

# Real option theory from finance to batch distillation

Vicente Rico-Ramirez<sup>a</sup>, Urmila M. Diwekar<sup>b,\*</sup>, Benoit Morel<sup>c</sup>

<sup>a</sup> Instituto Tecnológico de Celaya, Ave. Tecnológico y GarciaCubas SN, CP 38010, Celaya, Gto., Mexico

<sup>b</sup> CUSTOM, Center for Uncertain Systems, Department of Chemical Engineering, Institute for Environmental Science and Policy, University of Illinois at Chicago, Chicago, IL 60607, USA

<sup>c</sup> Department of Engineering and Public Policy, Carnegie Mellon University, Pittsburgh, PA 15213, USA

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## Abstract

Batch distillation processes have gained renewed interest because of the recent development in small-scale industries producing high-value-added, low-volume specialty chemicals. The flexibility and unsteady state nature of batch distillation constitute a challenge for the designer. A particularly difficult problem is the optimal control problem involving open loop solution for the reflux ratio profile. This is because of the complexity of the formulation and the large computational effort associated to its solution. The mathematical and numerical complexities of the optimal control problem get worse when uncertainty is present in the formulation. In this work, by applying the optimality conditions from the real option theory based on the Ito's Lemma [Investment under uncertainty (1994); *Memoirs Am. Math. Soc.* 4 (1951) 1; *Appl. Math. Opt.* 4 (1974) 374], the mathematical tools needed to solve optimal control problems in batch distillation columns when uncertainties in the state variables are present have been developed. Furthermore, the coupled maximum principle and NLP approach developed by Diwekar [*Am. Inst. Chem. Eng. J.* 38 (1992) 1551] has been extended for solving the optimal control problem in the uncertain case. This new algorithm has been implemented in the MultiBatchDS batch distillation process simulator. Finally, a numerical case-study is presented to show the scope and application of the proposed approach.

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## 1. Introduction

Optimal control problems in batch distillation have received considerable attention in the literature. In general, solution to these problems involves finding the time-dependent reflux profile (for the conventional batch column) so as to optimize a particular performance index. The dynamic nature of these decision variables makes these problems much more difficult to solve compared to normal optimization where the decision variables are scalar. Optimal control problems in batch distillation can be classified as (Diwekar, 1994):

- 1) Maximum distillate problem—where the amount of distillate of a specified concentration for a specified time is maximized (Converse & Gross, 1963; Diwe-

kar, Malik & Madhavan, 1987; Logsdon, Diwekar & Biegler, 1990; Farhat, Czernicki, Pibouleau & Domench, 1990).

- 2) Minimum time problem—where the batch time needed to produce a prescribed amount of distillate of a specified concentration is minimized (Hansen & Jorgensen, 1986; Mujtaba & Macchietto, 1988).
- 3) Maximum profit problem—where a profit function for a specified concentration of distillate is maximized (Kerkhof & Vissers, 1978; Logsdon et al., 1990).

It has been shown (Diwekar, 1992) that these optimal control problems, encountered in batch distillation, are not different from each other but essentially involve the solution of the maximum distillate problem.

The general mathematical techniques used to solve optimal control problems include the calculus of variations, dynamic programming, Pontryagin's maximum principle, and nonlinear programming optimization

\* Corresponding author.

E-mail address: [urmila@uic.edu](mailto:urmila@uic.edu) (U.M. Diwekar).

(NLP). The first three methods treat the decision variables as vectors, while the NLP approach requires the variables to be transformed into scalars. The choice of the appropriate or the best optimization technique is generally problem-dependent.

Traditionally, the models used in the optimal control of batch distillation have been deterministic in nature. However, in many realistic situations one cannot neglect the associated uncertainties. The presence of uncertainties in optimal control problems results in stochastic optimal control problems.

Stochastic processes do not have time derivatives in the conventional sense and, as a result, they cannot always be manipulated using the ordinary rules of calculus. As a consequence, the typical mathematical techniques used to solve optimal control problems (calculus of variations, dynamic programming, Pontryagin's maximum principle, and NLP) cannot be directly applied. To work with stochastic processes, one must make use of Ito's Lemma. This Lemma (Ito, 1951, 1974), called the Fundamental Theorem of Stochastic Calculus, allows to differentiate and to integrate functions of stochastic processes.

Dixit and Pindyck (1994) described optimal investment rules developed for pricing options in financial market and Ito's Lemma to generalize the Bellman equation (optimality conditions using dynamic programming) for the stochastic case. This new equation constitutes the base of the so called Real Option Theory.

Although such a theory was developed in the field of economics, it certainly can be applied to engineering problems and this is the focus of the current endeavor. Real options analysis focuses on the temporal aspects of risk, attempting to accurately capture the potential for future value in investments and decisions made today (Amram & Kulatilaka, 1999). There are similarities between acquiring options in the world of finance and making strategic business decisions, and optimal operating strategies for batch processing: both deal with dynamic uncertainties and both attempt to respond to time dependent changes.

In this paper it is shown how this theory can be applied to find the solution of a maximum distillate problem in batch distillation when uncertainties in the state variables of the model are present. It is also demonstrated that, when no uncertainty exists in the problem, this theory provides the same solution as the other mathematical techniques traditionally employed.

The paper is divided into seven sections. Section 2 presents the previous work on batch distillation optimal control, including the solution to the deterministic maximum distillate problem and the derivation of the expression for optimal reflux ratio profile obtained by using the maximum principle. Section 3 starts by describing the different types of uncertainties that may be present in a batch distillation process (as an instance

of a dynamic process) and then is devoted to the theory of stochastic calculus: the Ito's Lemma, and the real option theory. The contributions of the paper are presented in Sections 4–7. Section 4 presents the application of real option theory to the stochastic maximum distillate problem in batch distillation. First, it is shown that, by applying the generalization of the Hamilton–Jacobi–Bellman (HJB) equation to the deterministic version of the maximum distillate problem, the solution obtained is the same as that obtained by traditional techniques. The section then includes the derivation of an expression for computing the optimal reflux ratio profile in the uncertain case and proposes an extension of the previous approach for solving the resulting stochastic optimal control problem. Section 5 describes how the uncertainty in thermodynamic modeling of batch distillation systems can be represented by using the concept of an Ito process. A numerical case-study to support the assumption made is also presented. Section 6 presents an example of the calculation of an optimal reflux ratio policy under uncertainty to emphasize the impact of the proposed approach. Finally, Section 7 concludes the paper.

## 2. The deterministic maximum distillate problem

The maximum distillate problem without stochasticity described in the literature as early as 1963 (Converse & Gross, 1963) can be represented as follows:

$$\text{Maximize}_{R_t} J = \int_0^T \frac{dD}{dt} dt = \int_0^T \frac{V}{R_t + 1} dt, \quad (1)$$

Subject to:

$$x_{D_{ave}} = \frac{\int_0^T x_D^{(1)} \frac{V}{R_t + 1} dt}{\int_0^T \frac{V}{R_t + 1} dt} = x_D^* \quad (2)$$

$$\frac{dx_t^1}{dt} = \frac{dB_t}{dt} = \frac{-V}{R_t + 1}, \quad x_0^1 = B_0 = F, \quad (3)$$

$$\frac{dx_t^2}{dt} = \frac{V}{R_t + 1} \frac{(x_B^{(1)} - x_D^{(1)})}{B_t}, \quad x_0^2 = x_F^{(1)} \quad (4)$$

In the above equations, the following notations are used:  $R_t$  is the control variable vector, reflux ratio (function of time);  $V$ , the molar vapor boilup rate (mol h<sup>-1</sup>);  $t$ , time (h);  $T$ , the total batch time (h);  $D$ , the molar distillate product (mol);  $x_D^{(1)}$ , the overhead or distillate composition for the key component 1 (mole fraction);  $x_{D^*}$ , the average specified distillate composition for the key component 1 (mole fraction);  $F$ , the initial feed (mol);  $x_t^1$ , a state variable at time  $t$  representing quantity of charge remaining in the still,  $B_t$  (mol);  $x_t^2$ , a state variable representing the composi-

tion of the key component in the still at time  $t$ ,  $x_B^{(1)}$  (mole fraction), and  $L, J$ , objective function to be maximized. The objective function can be rewritten by using the Lagrangian formulation (assumption of convexity implied):

$$\text{Maximize } L = \int_0^T \frac{V}{R_t + 1} [1 - \lambda(x_D^* - x_D^{(1)})] dt \quad (5)$$

Subject to Equations 3, 4, and the time-implicit model equations that link the state variables ( $x^1$  and  $x^2$  to other parameters and design variables).

### 2.1. The time implicit model

As in most of the models used to solve the optimal control problems in batch distillation, the discussions are restricted to negligible holdup models. Furthermore, the batch distillation model assuming quasi-steady state approximation for the column with dynamics of the reboiler (resulting in the above two differential equations) is considered, which is also consistent with numerous problems reported in the literature. Diwekar (1992) suggested further simplification for multicomponent systems, wherein the quasi-steady state approximation extends to components in the reboiler other than the key component. These other state variables are assumed to be in a quasi-steady state and may be obtained using time-implicit equations (either the plate-to-plate model or the shortcut method equations). The quasi-steady state approximation reduces the dimensionality of the problem, since the number of additional variables and additional equations required for these techniques does not increase with the number of components. The short-cut method based time implicit model is presented in Table 1.

