

# **Evaluation of 1,3-Butadiene Thermal Stability: Dimerization and Secondary Reactions**

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## **ABSTRACT**

Thermal stability evaluation of exothermic chemical reactions is of great importance to the design and operation of chemical processes. Dominant reaction stoichiometries and their thermochemistry parameters are key elements in the evaluation process. Identification of main reaction pathways under operating conditions will lead to an understanding of the overall thermodynamic and kinetic behavior.

The kinetics of 1,3-butadiene (BD) is an excellent example of dienes that undergo addition reactions. At elevated temperatures, BD monomers may dimerize exothermally, and as temperature increases secondary exothermic reactions will take place. The very high temperature and pressure rates of these reactions may lead to a reaction runaway or even a thermal explosion scenario. BD is a gas at ambient conditions and is very toxic, so the experimental evaluation is very difficult and hazardous.

In this paper, the thermal stability of BD is evaluated. Dimerization and other secondary reactions are investigated by experimental thermal analysis using an Automatic Pressure Adiabatic Calorimeter (APTAC<sup>®</sup>), by theoretical computational quantum chemistry methods, and empirical thermodynamic-energy correlations. A theoretical approach is conducted to predict some of the BD reaction behavior. Results are compared to other literature data obtained using different experimental methods.