MULTIOBJECTIVE NONLINEAR MODEL PREDICTIVE CONTROL OF THE WILLIAMS OTTO PROCESS

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ABSTRACT

A rigorous multiobjective nonlinear model predictive control is performed on the Williams Otto chemical process maximizing the product and minimizing the waste substance. This strategy does not involve additional constraints or functions. The optimization language PYOMO was used in conjunction with the state-of-the-art optimization solvers, IPOPT and BARON. Two strategies areused with two different configurations for each strategy. Forboth these strategies it is shown that one configuration produces a larger amount of the required product while the other configuration produces a product of greater purity.

KEYWORDS

Williams Otto Process, optimal control. Multiobjective

1. WILLIAMS OTTO PROCESS

The Williams-Otto process is a chemical process that is complex and exhibits a considerable amount of nonlinearity(1-5). In this process, two substances A and B are fed into the reactor. The mass flow rates of these two substances are F_{fA}, F_{fB} . The reactions occurring are

$$\begin{aligned} &A + B \rightarrow C \\ &B + C \rightarrow P + E \\ &P + C \rightarrow G \end{aligned} \tag{1}$$

The required product is P while the waste product is G. A , B,C, E, P and G are proprietary chemicals whose names cannot be revealed.

The equations representing the Williams-Otto process model are

$$\frac{dm_A}{dt} = F_{fA} + \{(1-\eta)\mu - \mu\}\frac{m_A}{m} - k_1(\frac{m_A m_B}{V}) \tag{2}$$

$$\frac{dm_B}{dt} = F_{fB} + \{(1-\eta)\mu - \mu\}\frac{m_B}{m} - k_1(\frac{m_A m_B}{V}) - k_2(\frac{m_B m_C}{V}) \tag{3}$$

$$\frac{dm_C}{dt} = \{(1-\eta)\mu - \mu\}\frac{m_c}{m} + 2k_1(\frac{m_A m_B}{V}) - 2k_2(\frac{m_B m_C}{V}) - k_3(\frac{m_C m_P}{V}) \tag{4}$$

$$\frac{dm_E}{dt} = \{(1-\eta)\mu - \mu\}\frac{m_E}{m} + 2k_2(\frac{m_B m_C}{V}) \tag{5}$$

$$\frac{dm_P}{dt} = \{0.1(1-\eta)\mu\}\frac{m_E}{m} - -\mu\frac{m_P}{m} + k_2(\frac{m_B m_C}{V}) - 0.5k_3(\frac{m_C m_P}{V}) \quad (6)$$

$$\frac{dm_G}{dt} = -\mu\frac{m_G}{m} + 1.5k_3(\frac{m_C m_P}{V}) \quad (7)$$

$$m = m_A + m_B + m_C + m_E + m_P + m_G \quad (8)$$

$$V = \frac{m}{\rho} \quad (9)$$

$$k_i = \frac{a_i}{\rho}\exp(-\frac{b_i}{T}) \quad i = 1,2,3 \quad (10)$$

The masses of the species in the reactor for the species A, B, C, E, P, G are given by $m_A, m_B, m_C, m_E, m_P, m_G$. μ is the total mass stream leaving the reactor and η is the split fraction. The parameter values are given by

$$a_1 = 5.9755e+09(h^{-1}) \quad a_2 = 2.5962e+12(h^{-1}) \quad a_3 = 9.6283e+15(h^{-1})$$
$$b_1 = 12000^0 R \quad b_2 = 15000^0 R \quad b_3 = 20000^0 R \quad \rho = 50lb/ft^3$$

2. MNLMPC (MULTIOBJECTIVE NONLINEAR MODEL PREDIOTIVE CONTROL) METHOD

The multiobjective nonlinear model predictive control (MNLMPC) method was first proposed by Flores Tlacuahuaz et al(6) and used by Sridhar (7) . This method is rigorous and it does not involve the use of weighting functions not does it impose additional parameters or additional constraints on the problem unlike the weighted function or the epsilon correction method (Miettinen; (8)). For a problem that is posed as

$$\begin{aligned} &\min J(x,u) = (x_1, x_2....x_k) \\ &subject\ to\ \frac{dx}{dt} = F(x,u); h(x,u) \le 0; x^L \le x \le x^U; u^L \le u \le u^U \end{aligned} \quad (11)$$

