New Method and Software for Computer-Aided Flowsheet Design and Analysis - DTU Orbit (04/08/2019)

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Process synthesis-design involves identification of the best processing route to produce a desired product from a specified set of raw materials. In this work a systematic, multistage method and corresponding software (ProCAFD) is developed for sustainable process synthesis-design and analysis of chemical and biochemical processes. The developed method is capable of generating all the alternatives for a synthesis problem covering the entire search space of alternatives. The synthesis method is based on a group contribution based hybrid approach, where chemical process flowsheets are synthesized in the same way as atoms or groups of atoms are synthesized to form molecules in computer aided molecular design (CAMD) techniques. Another important aspect of this method is the integration of economic, sustainability and LCA analyses in the early stages of process synthesis to identify process hotspots and further improve the process using innovative design strategies. An overview of the key concepts and the method is presented along with a case study to generate sustainable designs for production of benzene from toluene and hydrogen.

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