The nomenclature for the additional variables in Table 1 is given below.  $x_{B_{old}}^{(i)}$ , composition of the  $i$ -th component in the still at the initial time of a finite difference interval;  $x_{B_{new}}^{(i)}$ , composition of the  $i$ -th component in the still at the final time of a finite difference interval (also the initial of the next interval);  $C_1$ , the constant in Hengestebeck–Geddes’ (HG) equation;  $H$ , Hamiltonian function;  $N$ , the theoretical number of plates in the column;  $N_{min}$ , minimum number of plates;  $R_{min}$ , minimum reflux ratio;  $R_{min,g}$ , minimum reflux ratio calculated using Gilliland’s equation;  $R_{min,u}$ , minimum reflux ratio calculated using Underwood equations; Greek symbols:  $\alpha_i$ , the relative volatility of component  $i$ ;  $\phi$ , constant in the Underwood equations.

At any instant of time there is a change in still composition of the key component (state variable,  $x_t^1$ ), resulting in changes in the still composition of all other components calculated by the finite difference material balance equations given in Table 1. The HG equation relates the distillate composition to the new still

Table 1  
Time implicit model equations for the shortcut method

Finite difference material balance equation

$$x_{B_{new}}^{(i)} = x_{B_{old}}^{(i)} + \frac{\Delta x_B^{(i)} (x_D^{(i)} - x_B^{(i)})_{old}}{(x_D^{(1)} - x_B^{(1)})_{old}}, \quad i = 2, \dots, n$$

Hengestebeck–Geddes (HG) equation

$$x_D^{(i)} = \left(\frac{\alpha_i}{\alpha_1}\right) C_1 \frac{x_D^{(1)}}{x_H^{(1)}} x_B^{(i)}, \quad i = 2, 3, \dots, n$$

Unknowns  $R, C_1, x_D^1$

Summation of fractions  $\sum_{i=1}^n x_D^{(i)} = 1, x_D^{(1)}$  estimation,

$$x_D^{(1)} = \frac{1}{\sum_{i=1}^n \left(\frac{\alpha_i}{\alpha_1}\right) C_1 \frac{x_B^{(i)}}{x_B^{(1)}}}$$

Fenske equation  $N_{min} \approx C_1$

Underwood equations  $\sum_{i=1}^n \frac{\alpha_i x_B^{(i)}}{\alpha_i - \phi} = 0; \quad R_{min,n} + 1 = \sum_{i=1}^n \frac{\alpha_i x_D^{(i)}}{\alpha_i - \phi}$

Gilliland correlation  $C_1$  estimation,

$$R_{min,g} = F(N, N_{min}, R), \quad \frac{R_{min,g}}{R} - \frac{R_{min,u}}{R} = 0$$

$R$  estimation  $R = F(\text{Minimum } H)$

composition in terms of the constant  $C_1$ . This constant  $C_1$  in the HG equation is equivalent to the minimum number of plates  $N_{min}$  in the Fenske equation. At this stage,  $R, C_1$  and  $x_D^{(1)}$  are the unknowns. Summation of distillate composition can be used to obtain  $x_D^{(1)}$  and the Fenske–Underwood–Gilliland (FUG) equations to obtain  $C_1$ . The unknown  $R$  is the optimal reflux control variable and can be calculated using the Pontryagin’s maximum principle (or other methods) by minimizing the Hamiltonian. This formulation is described in the next subsection.

### 2.2. Solution using the Pontryagin’s maximum principle

The maximum principle was first proposed in 1956 by Potryagin (1957). The maximum principle has been used to solve optimal control problems. Application of the maximum principle to an optimal control problem involves addition of a number of adjoint variables (one adjoint variable per state variable) and adjoint equations (same number as the state variables), and a

Hamiltonian (Diwekar, 1994). The optimal decision vector is obtained by extremizing this Hamiltonian.

To solve the maximum distillate problem, an additional state variable  $x_t^3$  is introduced which is given by:

$$x_t^3 = \int_0^t \frac{V}{R_t + 1} [1 - \lambda(x_D^* - x_D^{(1)})] dt \quad (6)$$

Then, the problem can be rewritten as:

$$\text{Maximize}_{R_t} x_T^3 \quad (7)$$

subject to the time implicit model for the rest of the column, the differential equation for the state variable  $x_t^3$ :

$$\frac{dx_t^3}{dt} = \frac{V}{R_t + 1} [1 - \lambda(x_D^* - x_D^{(1)})] \quad (8)$$

and the differential equations (3) and (4). The Hamiltonian function is:

$$H_t = -\mu_t^1 \frac{V}{R_t + 1} + \mu_t^2 \frac{V(x_t^2 - x_D^{(1)})}{(R_t + 1)x_t^1} + \mu_t^3 \frac{V}{R_t + 1} \times [1 - \lambda(x_D^* - x_D^{(1)})] \quad (9)$$

and the differential equations for the adjoint variables,  $\mu_t$ , are (see Thompson & Sethi, 1994 for the theory about the derivation):

$$\frac{d\mu_t^1}{dt} = \mu_t^2 \frac{V(x_t^2 - x_D^{(1)})}{(R_t + 1)(x_t^1)^2}, \quad \mu_T^1 = 0, \quad (10)$$

$$\frac{d\mu_t^2}{dt} = -\mu_t^2 \frac{V \left(1 - \frac{\partial x_D^{(1)}}{\partial x_t^2}\right)}{(R_t + 1)x_t^1} - \mu_t^3 \lambda \frac{V}{(R_t + 1)} \left(\frac{\partial x_D^{(1)}}{\partial x_t^2}\right), \quad (11)$$

$$\mu_T^2 = 0$$

$$\frac{d\mu_t^3}{dt} = 0, \quad \mu_T^3 = 1 \quad (12)$$

Equation (12) gives:

$$\mu_t^3 = 1, \quad (13)$$

By substituting (13) in (9), the Hamiltonian can be written as:

$$H_t = -\mu_t^1 \frac{V}{R_t + 1} + \mu_t^2 \frac{V(x_t^2 - x_D^{(1)})}{(R_t + 1)x_t^1} + \frac{V}{R_t + 1} \times [1 - \lambda(x_D^* - x_D^{(1)})] \quad (14)$$

and Equation (11) becomes:

$$\frac{d\mu_t^2}{dt} = -\mu_t^2 \frac{V \left(1 - \frac{\partial x_D^{(1)}}{\partial x_t^2}\right)}{(R_t + 1)x_t^1} - \lambda \frac{V}{(R_t + 1)} \left(\frac{\partial x_D^{(1)}}{\partial x_t^2}\right), \quad (15)$$

$$\mu_T^2 = 0$$

Finally, from the first order condition,  $\partial H/\partial R_t = 0$ , it follows that:

$$R_t = \frac{\left[ \frac{\mu_t^2}{x_t^1} (x_t^2 - x_D^{(1)}) - \mu_t^1 - \lambda(x_D^* - x_D^{(1)}) + 1 \right]}{\frac{\partial x_D^{(1)}}{\partial R_t} \left( \lambda - \frac{\mu_t^2}{x_t^1} \right)} - 1 \quad (16)$$

which represents an explicit equation for the calculation of  $R_t$  in terms of the adjoint and state variables. Notice that the adjoint and state variables can be calculated from the integration of equations (3), (4), (10) and (11). At this point, it is convenient to remark that the maximum principle establishes that the partial derivative of the Hamiltonian ( $H_t$ ) with respect to the control variable ( $R_t$ ) is equal to zero. Moreover, the partial derivatives of the Hamiltonian ( $H_t$ ) with respect to the state variables ( $x_t$ ) are not equal to zero but equal to the derivatives of the adjoint variables ( $\mu_t$ ) with respect to time. That is,

$$\frac{\partial H_t}{\partial R_t} = 0$$

$$\frac{\partial H_t}{\partial x_t^1} = \frac{d\mu_t^1}{dt}, \quad \frac{\partial H_t}{\partial x_t^2} = \frac{d\mu_t^2}{dt}, \quad \frac{\partial H_t}{\partial x_t^3} = \frac{d\mu_t^3}{dt}$$

### 3. Stochastic processes and real option theory

#### 3.1. Uncertainties in a dynamic process

In order to model a system under uncertainty, a quantitative description of the variations expected must be established. Consider a mathematical formulation of a dynamic process model as a set of differential algebraic equations (for details, please refer to Naf, 1994):

$$g(x, \dot{x}, u, \eta, t) = 0 \quad (17)$$

with the initial conditions:

$$x(t=0) = x_0 \quad (18)$$

where  $x$  are the state variables,  $u$  the input variables and  $\eta$  the model parameters, then qualitatively different sources of uncertainty may be located:

- 1) Uncertainty in the input variables  $u$ . This kind of uncertainty originates from the random nature and unpredictability of certain process inputs (e.g. feed composition uncertainty).
- 2) Variability in the initial conditions  $x_0$  (initial charge of a batch for instance).
- 3) Uncertainty with respect to the model parameters  $\eta$ . These parameters are a part of the deterministic

model and not in actual fact subject to randomness. Theoretically their value is an exact number. The uncertainty results from the impossibility of modeling exactly the physical behavior of the system.

