Water System Integration by the Process Superstructure Development

Ljubica Matijašević*, Damjan Spoja, Igor Dejanović Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, 10000 Zagreb, Croatia, ljmatij@fkit.hr

The methodology of mass and energy integration is widely applied for reduction of water consumption, which belongs to the area of mass integration, and is also energy integration problem if water is considered an energy source (cooling water and steam). This work presents a water-use reduction study, through process superstructure optimization.

1. Introduction

Present work describes tackling of the issues of the integrated system of water consumption where the water-related processes and wastewater treatment operations are integrated into a unique network so that the overall costs of fresh water consumption and the costs of wastewater treatment are minimized. The method is algorithmic and based on the superstructure that includes all potential solutions to water treatment, its re-use and recirculation. The procedure was based on relaxation of a non-convex non-linear programming problem into a mixed integer linear programming (MILP). The MILP model was further simplified using heuristic rules and solved by using MATLAB. A petroleum refinery water network was analysed, and a solution proposed that achieves the mentioned goals i.e. minimal fresh water and wastewater treatment costs. Three processes which use water, with three pollutants, were monitored and three potential treatment units were proposed.

2. General

A short report on industrial water use and graphical methods available for reduction of water consumption, has already been provided by many authors, such as Smith, 2005; Mann and Liu, 1999; Bagajewicz, 2000, and Gomes et al., 2005; Matijašević and Dejanović.,2007. The problem of optimal synthesis of an integrated water system is addressed by Yiqing and Xigang (2008). Optimization of water networks with multiple contaminants has been described by Galan and Grossmann (1998); Karuppiah and Grossmann (2006, 2008); Isafiade and Fraser (2009); Jeżowski and Wałczyk (2008); Tan et al. (2009); Teles et al. (2009) and Poplewski et al. (2010). In this paper the mathematical programming approach is based on heuristic rules which assist the formulation of the real industry process model in such a way that a mixed integer nonlinear programming problem can be derived for multiple contaminants.

Every operation which uses water is described by a mathematical model. Choice of an objective function depends on the model and its limitations. The limitations can refer to the mass and energy balances, thermodynamic conditions, environmental requirements, technical requirements, etc. Final results of optimisation are optimal parameters of every operation and optimal structure of the mass exchange network.

2.1 Synthesis of the water flows network

A superstructure is a process model which incorporates all possible operations and their possible interactions. These units are then linked by the mixing units (MUs) and splitter units (SUs) in a way that by manipulating the split ratios in MUs and SUs every conceivable network configuration can be achieved. The goal is to find a network configuration through optimization that will either minimize fresh water consumption and the number of waste streams or, generally and more frequently, minimize total construction costs and the network operation costs.

In the process units water is being polluted with certain amount of impurities which are removed in the treatment units. Balance of the substances in these units as well as of those in the splitting units and flow mixers, which help linking of the units, must be satisfactory. Other limitations are: concentration of impurities in the flows which shall not exceed the specification, and concentration of impurities which shall meet the requirements for release into environment.

2.2 Model development

First task is to choose an appropriate objective function. There are different possibilities, and the most common is to minimise total annualized cost of the water system. The system model taken into account is designed by balancing the substances for every plant separately. Balancing is usually made around branching point of the flows, when they are released from the process or treatment, i.e. either in the splitters or at the mixing point at the entry to the process unit or to the treatment unit i.e. in the mixers.

3. Motivation

Reduction of the process water consumption in the local oil refinery (Spoja, 2007). The analysis comprised three sub-systems which use process water. The first sub-system is a steam stripper; the second one is a hydrodesulphurisation plant which uses water in a high-pressure section, and the third one is a desalter unit which is part of a crude oil atmospheric distillation plant. Three major pollutants taken into consideration were hydrogen sulphide, oil and suspended particles. Figure 1 shows a superstructure with all possible combinations of the existing units. Limiting values for hydrogen sulphide, oil and suspended particles. Figure 1 shows are shown in Table 1. The flows in all units are fixed. The available treatment plants: sour water stripper (TU1) for removal of H₂S, oil separator (TU2) and a coagulation, sedimentation and filtering unit (TU3). Table 2 presents the data about the efficiency and costs.Considered are three process units. PU1 denotes a steam stripper, PU2 a high-pressure section of HDS and PU3 denotes a desalter. There are also three treatment units. TU1 denotes a sour water stripper (SWS), TU2 oil separator and TU3 coagulation, sedimentation and filtering



unit. The goal is to determine the flows and composition of impurities in every stream of the network so as to minimise total costs of the fresh water and wastewater treatment.

