant feedback. The simulated evolution of the melt stream topology up to disconnection is positively supported by related experimental results. The mechanism of the stagnation point formation proves to be very different from that predicted in conventional gas-only case studies. The peak pressure along the vertical centre line significantly varies once the melt stream becomes disconnected. The pressure gradient within the melt stream in the vertical direction contributes to the aspiration pressure, which is over-ambient with the specific parameters of this paper. This is the first time that direct numerical simulation has been used to investigate the melt–gas two-fluid flow in a real gas atomiser. Besides delivering a deep insight into the physical process involved, this new model has the potential to supply industrially applicable predictions.

1. Introduction

Gas atomisation is a very efficient processing route to powders in the powder metallurgy field. Compared with conventional manufacturing techniques, it can produce fine, clean, and spherical powders. By treating the Ni–50 wt.%Al powders with solvent, like concentrated sodium hydroxide, some aluminum atoms are removed and the Raney Ni–Al powders are obtained (Raney, 1927). Because of high porosity, the Raney powders are very good candidate catalysts for use in hydrogenation industry and can be sintered to produce Ni–Al fuel cell electrodes with the purpose of replacing expensive noble metals. Gas atomisation is also one of the key stages in the spray forming process. Atomisation affects the properties of spray formed product via its influence on the metal melt droplets and particles. The hydrodynamic and thermal interactions between melt stream, atomising gas jets and the chamber ambient gas, especially those near the nozzle of atomiser, are deserving of study since knowledge of such interactions permits prediction of the evolving flow and temperature field of the melt stream in the atomisation zone. Modelling and numerical simulation of gas atomisation has attracted the attention of many

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researchers because of its powerful potential to reveal the physical process, e.g. the melt–gas interface instability during atomisation, and to predict the atomisation result, e.g. the thermal history of droplets, and hence to help to find the optimum processing parameters (Fritsching, 2004).

Referring to the modelling of gas atomisation, the atomisation process can be roughly subdivided into three subprocesses. They are (i) the melt flow in the tundish and gas flow within the gas nozzles, (ii) melt stream disintegration caused by atomising gas jets which occurs in the atomisation zone near the melt orifice, and (iii) the droplet/particle spray in the chamber. Compared with the modelling of other subprocesses, treating the modelling of melt–gas dynamic interactions near the atomiser nozzle remains very challenging. The melt stream disintegration process includes strong melt–gas interactions, both hydrodynamic and thermal, which are very unsteady, complicated and coupled. Focused on the effects of gas flow on melt stream disintegration, many researchers have worked to simulate the gas flow in a gas-only case, in which the atomised liquid is not present. Fritsching and Bauckhage (1992) simulated the gas flow field near the nozzle of a free fall atomiser. Anderson et al. (Mi et al., 1996) examined the effects of parametric variation of gas atomising pressure on gas flow field. Ting and Anderson (2004) investigated the gas dynamics of the open-wake and closed-wake conditions of a close-coupled atomiser. Espina et al. (1998) simulated the effect of jet pressure ratio on the gas-only atomisation flow. Although, such gas-only studies can provide very helpful hints to investigate the mechanism of melt stream disintegration, it is far away from the status of the real gas atomisation process because of the strong feedback of the melt stream flow, which is caused by the high melt density (normally several thousand kg/m^3) and temperature (may be well over 1000 °C), significantly affecting the gas flow and makes the melt–gas interactions not negligible.

The conventional modelling methods of melt–gas interactions can be reduced to two categories. One is the analytical method to investigate the initialisation and growth of surface waves at the melt–gas interface by using linear stability analysis, such as the Taylor case (Rayleigh, 1878) and the Kelvin–Helmholtz (K–H) instability case (Bradley, 1973a,b). Markus et al. (2002) have analytically investigated the growth of surface waves on the gas–liquid boundary in a free fall atomiser by using such linear stability analysis. Although this analysis is of significant theoretical value, many assumptions and simplifications included in this method make it difficult to fit real experimental data. For example, in these analyses, the gas flow field close to the nozzles is extremely simplified and regarded as constant. The gas viscosity and gravity force are normally neglected. The second approach to simulating melt–gas interactions, with the purpose of industrial application, is an empirical one. In such an approach, the droplet size distribution is directly predicted according to variation of experimental parameters, like the material properties and operational settings. A famous droplet-size correlation is Lubanska's model (Lubanska, 1970). Although empirical models have often been successfully applied in industrial applications research, they cannot deliver a deep insight into the melt–gas dynamic interactions because they are not capable of analysis of the detailed physical process.

Nowadays, due to the rapid development of computer hardware, direct numerical simulation is becoming more and more applicable in the field of multi-fluid flow research. By modelling the K–H instability, accompanied by a variety of different interface tracing models, direct numerical simulation has been used by many researchers to investigate the melt–gas hydrodynamic interactions. The group of Zaleski (Scardovelli and Zaleski, 1999; Thomas et al., 2004; Li et al., 2007) has used the volume of fluid (VOF) model (Hirt and Nichols, 1981) to investigate melt ligament and droplet formation from a liquid sheet during the non-linear development of K–H instability. The group of Tryggvason (Tryggvason and Unverdi, 1999; Tauber and Tryggvason, 2000; Tauber et al., 2002) has used a front-tracking formulation to carry out simulation of the K–H instability, investigating the linear and non-linear evolution of surface waves in both 2D and 3D. In the above-mentioned research work, although different interface tracing models are used, the same simulation case study is used: liquid–gas parallel flow with periodic boundary condition. This case study totally excludes the complexity of gas flow near the nozzle of a close-coupled atomiser. In a real gas atomiser, the gas nozzles are not parallel to the melt nozzle but are inclined at an angle (typically 22.5° in a close-coupled atomiser). This gas nozzle arrangement, accompanied by feedback from the melt stream flow, makes the gas flow near the nozzle of atomiser very complex, turbulent and dynamic, especially at the start of the atomisation process when the gas first hits the melt stream. It is clear that such a gas flow field is essentially different from that of the aforementioned periodic liquid–gas parallel flow case and significantly affects the melt–gas interaction process.

The dynamic interactions between melt and gas in a real atomiser is very unsteady. Especially at the start of gas atomisation process, the status of the melt–gas flow significantly varies with time. The melt–gas dynamic interactions at the start of gas atomisation are of great research importance, because they are the origin of the whole atomisation process and, industrially, they will determine whether melt orifice choking occurs, which is very harmful to smooth process operation. In this paper, by using a front-tracking formulation, direct numerical simulation is carried out to investigate the melt–gas interactions near the nozzle of a close-coupled atomiser during the initial stage of gas atomisation of an intermetallic melt, within a simulation domain, of which some key geometric parameters are set to try to imitate a real atomiser design. In this work, all the fluids are assumed to be incompressible, viscous and Newtonian. The simulation is in 2D. The gas compressibility and 3D effects will be investigated in future research. Although modelling heat transfer is possible in the current model, the results of thermal interactions between melt and gas are not analysed here but they are included in Tong and Browne (2007) in detail. This paper concentrates on the hydrodynamic interactions between melt and gas during the initial stage of gas atomisation process.

2. Models and numerical formulation

Because complex interface geometry and significant and frequent interface topology changes are inherent to the nature