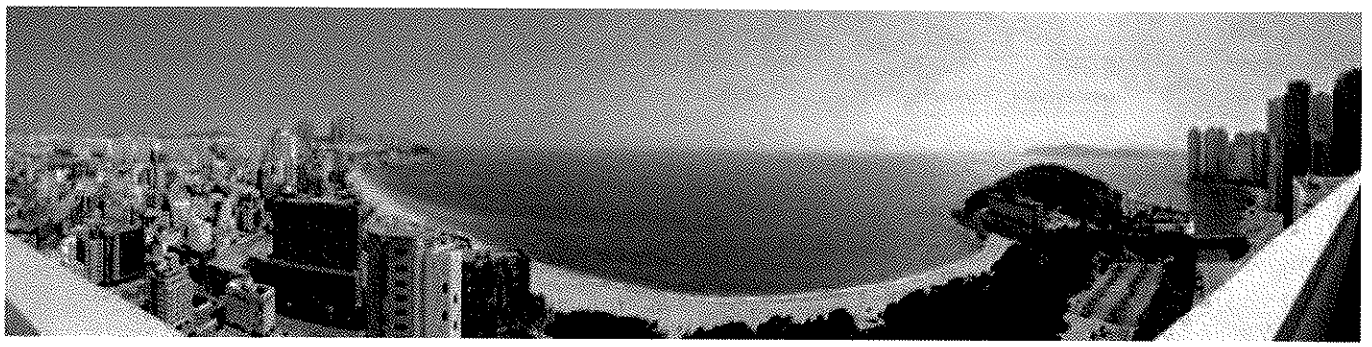
ICSST 17

The 11th International Conference on Separation Science and Technology

PROGRAM AND GENERAL INFORMATION



AIRRANE Gas Separation Membrane
Airrane Co., Ltd.

ATiK
ATI Korea Co., Ltd.

ABRC
Aquatic Biomass Research Center

CCP융합연구단
Center for Convergent Chemical Process

FCC
Functional Crystallization Center

GENS ENGINEERING
Gens Engineering Co., Ltd.

KCRC
Korea CCS R&D Center

PROTECH KOREA
Micrometrics Instrument Corp

SOLETEK
Soletek Trading Co., Ltd.

MicrotracBEL
MicrotracBEL Corp.

November 9 – November 11, 2017

Haeundae Grand Hotel, Busan, Korea

Organized by

The Division of Separation Technology, The Korean Institute of Chemical Engineers

The Society of Separation Process Engineers, Japan

사단법인 한국화학공학회
THE KOREAN INSTITUTE OF CHEMICAL ENGINEERS

SSPEJ

GENERAL TIMETABLE

Day 1. Thursday, November 9th

14:00-18:00	Registration
18:00-19:00	Chairmen's Meeting
19:00-20:30	Welcome Reception

Day 2. Friday, November 10th

09:00-09:30	Opening Ceremony				
09.30-10:30	Plenary Session 1 (Grand ball room)				
10:30-10:45	Coffee Break				
10:45-11:45	Plenary Session 2 (Grand ball room)				
12:00-13:30	Lunch (Hotel restaurant)				
13:30-15:30	Oral session1 (Studio G) Phase equilibria/ Transport Properties	Ora session2 (Ball room B) Distillation/Absorption	Oral session3 (Ball room C) Crystallization	Oral session4 (Ball room A) Adsorption/ Chromatography /Ion exchange	Poster Session 1 Membrane separation/Fluid-Solid Separation Extraction /Supercritical Fluid Technology New or Hybrid Separation Process & Material
15:30-15:50	Coffee break (This may vary with the sessions' schedule)				
15:50-17:30	Oral session1 (Studio G) Phase equilibrium/ Transport Properties	Oral session2 (Ball room B) Distillation/Absorption	Oral session3 (Ball room C) Crystallization	Flash PT for posters 1 (1/2) (Ball room A) Adsorption/ Chromatography /Ion exchange	
18:00-20:00	Banquet				

