Online model maintenance via output modifier adaptation

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Supporting Information for case study 2: Gas lifted oil well network

The model of the gas lifted oil well network is based on Krishnamoorthy et al.¹. It describes the dynamic behavior of a network containing two wells. Note that, since both Output Modifier Adaptation (MAy) and the methodology for selecting the model structure online are steady-state methods, only the steady-state solution of the nonlinear dynamic model is considered. No dynamics are included in the case study. Nevertheless, the original semiimplicit index-1 differential algebraic equations system is shown and the dynamic description is explicitly discarded:

$$\mathbf{0} = \mathbf{\dot{x}} = \mathbf{f}(\mathbf{x}, \mathbf{z}, \mathbf{u}, \mathbf{p}) \tag{1a}$$

$$\mathbf{0} = \mathbf{h}(\mathbf{x}, \mathbf{z}, \mathbf{u}, \mathbf{p}) \tag{1b}$$

$$\mathbf{y}_m = \mathbf{H} [\mathbf{x} \quad \mathbf{z}]^T \tag{1c}$$

in which, $\mathbf{x} \in \mathcal{R}^{n_x}$ are the differential states, $\mathbf{z} \in \mathcal{R}^{n_z}$ the algebraic states, $\mathbf{u} \in \mathcal{R}^{n_u}$ the

system inputs, $\mathbf{p} \in \mathcal{R}^{n_p}$ the model parameters, and $\mathbf{y}_m \in \mathcal{R}^{n_y}$ the process measurements. The set of nonlinear differential equations is $\mathbf{f} : \mathcal{R}^{n_x} \times \mathcal{R}^{n_z} \times \mathcal{R}^{n_u} \times \mathcal{R}^{n_p} \mapsto \mathcal{R}^{n_x}$ and $\mathbf{h} : \mathcal{R}^{n_x} \times \mathcal{R}^{n_z} \times \mathcal{R}^{n_z} \times \mathcal{R}^{n_u} \times \mathcal{R}^{n_p} \mapsto \mathcal{R}^{n_z}$ the set of algebraic equations. The output mapping \mathbf{H} is linear in relation to the states.

Given nominal values to the parameters \mathbf{p} , the steady-state solution of the system described in Equation (1) can be represented by a steady-state input-output mapping \mathbf{y} : $\mathcal{R}^{n_u} \mapsto \mathcal{R}^{n_y}$, which is adapted by the output modifier adaptation method $(\mathbf{y} \mapsto \mathbf{y}_{ad})$ like in Equation (1) of the main paper.

$$\mathbf{y}_m = \mathbf{y}(\mathbf{u}) \tag{2}$$

The system flowsheet is shown again in this section. The measurements (system pressures) are indicated now.



Figure 1: Network containing two gas lifted wells. Pressures, which are the measured states, are indicated. Adapted from: Krishnamoorthy et al.¹.

Nonlinear system model

The system mass balances, which are originally a differential equation set \mathbf{f} , are:

$$0 = \dot{m}_{ga,i} = w_{gl_i} - w_{iv_i} \quad i = 1, 2$$
(3a)

$$0 = \dot{m}_{gt,i} = w_{iv_i} - w_{pg_i} + w_{rg_i} \quad i = 1, 2$$
(3b)

$$0 = \dot{m}_{ot,i} = w_{ro_i} - w_{po_i} \quad i = 1, 2$$
(3c)

$$0 = j \widetilde{\mu_{gr}} = \sum_{i} w_{pg_i} - w_{tg} \tag{3d}$$

$$0 = \dot{p}_{or} = \sum_{i} w_{ro_i} - w_{to} \tag{3e}$$

where, m_{gr} and m_{or} are the total mass of gas and oil in the riser/manifold. $m_{ga,i}$ is the gas mass in the annulus of the well *i*. $m_{gt,i}$ and $m_{ot,i}$ are the total mass of gas and oil of the well *i*. For the *i*th well, w_{gl_i} is the gas lift injection rate; w_{iv_i} is the gas flow from the annulus into the tubing; w_{rg_i} is the gas flowrate from the reservoir; w_{ro_i} is the oil flowrate from the reservoir; and w_{pg_i} and w_{po_i} are the produced gas and oil flowrates from well *i*, respectively. Regarding the network, the total produced gas and oil flowrates are represented by w_{tg} and w_{to} . The mass flows are calculated using nonlinear relations explained in the following sections. Note that, i = 2 in the case study.

