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Including Fluctuations of Water Content in Feed Streams and Products for the Optimal Management of Water Resources

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In the food industry, water is frequently used both as a system utility and as a component that enters products and sub products. In other words, fresh water entering the process exits it either in the wastewaters or in the products. Consequently, the usual optimisation techniques for minimizing the overall water consumption are to be modified accordingly. In particular, the presence of chemical reactions in the balance equations can give rise to severe nonlinearities which are to be taken into account in the preliminary reconciliation of the process measurements, as well as in the following optimisation step. Furthermore, the presence of bilinear terms (flow-rates multiplied by concentrations) results in the model being non-convex. The objective function employed is the overall NPV function that considers both capital and operation costs, using a conventional 5 % discount factor. If all treatment options for the wastewaters and all possible interactions among the units are considered for the overall optimisation, the resulting superstructure gives rise to a stochastic non-convex MINLP problem, which was solved by combining an order optimisation approach with the Baron algorithm in the GAMS environment, as well as with software available in the public domain. No substantial difference in accuracy and efficiency between the two algorithms was observed. The method is applied to a complex process for the manufacture of starches and starch products and analysed the reduction in fresh water consumption as a result of the optimisation procedure.

1. Introduction

Water networks optimisation has been the object of a large amount of both theoretical and applied research. It can be regarded as a special case of a mass exchanger network (MEN) problem as developed by the pioneer work of El-Halwagi and Manousiouthakis (1989). Their work was based on a generalization of pinch analysis for heat integration (Linnhoff and Hindmarsh, 1983). Specific water pinch analysis was developed in the seminal articles of Wang and Smith (Wang and Smith, 1994a), who presented systematic graphical methods for targeting and design (Wang and Smith, 1995). As an alternative or as a complement to pinch analysis (Chew et al., 2015), mathematical programming methods, based on a water network superstructure including all feasible alternatives, can be used (Takama et al., 1980). Their use has been extended to a number of industrial cases including wastewater minimisation (Wang and Smith, 1994b), heat recovery optimisation (Solisio et al., 2012), total site analysis (Čuček et al., 2014). An extensive review on the optimization of water resources has been provided by Klemes (2012).
As discussed by Biegler, Grossmann, and Westerberg (1997), the optimum design can be identified using an optimisation algorithm capable to deal with suitable nonlinear, generally nonconvex objective functions and constraints including both continuous and discrete variables. The latter correspond to binary variables which specify the presence/absence of the option associated with the variable in the superstructure. The resulting algorithm is an MINLP optimisation solver, the most frequently used of which is BARON (Tawarmalani and Sahinidis, 2005) which can provide the global optimum solution of the network.
In the food industry, there is generally a twofold use of water. Water streams can be and generally are part of the usual utility system but are frequently also incorporated in the products. Thus, there arise additional difficulties with respect to the case in which water is only a system utility, because the amount of contaminants transferred from process streams to the water streams is subject to a double constraint: the quality of products

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and wastewater concentration which may need regenerating before being discharged. As shown in Section 2, this requires a modification of the algorithms for both process monitoring and optimisation.
The article is organized as follows. In Section 2, the overall mathematical model is introduced with a view to emphasizing the differences to the processes where there is no additional uncertainty due to the presence of a fluctuating amount of water in the products. In Section 3, a general description of the layout of the plant considered is provided along with some results obtained using the procedure outlined in this paper: some limitations in the amount of information is due to confidentiality requirement. In Section 4, the conclusions are outlined.

2. The mathematical model

The mathematical model includes two steps. The first of them, outlined in Section 2.1, is a generalization of standard process data reconciliation to include fluctuating water sinks. The reconciliation procedure is necessary for the optimisation step to use actual process variables, which occasionally do not coincide with the nominal values.
The actual optimisation is examined in Section 2.2. Again, the extension to fluctuating water sinks in the products requires the introduction of adequate modifications in the usual process optimisation algorithms.