Day 3, Saturday, November 11th

09:00-11:00	Oral session5 (Ball room A) Membrane separation/ Fluid-Solid Separation	Oral session6 (Ball room A) Extraction/ Supercritical Fluid Technology	Oral session7 (Ball room C) New or Hybrid Separation Process & Material	Flash PT for posters 2 (2/2) (Studio G) Adsorption/ Chromatography /Ion exchange (09:00~10:00) Flash PT for posters 2 (Studio 2) Distillation/ Absorption (09:00~11:00)	Poster Session 2 Phase equilibria/ Transport Properties Distillation /Absorption (11:00-13:00) Crystallization Adsorption/ Chromatography/ Ion exchange (10:00-13:00)
11:00-11:20	Coffee break (This may vary with the sessions' schedule)				
11:20-13:00	Oral session5 Membrane separation/ Fluid-Solid Separation	Oral session6 Extraction/ Supercritical Fluid Technology	Oral session7 New or Hybrid Separation Process & Material		
13:00 -	Wrap-up				

BO-06	15:10-15:30 INTRODUCTION FOR BATCH DISTILLATION SIMULATION, UTILIZATION EXAMPL PHARMACEUTICAL PROCESS INDUSTRY Tomoyuki TAGUCHI(Chiyoda Co.)
	Coffee Break **15:30-15:40**

Session chairmen : Yeon Ki HONG(Korea Nat'l Univ. of Transpo
Mitsuhiro KANAKU

BO-07	15:40-16:00 DEVELOPMENT OF ENERGY-SAVING CO_2 CAPTURE PROCESS USING PHASE SEPARATION SOLVENT Hiroshi MACHIDA*, Takehiro ESAKI, Tsuyoshi YAMAGUCHI, Koyo NORINAGA(N Univ.), Akira KISHIMOTO, Akira MATSUOKA, Katsuya AKIYAMA and Makoto NISHIMURA (Kobe Steel)
BO-08	16:00-16:20 GLOBAL SENSITIVITY ANALYSIS FOR CRUDE OIL DISTILLATION USING A METAMODELING REGRESSION METHOD Le Quang MINH, Pham Luu Trung DUONG and Moonyong LEE*(Yeungnam U
BO-09	16:20-16:40 SEPARATION PERFORMANCE OF A HORIZONTAL TYPE DISTILLATION SYSTEM Yusuke SHIMADA, Ken-Ichiro SOTOWA*, Jesús Rafael ALCANTARA-AVILA and Toshihide HORIKAWA(Tokushima Univ.)
BO-10	16:40-17:00 CHEMICAL REACTION AND MASS TRANSFER RATES IN AMINE ABSORBER Young-Il Lim* and Dung A Dung(Hankyong National Univ.)
BO-11	17:00-17:20 DESIGN OF HEAT-INTEGRATED DISTILLATION COLUMNS (HIDiC) WITH COMPACT MULTI-STREAM HEAT EXCHANGERS Morihiro TANAKA, J. Rafael ALCANTARA-AVILA*, Ken-Ichiro SOTOWA, Toshih HORIKAWA(Tokushima Univ.) and Hao-Yeh LEE(National Taiwan Univ. of Scie Technology)
BO-12	17:20-17:40 DEVELOPMENT OF CFU SIMULATOR AND PHYSICAL PROPERTIES ESTIMATIO Hyun-Jung LEE and Jongkuk WON(Hanwha Total Petrochemical. Ltd)

GLOBAL SENSITIVITY ANALYSIS FOR CRUDE OIL DISTILLATION USING A METAMODELING REGRESSION METHOD

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INTRODUCTION

The crude oil, which contains a complex mixture of hydrocarbons, is separated into higher quality fractions like naphtha, kerosene, diesel and gas oil [1, 2]. To quantify the effect of the input uncertainty on the model output, uncertainty quantification (UQ) is particularly priority to a design of efficient process. Furthermore, to determine their quantity, a global sensitivity analysis (SA) is necessary.