Well $i \mod i$

The mass flowrates are computed by (note that, for convenience, the subscript i for indicating the i^{th} well has been removed from the equations):

$$w_{iv} = C_{iv} \sqrt{\rho_a \max(0, p_a - p_{wi})} \tag{4a}$$

$$w_{pc} = C_{pc} \sqrt{\rho_w \max(0, p_{wh} - p_m)} \tag{4b}$$

$$w_{pg} = \frac{m_{gt}}{m_{gt} + m_{ot}} w_{pc} \tag{4c}$$

$$w_{po} = \frac{m_{ot}}{m_{qt} + m_{ot}} w_{pc} \tag{4d}$$

$$w_{ro} = PI \times (p_r - p_{bh}) \tag{4e}$$

$$w_{rg} = GOR \times w_{ro} \tag{4f}$$

where, C_{iv} and C_{pc} are the value flow coefficients for the downhole injection value and the production choke, respectively. ρ_a is density of gas in the annulus and ρ_w is fluid mixture density in the tubing. p_a is the annulus pressure, p_{wi} is the pressure at the gas lift injection point, p_{wh} is the wellhead pressure, p_m is the manifold pressure, p_r is the reservoir pressure and p_{bh} is the bottom hole pressure (all the pressures are indicated in Figure 1). *GOR* is the gas/oil ratio of the reservoir and *PI* is the reservoir productivity index. As discussed in the paper, the productivity index value is used for emulating different well models in order to test the model structure adaptation methodology.

The gas density is given by:

$$\rho_a = \frac{M_w p_a}{T_a R} \tag{5}$$

And the fluid mixture density by:

$$\rho_w = \frac{m_{gt} + m_{ot} - \rho_o L_r A_r}{L_w A_w} \tag{6}$$

where, M_w is the molecular weight of the gas, R is the gas constant, T_a is the temperature

in the annulus, and ρ_o is the density of oil in the reservoir. L_{bh} and A_{bh} are the length and cross-sectional area of the well below the injection point. L_w and A_w are the length and cross-sectional area of the well above the injection point.

The pressures are computed by:

$$p_a = \left(\frac{T_a R}{V_a M_w} + \frac{g L_a}{L_a A_a}\right) m_{ga} \tag{7a}$$

$$p_{wh} = \frac{T_w R}{M_w} \left(\frac{m_{gt}}{L_w A_w + L_{bh} A_{bh} - \frac{m_{ot}}{\rho_o}} \right)$$
(7b)

$$p_{wi} = p_{wh} + \frac{g}{A_w L_w} (m_{ot} + m_{gt} - \rho_o L_{bh} A_{bh}) H_w + M_2$$
(7c)

$$p_{bh} = p_{wi} + \rho_w g H_{bh} \tag{7d}$$

where L_a and A_a are the length and cross sectional area of the annulus, H_{bh} and H_w are the vertical height of the well tubing below and above the injection point. T_w is the temperature in the well tubing and g is the acceleration of gravity constant. M_2 is used for representing the "block" related to frictional pressure drop in the model. Two different sub-models can be chosen for the model structure adaptation methodology:

$$M_{2} := \left\{ (m_{2,1}:0) \lor \left(m_{2,2}: \frac{128\mu_{oil}L_{w}w_{pc}}{3.14D_{w}^{4}(m_{gt}+m_{ot})p_{wh}M_{w}\rho_{o}}(m_{ot}p_{wh}M_{w}+\rho_{o}RT_{w}m_{gt}) \right) \right\}$$
(8)

where, μ_{oil} is the oil viscosity and D_w is the tubing diameter. $m_{2,2}$ equation is based on the the Darcy-Weisbach² equation for laminar flow regime.

Riser/manifold model

For the riser/manifold system, the flows are calculated by:

$$w_{pr} = C_{pr} \sqrt{\rho_r \max(0, p_{rh} - p_s)} \tag{9a}$$

$$w_{tg} = \frac{m_{gr}}{m_{gr} + m_{or}} w_{pr} \tag{9b}$$

$$w_{to} = \frac{m_{or}}{m_{gr} + m_{or}} w_{pr} \tag{9c}$$

where, C_{pr} is the value flow coefficient for the riser choke. ρ_r is fluid mixture density in the riser. p_{rh} is the riser head pressure and p_s is the separator pressure (upstream process). The density is calculated by:

$$\rho_r = \frac{(m_{gr} + m_{or})p_{rh}M_w\rho_{ro}}{m_{or}p_{rh}M_w + \rho_{ro}RT_rm_gr}$$
(10)

where, T_r is the riser temperature. ρ_{ro} is the density of oil in the riser/manifold.

