Errata: Heat Exchanger Network Cleaning Scheduling: From Optimal Control to Mixed-Integer Decision Making

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Abstract

Errata to the article by Al Ismaili et al. [1], on the optimal scheduling of cleaning actions for Heat Exchanger Networks under fouling, are presented. Errors present in the equations of the Pontryagin Minimum Principle analysis of the original article are indicated and rectified. It is noted that despite these errors, there is no change to the conclusions of the analysis given in Al Ismaili et al. [1],.

Keywords: Optimal control problem; Bang-bang control; Fouling; Optimisation; Scheduling; Heat exchanger networks;

In the article by Al Ismaili et al. [1], a Pontryagin Minimum Principle analysis is presented to show that the underlying optimal control problems of their formulation are bang-bang. The analysis has some algebraic errors and the following corrections are to be made. Despite these errors, it is noted that the conclusion of the analysis is correct as shown in the present note.

Equation (4) of Al Ismaili et al. [1] is to be written as:

$$u = ((u^{(1)}), (u^{(2)}), \ldots, (u^{(NP)}))^T \tag{4}$$

Proof that the control in the relaxed multistage MIOCP for cleaning scheduling is linearly related to the process variables is rewritten as follows:

The performance index in equation (3a) is modified such that the Euler Lagrange multipliers are introduced:

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$$
\begin{aligned}
\bar{O} = \sum_{p=2}^{NP} \Bigg\{ & \\
& \phi^{(p)}(x^{(p)}(t_p), y^{(p)}(t_p), u^{(p)}, t^{(p)}) \\
& + \left(\nu^{(p)}\right)^T \left(I^{(p)}(x^{(p-1)}(t_{p-1}), y^{(p-1)}(t_{p-1}), u^{(p)}) - x^{(p)}(t_{p-1})\right) \\
& + \int_{t_{p-1}}^{t_p} L^{(p)}(x^{(p)}(t), y^{(p)}(t_p), u^{(p)}, t)\, dt \\
& + \int_{t_{p-1}}^{t_p} \left(\lambda^{(p)}(t)\right)^T \left(f^{(p)}(x^{(p)}(t), y^{(p)}(t_p), u^{(p)}, t) - \dot{x}^{(p)}(t)\right)\; dt \\
& + \int_{t_{p-1}}^{t_p} \left(\mu^{(p)}(t)\right)^T \left(g^{(p)}(x^{(p)}(t), y^{(p)}(t), u^{(p)}, t)\right)\; dt \\
& \Bigg\} \\
& + \phi^{(1)}(x^{(1)}(t_1), y^{(1)}(t_1), u^{(1)}, t^{(1)}) \\
& + \left(\nu^{(1)}\right)^T \left(I^{(1)}(u^{(1)}) - x^{(1)}(t_0)\right) \\
& + \int_{t_0}^{t_1} L^{(1)}(x^{(1)}(t), y^{(1)}(t), u^{(1)}, t)\, dt \\
& + \int_{t_0}^{t_1} \left(\lambda^{(1)}(t)\right)^T \left(f^{(1)}(x^{(1)}(t), y^{(1)}(t), u^{(1)}, t) - \dot{x}^{(1)}(t)\right)\; dt \\
& + \int_{t_0}^{t_1} \left(\mu^{(1)}(t)\right)^T \left(g^{(1)}(x^{(1)}(t), y^{(1)}(t), u^{(1)}, t)\right)\; dt
\end{aligned}
\tag{6}
$$

Variations on the parameter set of stage p', of the form $\delta u^{(p')}$, which will result in variations in the state values at all times. This is shown in the equation below. Clearly, the state vector of stage p such that $p < p'$ will not be influenced, resulting in $\delta x^{(p)}(t) \triangleq 0$ and $\delta y^{(p)}(t) \triangleq 0$.

