Revista Internacional de Investigación e Innovación Tecnológica
Página principal: www.riiit.com.mx

Simulation of an aeroderivative gas turbine via a chemical reactor Gibbs type

Simulación de una turbina de gas aeroderivada vía un reactor químico de tipo Gibbs

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Technological innovation: Defininition of operating conditions of aeroderivative gas turbines represented by Gibbs reactor.

Industrial application area: Petroleum industry, exploitation and transportation of hydrocarbons.

Recibido: 11 febrero 2016.
Aceptado: 03 de agosto 2016.

Abstract

In recent years the use of software for rigorous process simulation in dynamic and steady state has been taking great importance in the industry because it can represent virtual stages of a process, or the entire process, for analysis and decision in the design, simulation and control of processes. The aim of this work is to study the behavior in open cycle of the combustion chamber of an aeroderivative gas turbine based on Brayton cycle using models of chemical reactors. In this process, to represent the combustion chamber of a gas turbine, a Gibbs type chemical reactor model was used. The model is available in the commercial simulators databases, namely PROII 9.2. In order to find the convergence of the solution of the proposed model, three numerical controllers were included to keep the operation conditions associated with the air excess, thermal yield and expansion efficiency. Numerical results show that not only the values of flue gases leaving the reactor have a good correlation with the chemical energy available in the gas turbine, but also the conversion efficiency to mechanical energy, residual thermal energy and energy loss corresponds to efficiency range reported in the technical and scientific literature.

Key Words: Aeroderivative gas turbine, Chemical reactor Gibbs type, Conversion efficiency, Numerical simulation.

Resumen

En los últimos años, el uso de software para simulación rigurosa de procesos en estado estable y dinámico ha tomado gran relevancia en las industrias, porque estas permiten representar de forma virtual las etapas de un proceso, o el proceso completo, para su análisis y toma de decisiones en el diseño, simulación y control. El objetivo de este trabajo es analizar el comportamiento operativo en ciclo abierto de la cámara de combustión de una turbina de gas aeroderivada que se basa en el ciclo Brayton, utilizando modelos de reactores químicos disponibles en un simulador de procesos. En este proceso, para representar la cámara de combustión de una turbina de gas, se usó un modelo de reactor químico tipo Gibbs disponible en las bases de datos en simuladores comerciales tales como PROII 9.2. Para obtener la convergencia de la solución del modelo propuesto, se incluyeron tres controladores numéricos para mantener las condiciones y principios de operación de la turbina de gas relacionados con el exceso de aire, rendimiento térmico y eficiencia de expansión. Los resultados numéricos muestran que los gases de combustión a la salida del reactor representan la energía química disponible en la turbina de gas, y que la eficiencia de conversión a energía mecánica, energía térmica residual y energía perdida corresponde al intervalo de eficiencia que se reporta en la literatura técnica y científica.

Palabras clave: Turbina de gas aeroderivada; Reactor químico tipo Gibbs; Eficiencia de conversión; Simulación numérica

1. Introduction

Gas turbines are machines that generally work based on an open cycle. A feature of this cycle is that it takes the ambient air (active substance) and reacts with fuel oil, in order to produce energy, then combustion gases produced at high temperature are returned to the environment. In recent years the performance of these turbomachinery has increased, due to advances in materials technology, combined cycle plants, new coatings, etc. This has driven out the use of aeroderivative turbines, which are used in aviation, because they have a compact, lightweight system with a high ratio of potency. On these grounds since several years the gas turbines are used industrially (García et al, 2009; Leza et al, 2006). In the other hand, simulation is a powerful tool that has been used in recent years in several areas of research and application in industry to carry out the rigorous simulation of steady state (Muriel et al, 2008). In this work the processes simulator PRO II 9.2 was used.

The Brayton Cycle.

The first attempt to systematize the study of gas turbines based on the Brayton cycle was given by Hougen *et al* in 1959. Recently Razak (2007) and Boyce (2012) studied the cycle gas turbine behavior by means of temperature-entropy change diagrams. The Brayton cycle is an ideal thermodynamic cycle that consists of two isobaric processes and two isentropic processes (Boyce, 2012), as follows, Figures 1 and 2:

1. Air passes through an axial compressor where the pressure and temperature change (isentropic process).
2. The flow reaches the combustion chamber where the reaction takes place at constant pressure (isobaric process).
3. The flue gas flow undergoes an expansion process where the temperature and pressure change (isentropic process).
4. The combustion gases are sent into the atmosphere and cooled (isobaric process).