The riser pressure p_{rh} and the manifold pressure p_m are given by:

$$p_{rh} = \left(\frac{RT_r}{M_w}\frac{m_{gr}}{L_rA_r} - \frac{m_{gr} + m_{or}}{L_rA_r}\frac{gH_r}{2}\right)$$
(11a)

$$p_m = p_{rh} + \frac{g}{A_r L_r} (m_{or} + m_{gt} H_r + M_1)$$
(11b)

where L_r and A_r are the length and cross sectional area of the riser, H_r is the riser vertical height. As in the previous section, M_1 is used for representing the "block" related to frictional pressure drop in the model. Two different sub-models can be chosen for the model structure adaptation methodology:

$$M_{1} := \left\{ \left(m_{1,1} : 0 \right) \lor \left(m_{1,2} : \frac{128\mu_{oil}L_{r}w_{pr}}{3.14D_{r}^{4}(m_{gr} + m_{or})p_{rh}M_{w}\rho_{ro}} (m_{or}p_{rh}M_{w} + \rho_{ro}RT_{r}m_{gr}) \right) \right\}$$
(12)

where, D_r is the riser diameter. $m_{1,2}$ equation is based on the Darcy-Weisbach² equation for laminar flow regime.

Complete system model

Given the relations above for the wells and riser/manifold, the complete system model states x, measurements y and decision variables u for the 2-well network are:

$$\mathbf{x} = [m_{ga_1}, m_{ga_2}, m_{gt_1}, m_{gt_2}, m_{ot_1}, m_{ot_2}, m_{gr}, m_{or}]^T$$
(13a)

$$\mathbf{y} = [p_{a_1}, p_{a_2}, p_{wi_1}, p_{wi_2}, p_{wh_1}, p_{wh_2}, p_{bh_1}, p_{bh_2}, p_m, p_{rh}]^T$$
(13b)

$$\mathbf{u} = [w_{gl_1}, w_{gl_2}]^T \tag{13c}$$

Table 1 contains the values of the parameters used in the simulation.

Finally, there is a third "block", which is used to represent the reservoir model. The differences between the reservoir models lie in the *PI* value:

$$M_3 := \left\{ \left(m_{3,1} : PI = [5,5]^T \right) \lor \left(m_{3,2} : PI = [7,7]^T \right) \right\}$$
(14)

Plant model

Two different plant behaviors are formulated to test the ability of the methodology to track changes in the plant. Two regions are defined, each one presenting a different behavior. The regions are delimited by the values of the inputs u as shown in Figure 2. In Region A, pressure loss due to friction is taken into account in both wells and in the riser. In turn, Region B does not consider frictional pressure drop (i.e. the pressure difference between the top and bottom is related only with the static pressure exerted by the liquid column). Therefore, two different plant models are developed, one for Region A and one for Region B.

In order to obtain a smooth transition, a 2-D sigmoidal function is used for connecting

Table 1: Parameter values. Arrays indicate that each well has a different parameter value. In turn, if a scalar value is shown, it indicates that both wells have the same parameter value.

	Variable (symbol) [unit]	value
GOR	gas-oil ratio in the reservoir	$[0.1, 0.12]^T$
p_{res}	reservoir pressure $[bar]$	$[150, 155]^T$
p_s	separator pressure $[bar]$	20
T_a	annulus temperature $[^{o}C]$	28
T_r	riser temperature $[^{o}C]$	30
T_w	well temperature $[^{o}C]$	32
L_a	annulus length $[m]$	1500
H_a	annulus height $[m]$	1000
D_a	annulus diameter $[m]$	0.189
L_{bh}	well lenght below injection point $[m]$	500
H_{bh}	well height below injection $point[m]$	500
D_{bh}	well diameter below injection point $[m]$	0.121
L_r	riser length $[m]$	500
H_r	riser height $[m]$	500
D_r	riser diameter $[m]$	0.121
L_w	well length $[m]$	1500
H_w	well height $[m]$	1000
D_w	well diameter $[m]$	0.121
C_{iv}	injection value $[m^2]$	0.0001
C_{pc}	production valve $[m^2]$	0.0002
C_{pr}	riser valve $[m^2]$	0.001
ρ_o	oil density in the wells $[kg/m^3]$	800
ρ_{ro}	oil density in the riser $[kg/m^3]$	800
μ_{oil}	oil viscosity $[Pa \cdot s]$	0.001
M_w	average molecular weight $[kg/mol]$	0.02

the two regions. To illustrate its effect, Equation (11) is used:

$$p_m = p_{rh} + \frac{g}{A_r L_r} (m_{or} + m_{gt} H_r + \Omega)$$
(15)

Note that, Ω is used for representing the plant while M_1 represents the model, which is used in the economic optimization and model structure adaptation methodology. In addition, the value of Ω changes according to the model input values as shown below. In turn, M_1 represents a set of equations related to either sub-model $m_{1,1}$ or $m_{1,2}$. After choosing a



(a) Plant surface. Regions A and B as well as plant optimum are highlighted.