2.1 The reconciliation of process data

The reconciliation of steady-state processes is frequently carried out using adequate statistical objective functions (typically a likelihood function) which are optimised subject to constraints due to steady-state equations provided by material balances. If, additionally, only one component is considered (which is precisely the case if water resources are examined), the mass balances provide a set of linear equations and the maximization can be carried out analytically, which makes it possible to detect and remove gross errors.

Suppose $\boldsymbol{x}'$ are measurements of process water flow-rates and $\hat{\boldsymbol{x}}$ are the corresponding rectified values. They satisfy the set of steady-state material balances

$$A\hat{x} = 0 \tag{1}$$

where A is the incidence matrix and $\boldsymbol{x}$ the flow rates of all the water streams of the process. The number of rows of A, *m*, is equal to the number of units for which a material balance is considered, whereas the number of its columns, *n*, is given by the total number of streams present in the process.
The element a_{ij} is given by

$$a_{ij} = \begin{cases} 1 \text{ if the stream j enters the unit i} \\ -1 \text{ if the stream j leaves the unit i} \\ 0 \text{ otherwise} \end{cases}$$

However, the fluctuating content of water in the products - which correspond to some of the $\hat{\boldsymbol{x}}$ in Eq(1) - is not measured online; rather, samples are periodically collected and subjected to a quality control procedure that determines the water content. Thus, their average statistical properties (including the components of their variance-covariance) over the interval of time corresponding to the sampling frequency are available, the relevant information cannot be used directly but has to be adequately adjusted.

Using the fluctuations detected in the quality control procedure, the relevant statistical information can be employed to construct an a priori likelihood function $p_0\left(\hat{x}_p\right) = p_0\left(y\right)$ which is supposed to be

$$p_0\left(y\right) \propto e^{-y^T V_p^{-1} y} \tag{2}$$

where the subscript p is the index for the product flow rate vectors.
The a priori likelihood function is combined with the distribution resulting from dynamic fluctuations (Guo et al., 2017) using Bayes' theorem, with the information provided by the measurements of x whose experimental errors are also supposed to be normally distributed. This provides the “a posteriori” likelihood function

$$e^{-\left(\hat{\boldsymbol{x}}-\boldsymbol{x}'\right)^T V^{-1}\left(\hat{\boldsymbol{x}}-\boldsymbol{x}'\right)} \cdot e^{-y^T V_p^{-1} y} \tag{3}$$

(where *V* is the variance-covariance matrix of the process) subject to $A\hat{x} = y$.
Equivalently, the solution is given by the minimum of

$$\left(\hat{\boldsymbol{x}}-\boldsymbol{x}'\right)^T V^{-1}\left(\hat{\boldsymbol{x}}-\boldsymbol{x}'\right)+y^T V_p^{-1} y \tag{4}$$

subject to

$$A\hat{x} = y \tag{5}$$

This problem can be solved in closed form for $\hat{\boldsymbol{x}}$

$$\hat{\boldsymbol{x}} = \left[A^T V_p^{-1} A + V^{-1}\right]^{-1} V^{-1} x' \tag{6}$$

If some measurements are missing, the procedure described by Crowe, Garcia Campos, and Hrymak (1983) can be used to reconcile the values that are identifiable.

While the matrix V_p is evaluated directly by the quality control system, a tuning procedure for the determination of the incidence matrix *V* can be established following the strategy proposed by Dovì and Del Borghi (2001) for hold-up fluctuations. Constraining the sum of squared deviations of a train of measurements (including *q* data sets) to satisfy the chi square distribution provides the optimisation criterion:

$$\Phi = \sum_q \varphi_q^2 = \sum_q \left\{ x_q^T \left[\left(A^T V_p^{-1} A + V^{-1}\right)^{-1} V^{-1} - I\right]^T V^{-1} \left[\left(A^T V_p^{-1} A + V^{-1}\right)^{-1} V^{-1} - I\right] x_q - \nu \right\}^2 = \min \tag{7}$$

where ν is the dimension of $\boldsymbol{x}$. The minimization with respect to the elements of *V* can be efficiently carried out using a Gauss-Newton algorithm.

