

# Improvement of Central Composite Design in Modeling and Optimization of Simulation Experiments

A. Nuchitprasittichai, N. Lerdritsirikoon, T. Khamsing

**Abstract**—Simulation modeling can be used to solve real world problems. It provides an understanding of a complex system. To develop a simplified model of process simulation, a suitable experimental design is required to be able to capture surface characteristics. This paper presents the experimental design and algorithm used to model the process simulation for optimization problem. The CO<sub>2</sub> liquefaction based on external refrigeration with two refrigeration circuits was used as a simulation case study. Latin Hypercube Sampling (LHS) was purposed to combine with existing Central Composite Design (CCD) samples to improve the performance of CCD in generating the second order model of the system. The second order model was then used as the objective function of the optimization problem. The results showed that adding LHS samples to CCD samples can help capture surface curvature characteristics. Suitable number of LHS sample points should be considered in order to get an accurate nonlinear model with minimum number of simulation experiments.

**Keywords**—Central composite design, CO<sub>2</sub> liquefaction, Latin Hypercube Sampling, simulation – based optimization.

## I. INTRODUCTION

PROCESS simulation is usually conducted when a real system is impractical or impossible due to high cost and time consume. Process simulation is important in process engineering. It can be applied in conceptual design and plant operation. The simulation involves the material and energy balance of the system, unit operations, thermodynamic libraries, and property databases that make the simulation a complex process [1]. Process simulation and optimization can help improve the productivity, energy consumption and product quality of industry – all the corresponding process variables are solved for the minimum or maximum target [2]. In the process optimization, the second order model (nonlinear model) represented the relationship between process parameters and a response is required for the optimization problem. Experimental design is applied to simulation experiments in screening design to determine the significant parameters which have high impacts on a response, and finding the combinations between parameter levels which show impacts on a response. A metamodel (simple model of the simulation model) is then developed based on the significant parameters and a response [3].

Several experimental designs such as full factorial,

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fractional factorial, CCD, Box – Behnken Design (BBD), and LHS have been used for modelling of simulation [3], [4]. Factorial design is usually used in screening design. CCD is the most common design used in modeling. It consists of a factorial design with an addition of a center point and axial points. Axial points are outside the cube in which they are sometimes beyond safe operating limits. In case of a simulation model with complex response surface, CCD may provide the metamodel with poor predictions [3]. BBD consists of sample points at the edges of experimental spaces and a midpoint. The design does not have any axial points so it is useful if the experiments cannot be performed out of the region of interest. LHS is widely used in the area of computer simulation [4]. The technique is a space – filling design, which attempts to distribute samples evenly over the experimental spaces. This technique is widely used in the area of computer simulation.

This paper studied an improvement of CCD in constructing the second order model for optimization with response surface methodology (RSM) application. The CO<sub>2</sub> liquefaction based on external refrigeration with two refrigeration circuits simulated with Aspen HYSYS version 10 was used as a case study. The algorithm of process modeling and optimization was developed. The steepest descent was performed to find the local optimal region of interest. Due to the complex response, additional LHS samples were included in the CCD samples to represent information over the entire interest area. The second order model was then constructed for using in process optimization. Two different parameter ranges (10 and 20 kPa) with three different number of additional LHS samples (10, 15, 21 samples) were studied. The difference in parameter ranges was studied to represent different studied region sizes, and the difference in number of LHS was studied to determine the suitable number of additional sample points.

The second order model represents the relationship between operating conditions and CO<sub>2</sub> liquefaction cost (\$ per ton CO<sub>2</sub>). The objective of the optimization problem is to minimize the CO<sub>2</sub> liquefaction cost.

## II. PROCESS SIMULATION AND ECONOMIC EVALUATION

### A. Process Simulation

The CO<sub>2</sub> liquefaction process was simulated using Aspen HYSYS Version 10. Fig. 1 shows the process flow diagram of CO<sub>2</sub> liquefaction based on external refrigeration with two refrigeration circuits [5]. In this process, 12.5 tons per hour of CO<sub>2</sub> feed gas at 200 kPa and 20°C is sent to the first separator for separation of water from feed gas. Table I shows the specifications of CO<sub>2</sub> feed gas. After compression at the first

compressor, the CO<sub>2</sub> stream is cooled down by cooling water and sent to the second separator to separate water. Then, the CO<sub>2</sub> stream is refrigerated by ammonia in the refrigeration system. After the first refrigeration circuit, the CO<sub>2</sub> stream is then passed through the second refrigeration circuit. The CO<sub>2</sub> stream is finally condensed into liquid phase as a CO<sub>2</sub> product (with the specifications of -50°C and 700 kPa).

