MULTI-OBJECTIVE OPTIMIZATION ANALYSIS OF THE IGCC SYSTEM WITH CHEMICAL LOOPING COMBUSTION

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Abstract

Integrated Gasification Combined Cycle (IGCC) system using coal gasification is an important approach for future energy options. This work focuses on understading the system operation and optimizing it in the presence of uncertain operating conditions using ASPEN Plus and CAPE-OPEN compliant stochastic simulation and multiobjective optimization capabilities developed by Vishwamitra Research Institute. The feasible operating surface for the IGCC system is generated and deterministic multiobjective optimization is performed. Since the feasible operating space is highly non-convex, heuristics based techniques that do not require gradient information are used to generate the Pareto surface. Accurate CFD models are simultaneously developed for the gasifier and chemical looping combustion system to characterize and quantify the process uncertainty in the ASPEN model.

Keywords

IGCC, gasifier, chemical looping combustion, uncertainty, multi-objective optimization.

Introduction

The U.S. Department of Energy (DOE) is investing heavily in Fossil Energy R&D programs to promote the development of advanced power generation systems that meet the Nation's energy needs while achieving a sustainable balance between economic, environmental, and social performance. Integrated Gasification Combined Cycle (IGCC) technology is becoming increasingly important in this effort, where low-cost opportunity feedstock such as coal, heavy oils and pet coke are the fuels of choice. IGCC technology produces low-cost electricity while meeting strict environmental regulations. Efficient gasification process and combined with excellent post-gasification processing such as chemical looping combustion makes this an exciting option.

To achieve performance targets and at the same time reduce the number of costly pilot-scale and demonstration facilities, the designers of these systems increasingly rely on high-fidelity process simulations to design and evaluate virtual plants. Developed by the DOE's National Energy Technology Laboratory (NETL), the Advanced Process Engineering Co-Simulator (APECS) is a virtual plant simulator that combines process simulation, equipment simulations, immersive and interactive plant walk-through virtual engineering, and advanced analysis capabilities (Zitney et al. 2006, Zintey 2006a). The APECS system uses commercial process simulation software (e.g., Aspen Plus®) and equipment modeling software (e.g., FLUENT® computational fluid dynamics) integrated with the process-industry CAPE-OPEN (CO) software standard (Braunschweig 2002, Zitney 2006b). Plug-and-play interoperability of analysis tools in APECS is also facilitated by the use of the CO standard.

This work presents the application of the CO-compliant stochastic modeling and multi-objective optimization framework for APECS for the analysis of an IGCC system with single-stage gasification and chemical looping combustion. This framework enables optimizing

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model complexities in the face of uncertainty and multiple and sometimes conflicting objectives of design. It also provides a decision support tool to address some of the key questions facing designers and planners of advanced process engineering systems

The paper is arranged as follows. The next section gives a brief review of the IGCC system analyzed in this work. The theory behind the multi-objective analysis and the analysis results are presented in the subsequent sections. The last section draws the important conclusions.

