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GAUSSIAN EMULATOR FOR STOCHASTIC OPTIMAL DESIGN OF A DOUBLE GLAZING SYSTEM

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ABSTRACT

This paper addresses development of a simple and quick prediction model based on the Gaussian Stochastic Process (GASP) requiring a far less computation time than dynamic whole Building Performance Simulation (BPS) tools. An emulator, which can be regarded as a surrogate model of BPS tools, was developed using Gaussian process regression model and Bayesian approach. In the paper, the authors exemplify the use of the emulator for optimal design of a double glazing system for a given office building. In general, it requires a significant simulation run-time for stochastic optimization. In this paper, it was presented to make a coupling between the Gaussian process regression model and an optimization routine in MATLAB optimization toolbox. It is found that the emulator reduces computation time significantly, produces results almost identical to BPS tools. In addition, quantitative appraisal using the stochastic optimization yields reliable results, and helps to improve confidence in stochastic optimization as well as make rational decision making.

INTRODUCTION

Building Performance Simulation (BPS) tools, which translate physical phenomenon into an elaborate mathematical model, have been widely used for performance assessment, optimal design, online/offline calibration, and controls, etc. However, most of the BPS tools bear inflexible and rigid input-output relationships and are likely to produce different simulation results influenced by modelling assumptions and modelling judgment of simulationists.

Since BS 2001 when the concept of uncertainty analysis was introduced (de Wit, 2001; Macdonald & Strachan, 2001; de Wit & Augenbroe, 2002; Macdonald, 2002), Monte Carlo simulation has been widely understood to account for the aforementioned uncertainty matter (Buswell, 2001; Wouters et al, 2004; Breesch & Janssens, 2005; Suter et al, 2005; Kotek et al, 2007; Hyun et al, 2008; Hopfe, 2009; Kim & Park, 2009a; de Wilde & Tian, 2010). Monte Carlo simulation runs are based on sampling methods (e.g. Simple Random Sampling [SRS], Quasi-Random Sampling [QRS], Latin Hypercube Sampling [LHS], etc.) and popular due to its capability to produce probability distribution of expected performance. Monte Carlo simulation executes a number of simulation runs using probability distribution of inputs. Since Monte Carlo simulation requires vast computational time and efforts for generating and running simulation cases as well as analysing simulation results, it is not easy to employ BPS tools for stochastic optimal design during real design process, which is usually under very tight budget and time schedule.

This paper addresses a stochastic optimal design using an emulator produced by Gaussian Stochastic Process (GASP). The emulator can be regarded as a surrogate model of the dynamic whole-building simulators (e.g. EnergyPlus, ESP-r, TRNSYS, etc.). The emulator is usually very quick to generate prediction and alleviates vast computational requirements (Rasmussen & Williams, 2006; Liu & West, 2009; Heo & Zavala, 2012). It can be effectively used for statistical optimization problem (Eisenhower et al, 2012).

In the paper, EnergyPlus was chosen to derive the emulator. Stochastic optimal design of a double glazing system was exemplify for a given office building. The two elements in the objective function were (1) total energy consumption and (2) Predicted Mean Vote [PMV], respectively. For this multi objective optimization problem, Genetic Algorithm (GA) and Pareto optimality were used. (Wright et al, 2002; Kim & Park, 2009b; Oh et al, 2011).

METHODS

Emulator

The BPS tools require a number of simulation inputs interwoven in complex relationships for reflecting thermodynamic nature of building systems. However, most inputs cannot be determined in a deterministic way since it is highly probabilistic nature (e.g. occupant's activity, probability of lights on/off, infiltration/ventilation rate, etc.). Accordingly, deterministic simulation prediction is like shooting a constantly moving target. For more rational decision making, a method must be introduced to reflect probabilistic nature of reality. To solve for such uncertainty problem, Monte Carlo simulation is widely used. However, when it is used for optimal design that requires iterative calculation over a significant solution space, it becomes too computationally demanding for real practice.

The concept of emulator can be a solution for stochastic optimization problem (Rasmussen & Williams, 2006; Liu & West, 2009; Heo & Zavala, 2012; Eisenhower et al, 2012).