However, minimizing Φ does not necessarily satisfy the chi-test (although the resulting distribution is as close as possible to the χ^2 distribution, it might be not close enough). To this purpose, the Kolmogorov-Smirnov test can be used (Dovì and Del Borghi, 2001) to verify whether there is enough experimental evidence or the number of the data sets in the training period is to be increased.

Thus, the overall procedure for process data reconciliation in the presence of an a-priori water content distribution in the products has been completely outlined.

2.2 The optimisation of water resources

The fluctuations in the physical-chemical properties and composition of the raw materials input to the plants make it necessary to consider stochastic variables in the optimal design of food processes.

Combined with the necessity of considering binary variables for the description of structure alternatives and continuous parameters for the other unknown parameters of the process, the uncertainty of the supply conditions gives rise to a stochastic mixed integer non linear programming problem. In other words, it is possible to formulate the optimal design problem as

$$\begin{aligned} &\underset{x,y}{opt}\ E_s\{f(x,y,s)\} \\ &s.t.\begin{cases} h(x,y,s)=0 \\ g(x,y,s)\le 0 \\ x\in\Re^m \\ y\in\Re^n \end{cases} \end{aligned} \tag{8}$$

where $s \in \Re^k$ is the vector of variables subject to a known probability distribution function, *f* is a scalar function, *h* is a vector that represents the equations of the process and *g* is a vector of inequalities introduced to exclude unsuitable or physically impossible solutions. The dependence of the functions *f,h,g* on decision variables *y*, operation variables x and stochastic parameters *s* is non convex and highly non linear.

The objective function *f* (to be minimized) is generally given by the annualized cost of freshwater consumption and regeneration of wastewater. While freshwater consumption due to the fluctuating content of water in the product depends only on the properties of supply input, the make-up due to evaporation and wastewater discharge after the necessary decontamination procedures depend on the process structure and on the adoption of water reuse and recycling strategies and is consequently the result of the overall optimisation task provided by Eq(8). For every instance of the vector ***s,*** an MINLP has to be solved. An analysis of the application of MINLP algorithm to water networks can be found in Ahmetović and Grossmann, 2011. Due to the problem being non convex, there can be more than one minimum with possibly largely different values of the objective function. As anticipated in the introduction, the presence of multiple minimum points, an algorithm capable of locating a global minimum has to be adopted. The possibly most frequently used software is the BARON code (Tawarmalani and Sahinidis, 2005) available in the GAMS environment. It implements a global optimisation strategy using the branch-and-bound approach coupled with a number of additional techniques for reducing ranges of variables) and is guaranteed to locate global optima under general assumptions, that are practically always satisfied, such as the existence of finite lower and upper bounds on the nonlinear terms contained in problem (7). In the study case described below, both BARON and COUENNE (an MINLP reformulation-based spatial branch & bound algorithm that uses branching, bound reduction, linearization and heuristics to find feasible solutions, Belotti et al., 2013) have been used for comparison. No substantial difference in terms of efficiency and robustness has been found, which is a significant result because COUENNE is available in the public domain, although the input file has to be provide using the AMPL syntax (Fourer et al., 1990). On the other hand, if the vector ***s*** is allowed to take up values corresponding to its probability distribution, full stochastic mixed integer non linear programming (SMINLP) has to be used. To this purpose, numerical integration methods, such as the one proposed by Novak and Kravanja (1999), use a discretisation of the probability distribution functions and Gaussian integration to obtain the variables in the resulting discrete distribution. Sample average methods provide another class of SMINLP algorithms and are generally based on Monte Carlo simulation techniques. Monte Carlo simulations use pseudo-random samples creating specific values of a probability distribution by inverse transformation of the cumulative distribution function. They provide one of the most widely used framework for a large number of problems in chemical engineering including process planning, reactor design, risk analysis (Fabiano et al., 2015). In the so-called internal sampling methods, such as the two-stage stochastic programs with recourse, samples are modified in the course of the optimisation procedure. On the other hand, external sampling approaches embed SMINLP into the framework of MINLP and in doing so transform stochastic problems into a sequence of deterministic problems, which can be solved using well-proven deterministic algorithms.