The Brayton cycle is performed in a gas turbine of open cycle. In some applications, to harness the energy carried by the flue gas a regenerator is placed, then the Brayton cycle changes its name to regenerative cycle. In this way combined cycle Gibbs reactor may be built (Garcia, 2012).

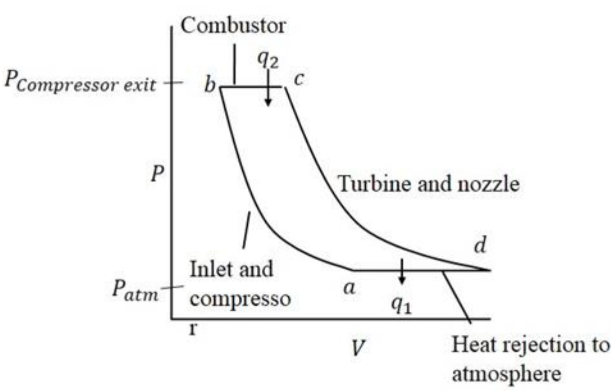

Figure 1. Brayton cycle, *P-V*.

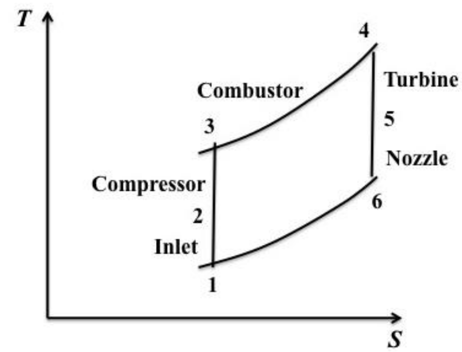

Figure 2. Brayton cycle, T-S.

Gibbs reactor.

To represent the combustion chamber, a Gibbs reactor model was used. This system is based on the reaction coordinate, which in turn is related to the equilibrium constant, K, which depends on reaction stoichiometry. To define whether it has reached equilibrium in the reaction, the criterion of minimization of the Gibbs free energy is used, as shown in the following equation:

$$\boldsymbol{(dG^t)_{T,P} = 0} \qquad \textbf{(1)}$$

where the temperature (*T*) and pressure (*P*) are constant and epsilon (ε) represents the reaction coordinate as shown in the graph of Figure 3 (Smith *et al.*, 2007).

In this paper the simulation of a chemical reactor type Gibbs is performed. Thermodynamic analysis and balances of matter and energy are developed to represent the combustion chamber of a gas turbine. Likewise the complete model of the gas turbine is constructed.

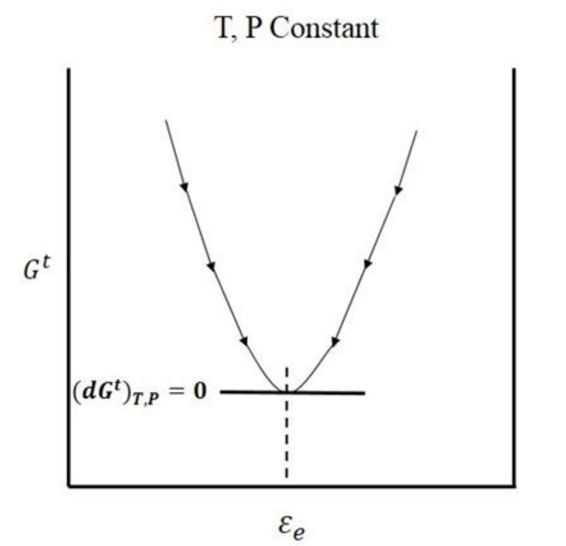

Figure 3. Criterion Gibbs free energy minimization.

2. Methodology

A. Process flow diagram of a gas turbine

To construct the model of a gas turbine the overall taxonomy presented in ISO 14224 (2006) was analyzed (Seider et al 2009). This standard includes accessories of industrial gas turbines and aeroderivative type. The features included in NRF-100-PEMEX (2009) were also considered.