$$
\begin{aligned}
\delta\bar{O} = \sum_{p=2}^{NP} \Bigg\{ & \\
& \left[\frac{\partial \phi^{(p)}}{\partial x^{(p)}(t_p)} \delta x^{(p)}(t_p) + \frac{\partial \phi^{(p)}}{\partial y^{(p)}(t_p)} \delta y^{(p)}(t_p) + \frac{\partial \phi^{(p)}}{\partial u^{(p)}} \delta u^{(p)}\right] \\
& + \left(\nu^{(p)}\right)^T \Bigg(\frac{\partial I^{(p)}}{\partial x^{(p-1)}(t_{p-1})} \delta x^{(p-1)}(t_{p-1}) + \frac{\partial I^{(p)}}{\partial y^{(p-1)}(t_{p-1})} \delta y^{(p-1)}(t_{p-1}) \\
& + \frac{\partial I^{(p)}}{\partial u^{(p)}} \delta u^{(p)} - \delta x^{(p)}(t_{p-1}) \Bigg) \\
& + \int_{t_{p-1}}^{t_p} \left(\frac{\partial L^{(p)}}{\partial x^{(p)}}(t) \delta x^{(p)}(t) + \frac{\partial L^{(p)}}{\partial y^{(p)}}(t) \delta y^{(p)}(t) + \frac{\partial L^{(p)}}{\partial u^{(p)}} \delta u^{(p)} \right) dt \\
& + \int_{t_{p-1}}^{t_p} \left(\lambda^{(p)}(t)\right)^T \left(\frac{\partial f^{(p)}}{\partial x^{(p)}}(t) \delta x^{(p)}(t) + \frac{\partial f^{(p)}}{\partial y^{(p)}}(t) \delta y^{(p)}(t) + \frac{\partial f^{(p)}}{\partial u^{(p)}} \delta u^{(p)} - \delta \dot{x}^{(p)}(t) \right) dt \\
& + \int_{t_{p-1}}^{t_p} \left(\mu^{(p)}(t)\right)^T \left(\frac{\partial g^{(p)}}{\partial x^{(p)}}(t) \delta x^{(p)}(t) + \frac{\partial g^{(p)}}{\partial y^{(p)}}(t) \delta y^{(p)}(t) + \frac{\partial g^{(p)}}{\partial u^{(p)}} \delta u^{(p)} \right) \; dt \\
& \Bigg\} \\
& + \left[\frac{\partial \phi^{(1)}}{\partial x^{(1)}(t_1)} \delta x^{(1)}(t_1) + \frac{\partial \phi^{(1)}}{\partial y^{(1)}(t_1)} \delta y^{(1)}(t_1) + \frac{\partial \phi^{(1)}}{\partial u^{(1)}} \delta u^{(1)}\right] \\
& + \left(\nu^{(1)}\right)^T \left(\frac{\partial I^{(1)}}{\partial u^{(1)}} \delta u^{(1)} - \delta x^{(1)}(t_0) \right) \\
& + \int_{t_0}^{t_1} \left(\frac{\partial L^{(1)}}{\partial x^{(1)}}(t) \delta x^{(1)}(t) + \frac{\partial L^{(1)}}{\partial y^{(1)}}(t) \delta y^{(1)}(t) + \frac{\partial L^{(1)}}{\partial u^{(1)}} \delta u^{(1)} \right) dt \\
& + \int_{t_0}^{t_1} \left(\lambda^{(1)}(t)\right)^T \left(\frac{\partial f^{(1)}}{\partial x^{(1)}}(t) \delta x^{(1)}(t) + \frac{\partial f^{(1)}}{\partial y^{(1)}}(t) \delta y^{(1)}(t) + \frac{\partial f^{(1)}}{\partial u^{(1)}} \delta u^{(1)} - \delta \dot{x}^{(1)}(t) \right) dt \\
& + \int_{t_0}^{t_1} \left(\mu^{(1)}(t)\right)^T \left(\frac{\partial g^{(1)}}{\partial x^{(1)}}(t) \delta x^{(1)}(t) + \frac{\partial g^{(1)}}{\partial y^{(1)}}(t) \delta y^{(1)}(t) + \frac{\partial g^{(1)}}{\partial u^{(1)}} \delta u^{(1)} \right) dt
\end{aligned} \tag{7}
$$

Integration by parts for the last term in the integrals involving $\delta \dot{x}^{(p)}$ is used to obtain equation (8):

