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Analysis and Optimization of the Williams-Otto Process by Geometric Programming

This paper applies the principles of geometric programming to the optimization of the well-known Williams-Otto process. Following the trend of the articles published on this subject, two different objective functions are considered and the results are compared to those of other investigators.

The dual geometric program is used to provide an answer to the question of why the optimal value of the objective function remains unchanged for perturbations in a certain variable.

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SCOPE

In this paper geometric programming is used to optimize the well-known Williams-Otto process. This process consists of a stirred-tank reactor and a separation system involving a cooler, a decanter, and a distillation column and has served as an example for a multitude of optimization studies.

The main purpose of this work is not to add another example to the rapidly expanding list of applications of geometric programming; neither is it to prove that geometric programming is another method for solving the Williams-Otto plant. The main goal is to shed some more light on various questions raised in connection with the optimization of the Williams-Otto plant and to examine in detail the observation made by Luus and Jaakola (1973) that the optimal value of the objective function remains unchanged under variations of a certain primal variable.

The theory of geometric programming is centered around some elegant and powerful primal-dual relations. The present paper shows that these relations not only provide a useful basis for computational algorithms, but that they also might be helpful in the analysis of the mathematical model describing the process to be optimized. Indeed an inconsistency in this model might cause numerical difficulties when applying an optimization procedure. These difficulties are then usually blamed on the optimization method, while in fact they are due to the model.

The dual geometric program contains valuable information on the primal problem and provides an answer to specific questions such as the occurrence in the model of redundant variables and redundant constraints. Hence a careful examination of this dual program prior to its optimization might safeguard the optimization procedure against pitfalls due to the mathematical model.

CONCLUSIONS AND SIGNIFICANCE

This paper derives the dual geometric programming constraints for the optimization of the classical Williams-Otto process. It shows how an examination of the linear so-called "orthogonality conditions" of geometric programming reveals a linear dependency among these conditions. Each of these conditions is related to a primal variable and their dependency means that the optimal value of the objective function remains unchanged under variations in a primal (redundant) variable. A further analysis of the orthogonality conditions and the nonlinear equilibrium conditions of the dual program makes clear that this redundancy is caused by an inconsistency in the primal mathematical model. Indeed both the objective function and the primal constraints can be written independently from a primal variable (for instance, the volume of the reactor). Clearly, under these conditions a completely arbitrary value can be assigned to this reactor volume without affecting the optimal value of the objective function.

Finally, the paper compares the optimal solution obtained by geometric programming to the results of other investigators for the two slightly different versions of this problem which have been circulating. Most processes in the chemical industry demonstrate the existence of optimal operating conditions so that a formal optimization of these processes is mandatory from an economical point of view. However, the application of such techniques might cause numerical difficulties, especially when the mathematical model simulating the operation of the plant becomes nonlinear.

It is a well established fact in the literature that for most engineering problems the above mentioned nonlinearities satisfy the formulation requirements of geometric programming (see, for instance, Rijckaert, 1973).

PRINCIPLES OF GEOMETRIC PROGRAMMING

Geometric programming deals with optimization problems that can be written as [Readers less familiar with the theory of geometric programming are referred to the basic textbook of Duffin, Peterson and Zener (1967), the textbook of Wilde and Beightler (1967) and to a recent article by Peterson (1973)]:

$$\min g_0 = \min \sum_{t=1}^{T_0} \sigma_{0t}\, c_{0t} \prod_{n=1}^{N} x_n^{a_{0tn}} \qquad (1)$$

$$\text{s.t. } \sigma_m\, g_m^{\sigma_m} = \sigma_m \left[\sum_{t=1}^{T_m} \sigma_{mt}\, c_{mt} \prod_{n=1}^{N} x_n^{a_{mtn}} \right]^{\sigma_m} \leq 1$$

$$m = 1, \ldots, M \qquad (2)$$

$$x_n > 0 \quad n = 1, \ldots, N$$

with a_{mtn} = exponents of the primal variables (real constants)

c_{mt} = coefficients of the primal terms (positive constants)

σ_{mt} = sign of the corresponding term

σ_m = sign of the corresponding constraint

To this primal program corresponds a quasidual one with linear constraints as reported by Passy and Wilde (1967). A precise description of the quasidual program requires the definition of a pseudomaximum which is a point satisfying the Kuhn-Tucker necessary conditions for a constrained local maximum. At such a pseudomaximum the objective function is maximal with respect to all variables which are zero but only stationary with respect to variables with positive values.

Hence an interior pseudomaximum with all variables positive is a stationary point which might even be a local minimum. The process of finding a pseudomaximum is called pseudomaximization.

The quasidual program looks for the T-dimensional vector $\boldsymbol{\omega}^0$ and the M-dimensional vector $\boldsymbol{\omega}_0^0$, pseudomaximizing the scalar function

$$v(\boldsymbol{\omega}) = \sigma_0 \left[\prod_{m=0}^{M} \prod_{t=1}^{T_m} \left(\frac{c_{mt}\, \omega_{m0}}{\omega_{mt}} \right)^{\sigma_{mt}\omega_{mt}} \right]^{\sigma_0} \qquad (3)$$

where $\sigma_0 = \text{sign}\,(g_0(\mathbf{x}^0))$

$$\omega_{00} = 1 \qquad (4)$$

subject to the following linear equality constraints:
normality condition

$$\sum_{t=1}^{T_0} \sigma_{0t}\, \omega_{0t} = \sigma_0 \qquad (5a)$$

orthogonality conditions

$$\sum_{m=0}^{M} \sum_{t=1}^{T_m} \sigma_{mt}\, a_{mtn}\, \omega_{mt} = 0 \quad n = 1, \ldots, N \tag{5b}$$

the equations

$$\sum_{t=1}^{T_m} \sigma_{mt}\, \omega_{mt} = \sigma_m\, \omega_{m0} \quad m = 1, \ldots, M \tag{5c}$$

and the nonnegativity conditions

$$\omega_{mt} \geq 0 \quad t = 1, \ldots, T_m; \quad m = 0, \ldots, M \tag{6}$$

The symbols $T = \sum_{m=0}^{M} T_m$, a_{mtn}, c_{mt}, σ_{mt} and σ_m were defined in the primal program. Only when all signum functions σ_{mt} and σ_m are positive, the global minimum of the primal coincides with the global linearly constrained maximum of the dual. In this case the polynomials (2) are called posynomials.