The emulator is usually made based on a Gaussian process regression model, a Bayesian approach and a dataset of observations. The emulator is developed in the follows steps:

- *Step 1 (training dataset)*: For the stochastic linear regression model, it needs to have a training dataset D of n observations, $D = \{(x_i, y_i) | i = 1, \ldots, n\}$, where x denotes an input vector of dimension D and y denotes a scalar output or target (Rasmussen & Williams, 2006). The training dataset is generated from a choice of sampling methods (e.g. SRS, QRS, LHS, etc.) used for Monte Carlo simulation.

- *Step 2 (Gaussian process regression model)*: The emulator is built using a linear regression model ($f(x_i)$) with Gaussian noise (ε_i) as shown in Equation (1). The linear regression model is formulated as Gaussian process with zero mean function and covariance matrix $\Sigma_{i,j} = k(x_i, x_j')$ (Equation (2)). The covariance matrix is constructed from a covariance function having two unknown parameters such as scaling parameter σ_{se}^2 and length-scale l_k (Equation (3)). The Gaussian noise follows an independent and identically distributed Gaussian distribution with zero mean and variance v_n (Equation (4)). The variance in the Gaussian noise is also an unknown parameter.

$$y_i = f(x_i) + \varepsilon_i \qquad (1)$$

$$f(x_i) \sim gp(0, k(x_i, x_j')) \qquad (2)$$

$$k(x_i, x_j') = \sigma_{se}^2 \exp(-\frac{1}{2}\sum_{k=1}^{d} \left| x_{i,k} - x_{j,k} \right|^2 / l_k^2) \qquad (3)$$

$$\varepsilon_i \sim N(0, v_n) \qquad (4)$$

- *Step 3 (Bayesian approach)*: Bayesian inference, based on Bayes' formula, obtains posterior estimates of three unknown parameters (scaling parameter, length-scale, and variance) by using conditional probability as shown in Equation (5). In general, a maximum of a posterior (MAP) estimate can be used to obtain a point estimate of three unknown parameters. The advantage of the MAP estimate is that it is relatively easy and fast to evaluate (Vanhatalo et al, 2011). In the stochastic optimal design using the emulator, the MAP estimate is more a suitable method than a Markov Chain Monte Carlo (MCMC) sampling which requires too much computational time if the uncertainty in parameters is not underestimated.

$$p(\sigma_{se}^2, l_{1:d}, v_n \left| y \right.) \propto p(y \left| \sigma_{se}^2, l_{1:d}, v_n \right.) p(\sigma_{se}^2, l_{1:d}, v_n) \qquad (5)$$

The emulator can be constructed from the aforementioned three steps, and it can mimic the stochastic behaviour of the dynamic whole-building simulators while being computationally cheap to run. It should be noted that the preparation work for generating training dataset with regard to a few critical parameters is anything but easy. However, if the trustworthy emulator was once built, it should provide a powerful solution for stochastic optimal design.

Simulation based optimal design

The simulation based optimal design needs to coupling of simulation models and optimization techniques (e.g. gradient search, Pattern Search [PS], Particle Swarm Optimization [PSO], and Genetic Algorithm [GA] etc.), and its approaches are classified as follows (Figure 1): (1) deterministic optimal design and (2) stochastic optimal design. The deterministic optimal design is a general approach to find optimal design based on deterministic simulation results. On the other hand, the stochastic optimal design finds optimal design based on post-processing simulation results whose values are reflect uncertainty propagation. The stochastic optimal design can explain uncertainty nature of simulation prediction, but it takes far more computational time than deterministic optimal design does. To solve the issue of the stochastic optimal design, a simple but accurate enough model, so called the emulator, should be introduced.

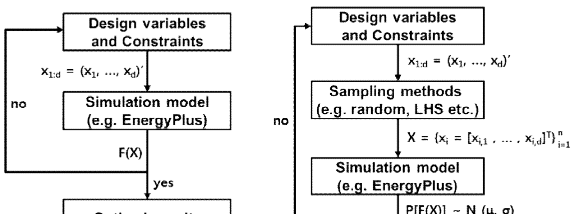


Figure 1 Comparison between deterministic (left) and stochastic (right) optimal design

SIMULATION MODEL & UNKNOWN INPUTS

In this paper, a main objective of the stochastic optimal design is to select double glazing systems minimizing total energy consumption and thermal comfort. A 5-story office building (floor area: 1,225m^2) having four perimeter zones and one interior zone in each story was selected, and it was modelled by EnergyPlus7.0 (Figure 2). Simulation inputs are categorised as known and unknown. The known inputs are as shown in Table 1. Regarding the schedule (people, lights, equipment, HVAC), the defaults defined in ASHRAE (2004) were used.

