

THERMODYNAMIC BASED RESPONSE TIME AS CONTROLLABILITY INDICATOR ON HEAT EXCHANGER NETWORKS.

Carmen De Leon Herrera, Camila B. Miranda, Cid M. G. Andrade and Mauro A. S. S. Ravagnani*

*Author for correspondence

Department of Chemical Engineering,
State University of Maringá,
Av. Colombo 5790, Maringá – PR, 87020900
Brazil,
E-mail: ravag@deq.uem.br

ABSTRACT

Nowadays, the interaction between process design and control has become the focus of research and development, because not always the best process design features the best dynamic performance, with implications in the controllability of the plant. The necessity in minimizing fixed investment and utilities consumption promotes integrated process design in energy and mass terms. These integrations are often designed without consideration of controllability and flexibility of these projects; creating difficulties in process control and resulting in more efficient designs with smaller gradients and reduced driving forces, which brings complications with disturbances rejection. Thermodynamics theory allows establishing relationships between physical quantities, giving an idea of how a system evolves in time. In this way, a thermodynamic analysis with a dissipative approach, can lead to an optimal point between process integration and controllability. The present paper proposes a simultaneous approach relating reversibility and control, obtaining a method to determine a thermodynamic index, relating the entropy and energy production in a new state function and establishing a response time index that serves as a guide to measure the process controllability. The method was applied to a known Heat Exchanger Network (HEN), resulting in smaller values for stages with high entropy production, when exposed to disturbance. The results were compared with the given by Relative Gain Array (RGA) and Disturbance Cost (DC) methods, showing consistency. With the proposed methodology, it is possible to relate the stages of process control and process design, with a base analysis of controllability based on the system thermodynamics.

INTRODUCTION

The interaction between process design and control has become one of the important focus in chemical and industrial processes research and development, considering that not always the best process design presents the best dynamic performance, with implications in the controllability of the plant.

A simultaneous analysis in the economic goals and controllability of the transient regime in the early stages of the project design is preferred over the classical sequential approach, where the process design is developed first based only on steady state information.

Mass and energy integrations are often designed without consideration of controllability and flexibility of the project; resulting in more efficient designs (closer to the reversible thermodynamic point of view), with smaller gradients, reducing the driving force and creating difficulties in process control.

A heat exchanger network (HEN) is an arrangement of heat exchangers whose purpose is to recover energy from hot streams to heat up cold streams, achieving the specified outlet target temperatures of the process stream. Process systems, as HEN, are described as a thermodynamic system with interconnection between process units. Thermodynamics theory allows establishing relationships between physical quantities although is not enough to describe complex interactions and behaviors it can give an idea of how a system evolves in time. [1]

Using the concept of passivity derived of the Second Law of Thermodynamics can be shown how conditions for evolution to a passive state can be derived using bounding properties of equilibrium thermodynamics, energy conservation and the Clausius-Planck inequality. [2]

Consequently, an optimal point, or near it, between process integration and controllability can be reached through thermodynamic analysis with a dissipative approach.

The concepts of thermodynamic applied to process control have been studied by some authors. [3] presents a stability and stabilizability analysis for plantwide chemical processes, applying the dissipativity analysis based on thermodynamics to dissipativity-based conditions suitable for process network analysis and generating a storage function in terms of temperatures and composition, this approach is used for the analysis of a cascade network of two continuous stirred tank reactors (CSTRs). [4] make use of dissipative approach for plantwide control, applied on the Tennessee Eastman Process.

[5] present a distributed control synthesis approach for plantwide processes based on dynamic supply rates, expressed as quadratic differential forms. [6] use a thermodynamic approach for analyzing the structural stability of process plants while [7] proposed a modeling framework for complex chemical process networks, using the concavity of the entropy function to define a storage function for passivity design.