When some primal signum functions are negative, pseudominima might occur. The quasiduality theorems of Passy and Wilde assure then that the global minimum of the primal equals the smallest pseudomaximum of the dual. The polynomials (2) are then called signomials instead of posynomials. Hence, if one prefers to solve the dual instead of the primal, the problem is transformed into one of finding stationary points of the dual program.

Such points are obtained by setting the Jacobians of the independent dual variables equal to zero, creating this way a set of nonlinear equations called equilibrium conditions:

$$\sum_{m=0}^{M} \sum_{t=1}^{T_m} \sigma_{mt}\, \nu_{mtd} (\log \omega_{mt} - \log \omega_{m0}) = \sum_{m=0}^{M} \sum_{t=1}^{T_m} \sigma_{mt}\, \nu_{mtd} \log c_{mt} \quad d = 1, \ldots, D \tag{7}$$

where $D = T - (N + 1)$: degree of difficulty
$\boldsymbol{\nu}_d$ are D linearly independent vectors orthogonal to normality and orthogonality conditions.

Adding these equilibrium conditions to the set of Equations (5) gives a dual program with exactly as many unknowns as equations, which is solved iteratively by a Newton-Raphson method.

It should be noted at this point that—as described by Peterson (1972)— inactive constraints in geometric programs can be treated by inserting simultaneously a slack-term in the objective function and in each constraint that might be inactive.

The program stated in (1) and (2) is then redefined as

$$\min g_0 = \min \left[\sum_{t=1}^{T_0} \sigma_{0t}\, c_{0t} \prod_{n=1}^{N} x_n^{a_{0tn}} + \sum_{j=1}^{P} b_j\, \epsilon_j^{-0.01} \right] \tag{8}$$

$$\text{s.t. } \sigma_m\, g_m^{\sigma_m} = \sigma_m \left[\sum_{t=1}^{T_m} \sigma_{mt}\, c_{mt} \prod_{n=1}^{N} x_n^{a_{mtn}} \right]^{\sigma_m} \leq 1$$

$$m = 1, \ldots, M - P - 1 \tag{9}$$

$$\sigma_j\, g_j^{\sigma_j} = \sigma_j \left[\sum_{t=1}^{T_j} \sigma_{jt}\, c_{jt} \prod_{n=1}^{N} x_n^{a_{jtn}} + \epsilon_j \right]^{\sigma_j} \leq 1$$

$$j = M - P, \ldots, M \tag{10}$$

where P is the number of inactive constraints and b_j are positive constants. This program (8, 9, 10) is called the augmented program. It can be solved in exactly the same way as program (1, 2).

Rijckaert and Martens (1973) showed that by a proper selection of b_j, $j = 1, \ldots, P$ the value of objective function (1) can be deduced from the value of objective function (8).

WILLIAMS-OTTO PROCESS

The optimization of the Williams-Otto process has gotten a lot of attention in the chemical engineering literature. Each investigator used a different technique and a variety of optimal conditions were found. However, part of this variety is caused by the fact that different forms for the objective function have been circulating. Mainly two types are frequently encountered. One of them results in an optimal return of nearly 50%. The other gives about 120%. Both versions will be discussed in this paper.

Formulation of the Process

A block diagram of the Williams-Otto process is shown in Figure 1. Although the plant is represented by a somewhat simplified model, this model stays sufficiently close to reality in order to be a meaningful representation of the real life process.

The process consists of a stirred-tank reactor, a separation system involving a cooler, a decanter, and a distillation column.

Two input streams A and B together with a recycle stream are fed into a perfectly stirred reactor, of which the temperature is controllable at any desired value. The plant is built to manufacture 18 143 696 kg/year (40 000 000 lb./yr.) of distillate P. In the reactor three irreversible exothermic second-order reactions take place

$$A + B \rightarrow C$$
$$C + B \rightarrow P + E$$
$$P + C \rightarrow G$$

The reaction coefficient of each individual reaction can be expressed in the classical Arrhenius form

$$k_i = Q_i \exp(-B_i/T) \quad i = 1, 2, 3 \tag{12}$$

where T is the temperature in °K. (Numerical values for Q_i and B_i are listed in Appendix A.)

The reactor effluent F_R contains six components: the raw materials A and B, the desired product P (to be removed by distillation), an intermediate C, an inert E, and a residu G. After the effluent is cooled, G becomes insoluble in it and is separated in the decanter. The desired product P forms an azeotropic mixture with the bottom of the distillation column so that the recovery of P will be incomplete. The concentration of inert E is controlled by discarding a portion of the bottom product. The remainder is recycled to the reactor.

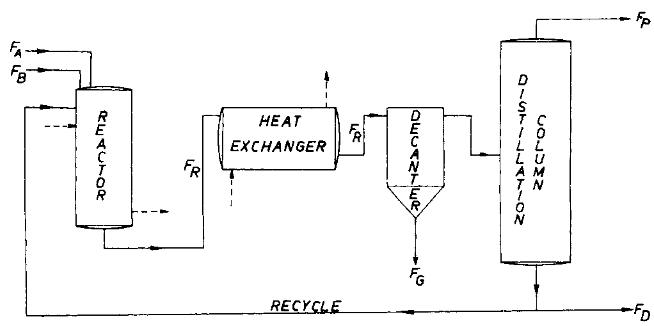

Fig. 1. Block diagram of the Willioms-Otto process.

The rate of reaction is found to be negligible below 322.22°K (580°R) and substantial decomposition occurs above 377.78°K (680°R). The density ρ of the reaction mixture can be considered constant at 240.28 kg/m^3 (50 lb./cu.ft.), while the molecular weights of the components are listed in Appendix A. In this appendix also the process constraints are formulated whereas in Appendix B the constraints are transformed into a more simple set by using the substitutions introduced by Luus and Jaakola (1973). The latter formulation is used here. The objective function for this process is then:

(a) either

Find max % return =

$$\max\left[\frac{100[8400X - 2.22F_R - 0.124(8400)(0.3F_P + 0.0068F_D - 60V\rho)]}{600\,V\rho}\right] \quad (13)$$

where

$$X = 0.3F_P + 0.0068F_D - 0.02F_A - 0.03F_B - 0.01F_G \quad (14)$$

Inserting X and F_B (A17) into (13) yields

max % return =

$$\max\left((84F_A - 201.96F_D - 336F_G + 1955.52F_P - 2.22F_R - 60V\rho)(6V\rho)^{-1}\right) \quad (15)$$

(b) or

Find max % return =

$$\max\left[\frac{100[8400X - 2.22F_R - 0.124(8400)(0.3F_P + 0.0068F_D) - (30V\rho + 1.3F_R)]}{300V\rho + 13F_R}\right] \quad (16)$$

Inserting X and F_B also into (16) gives

max % return =

$$\max\,(84F_A - 201.96F_D - 336F_G + 1955.52F_P - 3.52F_R - 30V\rho)(3V\rho + 0.13F_R)^{-1} \quad (17)$$

The two objective functions become identical if one could assume that $V\rho = 0.13/3\ F_R$.