The MNLMPC method first solves dynamic optimization problems independently minimizing/maximizing each x_i individually. The minimization/maximization of x_i will lead to the values x_i^* . Then the optimization problem that will be solved is

$$\begin{aligned} &\min \sqrt{\{x_i - x_i^*\}^2} \\ &subject\ to\ \frac{dx}{dt} = F(x,u); h(x,u) \le 0; x^L \le x \le x^U; u^L \le u \le u^U \end{aligned} \quad (12)$$

Thiscalculation will provide the control values for various times. The first obtained control value is implemented and the remaining is discarded. This procedure is repeated until the implemented and the first obtained control values are the same.

The optimization package in Python, Pyomo (Hart et al (9)) where the differential equations are automatically converted to a Nonlinear Program (NLP) using the orthogonal collocation method (Biegler, (10)) is commonly used for these calculations. The state-of-the-art solvers like IPOPT (Wachter and Biegler(11), 2006) and BARON (Tawaralmani and Sahinidis ; (12) are normally used in conjunction with PYOMO.

To summarize the steps of the algorithm are as follows

1. Minimize/maximize x_i subject to the differential and algebraic equations that govern the process using Pyomo and Baron. This will lead to the value x_i^*
2. Minimize $\sqrt{\{x_i - x_i^*\}^2}$ (multiobjective function) subject to the differential and algebraic equations that govern the process. This is the MOOC calculation and provide the control values for various times. If this calculation results in obtaining a value of zero for the multiobjective function then the Utopia point is obtained and the calculations are terminated. Otherwise, we proceed to step 3.
3. Implement the first obtained control values and discard the remaining.
4. Repeat steps 1 to 3 until there is insignificant difference between the implemented and the first obtained value of the control variables

3. Results and Discussion

3.1. MNLMPC of Williams Otto Process

The main aim of the multiobjective nonlinear model predictive control is to maximize the yield and minimize the waste.Strategies with two different kinds of objective function minimizations were used. In the first strategy, $\sum_{0}^{t_f} P(t)$ was maximized and $\sum_{0}^{t_f} G(t)$ was minimized. In the second strategy $P(t_f)$ was maximized and $G(t_f)$ was minimized. t_f is the final time. For each of these strategies to different configurations were used.

In the first configuration, the values of μ, η were maintained at the steady-state bias values (Schmid et al) of 129.5 and 0.2 while F_{fA}, F_{fB}, T were treated as of control variables. In the second configuration, μ, η was also a dynamic variables and the control variables were $F_{fA}, F_{fB}, T, \eta, \mu$.

Strategy 1,

This strategy involves the maximization $\sum_{0}^{t_f} P(t)$ and minimization of $\sum_{0}^{t_f} G(t)$

Configuration 1

In this configuration, the values of μ, η were maintained at the steady-state bias values (obtained by Schmid et al[5]) of 129.5 and 0.2 while F_{fA}, F_{fB}, T were treated as of control variables. The maximization of $\sum_{0}^{t_f} P(t)$ resulted in a value 696.78 and the minimization of $\sum_{0}^{t_f} G(t)$ led to a value of zero. The multiobjective optimal control problem involved the minimization of $\sqrt{(\sum_{0}^{t_f} P(t) - 666.2)^2 + (\sum_{0}^{t_f} P(t) - 0)^2}$ subject to the equations governing the William Otto process. The MNLMPC values obtained were (F_{fA}, F_{fB}, T = 20,5, 570) while the final values of m_P, m_G were 158.7849 and 11.9997. The profiles of the various mass streams are shown in figs. 1a and 1b.

Configuration 2

In this configuration, μ, η was also a dynamic variables and the control variables were $F_{fA}, F_{fB}, T, \eta, \mu$.