A flow diagram with the main components of an aeroderivative gas turbine, shown in Figure 4, is constructed.

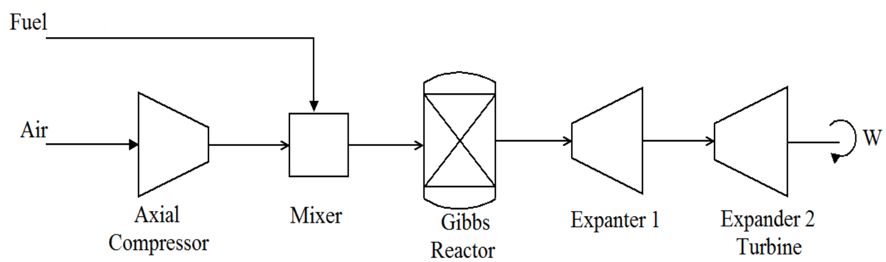

Figure 4. Flow diagram of a gas turbine.

Based on the diagram of Figure 4, the model of the gas turbine is built in the PRO II simulator.

Table 1. Items selected for the construction of model gas turbine.

Units	***Name***
C-101	Axial Compressor
M-101	Mixer
R.101	Gibbs Reactor
EX-101	Expander 1
EX-102	Expander 2 (Turbine)
CN1	Controller 1
CN2	Controller 2
CN3	Controller 3

It was necessary to use numerical controllers that are available in the PRO II process simulator to maintain the values of the mass and energy balances in the steady state, and the conditions and principles of operation of the turbine.

Table 1 shows each item of the PFD (Process Flow Diagram) and their nomenclature for identification in the flowchart. Also, the controllers for process variables are included.

Figure 5 shows the model of the gas turbine via the Gibbs reactor, which was built in the environment of the process simulator PRO II 9.2.

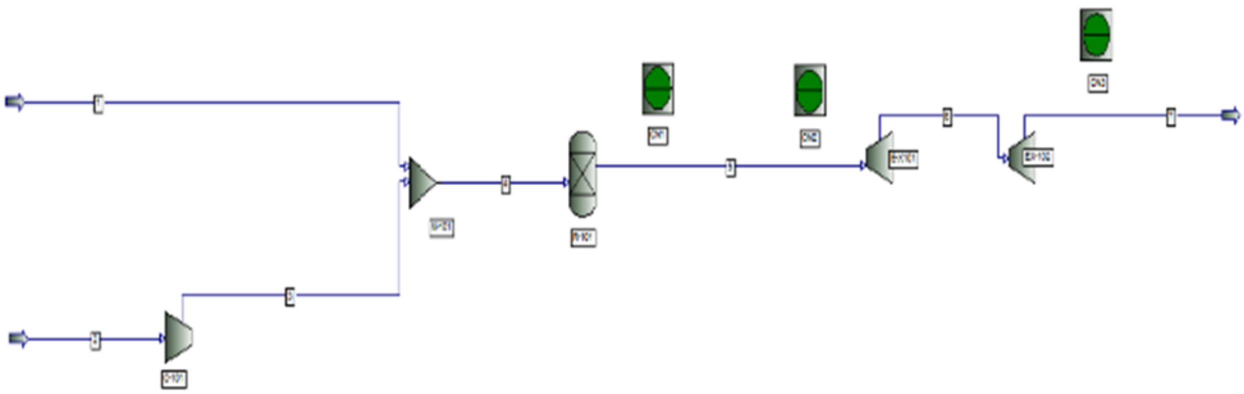

Figure 5. Gas turbine model in PRO II.

B. Simulation model of a gas turbine: Base Case

To carry out the rigorous simulation, Soave-Redlich-Kwong's (SRK) state equation was selected as the thermodynamic method, which was used by default for all input items in the PFD of Figure 5. Afterwards, the input streams were defined for numerical simulation. These streams are fuel gas (CH_4) and air. The input values of the air and flue gas flowrates are shown in Table 2. To define the parameters used in each item of the flow diagram, the heuristic rule of compressors was considered (Walas, 1990), Table 3. The inlet temperature was 922.04 K, according to the operating conditions reported in literature (Sierra *et al*., 2005).