This paper presents a thermodynamic approach based on the concepts presented in [8] relating exergy and controllability as well as the connection between thermodynamics (reversibility)

and control (dissipative effects), as presented in [9] and [2]. This approach will be used in a HEN base case.

In Section 2 it is presented the issues that motivate this approach and its description. In section 3 it is presented a case study applying the concepts previously described to a known HEN. Finally, section 4 presents the conclusions based on the results obtained.

NOMENCLATURE

| | | |
|--------------------|-------------------|---|
| A_j | [m ²] | Heat transfer area |
| A | [MW] | Helmholtz free energy |
| C_{pj} | [MW h/Kg K] | Specific heat capacity |
| dq | [MW/KgMol] | Specific heat variation |
| du | [MW/KgMol] | Specific internal energy variation |
| dw | [MW/KgMol] | Specific work |
| F_j | [KgMol/h] | Molar flow rate |
| f_j | [-] | Non-linear energy balance function |
| K | [-] | Area correction factor |
| $p(t, \tau)$ | [-] | Amount of system property produced during a process |
| $P_E(x)$ | [MW] | Energy production |
| $P_S(x)$ | [MW/K] | Entropy production |
| Q_j | [-] | Heat exchanged |
| S | [MW/K] | Entropy |
| $S(x(t))$ | [-] | Storage function |
| T | [K] | Absolut temperature |
| T_j | [K] | Hot stream temperature |
| U | [MW] | Internal energy |
| $u(x)$ | [-] | System input |
| U_j | [-] | Heat transfer coefficient |
| $w(u, y)$ | [-] | Supply rate |
| $x(t)$ | [-] | System state |
| $Y(x(t))$ | [-] | Lyapunov function |
| $y(t)$ | [-] | System output |
| Special characters | | |
| $\delta(t, \tau)$ | [-] | Inventory change of the system |
| θ_3 | [K] | Cold stream temperature |
| φ | [-] | By-pass fraction |
| ϕ_A | [-] | Net flow of Ydstie function quantity produced |
| $\phi(t, \tau)$ | [-] | Action applied to the system |
| $v(t)$ | [-] | Measured system property |
| $Y_A(x)$ | [-] | Ydstie function |
| $Y_{A0}(x)$ | [-] | Ydstie function constant |
| $Y_E(x)$ | [MW] | Energy function |
| $Y_S(x)$ | [MW/K] | Entropy function |
| Subscripts | | |
| $J=1,2,3$ | | Stream or heat exchanger identifier |
| o | | Reference point |

DEVELOPED APPROACH

Irreversible Thermodynamics and Stability in HEN

The First Law of Thermodynamic states that the change in the internal energy of a closed system (du) is equal to the amount of heat supplied to the system (dq), minus the amount of work done by the system on its surroundings (dw), as shown on Equation 1.

$$dq = du + dw \quad (1)$$

Clausius inequality is known as the Second Law of Thermodynamic, it states that for a process the entropy variation of a body undergoing a transformation from an equilibrium state to another via heating is greater or equal than the incremental heating and the absolute temperature ratio.

$$S_2 - S_1 \geq \int_1^2 \frac{dq}{T} \quad (2)$$

A dynamic system is irreversible if there is no control action that returns the system to its original condition or steady state. Entropy an energy can be related combining the first and the second laws, through the definition of the Helmholtz Free Energy. Defining the reference system at absolute zero it is established a lower bound for the Helmholtz energy and it can be used as a storage function candidate for control system design [10].

$$A = U - TS \quad (3)$$

An isolated system, without any exchange with the surroundings tend to the equilibrium, involving an entropy increase. If a mass or energy exchange occurs, it is named as action on the system, which can be time dependent and prevent the reach of equilibrium state with minimum dissipation.

In [11] is postulated that the entropy production should be minimized for stable stationary states. [12] presented a discussion and a proof on that idea, and suggested a Hamiltonian formulation of thermodynamics of stationary states, which, when applied as a storage function to two comparison systems showed that they converge to the same measure.