IGCC System

The system is based on the General Electric (GE) Energy gasifier (single stage entrained-flow), two Advanced F-Class gas turbines partially integrated with an elevated pressure Air Separation Unit (ASU). Syngas desulfurization is provided by a Selexol Acid Gas Removal (AGR) system and a two-bed Claus Unit with Tail Gas Recycle to Selexol, and a chemical looping combustion system. In chemical looping combustion, metal oxide particles (oxygen carrier) are used for the transfer of oxygen from the combustion air to the fuel, thus the combustion products CO_2 and H_2O (or pure H_2) are obtained in a separate stream (Lyngfelt et al. 2001). The flowsheet for chemical looping combustion combined cycle system is separated into sections like coal gasification, water gas shift reaction, sorbent energy transfer system and power generation. The coal gasification the process is modeled with two reactors, the first reactor decomposes the stream of coal into its elemental constituents (C, H_2, N_2, O_2, S, H_2O and Ash as a yield reactor) and the second reactor generates the fuel comprising CH_4, H_2, CO, NH_4, H_2S and CO_2 (plus unreacted N_2, O_2, H_2 and H_2O) by minimizing the total Gibbs free energy of the system (Gibbs reactor). The products of the gasification process are fed to the water gas shift (WGS) reactor section to complete the oxidation of CO with the simultaneous production of hydrogen. The reaction takes place in two adiabatic reactors in series simulated as Gibbs reactors with intermediate heat exchangers. Sulfur and Ammonia removal unit is located downstream the WGS section. H_2S is removed by an absorber using methanol or glycol. The removal of Ammonia is carried out with a reactive absorption process on sulfuric acid. Both separations are modeled in one single unit as a simple component separator. This section of the process is finished with a pressure swing adsorption (PSA) unit to purify the hydrogen that is fed to the gas turbine. The pure hydrogen stream and the fuel gas stream from the PSA are fed to the sorbent energy transfer system (SETS) which uses a chemical looping principle to purify CO2 and to recover the energy from the oxidation processes. The reduction reactor, the oxidation reactor and the combustion chamber are modeled as adiabatic Gibbs reactors. The metal carrier used in this case is 25% NiO in Al_2O_3. Please refer to DOE/NETL (2006) and Maurstad (2005) for further details related to the process. Aspen Plus model for the IGCC system has been developed by the Department of Energy in order to conduct system level analysis of the process. The Aspen Plus modeling details (including the modeling approximations and configuration) is explained in DOE/NETL (2006) and not discussed here for the sake of brevity.

Multi-objective Analysis: Theory

Multiobjective problems appear in virtually every field and in a wide variety of contexts (Diwekar 2003). Conventional process models (such as the IGCC Aspen Plus model) now in use are largely based on a deterministic computational framework used for simulation of a specified flowsheet. An important shortcoming of these models is their inability to analyze uncertainties rigorously. Uncertainty analysis is especially important in the context of advanced energy systems, since available performance data typically are scant, accurate predictive models do not exist, and many technical as well as economic parameters are not well established. The work, therefore, goes beyond a deterministic analysis and studies multi-objective optimization in the presence of uncertainty. A generalized multi-objective optimization problem is of the form:

Minimize:

$$f_i(\vec{x}), i = 1, \ldots, k, k \geq 2$$

Subject to:

$$\begin{aligned} & h_l(\vec{x}) = 0, I \geq 0 \\ & g_J(\vec{x}) \leq 0, J \geq 0 \\ & l_j \leq x_j \leq u_j, \quad j = 1, \ldots, n, \\ & \vec{x} = (x_1, \ldots, x_n) \end{aligned} \tag{1}$$

The problem under consideration involves a set of n decision variables represented by the vector $\vec{x} = (x_1, x_2, \ldots, x_n)$. The equality constraints $h_I(\vec{x}), I \geq 0$: $\mathbf{R^n} \rightarrow \mathbf{R}$, and inequality constraints $g_J(\vec{x}) \leq 0, J \geq 0$: $\mathbf{R^n} \rightarrow \mathbf{R}$ are real-valued (possibly nonlinear) constraint functions, and l_j and u_j are given lower and upper bounds of decision variable x_j (allowed to be - ∞ and/or + ∞). If $I = 0$ and $J = 0$, the problem becomes unconstrained. The problem involves k (≥ 2) continuously differentiable nonlinear objective functions f_k : $\mathbf{R}^n \rightarrow \mathbf{R}$. Without loss of generality, we assume that all the objective functions are to be minimized simultaneously.

The solution of a multi-objective optimization problem is a set of solution alternatives called the Pareto set. For each of these solution alternatives, it is impossible to improve one objective without sacrificing the value of another relative to some other solution alternatives in the set. There are usually many (infinite in number) Pareto optimal solutions. The collection of these is called the Pareto set. The result of the application of a nonlinear multi-objective technique to a decision problem is the Pareto set for the problem, and it is from this subset of potential solutions that the final, preferred decision is chosen by the decision-makers.