The representation of uncertainties for the three categories is usually in terms of distribution functions.

### 3.1.1. Motivation: uncertainties in batch distillation

There are instances of all the three sources of uncertainties in batch distillation.

The first type of uncertainty results from uncertainties in the input variables. In batch distillation, this type of uncertainty is observed in parameters such as the vapor boilup rate  $V$ . Although  $V$  is commonly assumed as constant, this value depends on the heat load  $Q$  to the system. Fluctuations of the load  $Q$  and composition changes will result in variations of the vapor boilup rate, hence, the operation of the batch distillation column cannot be captured efficiently by the deterministic model especially if the model is simplified. By determining an appropriate distribution for  $V$ , it is possible to incorporate this type of uncertainty in the model.

The second type of uncertainty can be observed in initial variables, such as the variability in feed for different batches. In this case, the value of total feed and/or the feed composition varies from batch to batch. Since the calculations of the dynamic behavior of the column are performed based on this initial value, the uncertain nature of this implies that the profile determined for  $R$ , might need to be shifted to a new starting point and re-evaluated for the accurate, optimum performance.

Finally, the uncertainty with respect to the model parameters, the third type of uncertainty, will be the focus of this work. In general, optimal control problems are considered to be open loop control problems where the optimal reflux profile is generated a-priori using the model and then the controller is asked to follow this trajectory. This trajectory would be optimal when the model is an exact replica of the physical phenomena. However, very often this is not the case, and on-line updating of the profile is necessary. This calls for use of simplified models like the short-cut model described earlier. In short-cut methods for batch distillation columns, one of many assumptions is fixing the value of the relative volatility and considering this value as a constant throughout the operation. This relative volatility parameter,  $\alpha$ , in practice is varying with respect to number of plates in a column as well as with respect to time. So, how can one be sure of as to what (assumed constant) value is accurate for the simulation? In general, one cannot be. One cannot even try to calculate the changes of the relative volatility a-priori because its value depends on the reflux ratio profile, and the reflux ratio profile is what needs to be obtained. Therefore, the

main uncertainty in the short-cut model is related to the assumption of constant relative volatility throughout the operation of a batch distillation column. This work focuses on handling uncertainty in this important thermodynamic parameter. It will be shown later that the behavior of the relative volatility can be captured by the Geometric Brownian motion representation. Note that with such a representation, our approach not only captures the uncertainty in this crucial parameter (with respect to the assumption of a constant value) but also gains all the advantages of using the short-cut model for faster optimal control calculations and efficient on-line updating. However, this results in a stochastic optimal control problem and one has to deal with stochastic calculus. The remaining of this section defines some concepts commonly used in stochastic analysis and provides a description of the mathematical tools that will be applied for solving stochastic optimal control problems in batch distillation.

### 3.2. Stochastic processes

In a stochastic process there exists a variable that evolves over time in an uncertain way. A stochastic process in which the time index,  $t$ , is a continuous variable is called a continuous-time stochastic process. Otherwise, it is called a discrete-time stochastic process. Similarly, according to the conceivable values for the stochastic variable,  $x_t$  (called the states), a stochastic process can be classified as being continuous-state or discrete-state. One of the simplest examples of a stochastic process is the random walk process. Wiener process or also called a Brownian motion is a continuous limit of the random walk and is a continuous time stochastic process. Wiener process can be used as a building block to model an extremely broad range of variables that vary continuously and stochastically through time. For example, consider the price of technology stock, it fluctuates randomly, but over a long time period has a positive expected rate of growth that compensates investors for risk in holding the stock. Can the stock price be represented as a Wiener process? The following paragraph establishes that stock price can be represented as a Wiener process.

A Wiener process has three important properties:

- 1) It satisfies the Markov property. The probability distribution for all future values of the process depends only on its current value. Stock prices can be modeled as Markov processes, on the grounds that public information is quickly incorporated in the current price of the stock and past pattern has no forecasting values.
- 2) It has independent increments. The probability distribution for the change in the process over any



time interval is independent of any other time interval (non-overlapping).

- 3) Changes in the process over any finite interval of time are normally distributed, with a variance that increases linearly with the time interval.

From the example of the technology stock above, it is easier to show that the variance of the change distribution can increase linearly, however, given that stock prices can never fall below zero, price changes cannot be represented as a normal distribution. Nevertheless, it is reasonable to assume that changes in logarithm of prices are normally distributed. Thus, a stock price can be represented by logarithm of a Wiener process.

Stochastic processes do not have time derivatives in the conventional sense and, as a result, they cannot be manipulated using the ordinary rules of calculus as needed to solve the stochastic optimal control problems. Ito (1951, 1974) provided a way around this by defining a particular kind of uncertainty representation based on the Wiener process as a building block.

An Ito process is a stochastic process on which the increment of the stochastic variable,  $dx$ , is represented by the equation:

$$dx = a(x, t)dt + b(x, t)dz \quad (19)$$

where  $dz$  is the increment of a Wiener process, and  $a(x, t)$  and  $b(x, t)$  are known functions.  $dz$  represents the increment of a Wiener process expressed in terms of an unit normal distribution and  $dt$ .

For a stochastic variable, the expected value or expectation is usually defined as the mean value of the variable and is represented through the expectation operator  $E$ .

With respect to Equation (19), by definition,  $E(dz) = 0$  and  $E[(dz)^2] = dt$  (see Appendix B), where  $E(dz)$  is interpreted as the expected value of  $dz$ .

The real option theory uses the Ito process representation of the stock prices to find the solution of stochastic optimal control problems (Dixit & Pindyck, 1994). For details of the theory and simple illustrative examples, the readers are referred to a recent text book from one of the authors (Diwekar, 2003).

### 3.3. The real option theory and the Ito's Lemma

In the real option theory, Dixit and Pindyck (1994) used stochastic calculus (Ito's Lemma) coupled with dynamic programming to study investment decisions under uncertainty. This approach uses Ito's Lemma, which is called the Fundamental Theorem of Stochastic Calculus and allows to differentiate and to integrate functions of stochastic processes.

#### 3.3.1. Ito's Lemma

Ito's Lemma is easier to understand as a Taylor series expansion. Suppose that  $x(t)$  follows the process of equation (19), and consider a function that is at least twice differentiable in  $x$  and once in  $t$ . In order to find the total differential of this function,  $dF$ , the usual rules of calculus define it in terms of first-order changes in  $x$  and  $t$ :

$$dF = \frac{\partial F}{\partial t} dt + \frac{\partial F}{\partial x} dx \quad (20)$$

But suppose that higher-order terms for changes in  $x$  are also included:

$$dF = \frac{\partial F}{\partial t} dt + \frac{\partial F}{\partial x} dx + \frac{1}{2} \frac{\partial^2 F}{\partial x^2} (dx)^2 + \frac{1}{6} \frac{\partial^3 F}{\partial x^3} (dx)^3 + \dots \quad (21)$$

In ordinary calculus, these higher-order terms all vanish in the limit. For an Ito process following Equation (19), it can be shown that the differential  $dF$  is given in terms of first-order changes in  $t$  and second-order changes in  $x$ . Hence, Ito's Lemma produces the following differential  $dF$ :

$$dF = \frac{\partial F}{\partial t} dt + \frac{\partial F}{\partial x} dx + \frac{1}{2} \frac{\partial^2 F}{\partial x^2} (dx)^2 \quad (22)$$

By substituting equation (19), an equivalent expression is obtained:

$$dF = \left[ \frac{\partial F}{\partial t} + a(x, t) \frac{\partial F}{\partial x} + \frac{1}{2} b^2(x, t) \frac{\partial^2 F}{\partial x^2} \right] dt + b(x, t) \times \frac{\partial F}{\partial x} dz \quad (23)$$

Compared with the chain rule for differentiation in ordinary calculus, Equation (20), Equation (22) has one extra term that captures the effect of convexity or concavity on  $F$ .

#### 3.3.2. Dynamic programming optimality conditions

The method of dynamic programming is based on the principle of optimality, as stated by Bellman (1957).

An optimal policy has the property that, whatever the initial state and initial decision are, the remaining decisions must constitute an optimal policy with regard to the state resulting from the first decision.

In short, for the deterministic case when no uncertainty is present, the principle of optimality states that the minimum value is a function of the initial state and the initial time. The dynamic programming is best suited for multistage processes. However, the application of

the dynamic programming technique to a continuously operating system leads to nonlinear partial differential equations—the Hamilton–Jacobi–Bellman (HJB) equation. The HJB equation states that, for the optimal control problem:

$$\text{Maximize}_{\theta_i} L = \int_0^T k(\bar{x}_t, \theta_t) dt \quad (24)$$

Subject to:

$$\frac{d\bar{x}_t}{dt} = f(\bar{x}_t, \theta_t) \quad (25)$$

The optimality conditions are given by:

$$0 = \frac{\partial L}{\partial t} + \text{Maximize}_{\theta_i} \left[ k(\bar{x}_t, \theta_t) + \frac{dL}{dt} \right] \quad (26)$$

$$0 = \frac{\partial L}{\partial t} + \text{Maximize}_{\theta_i} \left[ k(\bar{x}_t, \theta_t) + \sum_i \frac{\partial L}{\partial x_i^t} \frac{dx_i^t}{dt} \right] \quad (27)$$

where  $i$  is the number of state variables in the problem. Note that in Equation (24)  $x$  are the state variables and  $\theta$  are the control variables.