Using extensive system properties as inventories thermodynamics can help develop a theory of process control. Considering $v(t)$ a measure, continuous on t , it is the inventory of property v in the system V at time t . In this case, the inventory considered is the energy (E), measure that is additive over different network nodes, non-negative and related to a state of the system. The change of inventory from time t to time $t + \tau$ is given by:

$$\delta(t, \tau) = v(t + \tau) - v(t) \quad (4)$$

If an action $\phi(t, \tau)$ that implies the supply of v to the system, takes place, taking the system to a new state. The new inventory balance is:

$$v(t + \tau) - v(t) = p(t, \tau) + \phi(t, \tau) \quad (5)$$

Where $p(t, \tau)$ is the amount of v produced along the process P in going from state 1 to state 2. This inventory control model introduced by [15] will be used as base to determine the controllability, as will be shown later in this paper.

a. Lyapunov functions and supply rate

With the concepts of of Lyapunov functions and supply rate it is possible to relate them with the energy as a storage function of the system, which is wanted to be asymptotically stable around a desire point.

A Lyapunov function is a function defined on an environment large enough which takes non-negative real values and whose first derivative is negative. This can be mathematically described as:

$$Y(x(t)) \geq 0 \quad (6)$$

$$\dot{Y}(x(t)) \leq 0 \quad (7)$$

If there is a state $x(t)$ in a dynamic system that can be described with a Lyapunov function, then x is a stable state that can be reached asymptotically.

The supply rate is a scalar function of the system inputs and outputs $w(u, y)$, that satisfies:

$$\int_t^{t+\tau} |w(u, y)| dt < \infty \quad (8)$$

A dissipative system is a dynamic system with states ($x(t)$), inputs ($u(x)$) and outputs ($y(t)$) that counts with a storage function ($S(x(t))$), that meets to be a Lyapunov function. In a dynamic system, the variation in the storage function cannot be higher than the supply rate

System Passivity and Ydstie Function

A dissipative system where the net supply of stored quantity is a function of the measured outputs and manipulated inputs only is defined as a passive system. This system cannot deliver more energy than the stored energy, as defined by [13].

Passivity and thermodynamics are related, as demonstrated by [2]. This property motivates the use of passivity-based methods for chemical process control since it suggests that it may be possible to derive process control systems directly from process physics.

As the dissipative storage function is a Lyapunov function, passive systems can be proven to be asymptotically stable. Hence, if an arbitrary dynamic system can be made passive, the system can be stabilized. [2] have proven that for process systems a storage function exists that leads to a passive system. This storage function is called the Ydstie Function and is constructed from variables already available in the thermodynamic description. It is given by:

$$Y_A(x) = Y_E(x) - T_0 Y_S(x) + Y_{A0}(x) \quad (9)$$

Where $Y_A(x)$ is the Ydstie function, $Y_E(x)$ is the energy and Y_{A0} is a constant, whose appropriate selection will guarantee that $Y_A(x) \geq 0$. The general balance for $Y_A(x)$ is given by:

$$\frac{dY_A(x)}{dt} = \phi_A + P_E(x) - T_0 P_S(x) \quad (10)$$

Where ϕ_A is the net flow of the quantity Y_A and T_0 is the reference temperature. Since the energy is conservative, $P_E(x)$ is always zero, and when the system is in a steady state there is no variation in the Ydstie function. Thus, $\frac{dY_A(x)}{dt} = 0$ and:

$$\phi_A - T_0 P_S(x) = 0 \quad (11)$$

When the system is exposed to a step change in ϕ_A , $\Delta\phi_A$, will move from the state x_1 to another steady state, x_2 , experiencing a change in the entropy production $\Delta P_S(x)$:

$$\Delta\phi_A - T_0 \Delta P_S(x) = 0 \quad (12)$$

As ϕ_A is the net flow of $Y_A(x)$ one can say that in the amount of time τ , where the system moves from steady state 1 to steady state 2, making possible to describe the response time, τ , as a