$$
\begin{aligned}
\delta\bar{O} = \sum_{p=2}^{NP} \Bigg\{ & \\
& \left[\frac{\partial \phi^{(p)}}{\partial x^{(p)}(t_p)} \delta x^{(p)}(t_p) + \frac{\partial \phi^{(p)}}{\partial y^{(p)}(t_p)} \delta y^{(p)}(t_p) + \frac{\partial \phi^{(p)}}{\partial u^{(p)}} \delta u^{(p)} \right] \\
& + \left(\nu^{(p)} \right)^T \Bigg(\frac{\partial I^{(p)}}{\partial x^{(p-1)}(t_{p-1})} \delta x^{(p-1)}(t_{p-1}) + \frac{\partial I^{(p)}}{\partial y^{(p-1)}(t_{p-1})} \delta y^{(p-1)}(t_{p-1}) \\
& + \frac{\partial I^{(p)}}{\partial u^{(p)}} \delta u^{(p)} - \delta x^{(p)}(t_{p-1}) \Bigg) \\
& + \int_{t_{p-1}}^{t_p} \left(\frac{\partial L^{(p)}}{\partial x^{(p)}}(t) \delta x^{(p)}(t) + \frac{\partial L^{(p)}}{\partial y^{(p)}}(t) \delta y^{(p)}(t) + \frac{\partial L^{(p)}}{\partial u^{(p)}} \delta u^{(p)} \right) dt \\
& + \int_{t_{p-1}}^{t_p} \left(\lambda^{(p)}(t) \right)^T \left(\frac{\partial f^{(p)}}{\partial x^{(p)}}(t) \delta x^{(p)}(t) + \frac{\partial f^{(p)}}{\partial y^{(p)}}(t) \delta y^{(p)}(t) + \frac{\partial f^{(p)}}{\partial u^{(p)}} \delta u^{(p)} \right) dt \\
& + \int_{t_{p-1}}^{t_p} \left(\dot{\lambda}^{(p)}(t) \right)^T \delta x^{(p)}(t)\, dt \\
& + \left(\lambda^{(p)}(t_{p-1}) \right)^T \delta x^{(p)}(t_{p-1}) - \left(\lambda^{(p)}(t_p) \right)^T \delta x^{(p)}(t_p) \\
& + \int_{t_{p-1}}^{t_p} \left(\mu^{(p)}(t) \right)^T \left(\frac{\partial g^{(p)}}{\partial x^{(p)}}(t) \delta x^{(p)}(t) + \frac{\partial g^{(p)}}{\partial y^{(p)}}(t) \delta y^{(p)}(t) + \frac{\partial g^{(p)}}{\partial u^{(p)}} \delta u^{(p)} \right) dt \\
& \Bigg\} \\
& + \left[\frac{\partial \phi^{(1)}}{\partial x^{(1)}(t_1)} \delta x^{(1)}(t_1) + \frac{\partial \phi^{(1)}}{\partial y^{(1)}(t_1)} \delta y^{(1)}(t_1) + \frac{\partial \phi^{(1)}}{\partial u^{(1)}} \delta u^{(1)} \right] \\
& + \left(\nu^{(1)} \right)^T \left(\frac{\partial I^{(1)}}{\partial u^{(1)}} \delta u^{(1)} - \delta x^{(1)}(t_0) \right) \\
& + \int_{t_0}^{t_1} \left(\frac{\partial L^{(1)}}{\partial x^{(1)}}(t) \delta x^{(1)}(t) + \frac{\partial L^{(1)}}{\partial y^{(1)}}(t) \delta y^{(1)}(t) + \frac{\partial L^{(1)}}{\partial u^{(1)}} \delta u^{(1)} \right) dt \\
& + \int_{t_0}^{t_1} \left(\lambda^{(1)}(t) \right)^T \left(\frac{\partial f^{(1)}}{\partial x^{(1)}}(t) \delta x^{(1)}(t) + \frac{\partial f^{(1)}}{\partial y^{(1)}}(t) \delta y^{(1)}(t) + \frac{\partial f^{(1)}}{\partial u^{(1)}} \delta u^{(1)} \right) dt \\
& + \int_{t_0}^{t_1} \left(\dot{\lambda}^{(1)}(t) \right)^T \delta x^{(1)}(t)\, dt \\
& + \left(\lambda^{(1)}(t_0) \right)^T \delta x^{(1)}(t_0) - \left(\lambda^{(1)}(t_1) \right)^T \delta x^{(1)}(t_1) \\
& + \int_{t_0}^{t_1} \left(\mu^{(1)}(t) \right)^T \left(\frac{\partial g^{(1)}}{\partial x^{(1)}}(t) \delta x^{(1)}(t) + \frac{\partial g^{(1)}}{\partial y^{(1)}}(t) \delta y^{(1)}(t) + \frac{\partial g^{(1)}}{\partial u^{(1)}} \delta u^{(1)} \right) dt
\end{aligned}
\tag{8}
$$

For a stationary point, infinitesimal variations in the RHS should yield no change to the performance index, *i.e.* $\delta\bar{O} = 0$ and hence related terms must be chosen so that they always guarantee this. This leads to the following set of Euler-Lagrange equations and the Pontryagin et al. [2] Maximum (Minimum) Principle.