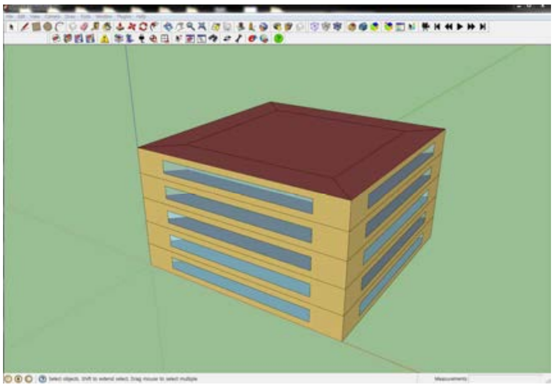


Figure 2 Target building (displayed in OpenStudio)

Table 1
Simulation inputs

INPUTS		DESCRIPTIONS
Weather file		Seoul (*epw)
Simulation period		January 1 – December 31
Construction materials	Exterior wall	100 mm brick,50 mm insulation, air space, 19 mm gypsum board
	Partition	19 mm gypsum board, air space, 19 mm gypsum board
	Floor	19.1 mm acoustic tile, air space, 100 mm HW concrete
	Roof/ ceiling	100 mm HW concrete, air space, 19.1 mm acoustic tile
Indoor load density	People	People per floor area: 0.215 (*person/m*^{2}) Activity level: 80 (*W/m*^{2})
	Lights	Watts per floor area: 18.22 (*W/m*^{2})
	Electric equipment	Watts per floor area: 16.15 (*W/m*^{2})
Infiltration rate		0.2 (air changes per hour)
Thermostat set-point		Heating air temp.: 20 (℃), Cooling air temp.: 26 (℃)
HVAC system		IdealLoadAir system
Outputs		Total energy consumption (*kWh/m*^{2}) Predicted Mean Vote

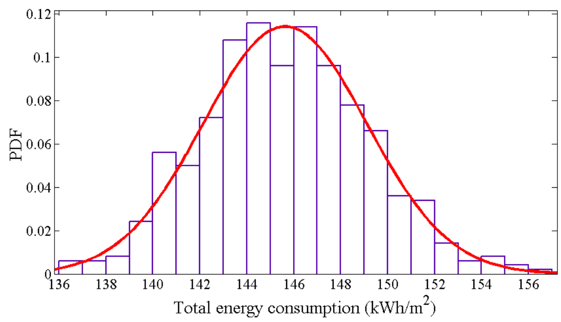
Eight unknown inputs are as follows: U-factor (*W/(m*^{2}*K)*) and Solar Heat Gain Coefficient (SHGC, *dimensionless*) of the double glazing system per each orientation (north, west, east, and south). This means that the optimal design problem in this paper is to find optimal U-factor and SHGC of the transparent envelopes in each orientation. The probability distribution of each unknown input is assumed to be a normal distribution. The mean values of U-factor and SHGC are respectively 2.67 (*W/(m*^{2}*K)*) and 0.705. The standard deviations of both are set to 0.267 (*W/(m*^{2}*K)*) and 0.0705, respectively. In this paper, we have not included any other uncertainties such as specification uncertainty, modelling uncertainty, numerical uncertainty, and scenario uncertainty as reported in de Wit (2001). It has been widely acknowledged that simulation prediction is strongly influenced by such uncertainty e.g. occupant behaviours (opening/closing windows, changing room set-point temperature, lights on/off, rolling up/down blinds/louvers, etc.). In this paper, the aforementioned uncertainty was purposefully excluded. Be noted that this study aimed to present a viable way of stochastic optimal design using Gaussian process regression model, Bayesian approach, GA and Pareto optimality.

With this in mind, it should be noted that if the uncertainty that was excluded in this study would be included in optimal solution search space of this study, the answer out of it would be very different from the one from this study.