(b) Profit contour lines for the plant, the feasible region is indicated with an arrow. Dashed blue line is the maximum gas production constraint and dashed black lines are the maximum gas lift flow rate for each well. The plant optimum is also indicated.

Figure 2: Plant surface

sub-model to compose the complete process model, the set of equations in M_1 is specified and do not change according to **u**.

In order to compute Ω , ω is determined based on the model inputs $w_{gl,1}$ and $w_{gl,2}$. Note that ω changes within the interval 0-1,

$$\omega(w_{gl,1}, w_{gl,2}) = \left(\frac{1}{1 + e^{-10w_{gl,1} + 17.5}}\right) \left(\frac{1}{1 + e^{-10w_{gl,2} + 17.5}}\right) \tag{16}$$

Then, the effects of the different models that represent Regions A and B are weighted based on Equation (17). Next, the value of Ω is added to Equation (15).

$$\Omega = \omega \times (0) |_{\text{Region A}} + (1 - \omega) \times \left(\frac{128\mu_{oil}L_r w_{pr}}{3.14D_r^4(m_{gr} + m_{or})p_{rh}M_w \rho_{ro}} (m_{or}p_{rh}M_w + \rho_{ro}RT_r m_{gr}) \right) \Big|_{\text{Region B}}$$
(17)

Gradient Estimation *

The method from Gao et al.⁴ is applied to estimate plant gradients, which are necessary for calculating the modifiers. They are estimated via quadratic approximations of the inputoutput mapping of Equation (2). The step-by-step description of the method can be seen in Figure 3.

For estimating the parameters of quadratic functions, it is necessary to obtain at least $n_r = (n_u + 1)(n_u + 2)/2 - 1$ measurements (with n_u equals to the number of inputs of the problem, which are the number of manipulated variables in our case). This measurements are required due to the number of coefficients that are adjusted in the multidimensional quadratic functions. In order to estimate the gradient while we do not have enough measurements to compute the quadratic approximations, Gao et al.⁴ apply finite-difference approximation (FDA) n_u times and uses iterative gradient-modification optimization and gradient estimation (IGMO) to generate the remaining $n_r - n_u$ measurements. FDA applies small perturbation (Δh) to the inputs in order to obtain the measurements around the current point. On the other hand, IGMO optimizes the plant using MA and estimates plant gradients with a variant of FDA,⁵ which uses setpoints of the past iterations to evaluate the gradients instead of further probing the plant.

$$\frac{\partial \mathbf{y}_p}{\partial \mathbf{u}} = [S_k]^{-1} \cdot [(y_{m,k} - y_{m,k-1}) \dots (y_{m,k} - y_{m,k-n_u})]$$
(18)

where, y_m are the process measurements at time instants $k, k-1, \ldots, k-n_u$. Note that, the input matrix $[S_k]^{-1} = [(u_k - u_{k-1}), \ldots, (u_k - u_{k-1})]^{-1}$ also contains only past information. However, $[S_k]^{-1}$ needs to be well-conditioned in order to obtain good approximations for the gradients. If it is not, IGMO perturbs the process in order to improve the input matrix conditioning. Clearly, IGMO is not as expensive as FDA, because it only perturbs the system when necessary.

^{*}This section is based on Matias et al.³



Figure 3: Flowsheet of MA with gradient estimation via quadratic approximation. Adapted from: Gao et al. 4 and Matias et al. 3

After obtaining n_r plant measurements, the gradients are calculated by the quadratic approximations. As the gradient is computed by differentiating the quadratic models, its quality depends on their precision. Thus, it is critical that the algorithm chooses welldistributed past operating points over the feasible space for estimating the parameters of the quadratic approximation. In order to do so, the set of past operating points, which is represented by U, is divides set in three subsets:

- 1. U_{nb} : Neighborhood of the current point, which is defined by a tuning parameter $\Delta \mathbf{u}$, $U_{nb} := {\mathbf{u} : ||\mathbf{u} - \mathbf{u}_{current}|| \le \Delta \mathbf{u}; \mathbf{u} \in U};$
- 2. U_{dist} : Set of points that are sufficiently distant from the current point, but sufficiently scattered and well-distributed to capture the plant curvatures;
- 3. U_{outer} : the points that do not belong to the other sets, i.e. $U_{outer} = U \setminus U_{nb}, U_{dist}$.

