Increasing the Computational Efficiency of Discrete-Continuous Coupled Methods: A Powder Metallurgy Case Study

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ABSTRACT

Powder Metallurgy (PM) is an evolving technology to produce metallic components from a starting powder phase. The PM products are of high interest because of the particular mechanical and thermal properties they can achieve. Herein, an advanced simulation framework, based on a discrete-continuous numerical concept [1], to address the various thermochemical processes arising in PM industry is proposed The model resolves powder as a discrete with the eXtended Discrete Element Method (XDEM); which predicts the thermodynamic state e.g. temperature and chemical reaction for each powder-particle. The gaseous powder surrounding is resolved with tailored computational fluid dynamics (CFD). Thus, the various heat and mass transfer between the gas phase and the powder is accurately determined. Predicted results track the thermodynamic history of each particle in conjunction with the gas temperature and composition.

The large amount of particles to be resolved in a powder -based scale makes it impractical to use conventional discrete element techniques. To tackle this challenge, this contribution introduces a new concept, the Agglomerated Particle Method (APM); which relies on the so-called Population Balance Method principle, as described by Marshall and Li [2]. In the concept, an agglomeration or particles-parcel is substituted by a single-effective-entity, for which, it is assumed that all the represented-particles (i.e. particles in a same neighbourhood) are under the same boundary conditions as the introduced effective-entity. Consequently, the entire powder space is divided into sub-domains, each of which is solved as an Agglomerated Particle (AP) within a unit cell. The thermochemical state of each AP is predicted as the above-cited XDEM. However, modifications for the intra-particle physical properties are applied. Thus, the numerical technique resolves fewer entities increasing computational efficiency and feasible time simulations.

In this contribution, in order to evaluate the capacity of the proposed technique, the industrial production of tungsten powder is presented and numerically studied. The industrial production of tungsten powders is a complex process that includes handling of powder, thermal treatment in a hydrogen atmosphere with a significant mass and heat transfer between the gaseous phase and the powder. Extensive research has shown that tungsten grain size distribution (W-GSD) is correlated to key material properties of tungsten-carbide based products. The detailed results uncover the underlying physics that allows to improve the process and to offer a wider examination for controlling the W-GSD.

REFERENCES

[1] A. A. Estupinan Donoso, “A Discrete-Continuous Approach to Model Powder Metallurgy Processes,” University of Luxembourg, 2016.

[2] J. S. Marshall and S. Li, *Adhesive Particle Flow: A Discrete-Element Approach*. Cambridge Univeristy Press, 2014.