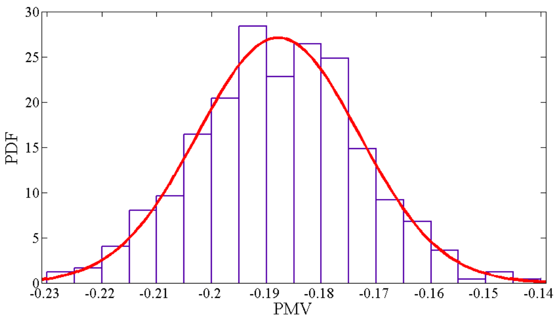
DEVELOPMENT AND VALIDATION OF THE EMULATOR

Training dataset

What follows is the description of how the authors made the training dataset for the emulator. The LHS method was used since it provides good convergence of the input space with relatively few samples compared to the standard brute force random sampling (Saltelli et al, 2004). The LHS method has been widely used for uncertainty analysis in building simulation (de Wit, 2001; Macdonald, 2002; Hyun et al, 2008; Kim & Park, 2009a; Hopfe, 2009; de Wilde & Tian, 2010). To obtain the training dataset, the propagated sampling was set to 500 simulation cases, which is well above the value of 10 × *k* (where, *k* is the number of unknown inputs. In this study, *k*=8) and confidence interval was set to 95%. Figure 3 shows the uncertainty results with regard to total energy consumption and PMV. The mean value and variance of the total energy consumption are 145.2 (*kWh/m*^{2}) and 12.18 (*kWh/m*^{2}), respectively, and the mean value and variance of the PMV are 0.19 and 0.0002, respectively.



(a) Total energy consumption



(b) PMV

Figure 3 Uncertainty results using LHS method

Gaussian process regression model

To build and analyze Bayesian model over Gaussian processes, GPstuff software made by M-scripts in MATLAB (Vanhatalo et al, 2011) was used. As noted above, Gaussian process regression model has three unknown parameters such as scaling parameter (σ_{se}^2), length-scale (l_k), and variance (v_n). MAP estimate was used to obtain point estimates of the three unknown parameters. In this study, a gradient-based optimization function was used (Equation (6)). The gradient-based optimization approach needs derivatives of a cost function and finds optimal solution quickly. However, it sometimes converges to a local minimum.

$$\begin{aligned}\{\hat{\sigma}_{se}^2, \hat{l}_{1:n}, \hat{v}_n\} &= \arg\max\ p(\sigma_{se}^2, l_{1:n}, v_n \mid D) \\ &= \arg\min[-\log p(D \mid \sigma_{se}^2, l_{1:n}, v_n) - \log p(\sigma_{se}^2, l_{1:n}, v_n)]\end{aligned} \tag{6}$$

Table 2 shows the point estimate results of the unknown parameters based on MAP estimate. MAP estimate took about 10 seconds to find the optimal solutions. The emulator built with the point estimate needs validation whether it is able to provide reliable prediction or not. In this paper, *k*-fold Cross-Validation (CV) was used. *k*-fold CV is an approach to validate the emulator by iteratively training on *k-1* subsamples and iteratively testing the remaining subsample of the *k* subsamples that is randomly divided into *k* equal size subsamples.

The default division of the training dataset was into 10 groups. The results of *k*-fold CV were calculated from Mean Absolute Error (MAE) and Root Mean Square Error (RMSE). As shown in Table 3, MAE and RMSE results of *k*-fold CV given the training dataset have considerably low values. In other words, the emulator built with the point estimate has reliable prediction. Table 4 shows comparison between EnergyPlus and the emulator for given different samples. The emulator is surprisingly close to prediction from EnergyPlus.

Figure 4 shows uncertainty results using Cumulative Distribution Function (CDF). The difference in mean values of total energy consumption and PMV between EnergyPlus and emulator is 0.27 (*kWh/m²*) and 0.01, respectively. The results of emulator are similar to those of EnergyPlus.

