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Abstract

Within the framework of elementary process functions (Freund and Sundmacher (2008)) an approach is developed to derive reactor-network candidates from the solution of a dynamic optimization of a batch process scheme by analyzing its optimal mass and energy control fluxes. Thereby, any characteristics of the reaction progress can be identified, e.g. benefits from mixing, back-mixing, recycling, heating, cooling, etc. The approach is used to (i) determine the attainable region for the modified, isothermal van-de-Vusse reaction, which matches literature results; and (ii) synthesize reactor-network candidates for the standard, non-isothermal van-de-Vusse reaction, which gives new insights compared to previous results from literature using superstructure optimization approaches. The results indicate how this approach can be used to determine the attainable region of a process and to rationally select candidates for detailed reactor design with, e.g. superstructure optimization. It further closes the gap between dynamic batch optimization and continuous reactor-network synthesis.