

## SIMULTANEOUS OPTIMIZATION OF SOLVENT, WATER, AND ENERGY CONSUMPTION: THE CASE OF CIMV ORGANOSOLV

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A.D. MOUNTRAKI(1,2), B. BENJELLOUN-MLAYAH(1), A.C. KOKOSSIS(2)

- ◆ (1) Compagnie Industrielle de la Matière Végétale (CIMV)  
109, rue Jean Bart – Diapason A  
31670, Toulouse, FRANCE  
e-mail : [a.mountraki@cimv.fr](mailto:a.mountraki@cimv.fr); [b.benjelloun@cimv.fr](mailto:b.benjelloun@cimv.fr)
  - ◆ (2) National Technical University of Athens (NTUA)  
9, Heroon Politechniou, Politechnioupoli, Zografos  
15780, Athens, GREECE  
e-mail : [mountrak@central.ntua.gr](mailto:mountrak@central.ntua.gr); [akokossis@mail.ntua.gr](mailto:akokossis@mail.ntua.gr)
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**Abstract.** The research addresses the simultaneous mass and energy integration problem using optimization methods and multiple resources considering regeneration. The problem is formulated as a mixed integer linear programming model (MILP) to calculate targets for savings in operating cost (savings in energy, water, and raw materials use and cost reduction in effluent treatment). The approach is applied for the design of an organosolv fractionation plant (CIMV - Compagnie Industrielle de la Matière Végétale). Results illustrate savings at 33% in the total cost, compared to sequential optimization results. Future work focuses on the role of the regeneration unit in integrated resource recycle/reuse networks.

**Key-words.** Optimization, Biorefinery, organosolv, Heat Integration, Mass Networks

### INTRODUCTION

Organosolv technologies hold a good potential to accomplish the multi-product biorefinery design because of their ability to fractionate the lignocellulosic biomass into its main constituents (cellulose, hemicellulose, and lignin) <sup>[1,2]</sup>. Nevertheless, this fractionation capacity comes with an additional cost: the solvent. Almost half of the energy required in these technologies goes for the regeneration of the solvent because of high prices and environmental restrictions, which call for its maximum reuse. Moreover, these processes have a considerable number of washing stages, which employs a significant amount of water. The combinatorial nature of the solvent, water and heat exchange network design calls for the development of a systematic methodology that can deal with the high dimensionality of the design problem.

Pinch analysis <sup>[3]</sup> set the basis for the systematic design of heat exchanger networks, utility networks, and total sites. Existing systematic methods deal with problems of grassroots or retrofit design, for continuous or batch operation <sup>[4,5]</sup>. More recently, the transshipment model <sup>[6]</sup> was extended for variable inlet and outlet temperatures <sup>[7]</sup> with options for fixed or variable flowrates <sup>[8,9]</sup>. Mass exchange networks analysis <sup>[10]</sup> combined with pinch analysis <sup>[11]</sup> systematized the design procedures for resource conservation networks focusing more on water-using systems <sup>[11,12,13,14]</sup>. The combined optimization of mass and energy networks is also addressed in the literature. Savulescu et al. <sup>[15]</sup>, combined direct and indirect heat transfer in water systems. Systematic methods for water using networks include graphical tools, mathematical models, or their combination, following a sequential or a simultaneous optimization approach <sup>[12,13;16]</sup>. Applications on bioprocesses include bioethanol production from either corn or lignocellulosic biomass and transesterification processes by heterogeneous or homogeneous catalysis (alkali, acid, or enzymes) <sup>[17]</sup> and Kraft pulping mill <sup>[18,19]</sup>. However, in solvent-using processes, the solvent is usually tangled with the water network, and, in some cases, the "contaminant" component may be the water.

This work extends existing methods to multiple-utility-using networks, accounting for the parallel regeneration of several resources. Network design does not pivot on a central resource type (water, H<sub>2</sub>, or solvent), but the role of the a priori peer resources is defined by their impact on the objective function. Given is a set J of utility-using locations (targets) with specified operating temperatures and certain constraints about the composition and/or the total flow of the inlet streams. Besides, a set I of utility-providing nodes (sources) with specified temperature, specific heat capacity, total flow, and composition is given. The objective is to determine the interconnections (i, j), the composition and the flowrate of each stream within the network by minimizing the total annual cost. It is assumed that appropriate stream mixing can do both, respect mass composition constraints and mitigate energy requirements.

