University of Alicante **Department of Chemical Engineering**

Handling of Uncertainty in Life Cycle Inventory by Correlated Multivariate Lognormal Distributions: Application to the Design of Supply Chain Networks

Juan A. Reyes-Labarta[a], Raquel Salcedo-Díaz[a], Rubén Ruiz-Femenia[a], Gonzalo Guillén-Gosálbez[b], Jose A. Caballero[a]

[a]*Department of Chemical Engineering, University of Alicante, Apdo. 99, Alicante (Spain) e-mail: ja.reyes@ua.es*

[b]*Departament d'Enginyeria Química, Universitat Rovira i Virgili, Tarragona E-43007, Spain*

Summary

In this work, we analyze the effect of incorporating life cycle inventory (LCI) uncertainty on the multi-objective optimization of chemical supply chains (SC) considering simultaneously their economic and environmental performance. To this end, we present a stochastic multi-scenario mixed-integer linear programming (MILP) coupled with a two-step transformation scenario generation algorithm with the unique feature of providing scenarios where the LCI random variables are correlated and each one of them has the desired lognormal marginal distribution. The environmental performance is quantified following life cycle assessment (LCA) principles, which are represented in the model formulation through standard algebraic equations. The capabilities of our approach are illustrated through a case study of a petrochemical supply chain. We show that the stochastic solution improves the economic performance of the SC in comparison with the deterministic one at any level of the environmental impact, and moreover the correlation among environmental burdens provides more realistic scenarios for the decision making process.

Introduction

Whether simulate a distillation column can be a challenging problem, especially for high non ideal mixtures, design a distillation column is even a much more complex problem. While in simulation problems it is necessary to specify the total number of stages, all the feeds locations, all the side draws as well as the operating conditions, when we design a distillation column we are interested in calculating the distillate and residue flows, the number of stages and the optimum feed(s) location for a specified separation of components in products, that is to say that the design methods focus on the best column configuration for a specified separation. Due to the inclusion of very efficient simulation algorithms in commercial packages the design of distillation columns has been usually performed by successive simulations [1,2]. However, this procedure is very time consuming and of doubtful utility when trying to evaluate optimal sequences of interrelated columns.

