

SUPPLEMENTAL MATERIAL

Globally Optimal Simultaneous Heat

Exchanger Network Synthesis and Basic

Heat Exchanger Design

Diego G. Oliva¹, Andre L. Nahes², Julia Lemos², André L.

H. Costa², Miguel J. Bagajewicz^{3,4,*}

¹INGAR Institute for Process Design and Development, INGAR UTN-CONICET, Santa Fe, Argentina.

²Institute of Chemistry, Rio de Janeiro State University (UERJ), Rio de Janeiro, RJ, Brazil

³School of Chemistry, Federal University of Rio de Janeiro, (UERJ), Rio de Janeiro, Brazil

⁴School of Chemical, Biological, and Materials Engineering, University of Oklahoma, Norman, Oklahoma 73019

(*) Corresponding Author: Miguel Bagajewicz: bagajewicz@ou.edu.

All the data needed to run the global optimization procedure is included in the body of the article. There is no additional data. The proposed approach is an adaptation of the enumeration procedure developed by Chang et al. (2020). We now add some details about the implementation of selected steps (0 to 8) of the revised procedure:

1. Step 1: This step calls for obtaining the first *MSTR*. The procedure to do this is to run the Synheat model (see Chang et al., 2020) and several other sources available. One of these sources is the .gms file available at https://www.gams.com/latest/gamslib_ml/libhtml/gamslib_synheat.html. This code needs to be modified to
 - a. Include a constraint that limits the number of exchangers to be less than or equal to the minimum number of exchangers. Specifically:

$$\text{sum}((i,j),z(i,j))+\text{sum}(i,zcu(i))+\text{sum}(j,zhu(j))=l=Nmin;$$
 - b. Replace the objective function with a dummy variable.
 - c. Use $EMAT=HRAT_{Min}$
2. Step 3: This step calls for calculating the minimum energy consumption. This is accomplished by modifying the Synheat model as follows:
 - a. Replace the objective function with the total hot utility consumption.
 - b. Use $EMAT=HRAT_{Min}$
 - c. Fix the binary variables representing the exchangers ($z(i,j)$, $zcu(i)$, $zhu(j)$) to be equal to the solution obtained in step 1.
3. Step 4: This step calls for calculating the maximum energy consumption. This is accomplished the same way as in Step 3, using $EMAT=HRAT_{Max}$
4. Step 5: Once the energy consumption and the matches defining the exchangers are defined, the heat load of each exchanger is obtained solving a linear system. As stated the design of each heat exchanger is obtained using Set Trimming followed by Sorting (Lemos et al., 2020).
5. Step 6: The Direct method (Jones and Martins, 2021) mentioned is available at <https://docs.scipy.org/doc/scipy/reference/generated/scipy.optimize.direct.html>. As in Step 5, the design of each heat exchanger is obtained using Set Trimming followed by Sorting (Lemos et al., 2020).

REFERENCES

- Chang, C.; Peccini, A.; Wang, Y.; Costa, A.L.H.; Bagajewicz, M.J. Globally Optimal Synthesis of Heat Exchanger Networks. Part I: Minimal Networks. *AIChE J.* 2020a, 66, e16267.
- Jones, D.R.; Martins, J.R.R.A. The DIRECT algorithm: 25 years later. *J. Glob. Optim.* 2021, 79, 521-566
- Lemos, J.C, Costa, A.L.H, Bagajewicz, M.J. Set trimming procedure for the design optimization of shell and tube heat exchangers. *Ind. Eng. Chem. Res.* 2020, 59, 14048–14054.