Numerical simulation of kinetic demixing and decomposition in a LaCoO$_3$-$\delta$ oxygen membrane under an oxygen potential gradient

A composition- and temperature-dependent mobility database of all ionic species in the LaCoO$_3$-$\delta$ phase was developed and combined with a La-Co-O thermodynamic database to simulate kinetic demixing and partial decomposition in LaCoO$_3$-$\delta$ oxygen membranes operated under a 0.0001/0.21 bar oxygen partial pressure difference at 1073 K for 1 year. Formation of La$_2$O$_3$, Co$_3$O$_4$, and CoO phases across the membrane is predicted. The kinetic demixing process can be divided into two stages, namely, establishment of the oxygen potential gradient (fast) and demixing of the cations (slow); the former is controlled by the mobility of oxygen ions, and the latter is determined by the higher mobility of Co ions as compared to the La ion in the ABO$_3$-type perovskite. A drift motion of both oxide surfaces towards the high PO$_2$ side occurs with the movement of cations.