To cancel $\delta x^{(1)}(t)$ and $\delta x^{(1)}(t_1)$ terms, the differential equations and final time stage conditions as shown in equations (9a) to (10) must hold, respectively:

$$\dot{\lambda}^{(1)}(t) = -\left[\frac{\partial f^{(1)}}{\partial x^{(1)}}(t)\right]^T \lambda^{(1)}(t) - \left[\frac{\partial g^{(1)}}{\partial x^{(1)}}(t)\right]^T \mu^{(1)}(t) - \left[\frac{\partial L^{(1)}}{\partial x^{(1)}}(t)\right]^T \tag{9a}$$

$$t_0 \leq t \leq t_1 \tag{9b}$$

$$\lambda^{(1)}(t_1) = \left[\frac{\partial \phi^{(1)}}{\partial x^{(1)}(t_1)}\right]^T + \left[\frac{\partial I^{(2)}}{\partial x^{(1)}(t_1)}\right]^T \nu^{(2)} \tag{10}$$

It is noted that equation (10) is an edited form of equation (10) in Al Ismaili et al. [1]. The term $\left[\frac{\partial I^{(2)}}{\partial x^{(1)}(t_1)}\right]^T \nu^{(2)}$ is not present in equation (10) of the original manuscript of Al Ismaili et al. [1].

Algebraic equations and final stage conditions (11a) to (12) must hold in order to cancel $\delta y^{(1)}(t)$ and $\delta y^{(1)}(t_1)$ terms;

$$\left[\frac{\partial f^{(1)}}{\partial y^{(1)}}(t)\right]^T \lambda^{(1)}(t) + \left[\frac{\partial g^{(1)}}{\partial y^{(1)}}(t)\right]^T \mu^{(1)}(t) + \left[\frac{\partial L^{(1)}}{\partial y^{(1)}}(t)\right]^T = 0 \tag{11a}$$

$$t_0 \leq t \leq t_1 \tag{11b}$$

$$\left[\frac{\partial \phi^{(1)}}{\partial y^{(1)}(t_1)}\right]^T + \left[\frac{\partial I^{(2)}}{\partial y^{(1)}(t_1)}\right]^T \nu^{(2)} = 0 \tag{12}$$

It is noted that equation (12) is an edited form of equation (12) in Al Ismaili et al. [1]. The coefficient of the term $\left[\frac{\partial I^{(2)}}{\partial y^{(1)}(t_1)}\right]^T$ should be $\nu^{(2)}$ and not $\lambda^{(2)}(t_1)$ as given in equation (12) of the original manuscript of Al Ismaili et al. [1].

The $\delta x^{(p)}(t)$ and $\delta x^{(p)}(t_p)$ terms are cancelled through the condition that the following differential equations and final time stage conditions are held;

$$\dot{\lambda}^{(p)}(t) = -\left[\frac{\partial f^{(p)}}{\partial x^{(p)}}(t)\right]^T \lambda^{(p)}(t) - \left[\frac{\partial g^{(p)}}{\partial x^{(p)}}(t)\right]^T \mu^{(p)}(t) - \left[\frac{\partial L^{(p)}}{\partial x^{(p)}}(t)\right]^T \tag{13a}$$

$$t_{p-1} \leq t \leq t_p \quad \forall p = 2, 3, \ldots NP \tag{13b}$$

$$\lambda^{(p)}(t_p) = \left[\frac{\partial \phi^{(p)}}{\partial x^{(p)}(t_p)}\right]^T + \left[\frac{\partial I^{(p+1)}}{\partial x^{(p)}(t_p)}\right]^T \nu^{(p+1)} \quad \forall p = 2, 3, \ldots NP - 1 \tag{14a}$$

It is noted that equation (13a) is an edited form of equation (13a) in Al Ismaili et al. [1]. The term $-\left[\frac{\partial g^{(p)}}{\partial x^{(p)}}(t)\right]^T \mu^{(p)}(t)$ is missing in equation (13a) of Al Ismaili et al. [1]. It is also noted that (14a) has not been numbered in the manuscript. In addition, in the equation, the coefficient of $\left[\frac{\partial I^{(p+1)}}{\partial x^{(p)}(t_p)}\right]^T$ should be $\nu^{(p+1)}$ and not $\lambda^{(p+1)}(t_p)$, as given in the original manuscript of Al Ismaili et al. [1].

For $p = NP$, the following holds:

$$\lambda^{(NP)}(t_{NP}) = \left[\frac{\partial \phi^{(NP)}}{\partial x^{(NP)}(t_{NP})}\right]^T \tag{14b}$$

To cancel $\delta x^{(p)}(t_{p-1})$ terms, the following conditions must hold:

$$\nu^{(p)} = \lambda^{(p)}(t_{p-1}) \quad \forall p = 2, 3, \ldots NP \tag{15}$$

It is noted that equations (14b) and (15) are not present in Al Ismaili et al. [1] and are to be added to the set of equations in the derivation.