## MATERIALS & METHODS

The basic problem to be dealt with is how to reuse internal streams, potentially containing contaminants in order to minimize the cost of fresh supply of both material and energy utilities, and the treatment cost of the effluents.

### Methodology Description

The problem of multiple-utility-using networks has been based on a superstructure of source-target representation (Figure 1). Source and target nodes are located on different unit types. Supply units provide the network with fresh utilities at a given cost. On the production units, the source nodes have known temperature, availability, composition, and specific heat capacities, while the target nodes require resources at a desired temperature, with limitations on the composition and the specific mass flow rate of their feeding stream. Treatment units accept all the non-reusable effluents to be treated and discarded at a known temperature. They have no predefined mass flow rate, nor required composition. Upgrade unit is used to improve the quality of the reusable streams. This unit introduces non-linear terms in the mathematical formulation because, normally, the input and output temperatures and compositions are unknown. To keep the model linear, it is assumed that it operates on steady state and with a constant performance, so that the temperatures and compositions of the regenerated streams are fixed.

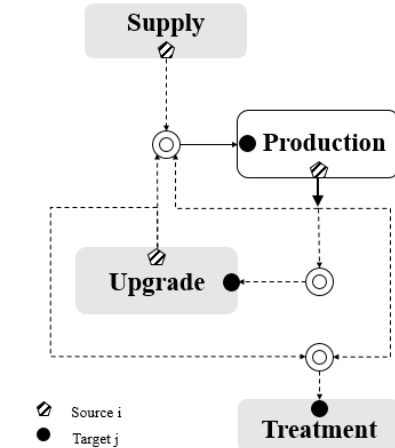


Figure 1. Utility Network Connectivity

Connecting sources and targets creates mass streams which can be considered also as heat streams with variable heat requirements. The energy network has been formulated as a transshipment problem [6] with variable inlet and outlet temperatures and variable flowrates [7, 8, 9]. But when both, flow rates and temperatures are variables, the heat network is described by non-linear equations. Therefore, an automate pre-characterization step as “hot” or “cold” for each match (i,j) is introduced to preserve the model linearity. To keep low the complexity of the resulted network and ensure its applicability, an integer constraint is introduced targeting for the minimum number of matches (i,j). The objective function takes into account the cost of mass utilities (water & solvent), energy utilities (heating & cooling), and effluent treatment:

$$Obj. \text{ minimize } TC = C^{UM} + C^{UE} + C^T$$

### Process Description

CIMV process has its origin in the manufacture of bleached paper pulp and its unique breakthrough is that it allows the clean fractionation of lignocellulosic biomass, without degradation, into intermediate products: biolignin<sup>TM</sup>, cellulosic pulp, and syrup of hemicelluloses [20-22].

The organic solvent used is an aqueous mix of acetic acid (AA) and formic acid (FA). The mass and energy balances are based on a simulation model, which has been developed in AspenPlus, but for space economy reasons cannot be presented here. The capacity has been set at 300kt/year of dry poplar with bark, and the operating year is set at 8.000 hr/year. CIMV has seven production units and a tank section for the intermediate storage of the solvent (Figure 2). The resource compounds to be conserved are water, AA, and FA, while solids account for either contaminants or neutral compounds, depending the target node.

