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Description of benchmarks homoazeo20 and homoazeo40

The homoazeo40.mod has three solutions corresponding to the lower concentration steady state (LSS), upper stable steady state or higher steady state (HSS), and unstable steady state (USS). The distillate molar flow rate, denoted by D, can be chosen as bifurcation parameter.

The homoazeo20.mod has a single solution, and also differs from homoazeo40.mod in the number of theoretical stages and in the feed stage location, besides the bifurcation parameter value.

The unstable steady state is missed by state-of-the-art methods such as the inside-out algorithm or the simultaneous correction procedure, even when supplied with a good initial guess obtained with case study. Bifurcation diagrams were computed with continuation methods earlier, for example:

Arjun Vadapalli, J. D. Seader;
A generalized framework for computing bifurcation diagrams using process simulation programs;
Computers and Chemical Engineering 25 (2001) 445–464

A. Kannan, Manish R. Joshi, G. Ramalinga Reddy, and Denish M. Shah;
Multiple-Steady-States Identification in Homogeneous Azeotropic Distillation Using a Process Simulator;
Ind. Eng. Chem. Res., 2005, 44 (12), 4386-4399; DOI: 10.1021/ie049443s

Güttinger, Dorn and Morari (see below) used the following software to compute the unstable steady state:

Doedel, E. J.; Wang, X. AUTO94: Software for Continuation and Bifurcation Problems in Ordinary Differential Equations; Computer Science Department of Concordia University: Montreal, Canada, 1994

Except the number of stages and the feed stage location, the model and its parameters correspond to the "Auto model" discussed in:

Thomas E. Güttinger, Cornelius Dorn, Manfred Morari;
Experimental Study of Multiple Steady States in Homogeneous Azeotropic Distillation;
Ind. Eng. Chem. Res. 1997, 36, 794-802

Solving this model with interval methods seems to be first discussed in:

A. Baharev, E. Rév;
A complete nonlinear system solver using affine arithmetic;
Interval Analysis and Constraint Propagation for Applications (IntCP 2009);
Workshop held in conjunction with the 15th International Conference on Principles and Practice of Constraint Programming (CP 2009);
Lisbon, Portugal, September 20th, 2009

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The above interval method finds the three solutions in 9 s without any user provided initial guesses.