measure of controllability of the process system, considering that for a better control a smallest value of τ is desirable. [14]

$$\tau = \frac{\Delta Y_A(x)}{T_0 \Delta P_S(x)} \quad (13)$$

RESULTS AND DISCUSSION

Case study

A system composed by three heat exchangers, used by [15] to measure controllability and resiliency using Relative Gain Array (RGA) and Disturbance Cost (DC) methods is used in this work to develop to determine the response time index, τ , based on the Ydstie function and the entropy, as explained above.

Figure 1 shows the HEN, where a hot stream (F_1) is cooled to 300 °F (422.04 K) using two cold streams (F_2 and F_3), whose feed temperatures are 300°F (422.04 K) and 200°F (366.48 K), respectively (θ_3 and θ_4). The system disturbances are the feed flowrate and temperature of the hot stream.

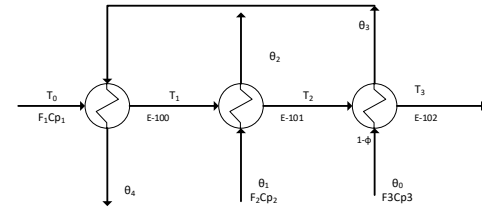


Figure 1: Studied HEN [15]

Equations 14 - 22 describe the energy balance of the HEN, it involves 15 variables, here the variables θ_0 and θ_1 are considered fixed and F_1 and T_0 are the external disturbances. In this way, the system presents 15 variables, 4 variables externally defined and 9 equations. Performing a degree of freedom analysis, the number of manipulated variables is: $15 - 4 - 9 = 2$. The RGA method can be used to establish the pairing of these variables, as presented by [15].

$$f_1(x) = Q_1 - F_1 C_{p1} (T_0 - T_1) = 0 \quad (14)$$

$$f_2(x) = Q_1 - F_3 C_{p3} (\theta_4 - \theta_3) = 0 \quad (15)$$

$$f_3(x) = Q_1 - U_1 A_1 \frac{(T_0 - \theta_4) - (T_1 - \theta_3)}{\ln[(T_0 - \theta_4)(T_1 - \theta_3)]} = 0 \quad (16)$$

$$f_4(x) = Q_2 - F_1 C_{p1} (T_1 - T_2) = 0 \quad (17)$$

$$f_5(x) = Q_2 - F_2 C_{p2} (\theta_2 - \theta_1) = 0 \quad (18)$$

$$f_6(x) = Q_2 - U_2 A_2 \frac{(T_1 - \theta_2) - (T_2 - \theta_1)}{\ln[(T_1 - \theta_2)(T_2 - \theta_1)]} = 0 \quad (19)$$

$$f_7(x) = Q_3 - F_1 C_{p1} (T_2 - T_3) = 0 \quad (20)$$

$$f_8(x) = Q_3 - F_3 C_{p3} (\theta_3 - \theta_0) = 0 \quad (21)$$

$$f_9(x) = Q_3 - U_3 A_3 \frac{(T_2 - \theta_3) - (T_3 - \theta_0)}{\ln[(T_2 - \theta_3)(T_3 - \theta_0)]} = 0 \quad (22)$$

The product of the global heat exchanger transfer coefficients (U_i) and heat transfer areas (A_i) for each exchanger are respectively 0.0427 MW / K, 0.1668 MW / K and 0.0731 MW / K.

Exposing the system to a disturbance $d = [F_1 T_0] = [5\% \ 2.778 \text{ K}]^T$, will move it from one steady state to another, resulting in variation in the heat and in the entropy production is used. The state variables values $x = [T_1, T_2, T_3, \theta_2, \theta_3, \theta_4, Q_1, Q_2, Q_3]^T$ are determined using the Newton-Raphson method, where the nonlinear state equations $f_i(x) = 0$ are solved considering nominal values the manipulated variables, disturbances and fixed variables.