Table 2
Approximated results of unknown parameters using MAP estimate

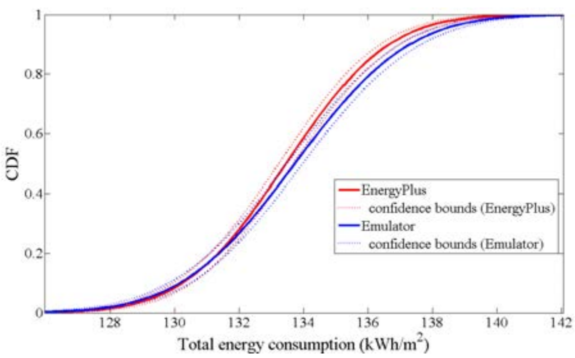
UNKNOWN PARAMETERS	INITIAL VALUES	ENERGY	PMV
scaling parameter	0.04	0.00067	6.0E-10
length-scale #1	1.0	13.86	17.61
length-scale #2	1.2	1.49	0.66
length-scale #3	1.0	14.12	18.98
length-scale #4	1.2	1.44	1.72
length-scale #5	1.0	13.78	15.55
length-scale #6	1.2	1.45	1.83
length-scale #7	1.0	10.95	14.76
length-scale #8	1.2	0.50	0.57
variance	0.04	1,756.97	0.05

Table 3
Results of k-fold Cross-Validation

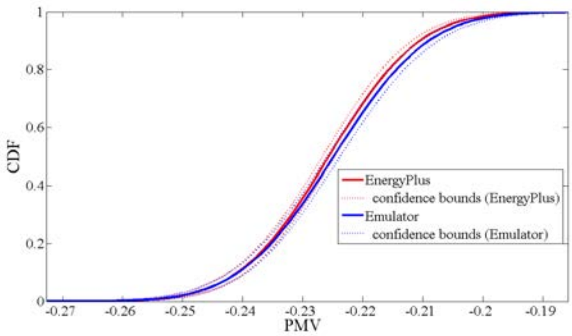
VALIDATION METHODS			VALUES
Total energy consumption (*kWh/m²*)	MAE	Mean	0.0248
		Variance	7.47E-07
	RMSE	Mean	0.0317
		Variance	1.37E-06
PMV	MAE	Mean	8.07E-05
		Variance	1.85E-11
	RMSE	Mean	0.000104
		Variance	2.93E-11

Table 4
Stochastic comparison between EnergyPlus and Emulator

STOCHASTIC RESULTS		ENERGY PLUS	EMULATOR
Total energy consumption (*kWh/m²*)	Mean	133.46	133.73
	Variance	6.26	7.79
PMV	Mean	-0.23	-0.22
	Variance	0.00014	0.00015



(a) Total energy consumption (kWh/m²)



(b) PMV

Figure 4 Uncertainty results (EnergyPlus vs. emulator)

STOCHASTIC OPTIMAL DESIGN

Design variables and objective function

For stochastic optimal design of the double glazing system, elements in the objective function are mean values of total energy consumption and PMV (Equation (7)). The objective function is constrained by a set of inequality equations so called a coefficient of variation. The coefficient of variation is a normalized measure of dispersion of a probability distribution. In this study, a convergence criterion of the coefficient of variation was set to 0.05 reported by Billinton & Li (1994) and Hu (2009). The optimal design problem is to find a Pareto set of optimal double glazing systems that minimize the objective function.

$$\begin{aligned} & MIN\ F(X) = E\left[f_1, abs(f_2)\right] \\ & s.t.\ \mathrm{Var}\left[f_1\right]^{1/2} / E\left[f_1\right] \le 0.05 \\ & \qquad \mathrm{Var}\left[abs(f_2)\right]^{1/2} / E\left[abs(f_2)\right] \le 0.05 \end{aligned} \tag{7}$$

where,

$f_1 = Total\ energy\ consumption\ (kWh/m^2)$

$f_2 = PMV$

$Var = Variance$

$E = Expected\ value\ or\ mean\ value$

$abs = absolute\ value$

143 double glazing systems appeared by DOE (2011) were used for optimal search space. Two thermal properties (U-factor and SHGC) were used in the optimization formulation. The properties were assumed to be a normal distribution.

Genetic algorithm and Pareto optimality

The objective function with inequality constraints is a multi-objective optimization problem. There are three approaches to handle the multi-objective optimization problem based on relationship between decision and search (van Veldhuizen & Lamont, 2000; Miettinen, 2001): [1] a prior preference articulation (decide → search), [2] progressive preference articulation (decide ↔ search), and [3] a posteriori preference articulation (search → decide).