Surrogate models, also known as meta-models, can become approximations of detailed mechanistic models which are capable of simplifying highly nonlinear and computationally expensive problems. The Kriging technique, which originates from interpolating the geographic data in mining, is known as Gaussian process modeling [3].

This study proposed a two-stage approach to handle the UQ of the crude oil distillation. First, a multiplicative dimensional reduction method was used to identify the influential factors on the model output. The UQ of Gaussian prediction regression modeling of the identified important factors from the previous step was then facilitated. The aim is to explain the efficient and practical framework and the typical steps involved SA and UQ.

METHODOLOGIES

Multiplicative dimensional reduction method

This section briefly describes the multiplicative dimensional reduction method (M-DRM) for the global sensitivity analysis from Zhang and Pandey [4].

A steady state process with m outputs

$$y = [y(\xi, t=1), ..., y(\xi, t=m)]^T \quad (1)$$

which is described in the form of nonlinear equations:

$$y = h(\xi, t) \quad (2)$$

where $t \in \{1, ..., m\}$ is index variable, y is the vector of process outputs.

Global sensitivity analysis is based on a decomposition of the computational model in Eq. (2), as follow [5].

$$y(\xi,t) = y_0(t) + \sum_{i=1}^{N} y_i(\xi_i, t) + \sum_{i=1}^{N-1}\sum_{j>i}^{N} y_{ij}(\xi_i, \xi_j, t) + \ldots + y_{i_1 \ldots i_N}(\xi_i, \ldots, \xi_N, t) \quad (3)$$

where $y_0(t) = \mu_y(t)$.

The first order Sobol's sensitivity index is

$$S_i(t) = \frac{D_i(t)}{D_Y(t)} \approx \frac{\theta_i(t)/\rho_i^2(t) - 1}{\left(\prod_{k=1}^{N} \theta_k(t)/\rho_k^2(t)\right) - 1} \quad (4)$$

The Sobol's total effect functions quantify the total impact of the factor, ξ_i , including all of its interactions with the other inputs:

$$T_i(t) = \frac{\mathbf{E}(\mathrm{var}(y(\xi,t)|\xi_{-i}))}{D_y(t)} \approx \frac{1 - \rho_i^2(t)/\theta_i(t)}{1 - \left(\prod_{k=1}^{N} \rho_k^2(t)/\theta_k(t)\right)} \quad (5)$$

Nq total number of functional evaluations are required for the complete SA.

Uncertainty quantification with Gaussian prediction regression modeling

In order to quantify the uncertainty of the model output, the Gaussian prediction regression modeling (GPR) is used.

A GPR model is defined as,

$$y(\xi_m) = h(\xi_m)^T \beta + f(\xi_m) \quad (6)$$

where $f(\xi_m)$ is a zero Gaussian random process with covariance function k, and $h(\xi_m)$ is a set of basic function or trend that transform the original input space into a new feature vector $h(\xi_m)$ in R^m, which is the vector of basis coefficients.

In this paper, the automatic relevance determination (ARD) squared exponential is defined by:

$$k(\xi_m^{(i)}, c^{(j)} \mid \boldsymbol{\theta}) = \theta_f \exp(-\frac{1}{2}\sum_{l=1}^{m}(x_l^{(i)} - x_l^{(j)})^2 / \theta_l) \quad (7)$$

where $\boldsymbol{\theta} \in R^{m+1} = (\theta_f, \theta_1, ..., \theta_m)$ is the vector of hyper parameters.

