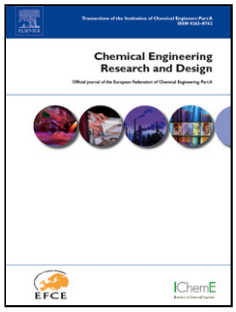

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PII: S0263-8762(14)00161-0
DOI: http://dx.doi.org/doi:10.1016/j.cherd.2014.04.003
Reference: CHERD 1546

To appear in:

Received date: 20-6-2013
Revised date: 22-3-2014
Accepted date: 2-4-2014

Please cite this article as: Szilágyi, B., Muntean, N., Barabás, R., Ponta, O., Lakatos, B.G.,Reaction precipitation of amorphous calcium phosphate: population balance modelling and kinetics, *Chemical Engineering Research and Design* (2014), http://dx.doi.org/10.1016/j.cherd.2014.04.003

Reaction precipitation of amorphous calcium phosphate: population balance modelling and kinetics

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Abstract

Precipitation of amorphous calcium phosphate being a precursor of hydroxy-apatite is investigated using a Y-mixer-tubular reactor device and a population balance model including nucleation, growth and agglomeration of particles. The set of moment equations generated by the population balance equation is solved using the direct quadrature method of moments. The population density function is approximated by gamma distribution with the Laguerre polynomial correction terms. The model parameters are estimated by fitting the population density function to experimental particle size distribution data using the least squares method. Identification of the kinetic parameters and the population density function proves to be satisfactory. The results of sensitivity analysis obtained by simulation with the estimated parameters show similar tendencies as those of experiments. The results demonstrate well that nano-scaled amorphous calcium phosphate can be obtained applying high temperature and high calcium ion concentrations.

Keywords: Amorphous calcium phosphate, Reaction precipitation, Population balance model, DQMOM, Parameter estimation, Simulation

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