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Optimal design of mixture experiments at Effex

Mixture experiments are commonplace in the chemical industry, where some or all the factors are components of a mixture expressed as percentages. These components are subject to a linear equality constraint, which forces the sum of the proportions to equal one. In most cases, the components are box-constrained, meaning there are constraints on the minimum and maximum concentrations of each component. Finally, multicomponent linear constraints involving several factors may also be present. All these constraints define a polytope in certain dimension (bounded convex polyhedron). At Effex, we have implemented a robust optimal design algorithm that uses point exchange for constrained factors, combined with an efficient enumeration of the polytope vertices, and coordinate exchange for other factors (e.g. factors associated with process parameters). The Effex algorithm has the advantage of finding optimal designs for problems involving a large number of components and complex scenarios such as mixture of mixtures problems, hard-to-change factors and blocking.

Special/ Invited session

Software Session

Classification

Mainly application

Keywords

Primary author: NUNEZ ARES, Jose (EFFEX)

Presenter: NUNEZ ARES, Jose (EFFEX)

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