To cancel $\delta y^{(p)}(t)$ and $\delta y^{(p)}(t_p)$ terms, the following algebraic equations must hold:

$$\left[\frac{\partial f^{(p)}}{\partial y^{(p)}}(t)\right]^T \lambda^{(p)}(t) + \left[\frac{\partial g^{(p)}}{\partial y^{(p)}}(t)\right]^T \mu^{(p)}(t) + \left[\frac{\partial L^{(p)}}{\partial y^{(p)}}(t)\right]^T = 0 \tag{16a}$$

$$t_{p-1} \leq t \leq t_p \quad \forall p = 2, 3, \ldots NP \tag{16b}$$

$$\left[\frac{\partial \phi^{(p)}}{\partial y^{(p)}(t_p)}\right]^T + \left[\frac{\partial I^{(p+1)}}{\partial y^{(p)}(t_p)}\right]^T \nu^{(p+1)} = 0 \quad \forall p = 2, 3, \ldots NP - 1 \tag{17a}$$

And for $p = NP$, the following holds:

$$\left[\frac{\partial \phi^{(NP)}}{\partial y^{(NP)}(t_{NP})}\right]^T = 0 \tag{17b}$$

It is noted that equation (17b) is not present in Al Ismaili et al. [1] and is to be added to the set of equations in the derivation.

The terms $\delta u^{(1)}$ and $\delta u^{(p)}$ are cancelled on the condition that equations (18a) to (19b) hold. These are equivalent to the Hamiltonian gradient condition:

$$\begin{aligned}\frac{\partial H^{(1)}}{\partial u^{(1)}} &= \left[\frac{\partial \phi^{(1)}}{\partial u^{(1)}}(t_1)\right]^T + \left[\frac{\partial I^{(1)}}{\partial u^{(1)}}\right]^T \nu^{(1)} \\ &+ \int_{t_0}^{t_1} \left\{ \left[\frac{\partial L^{(1)}}{\partial u^{(1)}}(t)\right]^T + \left[\frac{\partial f^{(1)}}{\partial u^{(1)}}(t)\right]^T \lambda^{(1)}(t) + \left[\frac{\partial g^{(1)}}{\partial u^{(1)}}(t)\right]^T \mu^{(1)}(t) \right\} dt \\ &= 0\end{aligned} \tag{18a}$$

$$t_0 \leq t \leq t_1 \tag{18b}$$

$$\begin{aligned}\frac{\partial H^{(p)}}{\partial u^{(p)}} &= \left[\frac{\partial \phi^{(p)}}{\partial u^{(p)}}(t_p)\right]^T + \left[\frac{\partial I^{(p)}}{\partial u^{(p)}}\right]^T \nu^{(p)} \\ &+ \int_{t_{p-1}}^{t_p} \left\{ \left[\frac{\partial L^{(p)}}{\partial u^{(p)}}(t)\right]^T + \left[\frac{\partial f^{(p)}}{\partial u^{(p)}}(t)\right]^T \lambda^{(p)}(t) + \left[\frac{\partial g^{(p)}}{\partial u^{(p)}}(t)\right]^T \mu^{(p)}(t) \right\} dt \\ &= 0\end{aligned} \tag{19a}$$

$$t_{p-1} \leq t \leq t_p \quad \forall p = 2, 3, \ldots NP \tag{19b}$$

It is noted that equations (18a), (18b), (19a) and (19b) are labelled as (15a), (15b), (16a) and (16b), in the original manuscript of Al Ismaili et al. [1] and have to be renumbered. In addition, the coefficients of $\left[\frac{\partial I^{(1)}}{\partial u^{(1)}}\right]^T$ and $\left[\frac{\partial I^{(p)}}{\partial u^{(p)}}\right]^T$ in equations (15a) and (16a) of Al Ismaili et al. [1] should be $\nu^{(1)}$ and $\nu^{(p)}$ and not $\lambda^{(1)}(t_0)$ and $\lambda^{(p)}(t_{p-1})$ respectively, as given in the original manuscript.

When the functions appearing in equations (18a) and (19b) are linearly related to the control, the optimal control for the relaxed MIOCP will exhibit bang-bang behaviour (with potential singular arcs).

Further, the equations (17) to (30) in the original manuscript of Al Ismaili et al. [1] should be renumbered accordingly to take into account the changes in the numbering caused by the above corrections.

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