The maximization of $\sum_{0}^{t_f} P(t)$ resulted in a value of 609.4568and the minimization of $\sum_{0}^{t_f} G(t)$ led to a value of 0.007855. The multiobjective optimal control problem involved the minimization of $\sqrt{(\sum_{0}^{t_f} P(t) - 641.065)^2 + (\sum_{0}^{t_f} P(t) - 0.007855)^2}$ subject to the equations governing the William Otto process.The MNLMPC values of the control variables $F_{fA}, F_{fB}, T, \eta, \mu$ obtained were (5, 5, 580, 0,40) while the final values of m_P, m_G were (140.90, 2.7576). The profiles of the various mass streams are shown in figs. 2a and 2b.

It is seen from the values of m_P, m_G [(158.7849, 11.999)and ((140.90, 2.7576) that there is a trade-off between the amount of product and the amount of waste obtained. The percentage of waste in the three cases is 7.026, 1.1919 respectively. Hence, the second configuration should be implemented if the objective is to get a high-purity product. On the other hand, if a large amount of product is required then the first configuration should be used.

Strategy 2,

This strategy involves the maximization $P(t_f)$ and minimization of $G(t_f)$

Configuration 1

In this configuration, the values of μ, η were maintained at the steady-state bias values of 129.5 and 0.2 (obtained by Schmid et al [5]) while F_{fA}, F_{fB}, T were treated as of control variables. The maximization of $P(t_f)$ resulted in a value 166.2 and the minimization of $G(t_f)$ led to a value of zero. The multiobjective optimal control problem involved the minimization of $\sqrt{(P(t_f) - 166.2)^2 + (G(t_f) - 0)^2}$ subject to the equations governing the William Otto process. The MNLMPC values obtained were (F_{fA}, F_{fB}, T = 17.21 ,5, 589.94) while the final values of m_P, m_G were almost the same as in strategy1 configuration 1, 158.7849 and 11.9997. The profiles of the various mass streams are shown in figs. 3a and 3b.

Configuration 2

In this configuration, μ, η was also a dynamic variables and the control variables were $F_{fA}, F_{fB}, T, \eta, \mu$. The maximization of $P(t_f)$ resulted in a value 148.32 and the minimization of $G(t_f)$ led to a value of 0.00908. The multiobjective optimal control problem involved the minimization of
$\sqrt{(P(t_f)-148.32)^2 + (G(t_f)-0.00908)^2}$ subject to the equations governing the William Otto process.

The MNLMPC values of the control variables $F_{fA}, F_{fB}, T, \eta, \mu$ obtained were (5, 5, 590, 0,40) while the final values of m_P, m_G were (147.97, 3.316). The profiles of the various mass streams are shown in figs. 4a and 4b.

It is seen from the values of m_P, m_G [(158.7849, 11.999) and ((147.90, 3.316) that there is a trade-off between the amount of product and the amount of waste obtained. The percentage of waste in the three cases is 7.026, 2.192 respectively. Hence, the second configuration should be implemented if the objective is to get a high-purity product. On the other hand, if a large amount of product is required then the first configuration should be used.

4. SUMMARY OF RESULTS

Two strategies and two configurations were used.

Strategies

The two strategies that are implemented in the MNLMPC calculations are

1. maximization $\sum_{0}^{t_f} P(t)$ and minimization of $\sum_{0}^{t_f} G(t)$
2. maximization $P(t_f)$ and minimization of $G(t_f)$

Configurations

The two configurations used for each of these strategies are

1. μ, η were maintained at the steady-state bias values (Schmid et al) of 129.5 and 0.2 while F_{fA}, F_{fB}, T were treated as of control variables
2. $F_{fA}, F_{fB}, T, \eta, \mu$ are the control variables

Table 1 gives the summary of the results

Strategy	Configuration	$m_P(t_f)$	$m_G(t_f)$	% of waste
1	1	158.7849	11.9997.	7.026,
1	2	140.90,	2.7576	1.1919
2	1	158.7849	11.9997	7.026
2	2	147.90	3.316	2.192

It can be seen that if a higher amount of product is necessary, configuration 1 should be used. On the other hand, if greater purity is desirable configuration 2 should be more beneficial. This is true for both the strategies that were used.