Embedding either MINLP algorithms into a stochastic framework often implies an intractably high number of solutions of single MINLP problems. The computational difficulties are related to the computational burden resulting from a large (and possibly very large) number of binary variables (which are combinatorial in nature) and of uncertain variables subject to a known probability distribution function. The burden is associated with the optimisation being carried out on a cardinality basis, i.e. each optimum results from an accurate computation of cardinal values. Using ordinal optimisation reduces the overall computational effort considerably. The ordinal optimisation methodology has been developed with a view to tackling hard problems (including, but not limited to problems with uncertainties), whose solution requires a computational effort that grows exponentially with respect to the problem size. Typically, NP complete problems fall into this class.

The ordinal optimisation methodology is based on two main considerations (Wen et al., 2009): (1) it is less expensive to evaluate ‘‘order’’ than “cardinal value’’; (2) the goal of the optimisation task is not to identify the ‘‘best for sure’’, but rather a ‘‘good enough’’ solution. In other words, a reduced subset of solutions is identified using a shortcut procedure followed by a rigorous procedure to determine the optimum solution that belongs to the subset. The ordinal optimisation methodology can therefore be regarded as a general strategy (much the same as branch-and-bound techniques) that is instanced on a case-by-case basis by specifying the preliminary shortcut procedure necessary to reduce the domain of optimal solutions to a (possibly small) subset in which the actual solution is finally to be searched. In this paper, the simplifying procedure is a substantial relaxation of the integrality condition. Indeed, reducing the tolerance to a value of 0.1 makes it possible to abate the computational time of a SMINLP to a value comparable to that of a simple MINLP. Selecting the binary options (discrete variables) to the integer values closest to the values obtained reducing the tolerance transforms the original SMINLP problem into an SNLP problem whose solutions do not require a high computational burden. Defining the original SMINLP with relaxed integrality conditions as SRMINLP, the overall procedure can therefore be regarded as an SRMINLP followed by a reformulation of the original problem with fixed binary options (i.e. the structure is fixed), followed in turn by a final SNLP.

3. Case study

The algorithms described in the previous sections have been applied to an existing industrial plant. The case study considered represents a large-scale plant involving eleven water using units (corresponding to six processing phases), seven treatment units (four for incoming water preparation and three for waste water treatment) and one main contaminant. The plant is a biorefinery which transforms raw corn into starches, starch products, sugars and fermentations products that are marketed in several sectors like food, animal nutrition, chemical and pharmaceutical industry. The initial transformation phases are mainly characterised by physical

separation processes (wet milling for corn steeping and by-products separation, and dry milling for final starch products) while the following phases are characterised by physical-chemical, chemical or biochemical processes (acid and enzymatic starch liquefaction, hydrolysis and fermentation).
A simplified scheme of the global process is shown in Figure 1. Water is supplied to the plant from superficial and deep aquifers, from a nearby stream and to a lesser extent from public water supply. The incoming freshwater is subjected to different treatment depending on its origin and its use. In particular:

- Deep aquifer water is used to produce crude water for the production process.
- Superficial aquifer water gets purified through filtration to generate crude water (C) for the production process.
- Water from the stream is used for auxiliary purposes (e.g. cooling service).
- Crude water is treated in reverse osmosis and softener units, and demineralization columns (anionic, cationic, decarbonisation) to produce demineralised (D) and soft (S) water.
- Demineralised water is used to produce process steam (P).

The scheme reported in Figure 1 details the grade of water consumed by each unit (as per legend). Beyond the grades mentioned above the scheme highlights the production/consumption of recycled water streams (R) as well as evaporation losses (L) and wastewaters (W) generated by product washing treatments. Waste waters undergo anaerobic and aerobic treatments to reduce the contaminant concentration before being discharged.

