# STEADY STATE EXERGY "BACK OFF" IN PROCESS CONTROL SYSTEMS

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**Abstract** - Considering process economic along with operational and controllability requirements is the routine for recent control structure selections studies. One of well-known studies is the Back Off theory that denotes extent of economic loss due to unmanageable and unpredictable disturbances and uncertainties. Parallel to the economic Back Off theory as a measure of economy and controllability in process system an exergy-based back off calculation is developed in this work to have a measure of energy efficiency of process systems. This new idea was applied to a reactor-separator system and was found that an steady-state exergy loss of about 10% is for the maximum back off due to worst case feed temperature and composition disturbances.

**Keywords** - Back Off, Exergy, Process Systems, Control Structure Selection

## I. INTRODUCTION

Despite traditional approaches of control structure design that merely provide steady state and dynamic controllability objectives, modern control systems have an integrated link with other performance objectives like economy. By this viewpoint the better control structures most provide more economic benefits beside controllability and operability preliminaries. One of the early studies of this approach to control design is the back off of economic objective from optimal operating condition to overcome disturbance and uncertainties (Bahri et al 1994, 1995, 1996). In fact since optimal operating point is most probably on the intersection of some constraints, uncertainties in the process may push the process to the infeasible regions. Then for assurance of feasible operation at any condition a back off from the optimum point is needed. The theory of back off is developed by many researchers in the recent two decades for linear (Narraway and Perkines, 1993) and nonlinear (Heath et al. 2000) processes for both steady state (Bahri et al 1995) and dynamic (Psaltis et al 2013, Narraway and Perkins 1994) and also for plantwide scale problems(Psaltis et al 2013, 2014). Optimization algorithms of back off are also search field of some works (Kookos and Perkins 2001).

Recent emerging universal problem of global warming and other pollution catastrophes is the persuading factor of other potential control design objectives to be of interest. Exergy as an indication of process energy efficiency is one of these objectives. As it is stated by Szargut et al. (1988), economic and exergy have not always the same trends in process optimizations. In process design and operation, however economic is the more desirable factor but by growing tendency to save resources and especially more tightly environmental regulations that enforcelower greenhouse gases production, energy efficient plants are in attention. Therefore exergy consideration as a measure of energy efficiency is emerging nowadays. Most of exergy considerations in design of chemical plants however are in steady state area and few literature are published about exergy analysis in process control. A short review shows that publication can be classified at least in three major fields:

First and major works are about second law of thermodynamic application in nonlinear process systems. Passivity-based control strategy is the basis from control standpoint and classical irreversible thermodynamic ideas make the thermodynamic foundation with the first ideas of Ydstie and Alonso (1997).

Second, two papers by Tyreus (1999) that in which thermodynamic is applied in order to select dominant variables in a partial control strategy.Third, Relative Exergy Array (REA) idea recently proposed by Montelongo-Luna et al. (2011) which is an analogy to RGA.Themethod try to measure the exergetic effect of a selected paring. They suggest that both RGA and REA be checked for paring alternatives and ones with satisfying criteria (i.e. near unity elements of both RGA and REA matrix) are the best choices.

In this paper parallel to economic back off calculation an exergy back off calculation would be calculated. This back off calculation then can be used for control structure decisions and analyses.

## II. EXERGY IN PROCESS SYSTEMS

In thermodynamics, first and second law analysis for an open process system like Figure 1 would give the following relations:

$$\frac{d[mU]_{sys}}{dt} + \Delta[\dot{m}h]_{\text{flowing streams}} - \sum_i^{n_q} \dot{Q}_i - \sum_i^{n_w} \dot{W}_i = 0 \quad (1)$$

$$\frac{d[ms]_{sys}}{dt} + \Delta[\dot{m}s]_{\text{flowing streams}} - \sum_i^{n_q} \frac{\dot{Q}_i}{T_i} = \dot{S}_G \quad (2)$$

U is internal energy of the system, h and s are for the molar or specific enthalpy and entropy of flowing streams respectively. Usually in process systems

kinetic and potential energies are neglected as done in Equations 1 and 2 and inlets of work $\dot{W}$ and heat $\dot{Q}$to the system appointed as positive and their outlets as negative quantities.