Solution by Geometric Programming

The formulation of the Williams-Otto process developed by Luus and Jaakola (1973a) and described in Appendix B was the basis of the present geometric programming formulation. Two alterations are made, however.

1. The variables F_B and F_{RE} only appear in the constraints (B10) and (B11). They can be neglected during the calculation of the optimum since (A10) and (B4) assure that they will remain positive for all positive values of the other variables.

2. The temperature T is replaced as a variable by k_1 with

$$k_2 = 1.56268\,k_1^{1.25}$$

$$k_3 = 0.48932\,k_1^{1.67}$$

The geometric programming formulation becomes

$$\min g_0 = \min(-84F_A + 201.96F_D + 336F_G - 1955.52F_P + 2.22F_R)(6V\rho)^{-1} + 0.4\epsilon_1^{-0.01} + 0.4\epsilon_2^{-0.01} \quad (18)$$

$$g_1 = 0.73398k_1^{0.67}\,F_{RC}F_{RP}F_G^{-1}\,\beta \leq 1 \quad (19)$$

$$g_2 = -\,(-\,1.56268k_1^{0.25}F_{RC}F_{RA}^{-1} - 0.24466k_1^{0.67}F_{RC}F_{RB}^{-1}F_{RA}^{-1}F_{RP} - 0.15627k_1^{0.25}F_{RC}^2b^{-1}F_{RA}^{-1})^{-1} \leq 1 \quad (20)$$

$$g_3 = -\,(-\,1.25014k_1^{1.25}F_{RB}F_{RC}F_P^{-1}\beta + 0.24466k_1^{1.67}F_{RC}F_{RP}F_P^{-1}\beta)^{-1} \leq 1 \quad (21)$$

$$g_4 = 0.31254k_1^{1.25}F_{RB}F_{RC}F_D^{-1}b^{-1}\alpha\beta \leq 1 \quad (22)$$

$$g_5 = -\,(-\,k_1F_{RA}F_{RB}F_A^{-1}\beta - 0.31254k_1^{1.25}F_{RA}F_{RB}F_{RC}F_A^{-1}b^{-1}\beta)^{-1} \leq 1 \quad (23)$$

$$g_6 = \rho^{-1}\,\beta V^{-1}\,F_R^2 \leq 1 \quad (24)$$

$$g_7 = -\,(-\,F_{RP}b^{-1} + 1.25014k_1^{1.25}F_{RB}F_{RC}b^{-1}\beta - 0.24466k_1^{1.67}F_{RC}F_{RP}b^{-1}\beta)^{-1} \leq 1 \quad (25)$$

$$g_8 = \alpha F_R^{-1} + 0.73398k_1^{1.67}F_{RC}F_{RP}F_R^{-1}\beta + F_{RP}F_R^{-1} - bF_R^{-1} \leq 1 \quad (26)$$

$$g_9 = \alpha^{-1}F_{RC} + 0.24466k_1^{0.67}F_{RC}F_{RP}F_{RB}^{-1}\alpha^{-1} + 0.15627k_1^{0.25}F_{RC}^2b^{-1}\alpha^{-1} + F_{RB}\alpha^{-1}\,11b\alpha^{-1} + 1.5628k_1^{0.25}F_{RC}\alpha^{-1} \leq 1 \quad (27)$$

$$g_{10} = 0.00772k_1 + \epsilon_1 \leq 1 \quad (28)$$

$$g_{11} = 6.17975k_1^{-1} + \epsilon_2 \leq 1 \quad (29)$$

Since it is intended to manufacture 2160.46 kg/h (4763 lb./hr.) of distillate P, the variable F_P is fixed. [Luus and Jaakola (1973a,b) didn't keep F_P constant. In the next paragraph this will be discussed in more detail.] The above formulated optimization problem has 34 terms, 11 constraints and 15 variables. Its degree of difficulty is 18. This means that 18 equilibrium conditions have to be defined.

In the corresponding dual objective function (3) σ_0 equals -1 whereas the dual constraints are

Normality condition

$$-\,\omega_{01} + \omega_{02} + \omega_{03} - \omega_{04} + \omega_{05} + \omega_{06} + \omega_{07} = -\,1 \quad (30)$$

Orthogonality conditions

$$-\,\omega_{01} + \omega_{51} + \omega_{52} = 0 \quad (31)$$

$$\omega_{02} - \omega_{41} = 0 \quad (32)$$

$$\omega_{03} - \omega_{11} = 0 \quad (33)$$

$$1.67\omega_{11} - 0.25\omega_{21} - 0.67\omega_{22} - 0.25\omega_{23} - 1.25\omega_{31} + 1.67\omega_{32} + 1.25\omega_{41} - \omega_{51} - 1.25\omega_{52} + 1.25\omega_{72} - 1.67\omega_{73} + 1.67\omega_{82} + 0.25\omega_{96} + 0.67\omega_{92} + 0.25\omega_{93} + \omega_{101} - \omega_{111} = 0 \quad (34)$$

$$\omega_{05} + 2\omega_{61} - \omega_{81} - \omega_{82} - \omega_{83} + \omega_{84} = 0 \quad (35)$$

$$\omega_{01} - \omega_{02} - \omega_{03} + \omega_{04} - \omega_{05} - \omega_{61} = 0 \quad (36)$$

$$\omega_{11} - \omega_{21} - \omega_{22} - 2\omega_{23} - \omega_{31} + \omega_{32} + \omega_{41} - \omega_{52} + \omega_{72} - \omega_{73} + \omega_{82} + \omega_{91} + \omega_{92} + 2\omega_{93} + \omega_{96} = 0 \quad (37)$$

$$\omega_{11} - \omega_{22} + \omega_{32} - \omega_{71} - \omega_{73} + \omega_{82} + \omega_{83} + \omega_{92} = 0 \quad (38)$$

$$\omega_{11} - \omega_{31} + \omega_{32} + \omega_{41} - \omega_{51} - \omega_{52} + \omega_{61} + \omega_{72} - \omega_{73} + \omega_{82} = 0 \quad (39)$$

$$\omega_{21} + \omega_{22} + \omega_{23} - \omega_{51} - \omega_{52} = 0 \quad (40)$$

