World Academy of Science, Engineering and Technology
International Journal of Chemical and Materials Engineering
Vol:17, No:08, 2023

Mechanistic Modelling to De-risk Process Scale-up

Authors : Edwin Cartledge, Jack Clark, Mazaher Molaei-Chalchooghi

Abstract : The mixing in the crystallization step of active pharmaceutical ingredient manufacturers was studied via advanced modeling tools to enable a successful scale-up. A virtual representation of the vessel was created, and computational fluid dynamics were used to simulate multiphase flow and, thus, the mixing environment within this vessel. The study identified a significant dead zone in the vessel underneath the impeller and found that increasing the impeller speed and power did not improve the mixing. A series of sensitivity analyses found that to improve mixing, the vessel had to be redesigned, and found that optimal mixing could be obtained by adding two extra cylindrical baffles. The same two baffles from the simulated environment were then constructed and added to the process vessel. By identifying these potential issues before starting the manufacture and modifying the vessel to ensure good mixing, this study mitigated a failed crystallization and potential batch disposal, which could have resulted in a significant loss of high-value material.

Keywords : active pharmaceutical ingredient, baffles, computational fluid dynamics, mixing, modelling
Conference Title : ICCPMDEA 2023 : International Conference on Chemical Process Modeling, Design and Engineering Applications
Conference Location : Venice, Italy
Conference Dates : August 10-11, 2023