Controllability and resiliency analysis

The previously described HEN was analyzed by [15] initially performing a degree of freedom analysis, which concluded that two variables can be manipulated and controlled, selecting θ_2 and θ_4 as manipulated variables and leaving T_3 uncontrolled. The RGA determined that the diagonal pairing ($\theta_2 - F_2$ e $\theta_4 - F_3$), is preferred and almost provides perfectly decoupled answers.

Using the DC index to obtain the resiliency of the network for a set of disturbances the authors concluded that although the controlled variables show perfect rejection, the outlet hot stream temperature, T_3 , is significantly affected, especially when the disturbances on F_1 and T_0 occur I opposite direction.

In order to remove the variations in T_3 , to the exchanger E-102 was add a by-pass stream, as shown in Figure 2, this variation increments the process degrees of freedom and allows the regulation of all the outlet temperatures.

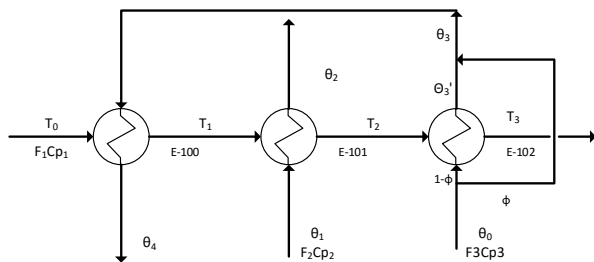


Figure 2 HEN with bypass in E-102 [15]

The exchanger area depends of the by-pass fraction, thus, the energy balance for E-102 exchanger transforms into Equations 23-25 with the addition of Equation 26, which expresses the energy balance for the streams mixer.

$$f_7(x) = Q_3 - F_1 C_{p1} (T_2 - T_3) = 0 \quad (23)$$

$$f_8(x) = Q_3 - F_3 C_{p3} (\theta'_3 - \theta_0) = 0 \quad (24)$$

$$f_9(x) = Q_3 - K_3 U_3 A_3 \frac{(T_2 - \theta'_3) - (T_3 - \theta_0)}{\ln[(T_2 - \theta'_3)(T_3 - \theta_0)]} = 0 \quad (25)$$

$$f_{10}(x) = (1 - \phi)\theta_0 + \phi\theta'_3 - \theta_3 = 0 \quad (26)$$

This way, the degree of freedom analysis results in three manipulated variables, and the RGA determined that the diagonal pairing is also preferred, and the sets of manipulated and controlled variables pairs is $\theta_2 - F_2, \theta_4 - F_3$ and $T_3 - \phi$, offering answers with interactions between the second and third control loop.

The DC index evaluated for a by-pass fraction of 0.10 resulted in values that exceeded the unity, which means a bas resiliency. The by-pass fraction of 0.15 offered a good trade-off between exchanger area and DC values.

Thermodynamic controllability analysis

Initially the state equations 14-22 are solved for nominal values of the manipulated variables, the worst response disturbances $d = [F_1, T_0]^T = [-5\% \ 2.78 \text{ K}]$, as shown in the previous analysis, and the constants θ_0 and θ_1 , to determine the states variables $x = [T_1, T_2, T_3, \theta_2, \theta_3, \theta_4]$.

With these values available for both cases, after and before applying the disturbances, the variation on the energy values and the entropy production is calculated and the values for the Ydstie function are determined for each stage of the network, allowing obtaining the response time index defined by equation 13.

After developing the thermodynamic analysis can be seen how the first unit of the HEN is considerably affected by disturbances, showing great difference on the values obtained for a set of disturbances, as shown on figure 3.