The most commonly used analytical techniques for multi-objective optimization problems (and to generate the Pareto surface) are: preference-based methods and generating methods (Diwekar 2003). Preference based methods require a-priori knowledge of the weights on different objectives and solves a single objective problem. Generating methods provide a great deal of information, emphasizing the Pareto optimal set or the range of choice available to decision-makers, and providing the trade-off information of one objective versus another. Generating techniques can be further divided into two sub-classes: no-preference methods and a posteriori methods. The selection of the appropriate method often depends on the optimization problem formulation.

It has been mentioned that this work performs multi-objective optimization in the presence of uncertainty. Uncertainty analysis consists of four main steps: (1) characterization and quantification of uncertainty in terms of probability distributions, (2) sampling from these distributions, (3) propagation through the modeling framework, (4) analysis of results (Diwekar et al. 1997). Once the uncertain parameters of a given model are identified in terms of their probability distributions, an efficient sampling techniques, such as the Hammersley Sequence Sampling (Kalagnanam and Diwekar 1997), is used to sample the uncertain space. The next important step is the propogation of uncertainty through the model. This work uses the Cape-Open compliance stochastic simulation capability to perform uncertainty analysis of the IGCC system and compute the feasible solution space.

IGCC System: Multi-objective Optimization Results

In this work, the non-dominated (Pareto) surface for the IGCC system is computed for following three important performance measures of the system, constituting the objectives for the system: Total plant efficiency (based on HHV of coal); Total CO_2 emissions measures in lb/hr; and Total SOx emission measured as volumetric fraction of the total flue gas volumetric flow rate. For multi-objective optimization, model parameters that have a significant impact on the system performance are first identified using the stochastic modeling PRCC (Partial Rank Correlation Coefficient) analysis for 11 different model parameters (Diwekar and Rubin, 1991). PRCC provides a major or unique or unshared contribution of each variable, and explains the unique relationship between two variables that cannot be explained in terms of the relations of these variables with any other variable. PRCC analysis identifies following critical parameters for the IGCC system: Gasifier operating temperature; Gasifier operating pressure; and Claus burner temperature. These parameters are used to analyze results of multi-objective optimization (used as decision variables).

The first step in the multi-objective analysis is to identify the feasible solution surface for the IGCC system for variations of the given decision variables. The feasible surface is generated through stochastic simulation by using 1000 samples of eleven different model parameters and propagating the uncertainty through the Cape-Open compliance stochastic simulation capability. The feasible surface is plotted as the values of the three objectives identified before and is shown in Figure 1. Here, the contours of one of the objectives (SOx) are plotted with respect to the values of the other two objectives for the 1000 samples. Please note that CO_2 emissions are measures in lb/hr while the SOx emissions are measures in volumetric fraction of the total exit gas volume as mentioned before. From the figure it is clearly evident that the trade-off surface is highly non-convex. One can observe multiple peaks and valleys in terms of one of the objectives when the other two objectives are varied.

