Electric-potential-assisted crystallisation of L-isoleucine: a study of nucleation kinetics and its associated parameters

ABSTRACT

The potential of producing L-isoleucine crystals with the aid of electric potential and its effect on the nucleation kinetics of L-isoleucine were probed using polythermal and isothermal crystallisation techniques, assisted with 5 V, 9 V, and 20 V electric potentials. The polythermal experiments were conducted with cooling rates of 0.1 °C/min–0.7 °C/min, whilst isothermal crystallisation was conducted with a supersaturation of 1.30–1.70, and both were carried out in a 200 mL temperature-controlled jacketed reactor. Prediction of the nucleation rate and its associated parameters for isothermal crystallisation was carried out using a molecular dynamics simulation. In both crystallisation techniques, electric potentials increased the nucleation rate, but the intensity of the electric potential had less impact on the measured parameters. Nucleation rates for 5 V isothermal crystallisation were in the order of 1010 higher than for polythermal crystallisation. Electric potential doubled the nucleation rates for polythermal crystallisation and increased the nucleation rates 12-fold in isothermal crystallisation. The isothermal technique produced the form B polymorph, but mixtures of forms A and B were produced in polythermal crystallisation. The predicted critical number of molecules, N*, and the critical radius, r*, were in good agreement with the experimental data, with a higher predicted nucleation rate in the order of 102

Keyword: Molecular dynamics simulation; Metastable zone width (MSZW); Nucleation rate; Polythermal and isothermal crystallisation; Homogeneous and heterogeneous nucleation; Nucleation kinetics; Critical radius; Electrocrystallisation