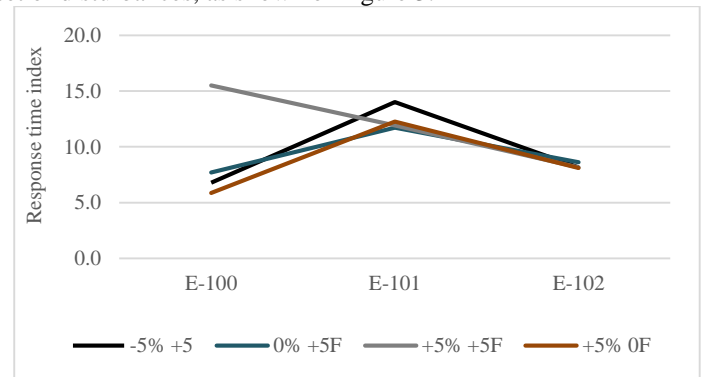


Figure 3 Response time for a set of variations $dist = [\pm 5\% \pm 2.778 \text{ K}]$.

The same procedure is applied is for the HEN with by-pass, initially evaluating the network with a by-pass fraction of 0.10. This modification increases the entropy production from -0.000036 MW/K to 0.000142 MW/ K, leading to a variation in the response time index from 8.15 to 0.82, the figure 4 shows the difference in the response time index of both cases.

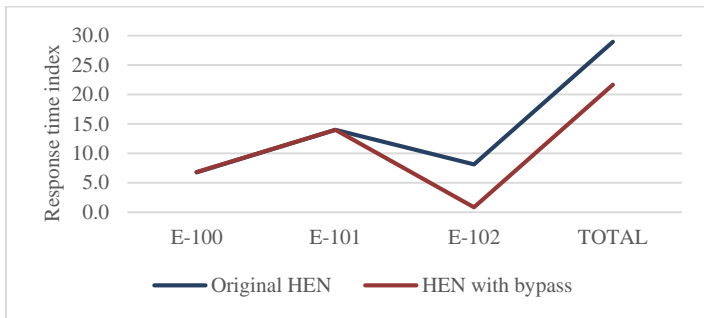


Figure 4 Response time for dist = [-5% 2.78 K] for original HEN and HEN with bypass $\phi = 0.10$

When analyzing the disturbances set, dist = [$\pm 5\%$ ± 2.78 K], it's visualized how the response time index decreases significantly on E-102 for all cases, as can be seen on figure 5.

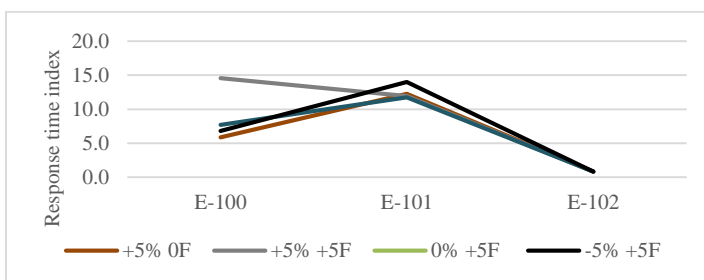


Figure 5 Response time for a set of variations dist = [$\pm 5\%$ ± 2.78 K]. (HEN with bypass)

When evaluating the relation between the response time and the bypass fraction, similarly as done by [15], can be seen how the index value slightly increases for E-100 and E-101 but decreases considerably for E-102, reducing this way the total value as the by-pass fraction increases. This behaviour is seen on figure 6.

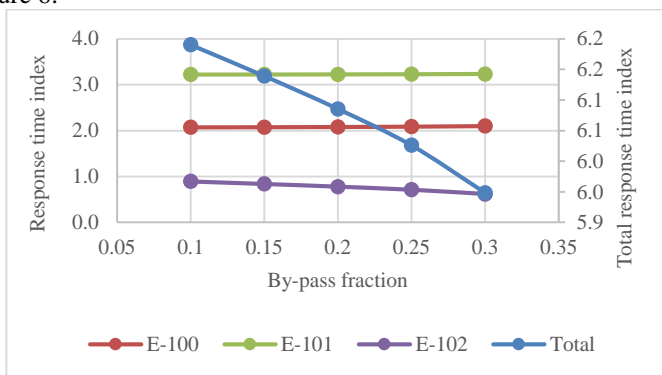


Figure 6 Response time variation with the by-pass fraction.