In the refrigeration system, the liquid ammonia is vaporized due to heat transfer from CO<sub>2</sub> stream. The vapor ammonia is

then compressed to 771 kPa, cooled and expanded to release the heat. The vapor ammonia becomes a liquid phase and is reused in the system. The pressure drop for all heat exchangers is assumed to be 50 kPa.

There are two studied operating parameters (decision variables) for the optimization problem, which are the pressure of CO<sub>2</sub> after the first compressor ( $x_1$ ), and the pressure of ammonia after expansion of the first refrigeration circuit ( $x_2$ ).

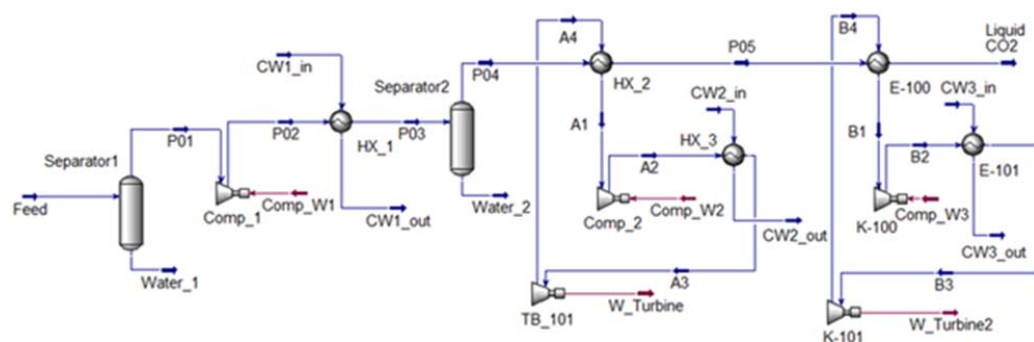


Fig. 1 Process flow diagram of CO<sub>2</sub> liquefaction based on external refrigeration with two refrigeration circuits

TABLE I  
SPECIFICATIONS OF CO<sub>2</sub> FEED STREAM

Parameters	Values
Temperature (°C)	20
Pressure (kPa)	200
Mass flow rate (ton per hour)	12.50
CO <sub>2</sub> content (percent by mass)	97.62
H <sub>2</sub> O content (percent by mass)	2.38

### B. Economic Evaluation

The economic analysis of the studied CO<sub>2</sub> liquefaction process includes both capital and operating costs. The analysis involves all major equipment (excluding piping) costs, utilities cost, and cash flow analysis. The capital cost was estimated based on equations and data from the capital equipment-costing program (CAPCOST) [6]. The capital cost was adjusted to the value in 2016 by using the Chemical Engineering Plant Cost Index (CEPCI) value of 541.7. All assumptions used in the economic analysis are the same as the work of [7], except the plant is expected to have a 10-year plant life.

### III. PROCESS MODELING AND OPTIMIZATION ALGORITHM

This section studied process modeling and optimization of CO<sub>2</sub> liquefaction based on external refrigeration with two refrigeration circuits. The objective is to minimize the CO<sub>2</sub> liquefaction cost. The algorithm was developed to incorporate the LHS samples to a data set to help represent more information in the studied region.

Fig. 2 represents the process modeling and optimization algorithm developed in this work. The algorithm starts with specifying range of each decision variable. Then, the two levels factorial design was used to construct the test matrix of

operating conditions. The data of CO<sub>2</sub> liquefaction cost were then collected from the process simulation coupled with the economic analysis. Data regression of the first order model (linear model) was performed. If the data fit the first order model (R-squared value is greater than 0.5), the steepest descent is performed to move the operating conditions to the region of lower CO<sub>2</sub> liquefaction cost. The steps keep repeating until there is no decreasing in CO<sub>2</sub> liquefaction cost. The operating conditions with the lowest liquefaction cost are then used as middle values for constructing the second order model. Then, additional sample points are generated using CCD for fitting the data with the second order model (a simple nonlinear model). If there is at least one significant interaction or quadratic term, the second order model is further used in the optimization problem. The significant term was determined under the criterion that the p - value is less than 0.05.

If all interaction or quadratic terms show insignificant, additional sample points generated from LHS are added to the data set. The numbers of additional samples in this study are 10, 15, and 21. Then, all the data are fitted with the second order model.

The optimization formulation, which uses the obtained second order model as the objective function, is shown as:

$$\begin{aligned} \text{MIN:} & \quad \text{Second order model} \\ \text{Decision variables:} & \quad x_1 \text{ and } x_2 \\ \text{Subject to:} & \quad -1.4142 \leq x_1 \leq 1.4142 \\ & \quad -1.4142 \leq x_2 \leq 1.4142 \end{aligned}$$

The Microsoft Excel nonlinear solver is used to solve this problem for the optimal operating conditions with the minimum CO<sub>2</sub> liquefaction cost.