By determining $\Delta \mathbf{u}$, U_{nb} is easily defined. Gao et al.⁴ proposed an optimization problem to compute U_{dist} , which determines at least n_r points using a criterion that minimizes the distance from the current point, while penalizes using points along the same direction. After determining the three subsets, U_{nb} and U_{dist} are used to estimate the parameters of the quadratic approximation.

In addition to the screening process, some extra steps are used to improve the quality of the quadratic approximation. First, a covariance-based constraint is imposed to the economic optimization problem in order to adjust the search space based on the previous iterations (e.g.: given that the past operating points are along a specific direction, the gradient is more reliably estimated in that direction). The parameter γ determines the size of ellipsoid center at the current input, u(k), $B(k) : (u - u(k))^T (cov(\mathcal{U}))^{-1}(u - u(k)) \leq \gamma^2$, which constraints the search space of the economic optimization problem. Note that lower values of γ are used to avoid unnecessary deterioration of the plant performance, preventing optimization moves in directions in which less data has been collected.

Second, an intermediary step is applied to improve the choice of the regression set (the block with colored background in Figure 3). This step determines if the calculated optimum, u^* , lies in the neighborhood of the current input. If so, the plant is probed in a different point, outside the neighborhood of the current point, in order to improve the quadratic

approximation. In the case that the new probing point does not improve the plant cost function, the iteration is considered unsuccessful, the probing point is included in the regression set and the screening algorithm is re-initiated. This step is based on the following logic: if the algorithm has calculated an optimal point that is in the neighborhood of the current operating point, it might be the case that the plant optimum is also in neighborhood of the current operating point. Therefore, additional plant probing points are taken in order to improve the information around the current point (by shrinking the regression region⁶), in order to avoid overshooting the plant optimal in the next moves.

Tuning parameters

The perturbation step size, Δh , is used in the finite-difference approximation (FDA). As described in Figure 3, FDA is executed only at the first step because in the case study $n_u = 2$. FDA applies small perturbation (Δh) to the inputs in order to obtain the measurements around the current point. Then, the measurements are used to estimate the plant gradients. Despite being simple, FDA becomes inefficient if the process measurements are noisy. Moreover, FDA might lead to constraint violations if operating close to a constraint.

After the initial step, Iterative gradient-modification optimization and gradient estimation (IGMO) is used for calculating the remaining $n_r - n_u$ measurements $(n_r - n_u = 3 \text{ in} \text{ our case})$. Thus, if the condition number is lower than δ_{IGMO} , the plant is probed around the current operating point in order to increase the conditioning of S_k . The third and fourth parameters are used in the screening process explained in the previous section. Δu defines the size of the U_{nb} and γ is the scaling parameter of the covariance-based constraint.

Table 2:	Parameters	and	variables	for	the	gradient	estimation	method.	Adapted	from:
Matias et	al. 3									

Description	Symbol	Value
Perturbation step size	Δh	0.1
Conditioning number of input matrix	δ_{IGMO}	0.1
Search space parameter	γ	1.9
Screening parameter	Δu	0.3

References

- Krishnamoorthy, D.; Foss, B.; Skogestad, S. Real-time optimization under uncertainty applied to a gas lifted well network. *Processes* 2016, 4, 52.
- (2) Perry, R. H.; Green, D. W.; Maloney, J. Perry's handbook of chemical engineering. Perry's Handbook of Chemical Engineering, pp. Top 1997, 2–65.
- (3) Matias, J. O.; Le Roux, G. A.; Jäschke, J. Modifier adaptation for real-time optimization of a gas lifted well network. *IFAC-PapersOnLine* **2018**, *51*, 31–36.
- (4) Gao, W.; Wenzel, S.; Engell, S. A Reliable Modifier-Adaptation Strategy for Real-Time Optimization. Computers & Chemical Engineering 2016, 91, 318–328.
- (5) Gao, W.; Engell, S. Iterative set-point optimization of batch chromatography. Computers
 & Chemical Engineering 2005, 29, 1401–1409.
- (6) Conn, A. R.; Gould, N. I.; Toint, P. A globally convergent augmented Lagrangian algorithm for optimization with general constraints and simple bounds. SIAM Journal on Numerical Analysis 1991, 28, 545–572.