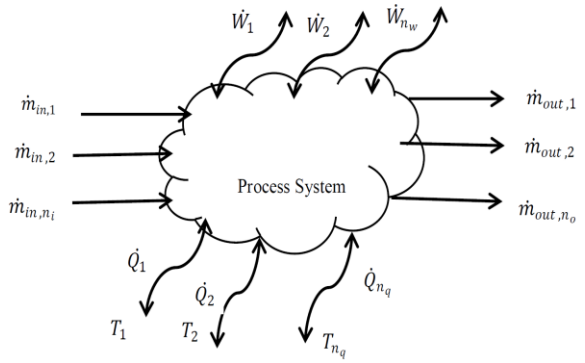



**Figure 1. Process system representation versus inputs and outputs of material and energy streams i=1,2,3,...**

In both Equations 1 and 2 $\Delta(.) = \sum_i^{n_o}$ output stream i $(.) - \sum_i^{n_i}$ input stream i $(.)$. $\dot{S}_G$ in Equation 2 is the rate of entropy generation due to irreversibility in the system ($\dot{S}_G = 0$ for reversible processes) and T is the heat source temperature which may be in cooling or heating duty. Multiplying Equation 2 by $-T_0$ (surrounding or dead state temperature) and summing with Equation 1 gives:

$$-\frac{d[m(b-Pv)]_{sys}}{dt} - \Delta[\dot{m}(b)]_{\text{flowing streams}} + \sum_i \left(1-\frac{T_0}{T_i}\right)\dot{Q}_i + \sum_i \dot{W}_i = \dot{I} \quad (3)$$

Where $b = h - T_0 s$ is the exergy function (Seider et al .2003) and $\dot{I} = T_0 \dot{S}_G$ is the lost work due to irreversibility inside system. For a steady state process Equation 3 becomes:

$$\dot{I} = -\Delta[\dot{m}(b)]_{\text{flowing streams}} + \sum_i \left(1-\frac{T_0}{T_i}\right)\dot{Q}_i + \sum_i \dot{W}_i \quad (4)$$

Some aspects of the exergy analysis of form Equation 4 rather than economic objective functions in process control are:

- In chemical processes manipulated variables are often of type of material flow rates ($\dot{m}$), heat flows $\dot{Q}$ (thermal duties) and rarely work supply $\dot{W}$ (pumps and compressors powers) that have simple and routine relations in lost work calculation. As can be seen later this is part of motivation of the method developed in this work.
- Lost work equation can be applicable to dynamic as well as the steady state analysis by taking into account the first right hand term of Equation 3.

## III. CALCULATION ALGORITHM OF EXERGY BACK OFF

The algorithm proposed by Bahri et al (1995) is selected in this work for calculation of exergy back off. That is a two-step method consists of outer and inner loops for optimization. In the outer loop for the predefined worst case disturbances $d^N$ the optimal exergetic operating conditions $u^*$ would be found. The objective function of this minimization is lost wok.

**Outer loop:**

$$\min_u \dot{I}$$
$$\text{S.t.} \quad h_i(x,u,d^N) = 0$$
$$g_j(x,u,d^N) \geq 0$$

In which $h_i$ and $g_j$ are equality and inequality constraints respectively. By this minimization problem the best operating point in presence of worst case disturbance can be found $\dot{I}_{opt}(d^N)$. But how can we find this $d^N$? Starting with nominal disturbances subsequent values of the possible range will be found in the inner loop.

**Inner loop:**
With a little modification to the original algorithm, in this loop it will be found disturbances that cause maximum violation of the objective function $(d) = \dot{I}_{opt}(d) - \dot{I}_{opt}(d^N)$ .

$$\max_d \varphi(d)$$
$$\text{S.t.} \quad h_i(x,u^*,d) = 0$$
$$g_j(x,u^*,d) \geq 0$$

Sent back to the outer loop, results from this loop, are the new values for probable worst case disturbances$d^N$.
The algorithm will terminate when in two successive iterations $d^N$became unchanged or the objective goes to zero. This new approach is more explained by a case study.

## IV. CASE STUDY: REACTOR-SEPARATOR SYSTEM

As the case study a simple liquid phase reaction in two phase separator (fig 2) is developed by some other simplifying assumptions such as:

1. Reaction is elementary $\{r_A = -k_1 x_A + k_2(1-x_A)^2\}$and just in the liquid phase.
2. Constant pressure and flow-driven condition (without any valve installed) and feed vapor fraction of 50% ($\phi = 0.5$).
3. Heat Q supplied only to the liquid phase and non-equilibrium vapor and liquid phases with simple mass transfer rate of $F_{vap,i} = K_i(x_i - x_i^*)$. For calculation of equilibrium the relation of $x^* =$

$y^*/\left((1-y^*)\alpha+y^*\right)$ with $\alpha = 0.4 + 10^{-4}T$ were used.