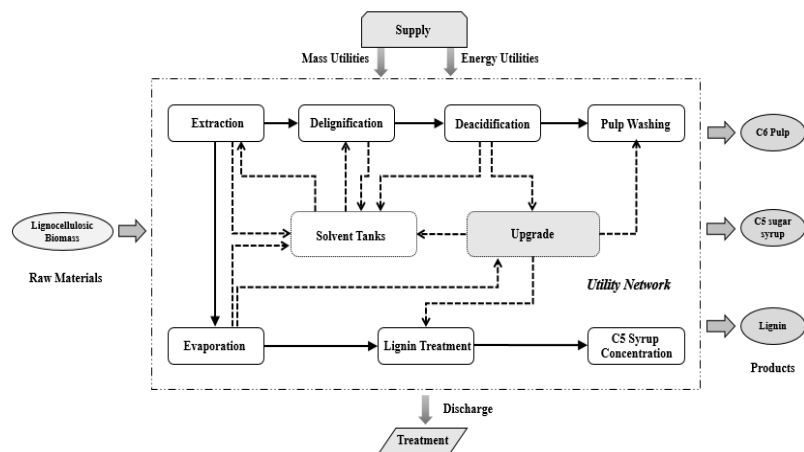


Figure 2. Utility Network of CIMV

## RESULTS

Three cases are used to demonstrate the capabilities of our model. The benchmark case applies sequential optimization: at first, the quantity of fresh solvent is minimized (AA and FA simultaneously), then the fresh water, and, finally, pinch analysis is used for the minimization of energy utility requirements. The case of centralized solvent management applies the simultaneous optimization framework on the original design of CIMV, where a tank is used for the intermediate storage and distribution of the solvent. In that case, the recycled solvent streams need to pass first through storage and come at 80°C (storage temperature), before re-entering the network. Lastly, the case of distributed solvent management applies the simultaneous optimization framework without intermediate storage.

### Benchmark Case

For the benchmark case, the resource network resulted in 22 matches and resource needs of 73.89tn/hr water, 0.94tn/hr AA, and 1.14tn/hr FA. A total quantity of 114.79tn/hr is entered in the regeneration technology (Distillation), which demands 97.63MWh of heating and 91.07MW of cooling utilities. The demand in energy utilities of the total process, before Pinch analysis are 184.19MW for heating and 181.66MW for cooling. After Pinch, the minimum energy utility requirements are 97.63MWh for heating and 95.11MWh for cooling. Table 1 summarizes the operating costs.

Table 1. Operating cost - Benchmark

TC [MMS/y]	C <sup>UM</sup> [MMS/y]	C <sup>UE</sup> [MMS/y]	C <sup>T</sup> [MMS/y]
64.15	11.25	52.90	0.00

### Centralized Solvent Management

The simultaneously optimized network of the centralized case came up with 20 matches and resource needs of 80.37tn/hr water, 3.49tn/hr AA, and 0.01tn/hr FA. The regeneration technology receives 80.08tn/hr inflow and needs 66.81MWh for heating and 62.68MWh for cooling. The total process utilities requirements are 66.81MWh for heating and 22.08MWh for cooling. The different contributions and the total operating cost are summarized in Table 2.

Table 2. Operating cost - Centralized

TC [MMS/y]	C <sup>UM</sup> [MMS/y]	C <sup>UE</sup> [MMS/y]	C <sup>T</sup> [MMS/y]
42.94	14.10	28.84	0.00

### Distributed Solvent Management

The optimized network of the distributed network has 25 matches and needs the same fresh mass utilities as those of the centralized case. The configuration of the regeneration unit is similar to the centralized. The process energy demand is 66.81MWh for heating and 21.95MWh for cooling. Table 3 shows the results of operating cost.

Table 3. Operating cost - Distributed

TC [MMS/y]	C <sup>UM</sup> [MMS/y]	C <sup>UE</sup> [MMS/y]	C <sup>T</sup> [MMS/y]
42.92	14.10	28.82	0.00

## Discussion

Compared to the benchmark, sequential, case, the simultaneously optimized cases have reduced the annual operating cost by 21MM\$. Even though the fresh supply cost is 25% higher, the utility cost is reduced by 46%. The total inflow allocated to the regeneration technology is 30% less, which is what caused the increase of fresh material supplies, but also the reduction of energy utility needs. The lower capacity of the regeneration unit may be accounted capital cost savings. The centralized configuration came up with two less connections than the benchmark case, while the distributed case came up with three more matches. Both, centralized and distributed cases have relatively similar results, because it is only one extra temperature interval that is imposed in the centralized case (the storage temperature). The slight difference in cooling utilities is due to the different thermal profiles because of the imposed storage temperature step. In that case, the buffer stage favors the configuration of both, mass and energy network. All cases come with zero treatment cost, because the upgrade unit in combination with appropriate stream mixing managed to reuse streams with high solid content.

## CONCLUSION

The simultaneous mass energy network optimization model presented here deals with multiple contaminants and with multiple material resources in need for parallel regeneration. Its application to CIMV organosolv process resulted in a 33% reduction of the total cost, compared to sequential optimization. The model chose to sacrifice some supply cost in order to improve the thermal profile of the network and reduce the total cost. The configuration of the regeneration technology is paramount to the consumption of fresh supply and utilities, but also to the capital investment cost. Future work will deal with debottlenecking the regeneration unit in integrated resource recycle/reuse networks.

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