In this paper, we used a posteriori preference articulation (search → decide). This approach presents a set of Pareto optimality to Decision Makers (DMs) (Wright et al, 2002; Kim & Park, 2009b; Oh et al, 2011). The solutions of Pareto optimality are termed as non-dominated Pareto optimal solutions. These means not being dominated by any other solutions in feasible region. The non-dominated Pareto optimal solutions are referred to as a “Pareto optimal set” or “efficient frontier” (Charnes et al, 1985). Decision Makers can pick their preferred optimal design.

This approach requires coupling of optimization techniques and Pareto optimality. In this study, Genetic Algorithm (GA) was used as an optimization technique. The GA uses a suitable random search technique to solve a nonlinear and non-differentiable problem. The coupling of GA and Pareto optimality has widely been used in building simulation. Wright et al (2002) showed a potential to find solutions by using multi-criterion works (GA + Pareto) in terms of optimum pay-off between energy cost and occupant thermal discomfort for HVAC system design. Kim & Park (2009b) reported that optimal design of ventilation systems (such as hybrid and total heat exchanger) was achieved using the GA and Pareto optimality. The stochastic optimal design was conducted in five steps as shown in Figure 5.

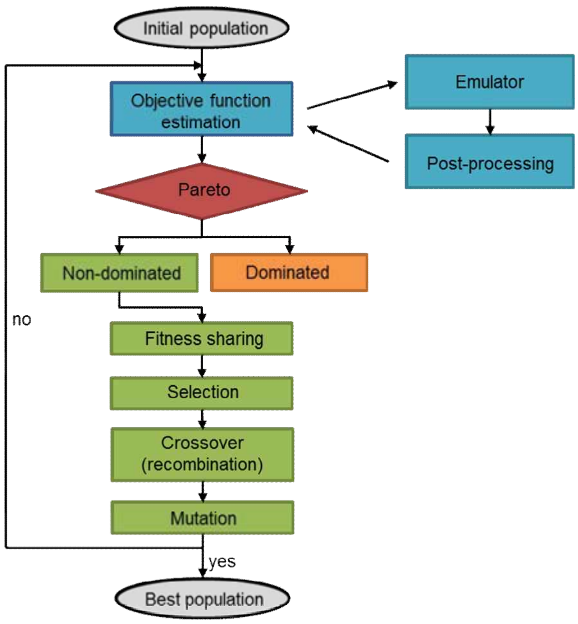


Figure 5 Stochastic optimal design using GA, Pareto optimality, and emulator

- *Step 1 (initial population)*: GA translates the design variables into binary values (0 or 1) by using an encoding process. The generation of initial population was set to 600 through five cycles of “trial and error”.

- *Step 2 (calculation of objective function)*: Uncertainty analysis using the emulator was implemented for the initial population in terms of total energy consumption and PMV. In this step, the emulator embedded in MATLAB platform runs a series of LHS simulation by varying design variables. As a result, the objective function was calculated.

- *Step 3 (fitness sharing)*: For the production of offspring, the individuals are selected according to their fitness. In this study, a non-dominated sorting genetic algorithm Ⅱ (NSGA-Ⅱ) method proposed by Deb et al (2000) was used.

- *Step 4 (selection)*: This step is to choose individuals for crossover (or mating). A tournament selection method was used.

- *Step 5 (crossover and mutation)*: The crossover and mutation produce new individuals by combining information contained in the parents and forcing changes in a bit of gene with low probabilities.

The stochastic optimal design iterates according to a number of generations until finding the non-dominated Pareto solutions from populations. At each generation, the same number of the fit offspring replaces a given number of the least fit parents. The number of generations was set to 1,000.

Optimal results

Table 5 shows 13 non-dominated Pareto solutions from option space of 418,161,601 (= 143 [north window] × 143 [west window] × 143 [east window] × 143 [south window]).

Optimal design #1 is superior to #2 in terms of total energy consumption, but optimal design #2 has lower PMV than #1. In other words, it cannot tell which one is better because it compares apples to oranges. To validate the non-dominate Pareto solutions, the authors compared optimal design #9 and five dominated Pareto solutions are randomly chosen as shown in Table 6. The dominated Pareto solutions have the same mean value for PMV as optimal design #9. However, the dominated Pareto solutions have greater total energy consumption than optimal design #9. The five dominated Pareto solutions are inferior to optimal design #9. In other words, the non-dominated Pareto solutions are always superior to dominated Pareto solutions.