$$\omega_{22} - \omega_{31} + \omega_{41} - \omega_{51} - \omega_{52} + \omega_{72} - \omega_{92} + \omega_{94} = 0 \quad (41)$$

$$\omega_{23} - \omega_{41} + \omega_{52} + \omega_{71} - \omega_{72} + \omega_{73} - \omega_{84} - \omega_{93} + \omega_{95} = 0 \quad (42)$$

$$\omega_{41} + \omega_{81} - \omega_{91} - \omega_{92} - \omega_{93} - \omega_{94} - \omega_{95} - \omega_{96} = 0 \quad (43)$$

$$-0.01\omega_{06} + \omega_{102} = 0 \quad (44)$$

$$-0.01\omega_{07} + \omega_{112} = 0 \quad (45)$$

The linear equations (5c) are

$$\omega_{11} - \omega_{10} = 0 \quad (46)$$

$$\omega_{21} + \omega_{22} + \omega_{23} - \omega_{20} = 0 \quad (47)$$

$$\omega_{31} - \omega_{32} - \omega_{30} = 0 \quad (48)$$

$$\omega_{41} - \omega_{40} = 0 \quad (49)$$

$$\omega_{51} + \omega_{52} - \omega_{50} = 0 \quad (50)$$

$$\omega_{61} - \omega_{60} = 0 \quad (51)$$

$$\omega_{71} - \omega_{72} + \omega_{73} - \omega_{70} = 0 \quad (52)$$

$$\omega_{81} + \omega_{82} + \omega_{83} - \omega_{84} - \omega_{80} = 0 \quad (53)$$

$$\omega_{91} + \omega_{92} + \omega_{93} + \omega_{94} + \omega_{95} + \omega_{96} - \omega_{90} = 0 \quad (54)$$

$$\omega_{101} + \omega_{102} - \omega_{100} = 0 \quad (55)$$

$$\omega_{111} + \omega_{112} - \omega_{110} = 0 \quad (56)$$

And the equilibrium conditions are

$$\prod_{m=0}^{M} \prod_{t=1}^{T_m} \nu_{mtd}\, \sigma_{mt} \log\left(\frac{\omega_{mt}}{\omega_{m0}}\right) = \prod_{m=0}^{M} \prod_{t=1}^{T_m} \nu_{mtd}\, \sigma_{mt} \log c_{mt} \qquad d = 1, \ldots, D \quad (57)$$

in which $\nu_{mtd} = 0$ for $t = 1, \ldots, T_m$; $m = 0, \ldots, M$; $d = 1, \ldots, D$ if its value is not listed in Table 1.

The solution of this dual program obtained by the aforementioned method is

$$\min g_0 = -120.73 - 0.80833 = -121.5383$$

The optimal dual variables are shown in Table 2.

After applying the correction described by Rijckaert and Martens (1973) for the use of slackterms, the objective function becomes

$$\min g_0 = -121.530 \pm 0.012$$

Note that the dual variables corresponding to each term of the constraints g_{10} and g_{11} into which slackvariables were added are of the same size. These constraints would have been inactive if no slackterm was introduced. Hence they could have been deleted without affecting the optimal solution, as done by Luus and Jaakola (1973a,b).

Nevertheless, this approach would have generated incorrect results if g_{10} and g_{11} were active in the optimum so that the use of slackvariables is a more secure procedure.

Table 3 shows the primal optimal solution of this problem together with the results of Luus and Jaakola (1973a) and with these of Adelman and Stevens (1972) corrected by Luus and Jaakola (1973a).

TABLE 1. ELEMENTS OF ν_{mtd} DIFFERENT FROM ZERO (OBJECTIVE FUNCTION 1)

d	$mt : \nu_{mtd}$									
1	01 : 1	06 : −1	21 : 1	51 : 1	61 : −1	81 : −2	91 : 4	94 : −1	96 : −5	102 : −0.01
2	01 : 1	07 : −1	21 : 1	51 : 1	61 : −1	81 : −2	91 : 4	94 : −1	96 : −5	112 : −0.01
3	01 : 1	03 : −1	11 : −1	22 : 1	51 : 1					
4	21 : −1	23 : 1	91 : −1	95 : 1						
5	01 : −1	04 : 1	21 : −1	31 : 1	51 : −1					
6	03 : 1	04 : −1	11 : 1	32 : −1						
7	01 : 1	02 : −1	21 : 1	41 : −1	51 : 1	95 : −1				
8	51 : −1	52 : 1	95 : 1	96 : −1						
9	01 : 1	03 : −1	11 : −1	21 : 1	51 : 1	71 : 1	91 : −1.67	94 : −1	95 : 1	96 : 1.67
10	01 : 1	05 : −1	21 : 1	51 : 1	72 : −1	81 : −1	95 : −1			
11	03 : −1	05 : 1	11 : −1	73 : 1	81 : 1	95 : 1				
12	03 : 1	05 : −1	11 : 1	82 : −1						
13	01 : −1	03 : 1	11 : 1	21 : −1	51 : −1	81 : 1	83 : −1	91 : 1.67	94 : 1	96 : −1.67
14	81 : −1	84 : 1	95 : −1							
15	01 : −1	03 : 1	11 : 1	21 : −1	51 : −1	92 : −1	96 : 1			
16	91 : 1	93 : −1	95 : −1	96 : 1						
17	91 : −4	96 : 4	101 : −1							
18	91 : 4	96 : −4	111 : −1							

TABLE 2. VALUES OF ω_{mt} AT THE OPTIMUM (OBJECTIVE FUNCTION 1)

m \ $t =$	1	2	3	4	5	6	7	0
0	1.012	6.540	0.962	8.308	0.733	0.042	0.042	1.000
1	0.962							0.962
2	0.843	0.124	0.452					1.012
3	10.170	1.866						8.308
4	6.540							6.540
5	0.656	0.356						1.012
6	1.084							1.084
7	2.872	0.867	0.159					2.164
8	2.839	0.025	0.151	0.114				2.001
9	0.202	0.150	0.055	3.805	4.144	1.024		9.379
10	0.002	$0.4(10^{-3})$						$0.3(10^{-3})$
11	$0.2(10^{-4})$	$0.4(10^{-3})$						$0.4(10^{-3})$