5. CONCLUSIONS

Two different strategies with two different configurations were used to perform a rigorous multiobjective nonlinear model predictive control on the WilliamsOtto chemical process, maximizing the product and minimizing the waste substance. For both these strategies one configuration provides a larger amount of product while the other configuration provides a product of better purity.

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APPENDIX

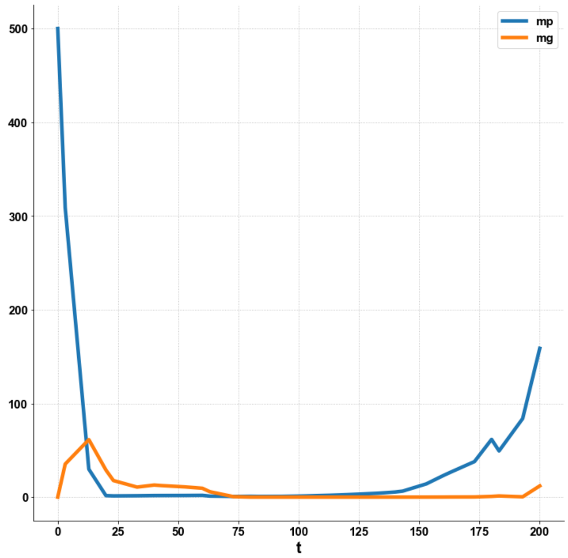


Fig. 1a

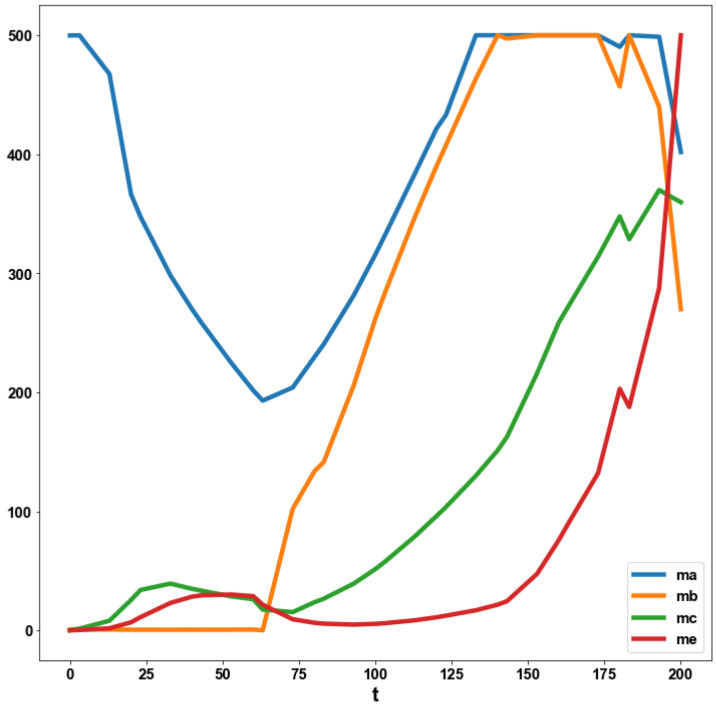
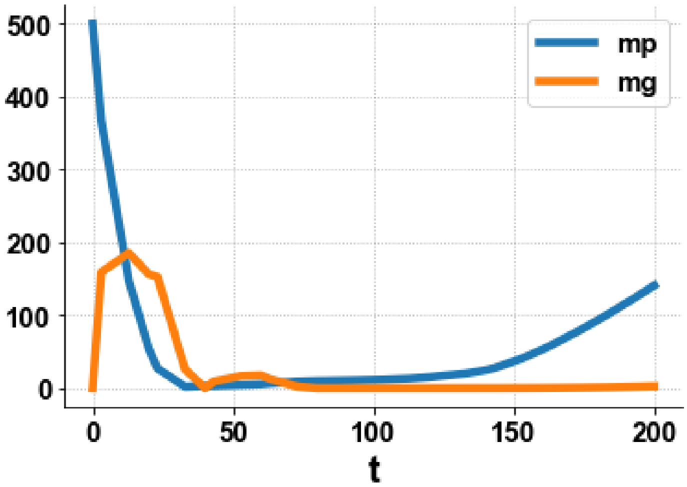


