

Decomposition of Ionic Liquids in Chemical Processing

M.C. Kroon^{1,2,S}, W. Buijs², C.J. Peters^{1,C} and G.-J. Witkamp²

¹*Department of Chemical Technology, Faculty of Applied Sciences, Delft University of Technology, Delft, Netherlands*
C.J.Peters@tudelft.nl

²*Department of Process and Energy, Faculty of Mechanical, Maritime and Materials Engineering, Delft University of Technology, Delft, Netherlands*

Ionic liquids have been described as novel environmentally benign solvents that can replace traditional volatile organic solvents. The long-term stability of ionic liquids with respect to operating conditions is of utmost importance for their industrial application. Ionic liquids decompose when high temperatures and/or high voltage differences are applied. An indication of the thermal stability is given by the height of the decomposition temperature, whereas the electrochemical stability is manifested by the width of the electrochemical window. However, little is known about the thermal and electrochemical decomposition mechanism, kinetics and products of ionic liquids. In this work the thermal and electrochemical breakdown of several ionic liquids is predicted using quantum chemical calculations and validated by experiments. The quantum chemical calculations showed to be an excellent method to predict the thermal and electrochemical decomposition reactions and products.