Computational analysis of unsteady heat and mass transfer in particulate systems

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Industrial production of many particulate materials is accomplished by means of crystallization from supersaturated solutions, supercooled melts or solutions under steady operating conditions when the injection of extra liquid volumes and the removal of a final particulate product are carried out continuously with constant rates during the whole process. The onset of instability in such a process with respect to small disturbances is often observed under certain conditions in the case of a sufficiently sharp dependence of the nucleation rate upon the supersaturation playing the role of a driving force of the process.

The present paper explains the mechanism of instability and a formation of unsteady regimes of heat and mass transfer in particulate systems. The following assumptions are put forward in order to develop a mathematical model. Physical properties of both the solution and the crystals are assumed to be independent of supersaturation and time. It is assumed that the supersaturation concentration, hydrodynamic conditions and supersaturation levels are such as to prevent any noticeable agglomeration or breaking of solid particles. The model is based on the mass balance equation together with the population balance equation expressed in terms of the crystal size distributed. This system of equations with distributed parameters is reduced to a single functional integro-differential equation describing the evolution of the supersaturation for arbitrary mass flux of a supersaturated solution into a volume under consideration, nucleation and crystal growth kinetics and withdrawal rate of crystals out of the volume. The mechanism of instability of a stationary crystallization process is studied. The neutral stability surface is calculated in terms of physical, chemical and processing parameters. Since the

instability is of oscillating nature, one has to expect that either and auto-oscillating or a chaotic pulsating regimes develops, depending on whether the break of stability of a stationary regime belongs to the “soft” or “hard” type. The bifurcation technique applied to the analysis of unstable steady states of continuous crystallization shows the instability to be established in the “soft” manner and to give rise to a regular auto-oscillating process which characteristics are studied details analytically and numerically. The model includes such effects as crystal growth rate fluctuations and a size-dependent crystal withdrawal rate. The good agreement of theoretical results with preciously reported experimental data proves the model developed to be quite adequate. The external periodic modulation of relevant processing parameters is shown to present powerful means of an expedient influence on a crystallization process giving an opportunity to change its properties in a desired direction. Frequency locking phenomena and quasiperiodic oscillations are demonstrated to be not only purely of theoretical concern, but also of prime importance from a practical point of view: in particular, examples are given providing that forced oscillations can yield a mass output exceeding that provided by auto-oscillations.

The significance of the general methods developed is by no means exhausted by their applications to the crystallization problems considered. They could as well be employed in analyzing the combustion of particulate solid and dropwise liquid propellants, numerous combustion processes in turbulent flows encountered in many technological schemes, systems with an exothermal chemical reaction whose rate is strongly dependent on the temperature and reagent concentrations.