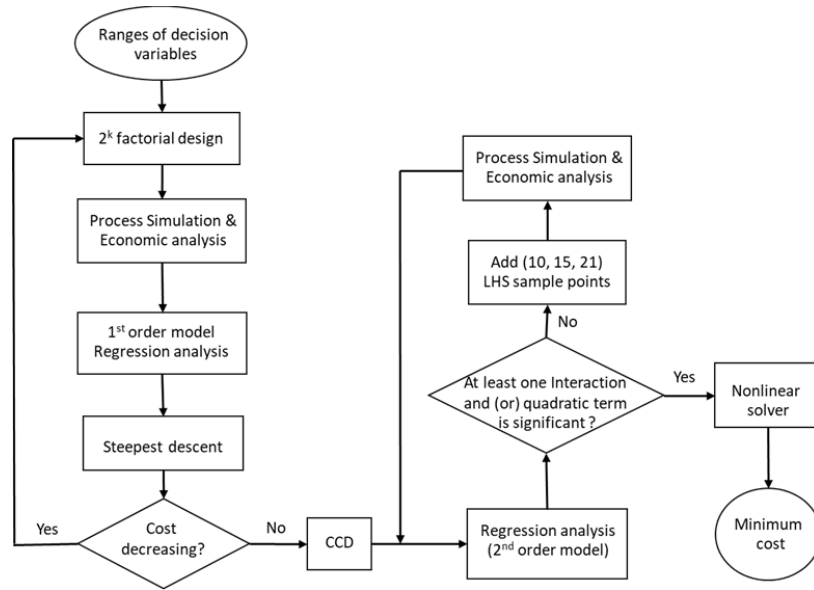


Fig. 2 Process Modeling and Optimization Algorithm

#### IV. RESULTS AND DISCUSSION

##### A. Steepest Descent

Steepest descent results of parameter ranges of 10 and 20 kPa are shown in Fig. 3.

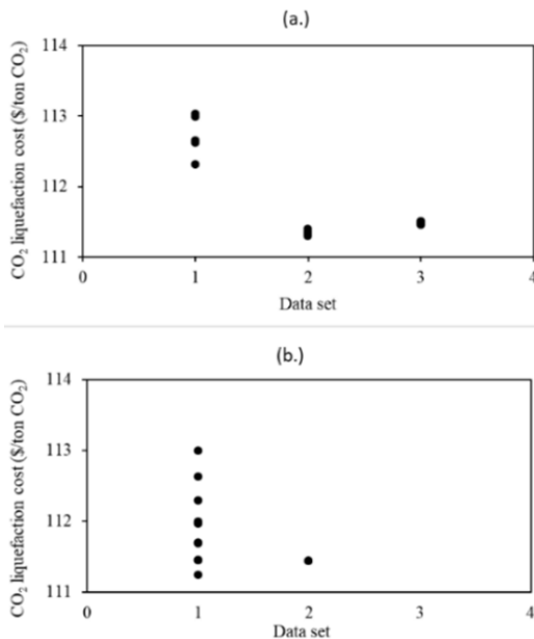


Fig. 3 Steepest descent results: (a) parameter range of 10 kPa, (b) parameter range of 20 kPa

For the range of 10 kPa, the lowest compression cost is at \$111.30/ ton CO<sub>2</sub> for data set 2, and the lowest cost is at \$111.45/ton CO<sub>2</sub> for data set 3. This means data set 2 get to the area of local minimum compression cost. For the range of 20 kPa, the lowest compression cost is at \$111.24/ ton CO<sub>2</sub> for the data set 2, and the lowest cost is at \$111.44/ton CO<sub>2</sub>. The results show that data set 1 get to the area of local minimum

compression cost. For both case studies, the operating conditions at the minimum liquefaction cost were used as the middle values in using CCD to construct the second order model.

##### B. Optimal Solutions

This section describes the results of model fitting and optimal solution of two case studies: The parameter range of 10 kPa and the parameter range of 20 kPa. Table II shows results of the model fitting with the data from CCD for both case studies. From the regression analysis of data from CCD (9 sample points), the interaction and quadratic terms do not show significant terms in the models for both case studies.