Sriram and Stevens (1973) and Ahlgren and Stevens (1966) solved the above optimization program with the second form of the objective function. If the term $(3V\rho + 0.13F_R)$ is replaced by τ, this alternative problem is related to the first one, and one gets

$$\max \% \text{ return} = \max(84F_A - 201.96F_D - 336F_G + 1955.52F_P - 2.22F_R)\,\tau^{-1} + 10 \quad (58)$$

with

$$g_6 = 3F_R{}^2\tau^{-1}\beta + 0.13F_R\tau^{-1} \leq 1 \quad (59)$$

All other primal constraints (19) to (23) and (25) to (29) remain unchanged. Constraint g_6 now contains two terms instead of one. In the corresponding dual program a new dual variable ω_{62} is introduced, so that the orthogonality conditions for F_R and τ become

$$\omega_{05} + 2\omega_{61} + \omega_{62} - \omega_{81} - \omega_{82} - \omega_{83} + \omega_{84} = 0 \quad (60)$$

$$\omega_{01} - \omega_{02} - \omega_{03} + \omega_{04} - \omega_{05} - \omega_{61} - \omega_{62} = 0 \quad (61)$$

The variable ω_{60} is now given by

$$\omega_{60} = \omega_{61} + \omega_{62} \quad (62)$$

Also another equilibrium condition needs to be added since the primal program is augmented by one term, while the number of variables remains unchanged.

A maximal percent return of 50.825 is obtained.

In Table 4 the results of this optimization problem are listed. They are also compared to the data of other investigators.

DISCUSSION OF THE FORMULATION AND THE OPTIMIZATION OF THE WILLIAMS-OTTO PROCESS

Value of the objective function and of the dual variables

The optimization problem as stated in Appendix B has 9 constraints and 14 variables. [As discussed before the inequality constraints (B12a) and (B12b) were omitted.] Its solution is not uniquely defined, neither for objective function 1 nor for objective function 2. This can be observed by an examination of the 14 orthogonality conditions of the dual program. Indeed these equations are not linearly independent. For instance, the orthogonality condition for β can be reproduced by adding all orthogonality conditions but the one for k_1.

Mathematically each orthogonality condition corresponds to a primal variable and is equivalent to putting the first derivative of the Lagrangian with respect to this variable equal to zero. The dependency of such conditions then implies that the stationary value of the Lagrangian remains constant with regard to one variable.

This variable can be chosen arbitrarily before performing the optimization, and its value will not affect the stationary value of the Lagrangian nor the optimal value of the objective function.

Since the plant is built to produce 2160.46 kg/hr. (4763 lb./hr.) of distillate P we will select F_P as arbitrarily to be chosen variable instead of β.

Following Luus and Jaakola F_P is given the values 2 160.46 (4763), 6.82 (15.04), 207 219.57 (456 840.93) kg/hr. (lb/hr.). Conform to the above theoretical remark, under each of these assumptions an optimal profit of

TABLE 3. PRIMAL OPTIMAL SOLUTION FOR OBJECTIVE FUNCTION 1

Var.	Present opt. sol. kg/hr.	lb./hr.	Opt. sol. Luus-Jaakola (73) kg/hr.	lb./hr.	Corrected opt. sol. Adelman-Stevens (72) kg/hr.	lb./hr.
F_A	6 125.90	13 505.29	6 130.85	13 516.20	6 127.22	13 508.20
F_B	13 962.67	30 782.41	13 962.64	30 782.36	13 905.41	30 656.17
F_D	16 471.01	36 312.35	16 475.34	36 321.90	16 431.13	36 224.43
F_G	1 457.10	3 212.35	1 457.26	3 212.70	1 440.77	3 176.35
F_P	2 160.46	4 763.00	2 160.90	4 763.96	2 160.93	4 763.60
F_R	168 016.00	370 411.86	168 474.94	371 423.65	163 797.59	361 111.84
F_{RA}	21 499.91	47 399.18	21 611.56	47 645.34	21 117.69	46 556.53
F_{RB}	66 695.79	147 039.03	66 874.86	147 433.81	64 765.97	142 784.52
F_{RC}	3 534.97	7 793.27	3 541.90	7 808.55	3 504.20	7 725.44
F_{RE}	66 042.24	145 598.20	66 207.70	145 962.99	64 371.12	141 914.02
F_{RP}	8 764.69	19 322.83	8 781.67	19 360.26	8 597.84	18 955.00
T	374.46°K	674.03°R	374.69°K	674.44°R	373.67°K	672.61°R
V	0.8707 m³	30.75 cu. ft.	0.8696 m³	30.71 cu. ft.	0.9093 m³	32.11 cu. ft.
g_0(%)	121.54		121.53		121.33	

TABLE 4. PRIMAL OPTIMAL SOLUTION FOR OBJECTIVE FUNCTION 2

Var.	Present opt. sol. kg/hr.	lb./hr.	Opt. sol. Sriram-Stevens (73) kg/hr.	lb./hr.	kg/hr.	lb./hr.	Opt. sol. Ahlgren-Stevens (66) kg/hr.	lb./hr.
F_A	5 673.08	12 507	5 610.48	12 369	5 603.23	12 353	5 697.12	12 560
F_B	13 054.39	28 780	13 081.15	28 839	13 025.36	28 716	13 126.96	28 940
F_D	15 174.48	33 454	15 136.83	33 371	15 063.80	33 210	15 254.31	33 630
F_G	1 392.98	3 071	1 394.34	3 074	1 404.32	3 096	1 416.57	3 123
F_P	2 160.46	4 763	2 160.46	4 763	2 160.46	4 763	2 160.46	4 763
F_R	65 525.05	144 458	65 159.91	143 653	66 703.94	147 057	67 458.26	148 720
F_{RA}	7 100.08	15 653	6 842.44	15 085	6 994.39	15 420	7 352.73	16 210
F_{RB}	23 883.00	52 653	23 892.07	52 673	24 331.15	53 641	24 689.49	54 431
F_{RC}	1 546.30	3 409	1 488.24	3 281	1 514.55	3 339	1 551.74	3 421
F_{RP}	4 840.28	10 671	4 831.67	10 652	4 914.67	10 835	4 924.65	10 857
F_{RE}	26 799.15	59 082	26 711.60	58 889	27 543.94	60 724	27 523.08	60 678
V	3.4547 m³	122.0 cu. ft.	3.4971 m³	123.5 cu. ft.	3.4660 m³	122.4 cu. ft.	3.2026 m³	113.1 cu. ft.
T	352.22°K	634.0°R	352.44°K	634.4°R	352.72°K	634.9°R	353.61°K	636.5°R
g_0	50.8%		50.8%		50.8%		46.0%	

121.54% was obtained.