Fig. 1b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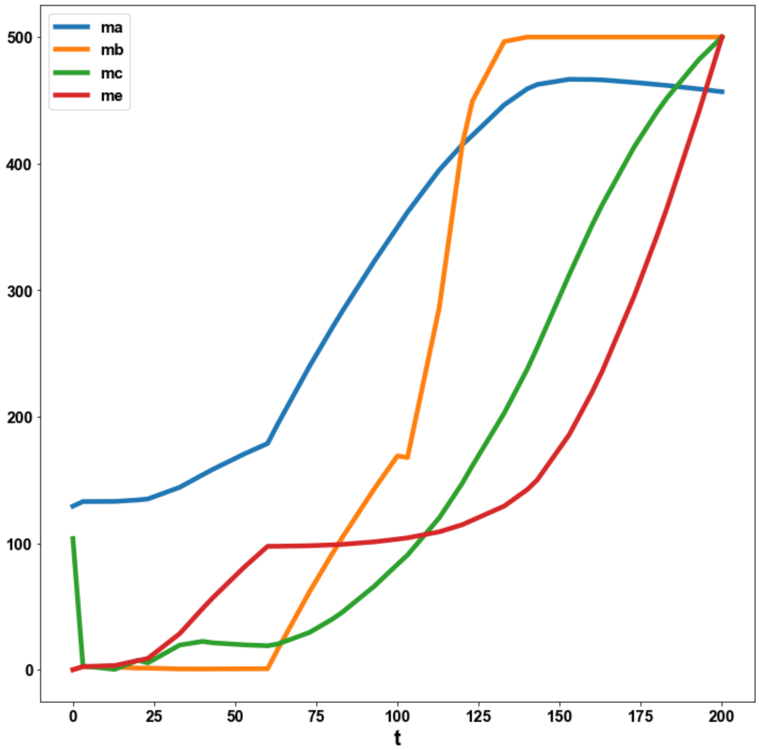
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Fig. 2b

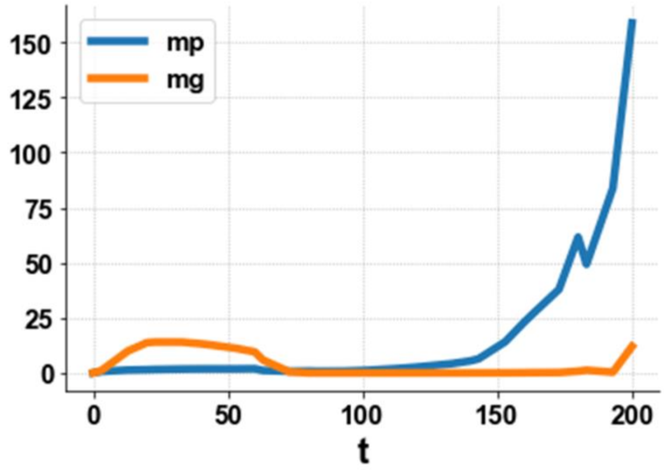
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Fig. 3a

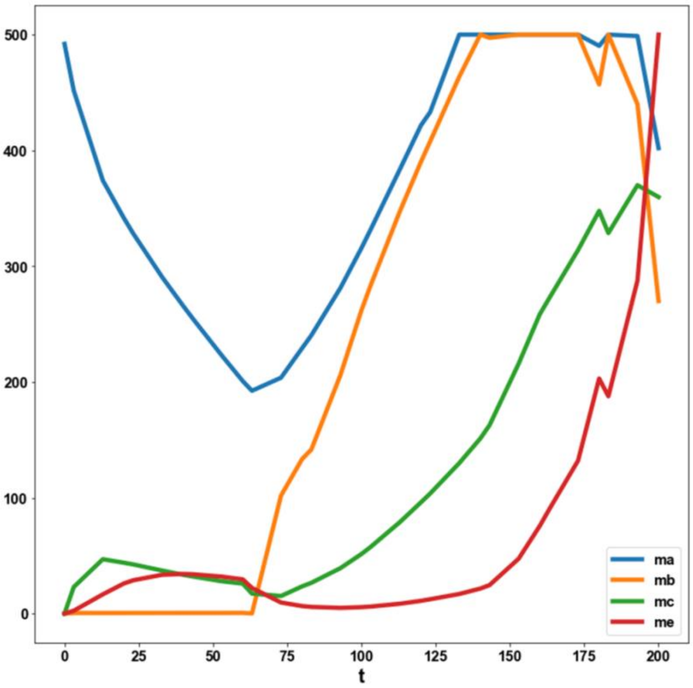
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Fig. 3b