Table 2. Values of the inlet streams.

Values considered for the base case simulation			
Streams	***Input Flows*** (Kg/sec)	***Temperature*** (K)	***Pressure*** (atm)
1 (CH4)	0.116	288.710	13.609
2 (Air)	13.864	288.710	1.000

C. Numerical controllers

To adjust and maintain constant values of the properties and flows in the steady state simulation, numerical controllers were used. These are found in the tool palette process simulator PRO II 9.2. In these numerical controllers, restrictions as the upper and lower limits are specified taking into account the stream that is adjusted.

Controller 1. The function is to adjust the required ratio of airflow to the reaction temperature: This controller adjusts the airflow to the defined value (or default) of the stream 5 (flue gas leaving the reactor Gibbs), and keeps the value of the reaction temperature. Controller 2. This sets the ratio between the pressure of the compressor and expander power 1. The compressor pressure ratio is adjusted so that the set value is the potency of expander 1, in order to maintain the required power. Here the potency in the base case is 4,989.4 hp.

Table 3. Rules of thumbs

Rules of thumbs (Walas, 1990)
To compress air from 310.960K, k = 1.4, compression ratio = 3,
Exit temperature should not exceed 449.850-477.624K; for diatomic gases (Cp/Cv = 1.4) this

Rules of thumbs (Walas, 1990)
corresponds to a compression ratio of about 4.
Compression ratio should be about the same in each stage of a multistage unit, ratio = $(P_n/P_1)^{1/n}$, with n stages
Efficiencies of reciprocating compressors: 65% at compression ratio of 1.5, 75% at 2.0, and 80-85% at 3-6.
Efficiencies of large centrifugal compressors, 6000-100,000 ACFM at suction, are 76-78%.
Rotary compressors have efficiencies of 70%, except liquid liner type which have 50%.

Controller 3 adjusts the fuel flow required to maintain the power of the gas turbine: Since the turbine power is concerned with the amount of incoming fuel, methane gas flowrate is adjusted to maintain the power of the gas turbine in order to keep the turbomachine efficiency.

D. **Setting values for Case 1 and Case 2**
Two additional simulations were performed, by changing the fuel and air input flowrates, as well as the temperature of the air stream, Table 4. These data are based on the behavior of a gas turbine at almost ideal conditions considering different location areas in the operation, such as Marine Region (Hernández, 2015) and the Southern Region (Teopa, 2015), both in Mexico.

Table 4. Specifications for case 1 and case 2.

Case	***Fuel Flow*** (Kg/sec)	***Air Flow*** (Kg/sec)	***Temperature*** (K)
1	0.0886	11.675	303.150
2	0.0886	11.675	288.710

3. Results and discussion

It was performed the steady-state simulation, according to PFD of the figure 4. When the convergence is reached the color of items turns to blue (figure 4 (b)), indicating there was no problem and that is managed to solve the mass and energy balances of process flow diagram. Numerical results shown in this section correspond to three cases considered in this work: i) base case, ii) case 1, and iii) case 2.

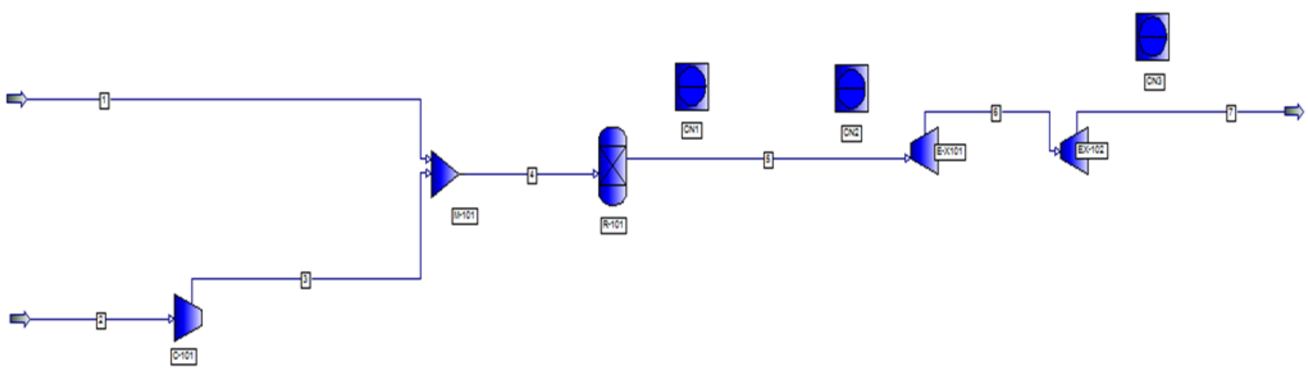

Figure 4 (b). Resolved model of the gas turbine (Convergence).

