

1. Record Nr.	UNINA9910647263703321
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Titolo	Simulation of Spray Polymerisation and Structure Generation in Spray Drying by Single Droplet Models / / Winfried Sackel
Pubbl/distr/stampa	Berlin, Germany : , : Logos Verlag Berlin GmbH, , 2022
ISBN	3-8325-5575-7
Descrizione fisica	1 online resource (328 pages) : illustrations
Disciplina	660.28426
Soggetti	Spray drying polymerization
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
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Sommario/riassunto

Spray polymerisation has a long time been discussed as a promising process, yet, with little knowledge on cause-and-effect relationships between drying and chemical reactions. This work develops a new single droplet model of combined solution drying and free radical homopolymerisation, based on the method of moments. New, consistent approaches for moments' diffusion and the reaction-diffusion system are derived to ensure conservation. Simulations reveal peculiarities of the process such as that, due to drying, polymerisation happens mostly in bulk and monomer evaporation leads to a poor yield. Various process variants and simulation models are discussed. The impact of process parameters is examined by means of numerical DoEs. The second part presents a novel approach for the simulation of structure evolution in suspension drying. The meshfree SPH method is used to model the relevant physical effects on a detailed scale during the first and second drying period. New implementations of physical effects are derived: heat and mass transfer based on linear driving forces, an implicit solution of the heat equation, several approaches for crust formation and a new formulation of surface tension by pairwise forces. The formation of dense structures as well as hollow granules can be simulated. Model parameters influence crust formation during the second drying period concerning shape and microporosity and can be interpreted in a physical sense.