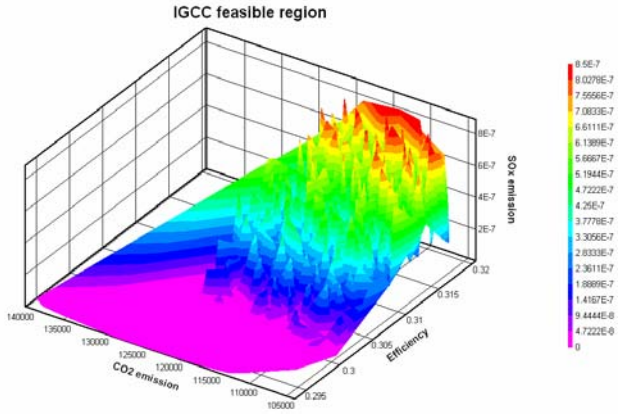

Figure 1. Feasible surface for IGCC system

Although constraint based methods or preference based methods give a good estimate of the Pareto surface, they require the use of gradient based techniques to determine the surface. However, since the feasible surface for the IGCC system is non-convex, it makes the use of the previous mentioned techniques very difficult. The 'No preference based methods' can successfully tackle such problems and hence are used in this case. The 'No preference based methods' include compromise programming (Yu 1985), Multi-objective Proximal Bundle (MPB) (Miettinen 1999), and feasibility-based methods, such as the parameter space investigation (PSI) methods (Osyczka 1984). They focus on generating a feasible solution or all the feasible solutions instead of the Pareto set (the best feasible solutions). In PSI methods the continuous decision space is first uniformly discretized using the Monte Carlo sampling technique; next a solution is checked with the constraints. If one of the constraints is not satisfied, the solution is eliminated and the objective values are finally calculated, but only for those feasible solutions. Therefore, a *discretized approximation* of the feasible objective region, instead of the Pareto set, is retained by the PSI method. The solutions of this feasibility-based method cover the whole feasible objective region rather than covering only the optimal solutions in the Pareto set. Because most of the feasible solutions are not Pareto optimal, a relatively small

number of the non-dominated (relatively better, but not necessarily Pareto optimal) solutions must be extracted from the whole feasible solution set to formulate an approximate representation of the Pareto set for feasibility-based methods. This justifies the use of PSI method to generate the approximate Pareto surface for the IGCC system. The feasible space shown in Figure 1 constitutes the output of the stochastic simulation which must be used for approximate identification of the Pareto surface.

Figure 2 shows the approximate Pareto surface in a 2-dimensional space where the Pareto surface is constituted by points A-B-C-D-E. The values of different objectives for the Pareto surface are reported in Table 1. The values of decision variables corresponding to this Pareto surface are shown in Table 2. The results illustrate that the optimal operating point changes based on the particular realizations of the uncertain parameters, and the decision variables can vary significantly for the optimal operating point.

Table 1. Approximate Pareto surface for IGCC System

Point	Efficiency	CO_2 emission (lb/hr)	SOx emission (volume fraction)
1.	0.30111	105430	0
2.	0.30578	117000	0
3.	0.31533	103950	0.00000031028
4.	0.32057	119110	0.00000076794
5.	0.31757	105580	0.00000073921
6.	0.31641	103960	0.00000024813

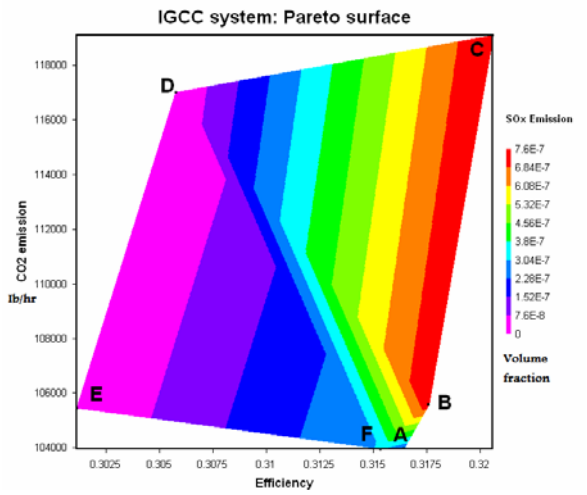

Figure 2. IGCC Pareto surface

Table 2. Decision variable values for the Pareto surface

Point	Gasifier operating temperature (F)	Gasifier operating pressure (psia)	Claus burner temperature (F)
1.	2295.7043	741.1281	2245.6123
2.	2376.7432	832.2906	2166.2783
3.	2589.1709	759.775	2307.2532
4.	2639.041	773.8	2590.3447
5.	2636.6433	886	2507.5862
6.	2615.0649	786.55	2242.1877

Conclusions

This work focused on the multi-objective optimization analysis of the IGCC system with a single stage coal gasifier. Initially, the important uncertain model parameters and the critical system objectives (performance indicators) are identified. The stochastic simulation of this system shows that the feasible solution is highly non-convex. Therefore, the PSI method is used to determine the approximate Pareto surface. The analysis of the results shows that uncertainty has a significant effect on the Pareto surface. It is also observed that there is a trade-off between the different objective functions of the system. Thus, Low SOx and CO2 emission often lead to low efficiency of the IGCC system.

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