CONCLUSION

This work developed a thermodynamic approach to measure process controllability on heat exchanger networks. This way, a response time index, based on thermodynamics properties of the system, is obtained and the outcome is compared with RGA and DC results.

The heat exchanger network and an alternative configuration, involving a bypass on the third unit is analyzed, the bypass addition improves entropy production on the final stage, reducing considerably the response time on this stage and overall the HEN.

Stages with smaller entropy production show a higher value for the response time index, which means difficulties to achieve a passive state and resulting on a less controllable system. In this way, the relation between irreversibility and the behavior of the system dynamics was achieved.

Results also shown that a higher bypass fraction results on a smaller response time, the results should be compared with the area increase of the heat exchanger in order to make a good decision on the process design stage.

Combined with the RGA and DC approaches in the process design stage, the method developed in this work can serve as a controllability indicator, making possible the integration process design and control.

REFERENCES

- [1] Tellez R. and Young B. Heat exchanger network optimization and controllability using design reliability theory. *Computers and Chemical Engineering*, Vol. 30 no. 4, 2006, pp. 1-2
- [2] Ydstie B. E., and Alonso A. A. Process systems and passivity via the Clausius-Planck inequality, *Systems & Control Letters* 30, 1997, pp. 253-256.
- [3] Hioe D., Bao J. and Ydstie B. E. Dissipativity analysis for networks of process systems. *Computers and Chemical Engineering*, v. 50, p. 207– 219, 2013.
- [4] Antelo L. T., Otero-Muras I., Banga J. R. and Alonso A. A. A Thermodynamic Based Plant-Wide Control Design Procedure of the Tennessee Eastman Process. *Computer Aided Chemical Engineering*, v. 21, p. 1413–1418, 2006.
- [5] Tippett M. and Bao J. Dissipativity Based Distributed Control Synthesis. *Journal of Process Control*, v. 23, p. 755– 766, 2013.
- [6] Hangos K. M., Alonso A. A., Perkins J. D. and Ydstie B. E. A thermodynamic approach to the structural stability of process plants. *AIChE Journal*, v. 45, p. 802-816, 1999.
- [7] Jillson K. R. and Ydstie B.E. Process Networks with Decentralized Inventory and Flow Control. *Journal of Process Control*, v. 17, p. 399-413, 2007.
- [8] Luyben W. L., and Tyréus B. D., *Plantwide Process Control*. McGraw-Hill. 1st. Edition, 1998, pp. 370-380.
- [9] Farschman C. A., Viswanath K. P., and Ydstie B. E., Process systems and inventory control, *AIChE Journal*, Aug. 1998, pp. 1841-1843, 1855.
- [10] Ydstie B. E., and Alonso A. A., Process systems, passivity and the second law of thermodynamics, *Computers chem. Eng. Vol. 20*, 1996 pp. S1119,S1124.
- [11] de Groot, W. P., and Mazur, P., *Non-equilibrium thermodynamics*. New York: Dover Publishing Company. 1985
- [12] Ydstie B. E., Passivity based control via the second law. *Computers and Chemical Engineering* 26, 2002, pp. 1037–1048.
- [13] Bao J., and Lee P. L., Process control: the passive systems approach, Springer-Verlag, 2007, pp. 5-12.
- [14] Meeuse F. M., and Grievink J., Thermodynamic controllability assessment in process synthesis, Elsevier B.V., 2004, pp. 146-165.
- [15] Seider W. D., Seader J. D., Lewin D. R., and Widagdo S., *Product and process design principles – Synthesis, analysis and evaluation*. 3rd edition. USA: Wiley, 2009, pp.766.