The reactions that determine the yield and selectivity of 1,3,5-trioxane

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Abstract

A rapid expansion of production capacities for 1,3,5-trioxane has occurred worldwide, which requires optimizing design and operation and developing new catalysts with high activity and selectivity. Such optimizing and developing need models of phase equilibrium of reaction mixture and of reaction kinetics. Both models have to consider intermolecular forces and chemical reactions accelerated by catalysts. Reported herein are the reactions that actually determine the equilibrium concentration of 1,3,5-trioxane and control the most important side reactions and, therefore, must be taken into consideration in phase equilibrium and reaction kinetic models. On the basis of these findings, new methods and the underlying mechanisms are established to successfully resolve the dilemma that increasing catalyst activity almost always decreases its selectivity to 1,3,5-trioxane. New salt additives are developed for the industrial catalyst H_2SO_4, which increase 1,3,5-trioxane concentration in distillate by 23% but decrease formic acid concentration in coexisting reaction solution phase by 34%.