On the other hand, when uncertainty is present in the calculation, the HJB equations are modified to obtain the following objective function:

$$\text{Maximize}_{\theta_i} L = E \left[ \int_0^T k(\bar{x}_t, \theta_t) dt \right]$$

where  $E$  is the expectation operator. If the state variable  $i$  can be represented as an Ito process given by equation (28) then, using stochastic dynamic programming, Merton and Samuelson (1990) found that the optimality conditions are given in terms of the expected value of  $dL$  by equation (29).

$$dx_t^i = f_i(\bar{x}_t, \theta_t) dt + \sigma_i dz \quad (28)$$

$$0 = \text{Maximize}_{\theta_i} \left[ k(\bar{x}_t, \theta_t) + \frac{1}{dt} E(dL) \right] \quad (29)$$

Following Ito’s Lemma equation (29) results in:

$$0 = \left[ k(\bar{x}_t, \theta_t^*) + \frac{\partial L}{\partial t} + \sum_i \frac{\partial L}{\partial x_i^t} f_i(\bar{x}_t, \theta_t^*) + \sum_i \frac{\sigma_i^2}{2} \frac{\partial^2 L}{(\partial x_i^t)^2} + \sum_{i \neq j} \sigma_i \sigma_j \frac{\partial^2 L}{\partial x_i^t \partial x_j^t} \right] \quad (30)$$

where  $\theta^*$  represents the optimal solution to the maximization problem.

In Equation (28),  $\sigma$  is the variance parameter of the state variable  $x^i$ . Note that this definition implicitly restricts the analysis for the cases in which the behavior of the state variables can be represented as an Ito process. Also, the extra terms in equations (30) come from the fact that second order contributions of stochastic state variables are not negligible (see equation (22) and Ito’s Lemma). Finally, note that the optimality

conditions derived by Merton are the stochastic generalization of the Bellman–Dreyfus fundamental equation of optimality (Dreyfus, 1965).

#### 4. Application to batch distillation

In this section the real option theory with the Bellman–Dreyfus fundamental equation for optimality is applied to batch distillation optimal control problems. First the parallel between the maximum principle approach, and the no uncertainty case of Bellman–Dreyfus equation described earlier is established. Then the application of this theory is extended to derive an analytical expression for the optimal reflux ratio profile when the uncertainties in the state variables are included in the problem formulation.

##### 4.1. Optimal reflux profile: deterministic case

For the deterministic case, the maximum distillate problem (Problem A) is expressed by Equation (5):

$$\text{Maximize}_{R_i} L = \int_0^T \frac{V}{R_i + 1} [1 - \lambda(x_D^* - x_D^{(1)})] dt$$

subject to Equations (3) and (4):

$$\frac{dx_t^1}{dt} = \frac{-V}{R_i + 1}, \quad x_0^1 = B_0 = F$$

$$\frac{dx_t^2}{dt} = \frac{V}{R_i + 1} \frac{(x_t^2 - x_D^{(1)})}{x_t^1}, \quad x_0^2 = x_F^{(1)}$$

As mentioned above, for the deterministic case, the optimality conditions (Equation (30)) reduce to the HJB equation (Equation (27)). Applying such conditions to Problem A results in:

$$0 = \frac{\partial L}{\partial t} + \text{Maximize}_{R_i} \left\{ \frac{V}{R_i + 1} [1 - \lambda(x_D^* - x_D^{(1)})] - \frac{\partial L}{\partial x_t^1} \frac{V}{R_i + 1} + \frac{\partial L}{\partial x_t^2} \left[ \frac{V(x_t^2 - x_D^{(1)})}{(R_i + 1)x_t^1} \right] \right\}$$

Then, simplifying:

$$0 = \left[ 1 - \lambda(x_D^* - x_D^{(1)}) - \frac{\partial L}{\partial x_t^1} + \frac{\partial L}{\partial x_t^2} \left( \frac{x_t^2 - x_D^{(1)}}{x_t^1} \right) \right] \times \left[ -\frac{V}{(R_i + 1)^2} \right] + \left[ \frac{V}{R_i + 1} \right] \left[ \lambda \frac{\partial x_D^{(1)}}{\partial R_i} - \frac{\partial L}{\partial x_t^2} \frac{1}{x_t^1} \frac{\partial x_D^{(1)}}{\partial R_i} \right]$$

So,

$$R_t = \frac{\frac{\partial L}{\partial x_t^2} \left( \frac{x_t^2 - x_D^{(1)}}{x_t^1} \right) - \frac{\partial L}{\partial x_t^1} - \lambda(x_D^* - x_D^{(1)}) + 1}{\frac{\partial x_D^{(1)}}{\partial R_t} \left( \lambda - \frac{\partial L}{\partial x_t^2} \right)} - 1 \quad (31)$$

Equation (31) is exactly the same result obtained by solving the maximum distillate problem using the maximum principle, and it is an equivalent solution to Equation (16) as follows:

$$\frac{\partial L}{\partial x_t^1} = \mu_t^1 \quad (32)$$

$$\frac{\partial L}{\partial x_t^2} = \mu_t^2 \quad (33)$$

#### 4.2. Case in which uncertainties are present

For this case, the stochastic optimal control problem (Problem B) is expressed as:

$$\text{Maximize}_{R_{tU}} L = E \left[ \int_0^T \frac{V}{R_{tU} + 1} [1 - \lambda(x_D^* - x_D^{(1)})] dt \right] \quad (34)$$

Subject to:

$$dx_t^1 = \frac{-V}{R_{tU} + 1} dt + x_t^1 \sigma_1 dz, \quad x_0^1 = B_0 = F \quad (35)$$

$$dx_t^2 = \frac{V}{R_{tU} + 1} \frac{(x_t^2 - x_D^{(1)})}{x_t^1} dt + x_t^2 \sigma_2 dz, \quad (36)$$

$$x_0^2 = x_F^{(1)}$$

and the optimality conditions developed by Merton and Samuelson (1990) can be stated as:

$$0 = \text{Maximize}_{R_{tU}} \left[ k(\bar{x}_t, R_{tU}) + \frac{1}{dt} E(dL) \right] \quad (37)$$

$$0 = \text{Maximize}_{R_{tU}} \left[ k(\bar{x}_t, R_{tU}) + \frac{\partial L}{\partial t} + \frac{\partial L}{\partial x_t^1} f_1(\bar{x}_t, R_{tU}) + \frac{\partial L}{\partial x_t^2} f_2(\bar{x}_t, R_{tU}) + \frac{\sigma_1^2}{2} (x_t^1)^2 \frac{\partial^2 L}{(\partial x_t^1)^2} + \frac{\sigma_2^2}{2} (x_t^2)^2 \frac{\partial^2 L}{(\partial x_t^2)^2} + \frac{\sigma_1 \sigma_2}{2} x_t^1 x_t^2 \frac{\partial^2 L}{\partial x_t^1 \partial x_t^2} \right] \quad (38)$$

Note that, assuming that the uncertainty terms in Equations (35) and (36) are not correlated, the last term can be eliminated. Hence, by substituting Equations (34)–(36) into Equation (38):

$$0 = \text{Maximize}_{R_{tU}} \left\{ \frac{V}{R_{tU} + 1} [1 - \lambda(x_D^* - x_D^{(1)})] + \frac{\partial L}{\partial t} - \frac{V}{R_{tU} + 1} \frac{\partial L}{\partial x_t^1} + \frac{V(x_t^2 - x_D^{(1)})}{(R_{tU} + 1)x_t^1} \frac{\partial L}{\partial x_t^2} + \frac{\sigma_1^2}{2} (x_t^1)^2 \frac{\partial^2 L}{(\partial x_t^1)^2} + \frac{\sigma_2^2}{2} (x_t^2)^2 \frac{\partial^2 L}{(\partial x_t^2)^2} \right\} \quad (39)$$

$$0 = \left[ 1 - \lambda(x_D^* - x_D^{(1)}) - \frac{\partial L}{\partial x_t^1} + \frac{x_t^2 - x_D^{(1)}}{x_t^1} \frac{\partial L}{\partial x_t^2} \right] \times \left[ -\frac{V}{(R_{tU} + 1)^2} \right] + \left[ \lambda \frac{\partial x_D^{(1)}}{\partial R_{tU}} - \frac{\partial x_D^{(1)}}{\partial R_{tU}} \frac{1}{x_t^1} \frac{\partial L}{\partial x_t^2} \right] \times \left[ \frac{V}{R_{tU} + 1} \right] + \sigma_1 \frac{\partial \sigma_1}{\partial R_{tU}} (x_t^1)^2 \frac{\partial^2 L}{(\partial x_t^1)^2} + \sigma_2 \frac{\partial \sigma_2}{\partial R_{tU}} (x_t^2)^2 \frac{\partial^2 L}{(\partial x_t^2)^2} \quad (40)$$