The optimal dual variables also happen to be independent of this variable F_P. Indeed if F_P is changed new optimal dual variables could be expected. However, this is not true since the right-hand sides of the equilibrium conditions are independent of F_P, as will be demonstrated.

Consider therefore the following expression for F_P, which can be derived from the other orthogonality conditions:

$$\sum_{m=0}^{M} \sum_{t=1}^{T_m} \sigma_{mt}\, a_{mtF_P}\, \omega_{mt} = 0 \tag{63}$$

This equation has the formal appearance of an orthogonality condition, but F_P is no longer a variable of the problem.

Since the vector $\boldsymbol{\nu}_d$, $d = 1, \ldots, D$ appearing in the equilibrium conditions satisfies each orthogonality condition individually, it also satisfies Equation (63):

$$\sum_{m=0}^{M} \sum_{t=1}^{T_m} \sigma_{mt}\, a_{mtF_P}\, \nu_{mtd} = 0 \quad d = 1, \ldots, \mathrm{D} \tag{64}$$

Mulltiplying each term of (64) by the constant factor ($\log F_P$):

$$\sum_{m=0}^{M} \sum_{t=1}^{T_m} \sigma_{mt}\, a_{mtF_P}\, \nu_{mtd} \log F_P = 0 \quad d = 1, \ldots, D \tag{65}$$

or

$$\sum_{m=0}^{M} \sum_{t=1}^{T_m} \sigma_{mt}\, \nu_{mtd} \log(F_P{}^{a_{mtF_P}}) = 0 \quad d = 1, \ldots, D \tag{66}$$

The right-hand side of each equilibrium condition in logarithmic form (57):

$$R_d = \sum_{m=0}^{M} \sum_{t=1}^{T_m} \sigma_{mt}\, \nu_{mtd} \log c_{mt} \quad d = 1, \ldots, D \tag{67}$$

can be split into one part containing F_P and another one independent of F_P:

$$R_d = A_d + B_d \quad d = 1, \ldots, D \tag{68}$$

with

$$A_d = \sum_{m=0}^{M} \sum_{t=1}^{T_m} \sigma_{mt}\, \nu_{mtd} \log(F_P{}^{a_{mtF_P}}) \quad d = 1, \ldots, D \tag{69}$$

$$B_d = \sum_{m=0}^{M} \sum_{t=1}^{T_m} \sigma_{mt}\, \nu_{mtd} \log c_{mt}' \quad d = 1, \ldots, D \tag{70}$$

$$c_{mt}' = c_{mt}\, F_P{}^{-a_{mtF_P}} \tag{71}$$

Obviously B_d doesn't contain F_P and Equation (66) shows that $A_d = 0$, $d = 1, \ldots, D$. The right-hand side of each equilibrium condition is thus independent of F_P and so are the dual variables and the primal terms. The expression for $v(\boldsymbol{\omega})$ can be split up in the same way to demonstrate its independence of F_P. However, this conclusion was already derived on other arguments.

Other formulation of the primal program

This section is meant to clarify the reasons for the redundancy of one orthogonality condition.

The linear dependency of these conditions can be expressed as

$$\sum_{n=1}^{N-2} a_{mtn}\, \sigma_{mt} = a_{mt\beta}\, \sigma_{mt} \quad t = 1, \ldots, T_m; \quad m = 0, \ldots, M \tag{72}$$

or

$$\sum_{n=1}^{N-2} a_{mtn} = a_{mt\beta} \quad t = 1, \ldots, T_m; \quad m = 0, \ldots, M \tag{73}$$

Each primal term has the form

$$u_{mt} = \sigma_{mt}\, c_{mt} \prod_{n=1}^{N} x_n{}^{a_{mtn}} \quad t = 1, \ldots, T_m; \quad m = 0, \ldots, M \tag{74}$$

Inserting (73) into (74) yields

$$u_{mt} = \sigma_{mt}\, c_{mt}\, k_1{}^{a_{mtk_1}}\, x_1{}^{a_{mt1}}\, x_2{}^{a_{mt2}} \ldots \ldots x_{N-2}{}^{a_{mt(N-2)}}\, \beta^{a_{mt1}+a_{mt2}+\ldots a_{mt(N-2)}}$$

$$u_{mt} = \sigma_{mt}\, c_{mt}\, k_1{}^{a_{mtk_1}}\, (x_1\beta)^{a_{mt1}}\, (x_2\beta)^{a_{mt2}} \ldots \ldots (x_{N-2}\beta)^{a_{mt(N-2)}} \tag{75}$$

$$\text{for} \quad t = 1, \ldots, T_m; \quad m = 0, \ldots, M$$

In the previous section every term has been proved constant for different choice of β. This also implies that k_1 doesn't vary since

$$u_{101} = 0.00772 k_1 \tag{76}$$

Equation (75) then becomes

$$\prod_{n=1}^{N-2} (x_n\beta)^{a_{mtn}} = \text{constant for every } \beta \tag{77}$$

This equation is satisfied if

$$x_n = \lambda_n \beta^{-1} \quad n = 1, \ldots, n-2; \quad \lambda_n \text{ being a constant} \tag{78}$$

Hence (78) shows that ($N - 2$) variables can be expressed as a function of β. The same discussion can now be repeated for every other variable (except k_1).

A further analysis of the problem is possible by substituting β by $\rho V/F_R{}^2$. Due to the deletion of constraints g_6, which prescribes the latter relation, the orthogonality conditions can be decomposed into two groups: one set for F_{RA}, F_{RB}, F_{RC}, F_{RP}, α, b and another for F_A, F_D, F_G, F_P, V. Multiplying the first set of orthogonality conditions by -1 and adding the resulting equations gives one part of the orthogonality condition for F_R. The other part of this condition is obtained by repeating the same operations on the second set of orthogonality conditions. Hence it is possible to express some variables in functions of F_R and others in function of V.

