

Methods Part 1 (Basics of industrial ecology data and accounting)

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IEooc_Methods1_Exercise2: Data reconciliation and inference

Goal: Understand data reconciliation and apply data reconciliation to a simple system. Use of mass balance to formulate constraints and to determine non-measured variables. Understand the basics of the maximum entropy principle

Reading: Chapter 1 in Narasimhan and Jordache and chapter 8 of the course material of the MIT course 6.050J/2.110J – Information, Entropy and Computation (cf. reference list below).

Part 1:

This exercise shall give you some hands-on experience on improving the quality of measurements by making them adhere to mass balance constraints using data reconciliation. It shall also help to understand how the system description can be reconciled in the case of missing data, and how the latter can be estimated. The techniques build on the basis explained in the lecture. They use some of the examples of chapter 1 in Narasimhan and Jordache (2000). The default software for obtaining a solution is Excel, but other software or manual calculations can be used, too.

The example will use the system in figure 1-2. There are six system variables and in the accompanying Excel file the measured values as well as the uncertainties of the measurements are given. The 'true' values are also given for your reference, but these are unknown to the people working in the plant.

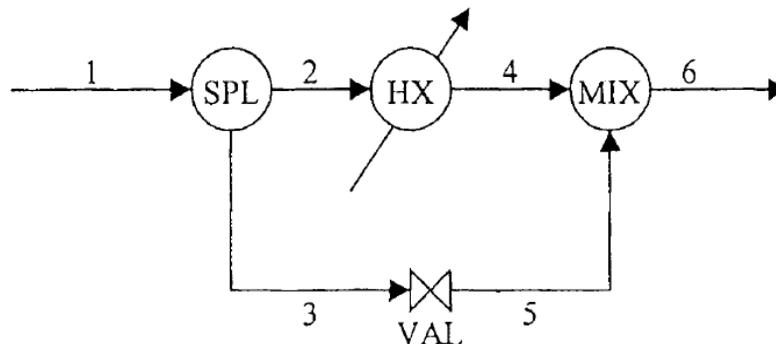


Figure 1-2. Heat exchanger system with bypass.

Figure 1-2: System definition of the example. SPL: Splitter, HX: heat exchanger, VAL: valve, MIX: Mixer. Only the mass flows of the reactant are shown. From Narasimhan and Jordache (2000).

Part II Methods

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The following questions shall be answered and the answers shall be documented, e.g., in an annotated Excel sheet.

- 1) How big are the mass balance mismatches for the processes in the system, both in absolute and in relative terms?
- 2) Determine a reconciled system solution using least square optimisation and the 'Solver' function of Excel (or any other optimisation tool). Assume that the deviation of each system variable has the same weight in the objective function. Do the reconciled data fulfil the mass balance? Calculate the absolute and relative changes of the flow values before and after reconciliation. Are the reconciled values the same as the 'true' values and why/why not?
- 3) Use the uncertainties of the measurements given to modify your objective function so that more certain parameters will change less! Then redo the reconciliation. Explain how the uncertainties enter the objective function and how the reconciled values differ from the case with equal weight.
- 4) Assume now that no measurements were performed for flows 3 and 4. Why is it still possible to reconcile the other measurements and to determine flows 3 and 4 from mass balance? Formulate a new set of constraints for the reduced set of measurements and reconcile the latter including the uncertainties given. Determine flows 3 and 4 from the results. How do the results differ compared to the case in task 3? What would have happened if flow 2 would not have been measured either?

Part 2:

- 1) Read the course chapter on statistical inference! What is the principle of maximum entropy and how could it be applied in the industrial ecology methods material flow analysis, life cycle inventory modelling, and input-output analysis?
- 2) Work through the example of Berger's Burgers (section 8.1.3 and 8.2)! Solve equation 8.26 numerically for $p(F)$ and confirm the results for $p(B)$ and $p(C)$ as well as the average calorie count of each meal and the percentage of meals served cold!

References:

Narasimhan, S., Jordache, C., 2000. Data Reconciliation & Gross Error Detection. An Intelligent Use of Process Data. Gulf Publishing Company, Houston, Texas.

MIT, Department of Electrical Engineering and Computer Science, Department of Mechanical Engineering, course 6.050J/2.110J – Information, Entropy and Computation. <http://www-mtl.mit.edu/Courses/6.050/2014/notes/chapter8.pdf>



(except for Figure 1-2.)