A. **Checking the Brayton cycle**

The changes that occur in a gas turbine are those of the Brayton cycle. The verification of this cycle was performed, according to the changes that were obtained in each item of the simulated PFD.

C-101: Axial compressor (isentropic). The first stage of the Brayton cycle is performed at the compressor, when the air is compressed so that its temperature rises to 551.070 K and reaches a pressure of 6.699 atm.

M-101: Mixer. This equipment was placed with the goal of making the air-fuel mixture in predefined proportions. Since air leaves the compressor with a temperature of 551.260 K and the fuel has a temperature of 288.710 K in the mixer it has a heat exchange and the resulting mixture is 545.570 K while the pressure was maintained at 6.699 atm.

R-101: Gibbs reactor (isobaric). Under isobaric conditions carried out the second stage of Brayton cycle, the pressure is 6.699 atm and the temperature of the reaction is conducted at about 922.040 K. The results obtained in the balance of the reaction show that the conversion fraction of methane is 1, indicating that all reactants are consumed in the reaction and therefore the Gibbs reactor can properly represent the combustion chamber of the gas turbine.

EX-101: Expander 1 and EX-102: Expander 2 (isentropic). In the EX-101 unit the flue gases leaving the reactor are expanded, which represents the chemical energy released in the reaction. By expanding the gases, the temperature decreases and thus the pressure (685.060 K and 1.656 atm).

The EX-102 unit is the expander of discharge; here occurs the last expansion of gases and conversion to mechanical energy seen as shaft work. The mass and energy balances show a shift to 618.900 K in the temperature of the combustion gases and a pressure of 1.054 atm.

The last change of the Brayton cycle is isobaric, this occurs in the output of combustion gases to the atmosphere, being an open cycle.

B. **Numerical Results of Controllers**

Controller 1. The values of parameters included in the controller, CN1, allow regulating the inlet airflow to maintain the required temperature in the reactor, and also comply with the mass and energy balances, Table 5.

Where the first value is the reaction temperature in K, and the second is the amount of air to the compressor inlet in Kgmol/sec. These values remain fixed at each cycle, which shows that there were not mismatches in the convergence and in the mass and energy balances.

Table 5. Numerical results of CN1 controller.

Controller CN1	
Cycles	Variables set by CN1
Vary value	
CYCLE 1	922.040 K
CYCLE 2	922.040 K
CYCLE 3	922.040 K
Vary value	
CYCLE 1	0.478 Kmol/sec
CYCLE 2	0.478 Kmol/sec
CYCLE 3	0.478 Kmol/sec

Controller 2. The results obtained by this numerical controller, CN2, are shown in Table 6. The power obtained in the expander is about 4,989.300 hp, whereas a pressure ratio of 6.7 in the compressor is reached. This unit allows keeping the thermal efficiency, because if the pressure ratio in the compressor decreases, then the temperature of the airflow also decreases, therefore it could enter to the reactor with a lower

temperature reducing the reaction temperature in the combustion chamber.

Table 6. Numerical results of CN2 controller.

Controller CN2	
Cycles	Variables set by CN2
Vary value	
CYCLE 1	4,989.370 hp
CYCLE 2	4,989.360 hp
CYCLE 3	4,989.350 hp
Vary value	
CYCLE 1	6.700 adim
CYCLE 2	6.700 adim
CYCLE 3	6.700 adim

Controller 3. With this controller it is possible to keep the mass balance and to obtain the necessary power in the last expansion, because the power is related to the amount of fuel entering the reaction. Furthermore this power must be maintained for turbine efficiency.

Controller CN3 not only adjusts the fuel and power, but also determines the amount of methane gas to be used for a specific power, i.e., it is only necessary to define the power and the controller will perform the calculations to estimate the amount of fuel that should be fed into the reaction.