Simplifying, an implicit equation for  $R_{tU}$  is obtained:

$$R_{tU} = \frac{\frac{\partial L}{\partial x_t^2} \frac{x_t^2 - x_D^{(1)}}{x_t^1} - \frac{\partial L}{\partial x_t^1} - \lambda(x_D^* - x_D^{(1)}) + 1}{\frac{\partial x_D^{(1)}}{\partial R_{tU}} \left[ \lambda - \frac{1}{x_t^1} \frac{\partial L}{\partial x_t^2} \right]} - \frac{\left[ \sigma_1 \frac{\partial \sigma_1}{\partial R_{tU}} (x_t^1)^2 \frac{\partial^2 L}{(\partial x_t^1)^2} + \sigma_2 \frac{\partial \sigma_2}{\partial R_{tU}} (x_t^2)^2 \frac{\partial^2 L}{(\partial x_t^2)^2} \right] \left[ \frac{(R_{tU} + 1)^2}{V} \right]}{\frac{\partial x_D^{(1)}}{\partial R_{tU}} \left[ \lambda - \frac{1}{x_t^1} \frac{\partial L}{\partial x_t^2} \right]} - 1 \quad (41)$$

Note that, assuming that  $\sigma_1 = 0$  (i.e. uncertainty exists only in  $x_t^2$  ( $x_B^{(1)}$ ), but does not exist in  $x_t^1$  ( $B$ )), the equation reduces to:

$$R_{tU} = \frac{\frac{\partial L}{\partial x_t^2} \frac{x_t^2 - x_D^{(1)}}{x_t^1} - \frac{\partial L}{\partial x_t^1} - \lambda(x_D^* - x_D^{(1)}) + 1}{\frac{\partial x_D^{(1)}}{\partial R_{tU}} \left[ \lambda - \frac{1}{x_t^1} \frac{\partial L}{\partial x_t^2} \right]} - \frac{\left[ \sigma_2 \frac{\partial \sigma_2}{\partial R_{tU}} (x_t^2)^2 \frac{\partial^2 L}{(\partial x_t^2)^2} \right] \left[ \frac{(R_{tU} + 1)^2}{V} \right]}{\frac{\partial x_D^{(1)}}{\partial R_{tU}} \left[ \lambda - \frac{1}{x_t^1} \frac{\partial L}{\partial x_t^2} \right]} - 1 \quad (42)$$

#### 4.3. Coupled maximum principle and non-linear programming approach for the uncertain case

Although the real option theory allowed to obtain an analytical expression for the reflux ratio profile, these equations are cumbersome and computationally inefficient to solve. One of the fastest and simplest method to solve optimal control problems in batch distillation with no uncertainty is the coupled maximum principle and nonlinear programming approach by Diwekar (1992). Such an approach can also be used in this work for the



solution of the optimal control problem in the uncertain case but, in order to do that, the derivation of the appropriate adjoint equations is required. Thompson and Sethi (1994) present a description of the mathematical basis of the maximum principle for the deterministic case. An analogous analysis is used in this work for the derivation of the adjoint equations in the uncertain case. The main difference with respect the technique provided by Thompson and Sethi and this work is the form of the Hamiltonian. As it can be observed in equation (38), in the uncertain case the Hamiltonian is augmented with terms involving second derivatives with respect to the state variables. The reason for the existence of such terms has been explained before (Ito's Lemma, Equation (22)). In a similar way, adjoint equations corresponding to uncertain state variables will contain an extra term, which accounts for the uncertain behavior of the state variable.

In this section, the maximum principle formulation, which results from the analysis of the uncertain case (similar to the formulation presented in Diwekar, 1992, the Lagrangian expression of the objective function is not included), is presented.

The problem is expressed as:

$$\text{Maximize}_{R_{IU}} -x_1^1 \tag{43}$$

Subject to:

$$\frac{dx_1^1}{dt} = \frac{-V}{R_{IU} + 1}, \quad x_0^1 = B_0 = F \tag{44}$$

$$dx_2^2 = \frac{V}{R_{IU} + 1} \frac{(x_1^2 - x_D^{(1)})}{x_1^1} dt + x_2^2 \sigma_2 dz, \tag{45}$$

$$x_0^2 = x_F^{(1)}$$

The Hamiltonian, which should be maximized, is:

$$H = \frac{V}{R_{IU} + 1} \frac{\partial L}{\partial x_1^1} + \frac{V}{R_{IU} + 1} \frac{(x_1^2 - x_D^{(1)})}{x_1^1} \frac{\partial L}{\partial x_2^2} + \frac{\sigma_2^2}{2} (x_2^2)^2 \times \frac{\partial^2 L}{(\partial x_2^2)^2} \tag{46}$$

The adjoint equations are:

$$\frac{d\mu_1^1}{dt} = \mu_1^2 \frac{V(x_1^2 - x_D^{(1)})}{(R_{IU} + 1)(x_1^1)^2}, \quad \mu_T^1 = -1 \tag{47}$$

$$\frac{d\mu_2^2}{dt} = -\mu_2^2 \frac{V \left(1 - \frac{\partial x_D^{(1)}}{\partial x_2^2}\right)}{(R_{IU} + 1)x_1^1} - \sigma_2^2 x_2^2 \frac{\partial_2 L}{(\partial x_2^2)^2}, \tag{48}$$

$$\mu_T^2 = 0$$

Recall that:

$$\frac{\partial L}{\partial x_1^1} = \mu_1^1$$

$$\frac{\partial L}{\partial x_2^2} = \mu_2^2$$

Also, by defining:

$$\frac{\partial^2 L}{(\partial x_2^2)^2} = \omega_2 \tag{49}$$

it can be shown that:

$$\begin{aligned} \frac{d\omega_2}{dt} = & -2\omega_2 \frac{V \left(1 - \frac{\partial x_D^{(1)}}{\partial x_2^2}\right)}{(R_{IU} + 1)x_1^1} + \mu_2^2 \frac{V \left(1 - \frac{\partial^2 x_D^{(1)}}{(\partial x_2^2)^2}\right)}{(R_{IU} + 1)x_1^1} - \omega_2 \sigma_2^2 \\ & - 2\sigma_2^2 x_2^2 \frac{\partial_3 L}{(\partial x_2^2)^3}, \end{aligned} \tag{50}$$

$$\omega_T = 0$$

The optimality condition on the reflux ratio results in:

$$\begin{aligned} R_{IU} = & \frac{-\frac{\partial L}{\partial x_2^2} \frac{x_1^2 - x_D^{(1)}}{x_1^1} + \frac{\partial L}{\partial x_1^1}}{\frac{\partial x_D^{(1)}}{\partial R_{IU}} \frac{1}{x_1^1} \frac{\partial L}{\partial x_2^2}} \\ & + \frac{\left[ \sigma_2 \frac{\partial \sigma_2}{\partial R_{IU}} (x_2^2)^2 \frac{\partial^2 L}{(\partial x_2^2)^2} \right] \left[ \frac{(R_{IU} + 1)^2}{V} \right]}{\frac{\partial x_D^{(1)}}{\partial R_{IU}} \frac{1}{x_1^1} \frac{\partial L}{\partial x_2^2}} - 1 \end{aligned} \tag{51}$$

Now, defining:

$$\xi = \frac{\frac{\partial^2 L}{(\partial x_2^2)^2}}{\frac{\partial L}{\partial x_1^1}} = \frac{\omega_2}{\mu_1^1} \tag{52}$$

$$\mu = \frac{\frac{\partial L}{\partial x_2^2}}{\frac{\partial L}{\partial x_1^1}} = \frac{\mu_2^2}{\mu_1^1} \tag{53}$$

and considering negligible third partial derivatives, without loss of information, Equations (47), (48), (50) and (51) can be reformulated as:

$$\frac{d\mu}{dt} = -\mu^2 \frac{V(x_1^2 - x_D^{(1)})}{(R_{IU} + 1)(x_1^1)^2} - \mu \frac{V \left(1 - \frac{\partial x_D^{(1)}}{\partial x_2^2}\right)}{(R_{IU} + 1)x_1^1} - \sigma_2^2 x_2^2 \xi, \tag{54}$$

$$\mu_T = 0$$

$$\frac{d\xi}{dt} = -2\xi \frac{V \left( 1 - \frac{\partial x_D^{(1)}}{\partial x_T^2} \right)}{(R_{IU} + 1)x_T^1} + \mu \frac{V \frac{\partial^2 x_D^{(1)}}{(\partial x_T^2)^2}}{(R_{IU} + 1)x_T^1} - \sigma_2^2 \xi - \xi \mu \frac{V(x_T^2 - x_D^{(1)})}{(R_{IU} + 1)(x_T^1)^2}, \quad (55)$$

$$\xi_T = 0$$

$$R_{IU} = \frac{x_T^1 - \mu(x_T^2 - x_D^{(1)})}{\frac{\partial x_D^{(1)}}{\partial R_{IU}} \mu} + \frac{x_T^1 \left[ \sigma_2 \frac{\partial \sigma_2}{\partial R_{IU}} (x_T^2)^2 \xi \right] \left[ \frac{(R_{IU} + 1)^2}{V} \right]}{\frac{\partial x_D^{(1)}}{\partial R_{IU}} \mu} - 1 \quad (56)$$

This representation allowed the use of the solution algorithm proposed by Diwekar (1992). In such an approach the Lagrangian formulation of the objective function is not used in the solution. Also, it introduces the quasi-steady state approximation to some variables, thereby reducing the dimensionality of the problem. Most important of all, the algorithm avoids the solution of the two-point boundary value problem for the pure maximum principle formulation, or the solution of partial differential equations for the pure dynamic programming formulation. Note that Equation (56) is obtained by maximizing the Hamiltonian (maximizing the distillate), that does not incorporate the purity constraint (Equation (2)). Hence, the use of the final boundary condition ( $\mu_T = 0$ ,  $\xi_T = 0$ ) provides the limiting solution resulting in all the reboiler charge instantaneously going to the distillate pot ( $R = -\infty$ ) with the lowest overall purity. Since in this approach the purity constraint is imposed external to the Hamiltonian, then the final boundary condition is no longer valid. Instead, the final boundary condition is automatically imposed when the purity constraint is satisfied. The algorithm involves solution of the NLP optimization problem for the scalar variable,  $R_0$ , the initial reflux ratio, subject to:

- 1) the dynamics of the state variables (Equations (44) and (45)),
- 2) the adjoint equations (Equations (54) and (55) and the initial conditions for these adjoint equations derived in terms of the decision variable  $R_0$  in the Appendix A, and
- 3) the optimality conditions for the control variable (Reflux Ratio, Equation (56)).