Using

$$F_A' = \frac{F_A}{\rho V}; \; F_D' = \frac{F_D}{\rho V}; \; F_G' = \frac{F_G}{\rho V};$$

$$F_R' = \frac{F_R}{\rho V}; \; F_P' = \frac{F_P}{\rho V} \tag{79}$$

and

$$C_{RA} = \frac{F_{RA}}{F_R}; \; C_{RB} = \frac{F_{RB}}{F_R}; \; C_{RC} = \frac{F_{RC}}{F_R};$$

$$C_{RP} = \frac{F_{RP}}{F_R}; \; C_\alpha = \frac{\alpha}{F_R}; \; C_b = \frac{b}{F_R} \tag{80}$$

the primal optimization problem is transformed into one with 8 constraints and 12 variables stated as

$$\min g_0 = \min(-14F_A' + 33.66F_D' + 56F_G' - 325.92F_P' + 0.37F_R') \quad (81)$$

$$g_1 \equiv 0.73398k_1^{1.67}C_{RC}C_{RP}F_G'^{-1} \leq 1 \quad (82)$$

$$g_2 \equiv -(-1.56268k_1^{0.25}C_{RA}^{-1}C_{RC} - 0.24466k_1^{0.67}C_{RA}^{-1}C_{RB}^{-1}C_{RC}C_{RP} - 0.15627k_1^{0.25}C_{RA}^{-1}C_{RC}^2C_b^{-1})^{-1} \leq 1 \quad (83)$$

$$g_3 \equiv -(-1.25014k_1^{1.25}C_{RB}C_{RC}F_P'^{-1} + 0.24466k_1^{1.67}C_{RC}C_{RP}F_P'^{-1})^{-1} \leq 1 \quad (84)$$

$$g_4 \equiv 0.31254k_1^{1.25}C_{RB}C_{RC}C_\alpha C_b^{-1}F_D'^{-1} \leq 1 \quad (85)$$

$$g_5 \equiv -(-k_1C_{RA}C_{RB}F_A'^{-1} - 0.31254k_1^{1.25}C_{RA}C_{RB}C_{RC}C_b^{-1}F_A'^{-1})^{-1} \leq 1 \quad (86)$$

$$g_6 \equiv -(-C_{RP}C_b^{-1} + 1.25014k_1^{1.25}C_{RB}C_{RC}C_b^{-1}F_R'^{-1} - 0.24466k_1^{1.67}C_{RC}C_{RP}C_b^{-1}F_R'^{-1})^{-1} \leq 1 \quad (87)$$

$$g_7 \equiv C_\alpha + 0.73398k_1^{1.67}C_{RC}C_{RP}F_R'^{-1} + C_{RP} - C_b \leq 1 \quad (88)$$

$$g_8 \equiv C_{RC}C_\alpha^{-1} + 0.24466k_1^{0.67}C_{RC}C_{RP}C_{RB}^{-1}C_\alpha^{-1} + 0.15627k_1^{0.25}C_{RC}^2C_b^{-1}C_\alpha^{-1} + C_{RB}C_\alpha^{-1} + 11C_bC_\alpha^{-1} + 1.56268k_1^{0.25}C_{RC}C_\alpha^{-1} \leq 1 \quad (89)$$

The variables C_{RA}, C_{RB}, C_{RC}, C_{RP}, C_α, C_b are concentrations of the components A, B, C, P, G, E, in the outlet stream F_R of the reactor, whereas F_A', F_D', F_G', F_P', F_R' are flow rates per unit mass of reactor.

The objective function (13) determines the maximal percent of return (= operating profit/total investment). Since the investment is assumed to be proportional to the mass of reactor ($600V\rho$), it follows that the objective function is also proportional to the operating profit per unit mass of reactor.

Moreover the operating profit is a linear function of ($V\rho$) so that the objective function is clearly independent of the mass of reactor. This, together with the fact that the constraints are mass balances and hence can be written independently from $V\rho$, [see for instance (82-89)] proves that the form of the objective function is responsible for the redundancy of one variable.

A remedy to avoid this redundancy is to use

$$\max g_0 = \max \left[\sum_{A,D,G,P,R} c_k F_k - c_v V \right] \quad (90)$$

as an objective function, where c_k and c_v are constants.

REMARKS

1. Analogue conclusions are valid if the second form of the objective function (17) is used.
2. Some investigators fix the reactor volume V and impose an inequality constraint

$$0 \leq F_P \leq 2\,160.46 \ (4763) \quad (91)$$

[See for instance Williams and Otto (1960), Jung, Mirosh and Ray (1971)]

If the assumed value of V is lower than the optimal found in the above section [$V \simeq 0.8782(31)$] (91) is satisfied as a strict inequality and the objective function is 121.54% at its optimum.

If on the other hand $V > 0.8782$ (31), the production rate F_P is fixed at its upper bound 2160.46 (4763) and an optimization problem is created with two fixed variables (V and F_P). The optimal value for the objective function of this problem can never exceed the value 121.54% obtained when no restrictions were imposed on F_P.

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APPENDIX A. Mathematical description of the Williams-Otto process

Three second-order irreversible reactions take place

$$A + B \to C \quad \text{reaction coefficient } k_1 \quad (A1)$$

$$C + B \to P + E \quad \text{reaction coefficient } k_2 \quad (A2)$$

$$P + C \to G \quad \text{reaction coefficient } k_3 \quad (A3)$$

The expressions for the chemical reaction rate are

$$r_1 = k_1F_{RA}F_{RB}\frac{V\rho}{F_R^2} \quad (A4)$$

$$r_2 = k_2F_{RB}F_{RC}\frac{V\rho}{F_R^2} \quad (A5)$$

$$r_3 = k_3F_{RP}F_{RC}\frac{V\rho}{F_R^2} \quad (A6)$$

where

$$k_i(i = 1, 2, 3) \quad \text{has the form} \quad k_i = Q_i \exp(-B_i/T) \quad (A7)$$

and

$Q_1 = 5.9755\ 10^9$/hr. wt fract A or B

$B_1 = 6\,666.67°K(12\,000°R)$

$Q_2 = 2.5962\ 10^{12}$/hr. wt fract B

$B_2 = 8\,333.33°K(15\,000°R) \quad (A8)$

$Q_3 = 9.6283\ 10^{15}$/hr. wt fract C

$$B_3 = 11\,111.11°\text{K}(20\,000°\text{R})$$

Process Constraints Equations

The process constraints are mainly material balances on each component and on the various processing units in the system.