Figure 1: A superstructure of the chosen example

Table 1 Limits for the flows and borderline levels of pollutants

	$C_{in} \ ppm \ H_2S$	Flowrate t/h	$egin{array}{c} C_{out} \ ppm \ H_2S \end{array}$	Δm kg/h H ₂ S	C _{in} ppm oil	C _{out} ppm oil	Δm kg/h oil	C _{in} ppm TSS	C _{out} ppm TSS	∆m kg/h TSS
Steam stripper	0	6	389	2.33	0	10	0.06	0	26	0.16
HDS	350	5.5	12300	65.73	20	116	0.53	50	70	0.13
Desalter	20	14	30	0.14	120	215	1.33	60	115	0.77

Table 2 The efficiency and investment and operating costs of the treatment units

	Removal ratio (%)			IC	OC	a	
	H_2S	oil	TSS	IC I	00	α	
TU1	99.9	0	0	16800	1	0.7	
TU2	0	95	20	12600	0.0067	0.7	
TU3	92	90	97	24000	0.033	0.7	

3.1 Design of a model

Design of a model takes into account overall flows and overall composition. Objective function was taken from Karuppiah and Grossmann, 2006, and is expressed by the Equation 1.

$$\min \phi = H C_{FW} FW + AR \sum_{\substack{t \in TU \\ t \in t_{k}}} IC^{t} \left(F^{i}\right)^{\alpha} + H \sum_{\substack{t \in TU \\ t \in t_{k}}} OC^{t} F^{i}$$
(1)

where: H - h of plant operation/y (h), C_{FW} - cost of fresh water (\$/t), FW freshwater intake into the system (t/h), AR – annualized factor for investment on treatment unit, IC^t

(Fⁱ) ^{α}- investment cost for treatment unit *t* (\$), OC^t Fⁱoperating cost for treatment unit *t* (\$/h), α –cost function exponent (0< $\alpha \le 1$). When the objective function is defined, the balances are made of the flow of substances from all the units under consideration which are mathematical models used in solving the problem. The problem is not a simple one. The initial NLP model is solved by the MILP model (Galan and Grossmann, 1998; Karuppiah and Grossmann, 2006).

3.2 Model solving

Solving of the given model requires a powerful optimization tool, such as GAMS. Due to unavailability of this support, the model has been simplified and solved using MATLAB. Solving of the tasks in MATLAB requires a number of assumptions and simplifications. Some assumptions require the data obtained by the graphical method (Matijašević and Dejanović, 2007): assumption 1- PU1 uses exclusively fresh water, assumption 2-Outlet concentration of H₂S from PU2 is too high to accomplish the return PU3 without pre-treatment, which increases the costs. Therefore, this option has not been taken into account, as supported by the solution obtained from the graphical method. Assumption 3 -The remaining flow from the treatment unit TU1 which is not returned to PU3 is channelled directly to TU3, given the fact that oil volumes are not high. Thus, the unit for oil removal need not be used. Assumption 4-The return from the treatment units TU1 and TU2 has not been taken into account because this would not satisfy the binding concentrations on release, due to very high concentrations of H₂S.

4. Results

Figure 2 shows the simplified superstructure after introduction of the assumptions and simplifications.



Figure 2: The superstructure after introduction of the assumptions and simplifications

The results obtained in the MATLAB (Table 3) have been used to design the optimal network of water flows (Figure 3).

Table 3 Water flows for the presented superstructure

Total consumption of freshwater	16.65 t/h	-
Total investment cost	621,135 \$ / y	

Consumption of freshwater for PU1	6 t/h
Consumption of freshwater for PU2	0.0004 t/h
Consumption of freshwater for PU3	10.64 t/h
Flowrate from PU1 to TU1	0.50 t/h
Return from PU1 to PU2	5.5 t/h
Flowrate from PU2 to TU1	5.5 t/h
Flowrate from TU1 to TU3	2.65 t/h
Return from TU1 to PU3	3.35 t/h
Flowrate from PU3 to TU2	2.25 t/h



Figure 3: Network of water flows after optimisation

The comparison of a base-case and optimised water system is given in Table 4.

Table 4 Comparison of the base-case with optimized network

	f _w (t/h)	$\Delta f_w(t/h)$	TIC	TCP
Base case	25.50	0.00	214,080	667,780
Optimal solution	16.65	8.85	145,870	621,135
Suitable for recipient No. V	16.65	8.85	133,150	592,649

5. Conclusion

This work presents the approach to optimization of water consumption in the oil processing industry. The optimization is achieved with a developed superstructure and by simplification of the non-convex, non-linear NLP model with partial linearization and transition into the MILP form. In order to unavailability of the adequate software for tackling such problems, the superstructure requires simplification, so as to carry out the optimization in the MATLAB. The simplifications are performed by the graphical method too. In our case the employed mathematical method with the superstructures, where we take into account several contaminants and known operating costs, shows to be more precise than the graphical one. Fresh water consumption is reduced and so are the operating costs. Legal constraints on the contaminants at the release into environment are met.

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