A computer implementation of this algorithm has been incorporated to the MultiBatchDS batch process

simulator (Diwekar, 1996)<sup>1</sup>. Note that the equations derived for the optimal reflux ratio profile (Equations (40) and (41)) and the proposed extension to the coupled approach in the uncertain case can be used whenever the assumption of the state variables of the maximum distillate problem, behaving as an Ito Process, holds. Next section describes how uncertainty in thermodynamic modeling of batch distillation systems can be captured using the concept of an Ito process. It is also shown that, for such a case, one of the state variables of the problem also behaves as an Ito process. Therefore, the tools developed in this work can be applied.

## 5. Uncertainty in the state variables of the maximum distillate problem

As mentioned before, when the model is not a replica of the physical phenomena and on-line updating of an optimal profile is necessary, in most of the cases it is required the use of simplified models like the short-cut model. Also recall, that the main uncertainty in the short-cut model is related to the assumption of constant relative volatility throughout the operation of a batch distillation column. In this section a numerical case-study is used to show that the behavior of the relative volatility can be captured by the Geometric Brownian motion representation. Furthermore, it is shown that the uncertainty in the value of the relative volatility affects the calculation of one of the state variables so that it can also be represented as an Ito process.

### 5.1. Relative volatility: an Ito process

Earlier, the behavior of the stock price was described as an example of a Wiener process. What is common between the technology stock price example given before and the uncertainty in the relative volatility parameter in the batch distillation models?

- 1) Both have time dependent variations. The technology stock fluctuates around the mean randomly, but over a long haul has a positive expected rate of growth. Relative volatility on the other hand fluctuates around the geometric mean across the column height, but over a time period the mean decreases.
- 2) Similar to the stock prices, relative volatility can be modeled as a Markov process since, at any time period, the value of relative volatility depends only

<sup>1</sup> MultiBatchDS is a trade mark of BPRC Inc. Educational version of this simulator is available through CACHE Corporation, e-mail: cache@uts.cc.utexas.edu.

on the previous value. The changes for both are non-overlapping.

- 3) Whether uncertainty in the relative volatility parameter can be represented by a Wiener process or not can be shown with a simple numerical case-study where data are generated from a rigorous simulation model (proxy for experiments) for various thermodynamic systems.

The results of a simple numerical case-study are presented next to show that the behavior of the relative volatility in a batch column can indeed be represented as an Ito process (specifically a Geometric Brownian motion). The example presented here corresponds to 100 kmol of an equimolar mixture of pentane and hexane being processed in a batch rectifier of ten internal theoretical stages at 1 atm of pressure. The vapor rate of the column is 50 kmol h<sup>-1</sup> and the molar holdup is assumed to be constant at 2 kmol for each plate. The batch time of the operation is 2 h. A rigorous simulation was performed in such a column to obtain the behavior of the relative volatility with respect to time. As expected, the relative volatility is different for each plate of the column at each point in time. Fig. 1 shows the behavior of the relative volatility with respect to time and number of plate for this Example.

It can be assumed that the behavior of the relative volatility with respect to time can be represented as a geometric Brownian motion (special instance of an Ito process), that is,

$$d\alpha = \alpha\beta dt + \alpha\sigma dz \tag{57}$$

where  $\beta$  and  $\sigma$  are constants.

Equation (57) establishes that the changes of the relative volatility are lognormally distributed with respect to time. In fact, by using Ito's Lemma, it can be shown that Equation (57) implies that the change in the logarithm of  $\alpha$  is normally distributed with mean  $(\beta - 1/2\sigma^2)t$  and variance  $\sigma^2t$  resulting in Equation (58).

$$d(\ln \alpha) = \left( \beta - \frac{1}{2} \sigma^2 \right) dt + \sigma dz \tag{58}$$

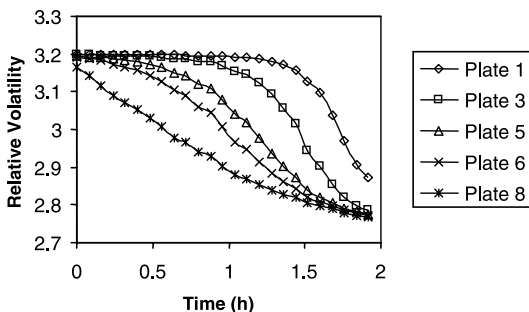


Fig. 1. Relative volatility as a function of time and the number of plate.

As before, in Equations (57) and (58),  $dz$  represents the increment of a Wiener process. This increment can be represented in terms of time as:

$$dz = \epsilon_t \sqrt{dt} \tag{59}$$

where  $\epsilon_t$  is drawn from a normal distribution with zero mean and unit standard deviation. The relationship given by Equation (59) is one of the main properties of a Wiener process and its derivation is presented in Appendix B.

Then, if Equation (57) applies and Equation (59) is substituted on it,  $\alpha(t)$  can be calculated by using the equation:

$$d\alpha = \alpha\beta dt + \alpha\sigma\epsilon_t \sqrt{dt} \tag{60}$$

For numerical purposes, Equation (60) can then be discretized to obtain:

$$\alpha_t = (1 + \beta\Delta t)\alpha_{t-1} + \sigma\alpha_{t-1}\epsilon_t \sqrt{\Delta t} \tag{61}$$

Assuming that  $\alpha$  obeys Equation (58), an analysis of the changes of the logarithm of relative volatility with respect to time for the mixture considered in this example (Fig. 2 shows a plot of the geometric mean (over all the plates of the column) of the relative volatility with respect to time) reveals that the variance of those changes is  $\sigma\Delta t = 0.008308504\Delta t$  and their mean is  $(\beta - 1/2\sigma^2)\Delta t = -0.0669125\Delta t$ . Note that no numerical fit or correlation has been used to calculate those parameters. Further, substituting these values of  $\sigma = 0.008308504$  and  $\beta = -0.06687799$  in Equation (61) results in predicting the uncertain behavior of  $\alpha$  as an Ito process given by the following equation (62).

$$\alpha_t = (1 - 0.06687799\Delta t)\alpha_{t-1} + 0.008308504\alpha_{t-1}\epsilon_t \sqrt{\Delta t} \tag{62}$$

Fig. 3 presents three sample paths and the 66% confidence interval ( $\pm 66\%$ ) for a forecast of  $\alpha$  with respect to time in hours. Notice that  $\epsilon_t$  is drawn from a normal distribution with zero mean and unit standard deviation, so,  $\epsilon_t$  is a random number. Each of those three paths in Fig. 3 is an instance of the calculation of  $\alpha$  based on Equation (62). Notice that the 66% confidence interval covers the deviation in  $\alpha$  in the column shown in

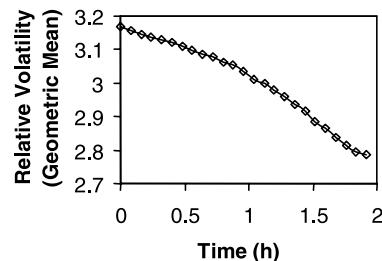


Fig. 2. Geometric mean of the relative volatility for the mixture pentane–hexane.

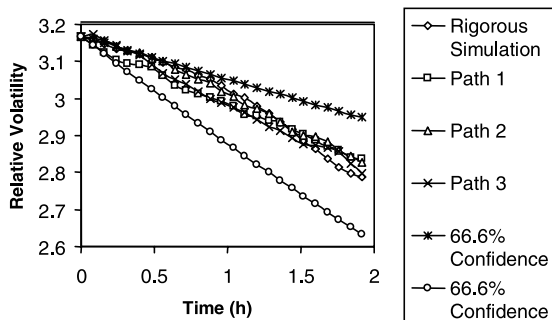


Fig. 3. Three sample paths and the confidence interval for the relative volatility assumed as an Ito process.