Thus, a GPR is defined by the coefficient vectors **β**, the hyper parameters and the measure of noise variance **σ**. The values will be updated and learnt from the given data by maximizing the log likelihood expressed in Eq. (8).

$$\log P(y \mid \xi_m, \boldsymbol{\beta}, \boldsymbol{\theta}, \sigma)$$
$$= \frac{1}{2}(\mathbf{y} - H\boldsymbol{\beta})^T \left[K(\xi_m, \xi_m^{'} \mid \boldsymbol{\theta}) + \sigma^2 I_p \right]^{-1} (\mathbf{y} - H\boldsymbol{\beta}) - \frac{p}{2}\log(2\pi)$$
$$-\frac{1}{2}\log\left| K(\xi_m, \xi_m^{'} \mid \boldsymbol{\theta}) + \sigma^2 I_p \right| \quad (8)$$

where I_p is an identity matrix of size p, and

$$X = \begin{pmatrix} (\xi_m^{(1)})^T \\ (\xi_m^{(2)})^T \\ \dots \\ (\xi_m^{(P)})^T \end{pmatrix}, \quad H = \begin{pmatrix} h(\xi_m^{(1)})^T \\ h(\xi_m^{(2)})^T \\ \dots \\ h(\xi_m^{(P)})^T \end{pmatrix}$$

$$\mathbf{y} = \begin{pmatrix} y^{(1)} \\ \dots \\ y^{(P)} \end{pmatrix} \quad (9)$$

$$K(\xi_m, \xi_m) = \begin{bmatrix} k(\xi_m^{(1)}, \xi_m^{(1)}) & \dots & k(\xi_m^{(1)}, \xi_m^{(P)}) \\ \dots & \dots & \dots \\ k(\xi_m^{(P)}, \xi_m^{(1)}) & \dots & k(\mathbf{x}^{(P)}, \xi_m^{(P)}) \end{bmatrix}$$

where $H_{p\times r}$ is the matrix of value of basis vector at training points, *r* is the number basis function, and *K* is the covariance matrix at training points.

RESULTS AND DISCUSSION

Here the UQ of a complex crude oil distillation unit is addressed by using HYSYS process simulator with MATLAB via the ActiveX/COM function. A set of 160 quadrature nodes was generated to HYSYS to calculate the operating revenue. The result of M-DRM method indicates three random variables, the flow rate of crude oil, naphtha, and diesel, were detected as being important. Other random variables can be fixed at the nominal values. Figure 1 compares the density functions of operating revenue obtained by the GPR with 500 training points and QMC method with three influential random inputs (flow rate of crude oil, naphtha, and diesel), and that by the QMC method with sixteen variables. The trained GPR model for the output model was {0.0304, 0.1202, and 0.0028}. It was observed in Figure 1 that the proposed method can achieve acceptable results with only a small computational cost (about 10 times less) in comparison with the Quasi-Monte Carlo method.

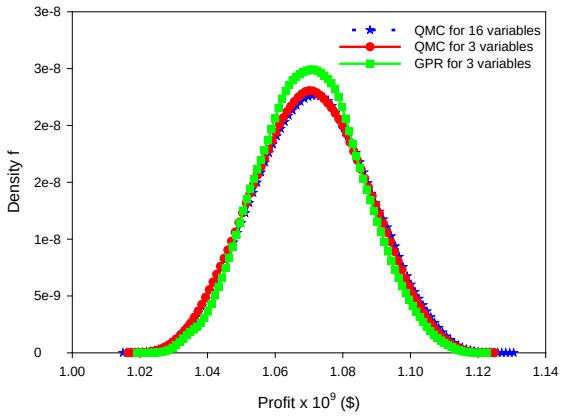

Figure 1. Density function plots of operating revenue obtained by GPR and QMC methods.

CONCLUSION

The purposes of this work focused on UQ and SA for the CDU to test the model robustness against uncertainties and obtaining a better understanding of the effects of inputs on the output. The proposed two-stage approach is superior to the popular QMC, primarily in terms of the computational efforts when a large number of random inputs is considered. The results are expected to handle for other complex chemical processes associated with a large number of uncertainties.

REFERENCES

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