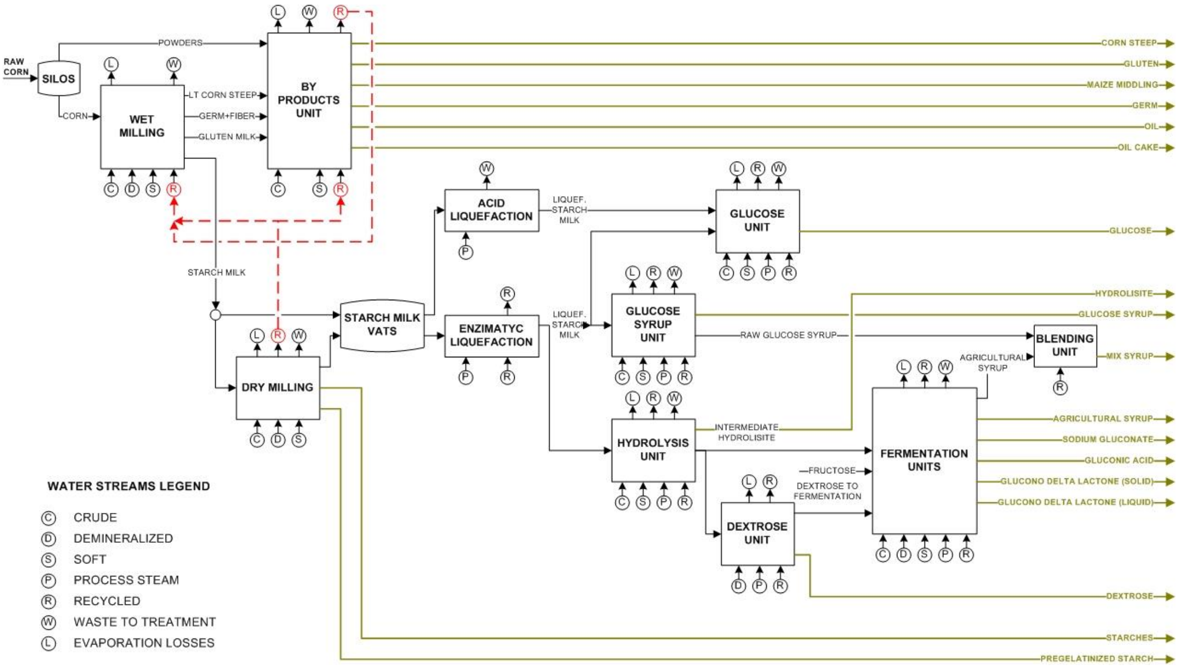

Figure 1: The whole process scheme

The final goal of the study consists in maximizing the amount of internal recycles in order to reduce the crude water demand. The first step of the study has been focused on Wet Milling, Dry Milling and By Product phases which globally account for the 65 % of the total demand of the bio-refinery. Water recycling is already in place from Dry Milling to Wet Milling/By-Product phases and from By-product to Wet Milling phase (see dashed red streams reported in Figure 1); the flowrates of these recycled streams are not directly measured and have been initially assessed with the reconciliation study and account roughly for the 40 % of the demand of the wet milling phase. Intermediate results make it possible to anticipate an approximate 40 % increase in the amount of the recycled stream flowrates which gives rise to an approximate 10 % reduction in the global consumption of water in the industrial complex. The detailed results are not reported in this publication because of the non-disclosure agreement in place with the company that provided the basic information used for this study, but the preliminary results confirm the validity of the approach outlined in the paper.

4. Conclusions

A general strategy for the optimisation of water resources has been outlined. The main differences to the usual procedures are the simultaneous presence of water in the utility system and in the products. This requires a modification of the well established algorithms for both process monitoring through reconciliation of process measurements and process optimisation. It has been shown that the former task can be performed by a straightforward extension of a previously developed algorithm to include fluctuations of water content in the products as measured by routine quality control procedures. On the other hand, the presence of fluctuating compositions in input raw materials and consequently in food products requires the generalization of well established mixed integer nonlinear programming (MINLP) algorithms to stochastic mixed integer nonlinear programming (SMINLP) algorithms. However, using a Monte Carlo approach would imply a prohibitive computational burden for all but the simplest flowsheets. An approximate strategy, based on ordinal optimisation, has been considered and applied to an industrial case involving the manufacture of starches and starch products. The preliminary results seem to confirm the overall validity of the algorithms developed.

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