Material balance on A

$$F_A - k_1 F_{RA} F_{RB} \frac{V\rho}{F_R^2} - \frac{F_D F_{RA}}{F_R - F_P - F_G} = 0 \quad (A9)$$

Material balance on B

$$F_B - (k_1 F_{RA} F_{RB} + k_2 F_{RB} F_{RC}) \frac{V\rho}{F_R^2} - \frac{F_D F_{RB}}{F_R - F_P - F_G} = 0 \quad (A10)$$

Material balance on C

$$\left(\frac{M_C}{M_B} k_1 F_{RC} F_{RB} - \frac{M_E}{M_B} k_2 F_{RB} F_{RC} - k_3 F_{RP} F_{RC} \right) \frac{V\rho}{F_R^2} - \frac{F_D F_{RC}}{F_R - F_P - F_G} = 0 \quad (A11)$$

Material balance on E

$$\frac{M_E}{M_B} k_2 F_{RB} F_{RC} \frac{V\rho}{F_R^2} - \frac{F_D F_{RE}}{F_R - F_P - F_G} = 0 \quad (A12)$$

Material balance on G

$$- F_G + \frac{M_G}{M_C} k_3 F_{RC} F_{RP} \frac{V\rho}{F_R^2} = 0 \quad (A13)$$

Material balance on P

$$- F_P + \left(k_2 F_{RB} F_{RC} - \frac{M_P}{M_C} k_3 F_{RC} F_{RP} \right) \frac{V\rho}{F_R^2} - \frac{F_D (F_{RP} - F_P)}{F_R - F_P - F_G} = 0 \quad (A14)$$

Constraint on flow rate in the reactor

$$F_{RA} + F_{RB} + F_{RC} + F_{RE} + F_G + F_{RP} - F_R = 0 \quad (A15)$$

Constraint on separation efficiency of the distillation column:

$$F_{RP} - 0.1\, F_{RE} - F_P = 0 \quad (A16)$$

Overall material balance

$$F_A + F_B - F_G - F_P - F_D = 0 \quad (A17)$$

Constraints on temperature

$$322.22\ (580) \leq T \leq 377.78\ (680) \quad (A18)$$

The overall material balance is not independent from the other balances. It can however be used instead of an other overall-component-material balance to simplify the objective function.

There are eight equality constraints, two inequality constraints, and twelve variables since F_P is fixed.

APPENDIX B. Formulation of Luus and Jaakola (1973a,b). Sense of the inequalities of the primal constraints.

Luus and Jaakola (1973a,b) showed that the constraints of Appendix A can be converted by a simple substitution into the following form:

$$F_A = k_1 F_{RA} F_{RB} \beta + F_D F_{RA} \alpha^{-1} \quad (B1)$$

$$F_{RA} = \frac{F_{RC}}{10 k_1 F_{RB}} (10 k_2 F_{RB} + 5 k_3 F_{RP} + k_2 F_{RB} F_{RC} b^{-1}) \quad (B2)$$

$$F_G = 1.5 k_3 F_{RC} F_{RP} \beta \quad (B3)$$

$$F_P = F_{RP} - b \quad (B4)$$

$$\alpha = F_{RA} + F_{RB} + F_{RC} + 11b \quad (B5)$$

$$b = F_{RP} - 0.2\ (4\beta k_2 F_{RB} F_{RC} - 2.5 k_3 \beta F_{RC} F_{RP}) \quad (B6)$$

$$\beta = \frac{V\rho}{F_R^2} \quad (B7)$$

$$F_R = \alpha + F_G + F_P \quad (B8)$$

$$F_D = 0.2 \alpha \beta k_2 F_{RB} F_{RC} b^{-1} \quad (B9)$$

$$F_B = F_G + F_P + F_D - F_A \quad (B10)$$

$$F_{RE} = 10(F_{RP} - F_P) \quad (B11)$$

$$322.22(580) \leq T \leq 377.78(680) \quad (B12)$$

This problem has 11 equality constraints, 2 inequality constraints, and 15 variables if F_P is fixed. As mentioned constraints (B10) and (B11) are deleted in defining the optimal value of the objective function.

The constraints (B1) to (B9) originally formulated as equalities are changed to mixed inequality constraints. The sense imposed on these inequalities is such that these constraints will be active in the optimum. Rules for selecting this appropriate direction of the inequalities are discussed by Blau and Wilde (1969). To facilitate the use of Blaus rule, the primal program was rearranged by algebraic substitutions so that a maximal number of primal variables appears exactly twice in the model—and if possible—once in the objective function and once in the constraints.

Applying this rule on the equalities (B1) to (B9) gives

(a) In (B1) F_D is replaced by (B9).
(b) In (B4) b is substituted by (B6).
(c) In (B8) F_G and F_P are substituted by (B3) and (B4).
(d) F_{RA} appearing in (B1), (B2) and (B5) is replaced in (B5) by (B2).
(e) Now F_A, F_G, F_P, F_D, F_{RA}, α appear only twice in the formulation of the problem.

The corresponding inequalities are

$$F_A \leq k_1 F_{RA} F_{RB} \beta + 0.2 \beta k_2 F_{RA} F_{RB} F_{RC} b^{-1} \quad (B13)$$

$$F_{RA} \leq k_2 k_1^{-1} F_{RC} + 0.5 k_3 k_1^{-1} F_{RC} F_{RP} F_{RB}^{-1} + 0.1 k_2 k_1^{-1} F_{RC}^2 b^{-1} \quad (B14)$$

$$F_G \geq 1.5 k_3 F_{RC} F_{RP} \beta \quad (B15)$$

$$F_P \leq 0.8 \beta k_2 F_{RB} F_{RC} - 0.5 k_3 \beta F_{RC} F_{RP} \quad (B16)$$

$$\alpha \geq k_2 k_1^{-1} F_{RC} + 0.5 k_3 k_1^{-1} F_{RC} F_{RP} F_{RB}^{-1} + 0.1 k_2 k_1^{-1} F_{RC} b^{-1} + F_{RB} + F_{RC} + 11b \quad (B17)$$

$$b \leq F_{RP} - 0.8 \beta k_2 F_{RB} F_{RC} + 0.5 k_3 \beta F_{RC} F_{RP} \quad (B18)$$

$$\beta \leq V\rho F_R^{-2} \quad (B19)$$

$$F_R \geq \alpha + 1.5 k_3 F_{RC} F_{RP} \beta + F_{RP} - b \quad (B20)$$

$$F_D \geq 0.2 \alpha \beta k_2 F_{RB} F_{RC} b^{-1} \quad (B21)$$

The sense of the inequality constraints (B13), (B15), (B16), and (B21) follows from the fact that these constraints contain variables that only appear in the objective function and in that particular constraint. The sense of (B19) can easily be found since V appears in each term of the objective so that the sum of these terms in the orthogonality condition for V is 1. Then (B19) is changed in such a way that the corresponding ω_{mt} must be subtracted to obtain zero. From (B19) and the objective the sense of (B20) is chosen so that the orthogonality condition for F_R is not restricted to only positive terms.

From (B13) the sense of (B14) is found easily and this is also true for (B17) from (B20).

About the sense of (B18) there can be some doubt. However, if an other sense for this inequality is selected, the orthogonality condition for F_{RP} would contain only one negative term out of 8.

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