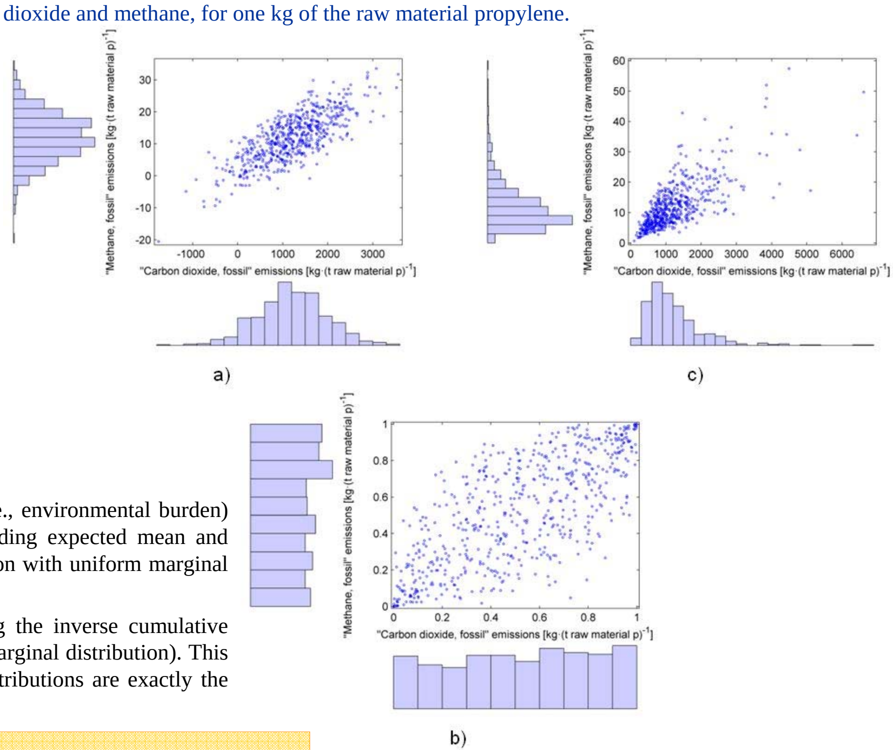
Methodology

We model the uncertainty in the LCI by a set of scenarios, generated by Monte Carlo sampling. Using the lognormal distribution, which is the default distribution for Ecoinvent database (Goedkoop et al., 1998), we implement a two-step transformation algorithm to generate the scenarios from a correlated multivariate random distribution function with the desired lognormal marginal distribution for each environmental burden in the LCI. Given are the mean expected value, the geometric standard deviation of each burden and the correlation matrix (whose entries range from -1 to 1, and 0 means no correlation). The geometric standard deviation is calculated from the uncertainty factors in conjunction with the pedigree matrix (Frischknecht et al., 2005). With these three inputs we compute the covariance matrix, whose diagonal elements contain the variances for each variable, while the off-diagonal elements contain the covariance among variables. Then, we use the probability density function of a multivariate normal distribution to generate a certain number of scenarios. Thus, a statistical dependence among each pair of variables is created, following each variable a normal marginal distribution (Figure 1a).Then we apply the 2 step algorithm:

Step 1: Apply a transformation separately to each random variable (i.e., environmental burden) using the normal cumulative distribution function with the corresponding expected mean and standard deviation. This transformation results in a correlated distribution with uniform marginal distribution on the interval (0,1) (Figure 1b).

Step 2: Transform each random variable (i.e., each burden) applying the inverse cumulative distribution function of a lognormal distribution (which is the desired marginal distribution). This transformation creates correlated random variables whose marginal distributions are exactly the lognormal distribution (Figure 1c).

➢ **Figure 1.** Correlated bivariate distributions with marginal: a) normal; b) uniform; c) lognormal distributions for two environmental burdens in the life cycle inventory, carbon dioxide and methane, for one kg of the raw material propylene.

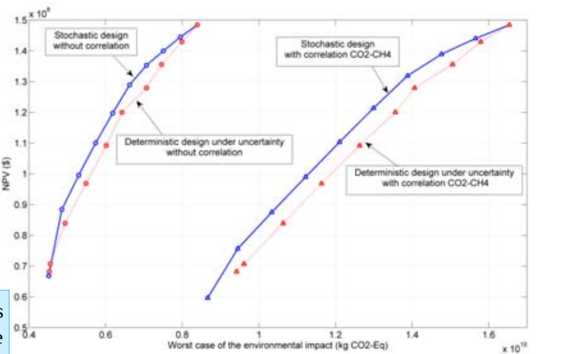


Mathematical model

The MILP formulation is based on that introduced by Guillén-Gosálbez and Grossmann (2009) for the case of petrochemical SC. It includes binary variables to represent the occurrence of the capacity expansion of manufacturing technology *i* at plant *j* in time period *t* $\left(X_{ijt}^{PL}\right)$, the capacity expansion of warehouse *k* in time period *t* $\left(X_{kt}^{WH}\right)$, and the establishment of transportation links between plant *j* and warehouse *k* in time period *t* $\left(Y_{jkt}^{PL}\right)$, whereas continuous ones denote the transportation flows, capacity expansions, storage inventories and production rates.

The model includes three main blocks of equations: **mass balances**, **capacity constraints** and **objective functions**: Economic performance represented by **net present value (NPV)**; and Environmental performance assessed according to the principles of Life Cycle Assessment (LCA) using the **global warming potential (GWP)** indicator as described by the IPCC 2007 (Intergovernmental Panel on Climate Change).

➢ **Figure 2.** Pareto set of solutions for the deterministic and stochastic design with no burden correlation and correlating the two contaminants with more contribution to the GWP



Conclusions

The results show how the incorporation of the correlation among the LCI entries that comprises the GWP, influences on the solution design of the supply chain. It has been proved that incorporating uncertainty in the LCI facilitates the decision-making process, providing a robust solution when burden emissions uncertainty reveals with different values from those nominal ones gathered in the environmental database

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