Figs. 1 and 2 especially for the initial part of the process. Remember that, in Fig. 1, initially the spread of  $\alpha$  is increasing and then it starts decreasing. However, to get high purity of more volatile component by changing reflux results in stopping the distillation process before it enters this second phase of Fig. 1 where the relative volatility spread is decreasing. Therefore, this Ito process shown in Fig. 3 where the spread of  $\alpha$  is increasing throughout the distillation is a good representation of variation of  $\alpha$ . From the analysis of Fig. 3, it can be seen that the variability in  $\alpha$  can be represented by an Ito process.

By assuming that the state variables of the maximum distillate problem can be represented by equations (35) and (36), an implicit equation (Equation (42)) that allows the calculation of the optimal profile for the reflux ratio has been obtained. For such derivations, it was assumed that the state variables of a maximum distillate problem behave as Ito processes. However, it was explained above that this work focuses on optimal control problems in which the uncertainty in the calculation is introduced by representing the behavior of the relative volatility as a Geometric Brownian motion (61)). If so, is it valid to solve this stochastic optimal control problem with an approach, which assumes uncertainty in the state variables? The answer to this question is given in the following section. By using Ito's Lemma, it is shown that the uncertainty in the calculation of the relative volatility affects the calculation of one of the state variables ( $x_t^2$ , which is the same as  $x_B^{(1)}$ ) so that it can also be represented as an Ito Process.

5.2. State variable and relative volatility: the two Ito processes

Recall that, in the quasi steady state method of batch distillation optimal control problems considered in this work, the integration of the state variables leads to the calculation of the rest of the variables assumed to be in quasi steady state (Diwekar, 1994). Also, recall that such

variables in quasi steady state are determined by applying shortcut method calculations.

Focus now on the expression for the dynamic behavior of the bottom composition of the key component, Equation (36):

$$dx_t^2 = \frac{V}{R_{tU} + 1} \frac{(x_t^2 - x_D^{(1)})}{x_t^1} dt + x_t^2 \sigma_2 dz$$

The question here is how to calculate the term corresponding to uncertainty in  $\alpha$ . To relate the relative volatility with the state variable  $x_t^2$  ( $x_B^{(1)}$ ), the HG equation which relates the relative volatility to the bottom composition  $x_B^{(1)}$  through constant  $C_1$  is used.

$$1 = \sum_{i=1}^n \left( \frac{\alpha_i}{\alpha_1} \right)^{C_1} \frac{x_D^{(1)}}{x_B^{(1)}} x_B^{(i)} \tag{63}$$

Note that the equation contains the relative volatility to the power of  $C_1$ . Rearranging,

$$1 = \frac{x_D^{(1)}}{x_B^{(1)}} \alpha_1^{-C_1} \sum_{i=1}^n \alpha_i^{C_1} x_B^{(i)} \tag{64}$$

Taking the derivatives of this expression implicitly with respect to  $x_B^{(i)}$  and  $\alpha_i^{C_1}$ ,

$$x_B^{(i)} d\alpha_i^{C_1} + dx_B^{(i)} \alpha_i^{C_1} = 0$$

$$\frac{d\alpha_i^{C_1}}{\alpha_i^{C_1}} = - \frac{dx_B^{(i)}}{x_B^{(i)}} \tag{65}$$

Since it was already shown that the relative volatility of the components of a mixture undergoing a batch distillation process can be considered as an Ito process (in particular as a Geometric Brownian motion), that is,

$$d\alpha = \alpha\beta dt + \sigma\alpha dz \tag{66}$$

Then, by using Ito's Lemma (Equation (22)):

$$dF = \frac{\partial F}{\partial t} dt + \frac{\partial F}{\partial x} dx + \frac{1}{2} \frac{\partial^2 F}{\partial x^2} (dx)^2$$

an expression for the relative volatility to the power of  $C_1$ ,  $\alpha^{C_1}$ , can be obtained:

$$d\alpha^{C_1} = \frac{\partial \alpha^{C_1}}{\partial \alpha} d\alpha + \frac{1}{2} \sigma^2 \alpha^2 \frac{\partial^2 \alpha^{C_1}}{\partial \alpha^2} dt \tag{67}$$

Simplifying:

$$d\alpha^{C_1} = C_1 \alpha^{C_1-1} d\alpha + \frac{1}{2} \sigma^2 \alpha^{C_1} C_1 (C_1 - 1) dt$$

and by substituting Equation (66):

$$\frac{d\alpha^{C_1}}{\alpha^{C_1}} = [C_1\beta]dt + C_1\sigma dz \tag{68}$$

Also, substituting Equation (68) in Equation (65) implies that,

$$\frac{dx_t^2}{x_t^2} = \frac{dx_B^{(1)}}{x_B^{(1)}} = -[C_1\beta]dt - C_1\sigma dz \quad (69)$$

Finally, substituting the relation for  $dx_t^2$ , Equation (36), and using Ito’s Lemma for such an expression, results in the following equation:

$$-[C_1\beta]dt - C_1\sigma dz = \left\{ \left[ \frac{V}{R_{tU} + 1} \frac{1}{B} \left( 1 - \frac{x_D^{(1)}}{x_t^2} \right) \right] - \frac{1}{2} \sigma_2^2 \right\} dt + \sigma_2 dz \quad (70)$$

Note that Equations (69) and (70) establish that the uncertain behavior for the relative volatility results in a similar behavior for the dynamics of  $x_t^2$ . That is, if  $\alpha$  is an Ito process then  $x_t^2$  can also be considered as an Ito process.

### 6. Solution of a stochastic optimal control problem

It has been established through a numerical case-study that the uncertainties in relative volatility of the mixture Pentane and Hexane can be represented as an Ito Process. It has been found that a number of mixtures, including non-ideal systems like ethanol–water, also follow the Ito process representation. For details of these case studies, please refer to Ulas, Diwekar & Rico-Ramirez (2003).

The system considered (Ulas, Diwekar & Rico-Ramirez, 2003) was 100 kmol of pentane–hexane mixture being processed in a batch distillation column at 1 atm pressure with ten internal theoretical stages, 70 kmol h<sup>-1</sup> vapor rate and the batch time of the operation was 3 h. The mean relative volatility of this mixture follows the uncertain behavior described by Fig. 4. For this problem, the purity constraint on the distillate was specified as 98%. The coupled maximum principle-NLP approach is used to obtain the two profiles, which are shown in Fig. 5. It can be seen that the reflux ratio profiles for the two cases are significantly different, the

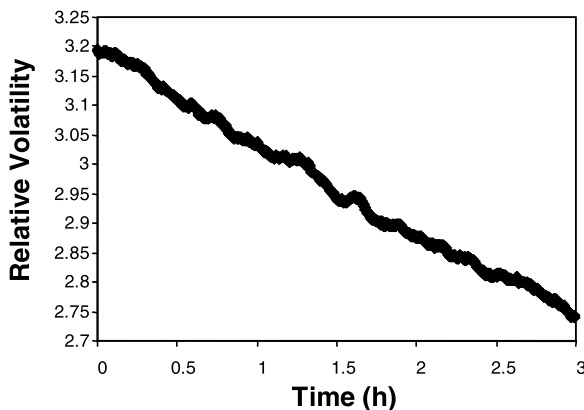


Fig. 4. Relative volatility assumed as a Brownian motion for example 2.

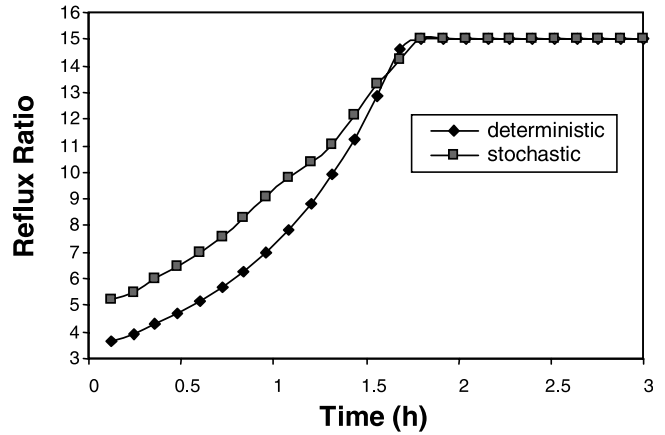


Fig. 5. Optimal reflux profiles for example 2.

uncertainty case having higher reflux ratio at any time as compared with the other two cases. This can be attributed to the fact that the relative volatility of the mixture decreases with time demanding higher reflux. Furthermore, the deviations between the two profiles increases representing the cumulative effect of uncertainties as time progresses. To validate the results, the column is simulated using rigorous model with the three profiles shown in the Fig. 5 and found that the profiles that do not take into consideration uncertainty in  $\alpha$  violates the purity constraint significantly (by 11% for deterministic case). While the stochastic reflux profile provides results closer to the specified purity. Fig. 6 show the distillate composition profiles for the two cases.

