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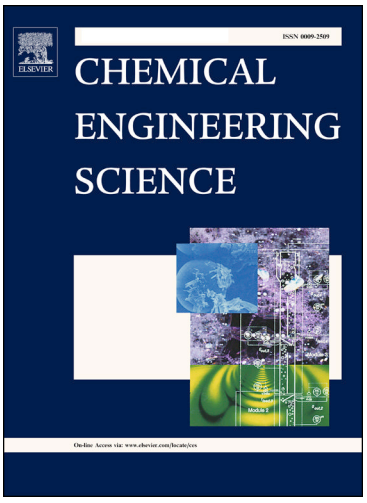

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STOICHIOMETRIC RESTRICTIONS ON OPERATING MODES IN CHEMICAL TECHNOLOGY

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ABSTRACT

It is shown that stoichiometric restrictions on the composition of the gross product stream diverted from the chemical-technological system (hereinafter refers to a chemical process structure where the reactor is considered the heart) define a reaction polyhedron located in a concentration space whose dimension is one less than the number of substances involved in the reaction mixture.

A geometric relationship is established between a reaction and a balanced polyhedron expressing the law of conservation of elements, of which molecules of reacting substances are composed. It is shown that a balanced polyhedron contains a reaction polyhedron and, if their dimensions are equal, they coincide (containing a reaction polyhedron). The main features of a chemical transformation are the degree of conversion of the reagents, the selectivity and yield of the target product, which are linear functions specified on the reaction polyhedron. These functions assume an extreme value at the vertices of the reaction polyhedron and on the faces constructed on the basis of these vertices. The algorithm outlined in this work allows localizing the sets of limiting stationary (steady) states characterized by extreme values of the parameters of chemical transformation, that listed above.

Keywords: stoichiometric analysis, analysis of the statics, limiting stationary states, reactive-distillation processes, reaction polyhedron, chemical interaction manifold (ChIM)

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