Table 6
Validation of Pareto optimal solution

DESIGN	TOTAL ENERGY CONSUMPTION		PMV	
	MEAN	STDEV	MEAN	STDEV
Non-dominated solution(Design#9)	**82.06**	**2.62**	**0.29**	**0.009**
Dominated solution #1	82.19	2.67	0.29	0.009
Dominated solution #2	82.57	2.76	0.29	0.010
Dominated solution #3	82.81	2.80	0.29	0.010
Dominated solution #4	83.17	2.80	0.29	0.011
Dominated solution #5	83.40	2.97	0.29	0.011

Table 5
Non-dominated Pareto solutions using stochastic optimal design

NON-DOMINATED PARETO SOLUTIONS												
OPTIMAL DESIGN	DESIGN VARIABLES								OBJECTIVE FUNCTION			
	X1 (NORTH WINDOW)		X2 (WEST WINDOW)		X3 (EAST WINDOW)		X4 (SOUTH WINDOW)		TOTAL ENERGY CONSUMPTION (*kWh/m²*)		PMV	
	U-factor	SHGC	U-factor	SHGC	U-factor	SHGC	U-factor	SHGC	MEAN	STDEV	MEAN	STDEV
1	2.431	0. 637	2.325	0.422	1.333	0.107	1.333	0.107	70.11	2.17	0.37	0.01
2	1.626	0.120	2.325	0.422	1.333	0.107	1.333	0.107	70.28	2.16	0.36	0.005
3	2.325	0.162	1.333	0.107	1.333	0.107	1.333	0.107	70.70	2.14	0.35	0.005
4	1.347	0.282	1.626	0.120	1.333	0.107	1.333	0.107	71.54	2.20	0.34	0.006
5	1.347	0.419	1.333	0.107	1.333	0.107	1.333	0.107	72.75	2.24	0.33	0.007
6	1.333	0.479	1.347	0.282	1.333	0.107	1.333	0.107	74.90	2.37	0.32	0.008
7	1.347	0.419	1.333	0.479	1.333	0.107	1.333	0.107	76.98	2.44	0.31	0.008
8	1.347	0.419	1.502	0.644	1.333	0.107	1.333	0.107	79.40	2.56	0.30	0.009
9	1.502	0.146	1.502	0.746	1.333	0.428	1.333	0.107	82.06	2.62	0.29	0.009
10	1.333	0.107	1.502	0.746	1.502	0.644	1.333	0.107	84.70	2.81	0.28	0.01
11	1.333	0.479	1.770	0.743	1.333	0.479	1.502	0.146	92.43	3.38	0.27	0.011
12	1.347	0.282	1.502	0.746	1.333	0.479	1.502	0.159	94.21	3.42	0.26	0.011
13	1.347	0.419	1.333	0.107	1.333	0.107	1.347	0.282	103.93	3.76	0.25	0.011

Figure 6 shows Probability Density Function (PDF) results of 13 non-dominated Pareto solutions by using multivariate normal distribution (3-dimensional plot, X-axis: total energy consumption, Y-axis: PMV, Z-axis: PDF).

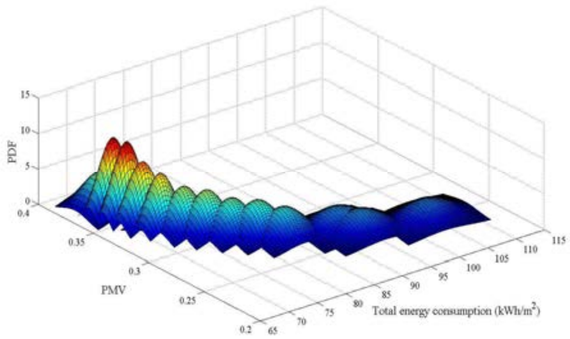


Figure 6 13 non-dominated Pareto solutions

CONCLUSIONS AND FUTURE WORK

Coupling of optimization and the emulator was presented for stochastic optimal design of double glazing system. The emulator was based on Gaussian process regression model using Bayesian approach. The emulator demands far less computational time and effort than whole-building simulation tools (e.g. EnergyPlus), and can be beneficially utilized for stochastic optimal design. It will help to improve confidence in rational decision-making since it can consider stochastic variation of prediction and deliver meaningful information. Future work may include the following:

- Stochastic optimal control: The emulator may be used for real-time whole-building simulation and control, considering stochastic nature of the system's response.

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