### 7. Conclusions

This paper presented the first step towards capturing the uncertainty effects on the optimal control profiles of a batch distillation system. Specifically, the commonly encountered uncertainties in such problems were considered; i.e. uncertainties in thermodynamics when a constant value for the relative volatility is considered. It

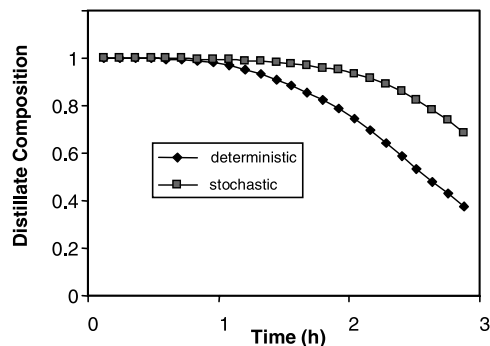


Fig. 6. Distillate composition for the deterministic and stochastic cases.



was shown that the uncertainties in the relative volatility of the system can be considered as an Ito process. Assuming quasi-steady state approximation and the short-cut method, Ito's Lemma is used to show that the uncertainty in the relative volatility parameter affects one of the state variables. This state variable uncertainty can also be represented as an Ito process. For the deterministic case, the real option theory and Merton's optimality conditions result in the same optimal reflux profile as that obtained by the traditional techniques. Finally, the efficient and unified approach of coupled maximum principle and nonlinear optimization technique for the deterministic optimal control problem was extended to the stochastic optimal control problem. The reflux profile obtained for the stochastic case is significantly different from that of the deterministic case.

As far as we know, this paper represents the first successful application of the real option theory from the finance literature to an engineering (chemical) problem.

In this paper the results and analysis for ideal thermodynamic systems where the deviations from the deterministic optimal reflux profile increase with time were presented. In future, some non-ideal and multi-component systems will be analyzed.

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### Appendix A: Initial value for the adjoint variable $\xi$

Assuming that at the initial conditions the effect of stochasticity is not present yet, the following equation applies for the reflux ratio:

$$R = \frac{-\frac{\partial L}{\partial x_t^2} \frac{x_t^2 - x_D^{(1)}}{x_t^1} + \frac{\partial L}{\partial x_t^1}}{\frac{\partial x_D^{(1)}}{\partial R} \frac{1}{x_t^1} \frac{\partial L}{\partial x_t^2}} \quad (\text{A.1})$$

Now, by defining:

$$\mu = \frac{\frac{\partial L}{\partial x_t^2}}{\frac{\partial L}{\partial x_t^1}} \quad (\text{A.2})$$

and substituting in Equation (A.1):

$$\mu = \frac{x_t^1}{(R + 1) \frac{\partial x_D^{(1)}}{\partial R} + (x_t^2 - x_D^{(1)})} \quad (\text{A.3})$$

Also, note that:

$$\begin{aligned} \frac{\partial \mu}{\partial x_t^2} &= \frac{\partial \left( \frac{\frac{\partial L}{\partial x_t^2}}{\frac{\partial L}{\partial x_t^1}} \right)}{\partial x_t^2} = \frac{\frac{\partial^2 L}{(\partial x_t^2)^2}}{\frac{\partial L}{\partial x_t^1}} - \frac{\frac{\partial L}{\partial x_t^2} \frac{\partial^2 L}{\partial x_t^2 \partial x_t^1}}{\left( \frac{\partial L}{\partial x_t^1} \right)^2} \\ &= \frac{\frac{\partial^2 L}{(\partial x_t^2)^2}}{\frac{\partial L}{\partial x_t^1}} - \frac{\frac{\partial L}{\partial x_t^2} \frac{\partial^2 L}{\partial x_t^2 \partial x_t^1}}{\frac{\partial L}{\partial x_t^1}} \end{aligned} \quad (\text{A.4})$$

Furthermore, by defining:

$$\xi = \frac{\frac{\partial^2 L}{(\partial x_t^2)^2}}{\frac{\partial L}{\partial x_t^1}} \quad (\text{A.5})$$

and substituting (A.2), it results in:

$$\frac{\partial \mu}{\partial x_t^2} = \xi - \mu \frac{\frac{\partial^2 L}{\partial x_t^2 \partial x_t^1}}{\frac{\partial L}{\partial x_t^1}} \quad (\text{A.6})$$

Then it is assumed that the second term of the right hand side of (A.2) can be neglected, since it involves the second derivative of the objective function  $L$  with respect to both  $x_t^1$  and  $x_t^2$ . Note that the same case does not apply for the second derivative of the objective function  $L$  with respect to  $x_t^2$ . That is because of the fact that the variable  $x_t^2$  is a stochastic variable behaving as an Ito process. So, (A.6) reduces to:

$$\frac{\partial \mu}{\partial x_t^2} = \xi \quad (\text{A.7})$$

It is important to emphasize that it is assumed that the equality given by (A.7) applies only as an initial condition, since as time progresses during the operation, the effect of stochasticity becomes important and has to be included in (A.1) (see Equations (66) and (67) of the paper).

Taking the derivative of (A.1) with respect to  $x_t^2$ :

$$\xi = \frac{\partial \mu}{\partial x_t^2} = - \frac{x_t^1 \left[ 1 - \frac{\partial x_D^{(1)}}{\partial x_t^2} \right]}{\left[ (R + 1) \frac{\partial x_D^{(1)}}{\partial R} + (x_t^2 - x_D^{(1)}) \right]^2} \quad (\text{A.8})$$

Therefore, the initial conditions for  $\mu$  and  $\xi$  are given from the substitution of the initial values for the variables in Equations (A.8) and (A.3):

$$\mu_0 = \frac{F}{(R_0 + 1) \frac{\partial x_D^{(1)}}{\partial R} \Big|_0 + (x_F^{(1)} - x_D^{(1)})} \quad (\text{A.9})$$

$$\xi_0 = - \frac{F \left[ 1 - \frac{\partial x_D^{(1)}}{\partial x_t^2} \Big|_0 \right]}{\left[ (R_0 + 1) \frac{\partial x_D^{(1)}}{\partial R} \Big|_0 + (x_F^{(1)} - x_D^{(1)}) \right]^2} \quad (\text{A.10})$$

### Appendix B: Derivation of the relationship between $dt$ and $dz$

The relationship between  $dt$  and  $dz$  can be derived as the continuous limit of a discrete-time random walk. This derivation has been taken from the book of Dixit and Pindyck (1994). In a discrete time random walk, time is divided into discrete periods of length  $\Delta t$ . Then, it is assumed that, in each period, the random variable can either move up a distance  $\Delta h$  with a probability  $p$  or down (a distance  $-\Delta h$ ) with a probability  $q = 1 - p$ . Note that from each period to the next,  $\Delta x$  is a random variable that can take the values of  $\pm \Delta h$ . For this process, the mean  $E[\Delta x]$  and the variance  $v[\Delta x]$  are given by:

$$E[\Delta x] = (p - q)\Delta h$$

$$E[(\Delta x)^2] = p(\Delta h)^2 + q(-\Delta h)^2 = (\Delta h)^2 \quad (\text{B.11})$$

$$v[\Delta x] = E[(\Delta x)^2] - (E[\Delta x])^2 = [1 - (p - q)^2](\Delta h)^2 = 4pq(\Delta h)^2 \quad (\text{B.12})$$

A time interval of length  $t$  has  $n = t/\Delta t$  discrete steps. Since successive steps of the random walk are independent, the cumulated change is a binomial random variable with mean:

$$n(p - q)\Delta h = t(p - q)\Delta h/\Delta t \quad (\text{B.13})$$

and variance:

$$n[1 - (p - q)^2](\Delta h)^2 = 4pqt(\Delta h)^2/\Delta t \quad (\text{B.14})$$

So far the probabilities  $p$  and  $q$  and the increments  $\Delta t$  and  $\Delta h$  have been chosen arbitrarily and shortly  $\Delta t$  will be let go to zero. As it does, the mean and the variance

should remain unchanged and independent of the particular choice of  $p$ ,  $q$ ,  $\Delta h$  and  $\Delta t$ . In addition, Equation (59) should be reached in the limit. All those conditions are met by setting:

$$\Delta h = \sigma \sqrt{\Delta t} \quad (\text{B.15})$$

and

$$p = \frac{1}{2} \left[ 1 + \frac{\beta}{\sigma} \sqrt{\Delta t} \right]$$

$$q = \frac{1}{2} \left[ 1 - \frac{\beta}{\sigma} \sqrt{\Delta t} \right]$$

Then

$$p - q = \frac{\beta}{\sigma} \sqrt{\Delta t} = \frac{\beta}{\sigma^2} \Delta h \quad (\text{B.16})$$

By substituting equations (B.15) and (B.16) into equations (B.11) and (B.12) and let  $\Delta t$  approach to zero ( $n$  goes to infinity), the binomial distribution converges to a normal distribution with mean:

$$t \frac{\beta}{\sigma^2} \Delta h \frac{\Delta h}{\Delta t} = \beta t \quad (\text{B.17})$$

and variance:

$$t \left[ 1 - \left( \frac{\beta}{\sigma} \right)^2 \Delta t \right] \frac{\sigma^2 \Delta t}{\Delta t} = \sigma^2 t \quad (\text{B.18})$$

Observe that those are exactly the values needed for Brownian motion as given by Equation (57),  $\beta$  is the drift and  $\sigma^2$  the variance. Also note that, in order to preserve equation (B.18), the relationship between  $\Delta h$  and  $\Delta t$  is not an arbitrary one. Using equation (B.15) is the only way to make the variance depend on  $t$  and not on the number of steps.

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