TABLE II  
REGRESSION ANALYSIS RESULTS OF CCD SAMPLES

Parameter ranges (kPa)	Number of sample points	Interaction and Quadratic terms
10	9	Insignificant
20	9	Insignificant

We then increased the sample points generated from LHS to represent more data in the studied region. There different numbers of additional sample points were studied, which are 10, 15, and 21 sample points. Table III shows the results of the second order model fitting after adding more sample points from LHS. In the table, the variable  $x_1$  is the first compressor outlet pressure (kPa), and  $x_2$  is the turbine outlet pressure at the first refrigeration circuit. The percent error was calculated from the difference between predicted value (obtained from the nonlinear model) and the actual value (obtained from Aspen HYSYS), divided by the actual value.

For the parameter range of 10 kPa, adding more sample points from LHS was able to capture the nonlinear characteristic in the studied region for all three different sample points. Adding 15 and 21 sample points gives higher model accuracy than the model of 10 additional sample points.

For parameter range of 20 kPa, adding 10 LHS sample points was not able to represent the nonlinear characteristic in the studied region - the interaction and quadratic are insignificant. When compared with the parameter range of 10 kPa, a larger region requires more sample points to represent the surface characteristic. Addition of 15 and 21 sample points was able to represent the nonlinear characteristic in this region. The model with 21 additional sample points shows higher accuracy than the model with 15 additional sample points. The optimal operating conditions for the parameter range of 10 kPa are as

follows – the first compressor outlet pressure: 884 kPa; and, the turbine outlet pressure at the first refrigeration circuit: 174 kPa with the local minimum liquefaction cost of \$111.29/ ton CO<sub>2</sub>.

The optimal operating conditions for the parameter range of 20 kPa are as follows – the first compressor outlet pressure: 917 kPa; and, the turbine outlet pressure at the first refrigeration circuit: 168 kPa with the local minimum liquefaction cost of \$111.22/ ton CO<sub>2</sub>. Different parameter ranges can yield in different local optimal conditions.

TABLE III  
OPTIMAL SOLUTIONS FROM THE MODELS USING CCD AND LHS SAMPLES

Parameter ranges (kPa)	Number of sample points		Decision variables		CO <sub>2</sub> liquefaction cost (\$/ton CO <sub>2</sub> )		Error (%)
	CCD	LHS	x <sub>1</sub> (kPa)	x <sub>2</sub> (kPa)	Predicted	Aspen HYSYS	
10	9	10	883.76	174.11	111.25	111.29	0.036
		15	883.76	169.11	111.30	111.31	0.009
		21	883.36	169.11	111.29	111.30	0.009
		10	insignificant interaction and quadratic terms				
20	9	15	916.75	167.61	111.15	111.23	0.072
		21	916.58	167.61	111.17	111.22	0.045

The second order models obtained from case studies in Table III are shown in (1)-(5) as follows. All x<sub>1</sub> and x<sub>2</sub> in the equations are in code variables – 1.4142 to 1.4142.

The parameter range of 10 kPa with a total of 19 samples:

$$111.318 - 0.080x_1 + 0.062x_1^2 \quad (1)$$

The parameter range of 10 kPa with a total of 24 samples:

$$111.328 - 0.087x_1 + 0.067x_1^2 \quad (2)$$

The parameter range of 10 kPa with a total of 30 samples:

$$111.319 - 0.085x_1 + 0.075x_1^2 \quad (3)$$

The parameter range of 20 kPa with a total of 24 samples:

$$111.228 - 0.061x_1 - 0.060x_2 + 0.045x_1^2 \quad (4)$$

The parameter range of 20 kPa with a total of 30 samples:

$$111.247 - 0.058x_1 - 0.058x_2 + 0.044x_1^2 \quad (5)$$

From (1)-(5), we can see that the results from all case studies agree that the quadratic term of the pressure of CO<sub>2</sub> after the first compressor (x<sub>1</sub>) shows significant impact on the CO<sub>2</sub> liquefaction cost. All obtained second order response surface models show accurate prediction as their percent errors are less than 0.1. For the parameter range of 20 kPa, the pressure of ammonia after expansion of the first refrigeration circuit (x<sub>2</sub>) also shows significant impact on the CO<sub>2</sub> liquefaction cost. We suspect that this is because of the different local optimal solution due to the different studied region boundary.

## V. CONCLUSION

The sampling techniques used in process modeling of simulation experiments were studied. The optimization of CO<sub>2</sub> liquefaction based on external refrigeration with two refrigeration circuits was used as a case study. The steepest descent was employed to find the minimum region of CO<sub>2</sub> liquefaction cost. An algorithm to incorporate LHS with CCD was developed. We found that, in case of complex response surface, LHS was able to represent more information in nonlinear region for constructing the second order model used in the optimization problem.

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