4. Enthalpy and entropy were determined by simple relations of $H = H_{form}\,(T_0) + \int_{T_0}^{T} C_P\,dT$ and $S = S_{form}\,(T_0) + \int_{T_0}^{T} \frac{C_P}{T}\,dT$ respectively and $H_{vap}$ was used to calculate enthalpy and entropy in the liquid phase. $T_0 = 25$ everywhere and $T_{out} = 80$.
- Neglecting interphase heat transfer

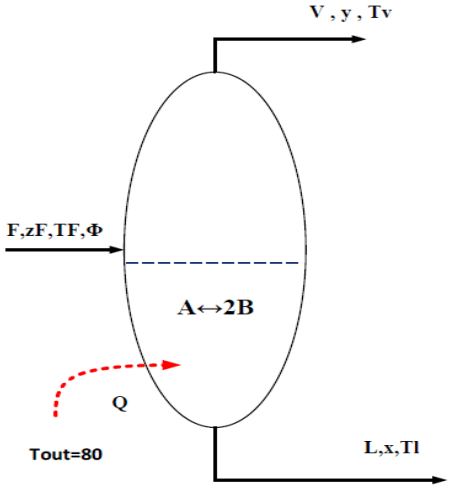



**Figure 2. Schematic of the reactor-separator system**

Physical parameters are showed in Table 1.

**Table 1 .physical properties for the case study**

| | Components | A | B |
|---|---|---|---|
| $C_P = a + bT$, a/b | Liquid | 300/0.1 | 200/0.2 |
| | Vapor | 0.3/0.6 | 0.25/0.4 |
| $H_{form}$ | | -1000 | -1500 |
| $S_{form}$ | | 103 | 150 |
| $H_{vap} = a + bT$ , a/b | | 200/0.23 | 140/0.43 |
| K | | 2 | 5 |
| Reaction forward/backward | | | |
| Rate constant: k | 2000/1000 | | |
| Activation energy: E | 200/300 | | |

## V. RESULTS AND DISCUSSION

Lost work equation 4 corresponding to this case study then will give:

$$\dot{I} = Fb_F - Vb_V - Lb_L + \left(1 - \frac{T_0}{T_{out}}\right)Q \qquad (5)$$

Lower and upper bonds of disturbances and MVs are shown in Table 2 and there is no other inequality constraint. For this simple case study the powerful MATLAB software was used, all equality constraints of optimization (energy and mole balances) were solved by "fsolve" and both optimization loops were done by "fmincon" function, Thrust Region algorithm was used for all calculations.

**Table 2, operational constraints and optimal conditions**

| | Feasible region | Optimal values for worst disturbances |
|---|---|---|
| MVs | | |
| F | 100-10000 | 100 |
| Q | 200-20000 | 8400 |
| V, y | | 55.3601 , 0.1465 |
| L, x | | 77.84 , 0.2442 |
| | | 46.45 , 60 |
| | | $2.3 \times 10^6$ , 0.0136 |
| Disturbances | | |
| $z_F$ | 0.81-0.99 | 0.99 |
| T | 45-55 | 45 |

As can be seen in table 2 the worst case disturbances are both at the margins and the optimal feed flow rate is an active constraint while heat duty is not an active one. Little positive value (0.0136) of inner loop optimization objective φ is due to calculation errors and theoretically must be zero. calculation for the optimal lost work $(2.1 \times 10^6)$ at nominal disturbances (d=[0.9 , 50]) shows a back off about $2 \times 10^5$due to worst case disturbances which is noticeable (about 10%).

## VI. CONCLUSION

A new approach for the back off theory in process control system was developed in this work and both objective function and calculation method were altered for this new approach. Exergy as an emerging discipline in nowadays physical systems serves as the objective function and a modification to the calculation strategy by Bahri et al 1995 is developed here. The approach shows the potential inclusion of exergy as an objective in process control optimizations. However not considered in this work this method can be used in all decision makings steps of process control from MVs and CVs selection to paring or tuning assortments. The other aspect of the method is simply application to dynamic problems by taking into account the unsteady term of exergy equation (first term of equation 3).

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