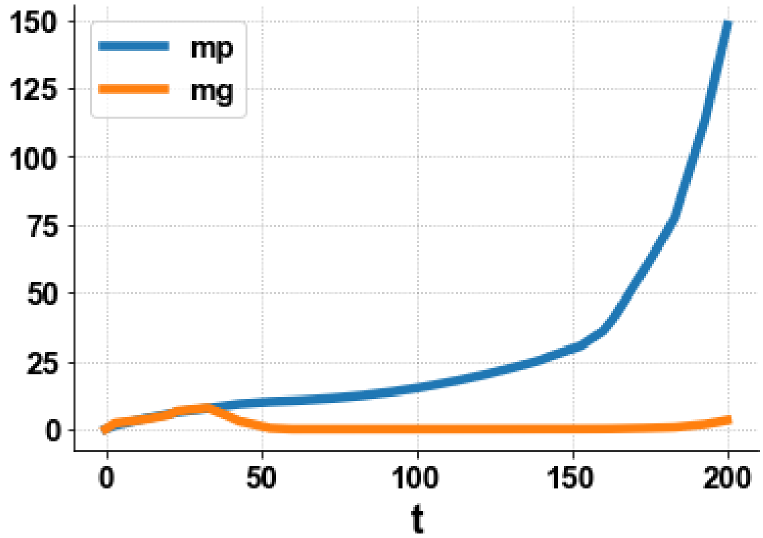
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Fig. 4a

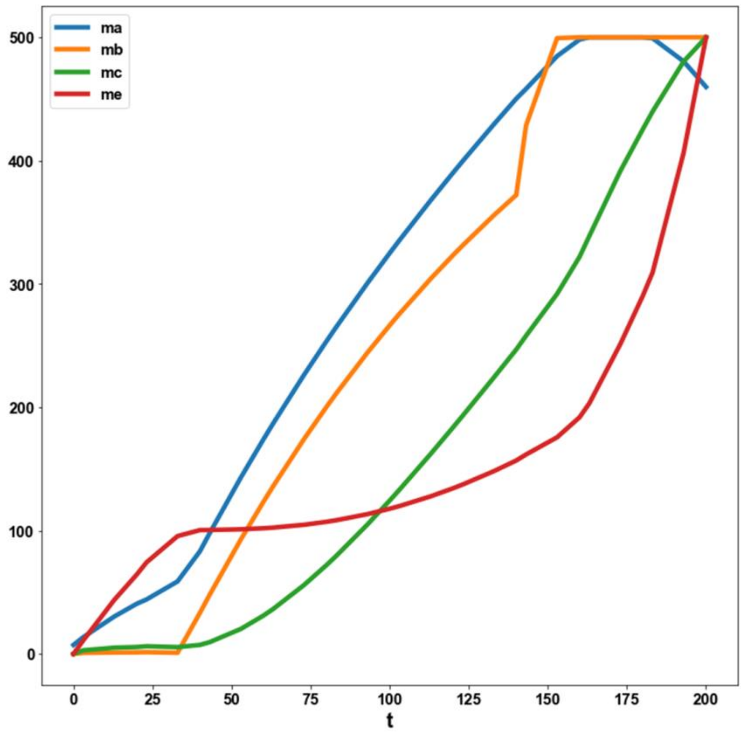
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Fig. 4b