The power of the turbine (expander 2) in base case is 1345.264 hp, and fuel flow is 0.007 Kgmol/sec, that is equivalent to 0.116 Kg/sec (Table 7).

Table 7. Numerical results of CN3 controller.

Controller CN3	
Cycle	Variables set by CN3
Vary value	
CYCLE 1	1,345.264 hp
CYCLE 2	1,345.264 hp
CYCLE 3	1,345.264 hp
Vary value	
CYCLE 1	0.007 Kgmol/sec
CYCLE 2	0.007 Kgmol/sec
CYCLE 3	0.007 Kgmol/sec

C. **Data comparison in base case, case 1 and case 2.**

Data from a company maker of gas turbines were taken to perform a comparative study. A gas turbine was picked based on the design values that were used in numerical simulation. Likewise, the comparative study was carried out using real data of this turbine in operation of an oil company and its installed offshore.

Table 8 shows data of air temperature, amount of methane gas, turbine output power, exhaust temperature and efficiency for each study case; and the reaction temperature is showed in Table 8.

Tables 8 and 9 also show that the values of case 2 are closed to the operation data and reaction temperature followed by the case 1 and to the base case.

Table 8. Manufacturer, operation and numerical simulation data.

	Manufacturer data of gas turbines for the model analyzed	**Operation data of a gas turbine for the model discussed in offshore facilities Hernández**	**Data obtained by the process simulator PRO II Base Case**	**Data obtained by the process simulator PRO II Case I**	**Data obtained by the process simulator PRO II Case 2**

			Arroyo, A. (2015)			
Airflow temperature	K	-233.150--- 323.150	303.150	288.710	303.150	288.710
Quantity of fuel (CH_4)	K/hr	Maximum: 399.520 Standard: 319.162	319.280	418.665	323.248	320.978
Output power W	Hp	400 ---1,590	1150	1345	1189	1156
Exhaust temperature	K	573.15 --- 794.26	ND	618.98	610.37	593.71
LHV (Lower Heating Value)	KJ/hr	844.045 --- 1,160.561	963.266	ND	ND	ND
Efficiency	%	24.5	ND	18	20	20

Table 9. Temperature data by numerical simulation and literature.

	Reaction temperature			
	Registered data Sierra *et al.* (2005)	**Data set to perform the simulation using the process simulator PRO II.- case base**	**Data set to perform the simulation using the process simulator PRO II.- case 1**	**Data set to perform the simulation using the process simulator PRO II.- case 2**
Temperature, K	873.150	922.040	910.090	885.930

4. Conclusions

The modeling and simulation of an aeroderivative gas turbine in steady state, via a chemical reactor type Gibbs showed effective results that are very close to the changes that occur theoretically in a turbine of open cycle known as Brayton cycle.

The use of numerical controllers in steady state simulation helps to keep the balance of matter and energy in each stream on gas turbine, i.e., to adjust the streams flow for work and efficiency to be satisfied according to the values reported in the literature, and also with data of turbomachinery manufacturers and with real data from offshore operations.

Also, we conclude that the results from numerical simulation in steady state compared with information from manufacturers and operating data of offshore.

Installations (Towler et al 2012) allowed the evaluation of the combustion chamber behavior of an aeroderivative gas turbine, by using a chemical reactor simulation of PRO II 9.2 process package, which fulfills the efficiency of reported parameters.

As perspectives of this work, it is to carry out the steady state simulation for energy integration of the flue gases through of a heat recovery system, with the gases that are sent into the atmosphere, placing a thermal oil closed circuit to transfer heat to a heat exchanger network (Puigjianer et al., 2006); using a dynamic process simulator to evaluate the gas turbine, (Serth et al 2014) with process controllers to regulate the temperature of the combustion gases (Capella et al 2000) (Turton el at 2012) and; performing the analysis of combined cycles in industrial plants (Kemp, 2007), (Picon M. *et al* 2005).

5. Acknowled gements

We appreciate the support of M.Sc. Alfonso Hernández-Arroyo for the information provided of the operation data of the process. H. Pérez-Pastenes gratefully acknowledges CONACYT the grant of his sabbatical stay at UAM-I.

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