**Chiral Symmetry Breaking and Deracemization of Sodium Chlorate in Taylor Vortex Flow**

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**Highlights**

* Taylor vortex flow promoted the chiral symmetry breaking and deracemization.
* Initial chiral symmetry breaking was enhanced by increasing the rotation speed.

**1. Introduction**

Due to the significant difference in pharmacological and biological effect of enantiomers of a chiral compound, the synthesis of chiral substance with a single chirality is of great value. A pioneer study for chiral symmetry breaking was reported by Kondepudi et al.[1] Enantiomerically pure crystals of sodium chlorate was obtained in evaporation crystallization with stirring, whereas symmetric chiral crystals were produced without stirring. Meanwhile, abrasive grinding using glass beads and temperature swing were demonstrated as highly effective techniques for promoting deracemization. [2] [3] According to Ahn et al study on the cooling crystallization of sodium chlorate, it was shown that the initial chiral symmetry breaking strongly depended on the turbulent fluid motion, because the turbulent eddy flow directly dictated the secondary nucleation during the induction period.[4] Thus, the initial chiral symmetry breaking was enhanced by increasing the agitation speed. Also, the final deracemization was determined by initial chiral symmetry breaking. So, the complete deracemization was achieved when the high initial chiral symmetry breaking occurred. It was already known that the periodic Taylor vortex flow was highly effective for the induction of nucleation and phase transformation in polymorphic crystallizations [5]. So, in the present study, Taylor vortex flow was applied to promote the chiral symmetry breaking and deracemization in cooling crystallization of sodium chlorate.

**2. Methods**

The cooling crystallization of sodium chlorate was carried out in a Couette-Taylor (CT) crystallizer. The feed solution of 96 g-NaClO3/100 ml was prepared at a saturated temperature of 26 ºC, and then filtered with micro-filter paper. The feed solution in CT crystallizer was cooled from 26 ºC to 13 ºC at a constant cooling rate for cooling crystallization. After the feed solution reached at 13 ºC, the CT crystallizer was further run for the deracemization. Suspension samples were taken intermittently and quickly ﬁltered using a vacuum pump, then dried in a convection oven. The chirality of crystals was analysed using polarized microscope (Olympus, BX53M, Japan). The crystal enantiomeric excess (CEE) was defined as (CEE = (N major – N minor) / (N major +N minor)), where N major and N minor meant crystal numbers of major and minor forms, respectively.

**3. Results and discussion**

The effect of the Taylor vortex flow on the chiral symmetry breaking and deracemization of sodium chlorate was investigated. As shown in Figure 1(a), initial chiral symmetry breaking (initial CEE) at low rotation speed of 100 rpm occurred at around 50%, and then, increased finally up to 80% (final CEE) by deracemization of chiral crystals. As increasing the rotation speed over 300 rpm, initial chiral symmetry breaking was enhanced over 80% and the complete deracemization was achieved within 7 hours. When considering the results in random turbulent flow, Taylor vortex flow was much effective for initial chiral symmetry breaking and deracemization of chiral crystal due to its unique periodic fluid motion. That is, Taylor vortex was much effective for the secondary nucleation during the induction period, resulting in high initial chiral symmetry breaking. Also, it promoted the deracemization of chiral crystals, bringing about the enantiomeric pure crystals within several hours. The cooling rate was also an influential factor in chiral symmetry breaking and deracemization, as shown Fig. 1(b). Initial chiral symmetry breaking was about 60% at high cooling rate of 0.295 °C/min, and it increased by decreasing the cooling rate. So, 91% of initial chiral symmetry breaking occurred at 0.0738 °C/min of cooling rate due to long induction period for the secondary nucleation. The deracemization also depended on cooling rate. Due to low initial chiral symmetry breaking at high cooling rate (0.295 °C/min), it took about 11 hours for complete of deracemization. However, it was reduced to 6 hours by decreasing the cooling rate to 0.0738 °C/min.

 

(b)

(a)

**Figure 1.** (a) Deracemization of sodium chlorate when varying rotation speed in cooling crystallization, The cooling rate was fixed at 0.197 °C/min; (b) Deracemization of sodium chlorate when varying cooling rate in cooling crystallization, The rotation speed was fixed at 500rpm [Calibri 9].

**4. Conclusions**

The Taylor vortex flow was highly effective for the secondary nucleation, resulting in high initial chiral symmetry breaking in the cooling crystallization of sodium chlorate. So, initial CEE was enhanced by increasing the rotation speed. As initial CEE increased, the deracemization was also facilitated. So, complete deracemization was achieved with initial CEE over 60%

**References**

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