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Dual response surface optimization with hard-to-control variables for sustainable gasifier performance

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Summary. Dual response surface optimization of the Sasol–Lurgi fixed bed dry bottom gasification process was carried out by performing response surface modelling and robustness studies on the process variables of interest from a specially equipped full-scale test gasifier. Coal particle size distribution and coal composition are considered as hard-to-control variables during normal operation. The paper discusses the application of statistical robustness studies as a method for determining the optimal settings of process variables that might be hard to control during normal operation. Several dual response surface strategies are evaluated for determining the optimal process variable conditions. It is shown that a narrower particle size distribution is optimal for maximizing gasification performance which is robust against the variability in coal composition.

Keywords: Desirability functions; Dual response surface; Gasification; Robustness studies

1. Introduction

Sasol, South Africa, gasifies approximately 30 million tons of bituminous coal per year to synthesis gas, which is converted to fuels and chemicals via the Fischer–Tropsch process. A total of 80 Sasol–Lurgi fixed bed dry bottom gasifiers have a combined production of approximately 4.6×10^6 m^3 n (normal) h^{-1} dry raw gas (RG), which is equivalent to approximately 3.2×10^6 m^3 n h^{-1} pure synthesis gas. The Secunda plant is the largest syngas production facility of its kind in the world.

Fixed bed coal gasification reactors are countercurrent devices in which a coal bed moves downwards by gravity flow through an upward flowing gas stream (Electric Power Research Institute, 1983). Steam and oxygen are fed at the bottom to provide the reactants for the combustion and gasification reactions. The composition and temperature of the product gas and the amount of unburnt carbon in the ash largely determine the thermal efficiency of the process. The product gas composition and temperature depend on the properties of the coal being processed and on operating parameters such as feed rates, feed temperature and reactor pressure. Since the Secunda coal-to-liquids facility delivers nearly 29% of the fuel requirements in South Africa, the continuous improvement of the gasification plant is of critical importance to the company.

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To optimize product yields further and to increase throughput, a thorough understanding is required of those process parameters that govern gasifier performance. Therefore, in 1998 Sasol decided to isolate one Sasol–Lurgi mark IV gasifier at the Secunda site as a test gasifier. This gasifier was equipped with additional instrumentation, which included a more sophisticated RG measurement and a dedicated coal feeding system.

17 comprehensive tests were conducted on the test gasifier. 10 of these tests were conducted according to a full 2^3 factorial design with two centre points in coal top size, coal bottom size and stone content (defined as the material that sinks at a relative density of 1.9), using only one coal source. Seven tests were performed with a blend of six coal sources. Additional process variables investigated were the gasifier oxygen load (oxygen feed rate (km^3 n h^{-1})) and the carbon dioxide (CO_2) in RG concentration (volume percentage). During each of the tests, loads were varied from low to medium to high, and at each load the CO_2 in RG concentration was adjusted between a high and a low value. It will be explained that the coal particle size distribution (PSD) is not uniquely determined by the planned top and bottom sizes. Therefore, three size fractions were selected to define the coal PSD, and, for the purposes of this paper, will be referred to as the coarse, medium and fine fractions. For the factorial design, Coetzer and Keyser (2003) developed statistical response surface models and evaluated the effect of the process parameters on gasifier performance in terms of carbon utilization and utility consumption.

However, the development of the models in Coetzer and Keyser (2003) was based on the assumption that all the test parameters are equally well controllable during normal operation. In practice the run-of-mine coal can be highly variable in certain coal seams, such as the stone or ash content in the coal. Controlling coal composition can result in significant capital investments for the coal-to-gas facility. Manipulation and control of the coal PSD, i.e. coal top and bottom sizes, can be accomplished at a marginal cost by effective screening of the run-of-mine coal before feeding to the gasification process (Coetzer and Keyser, 2003). Furthermore, operational conditions of varying PSD can occur under certain circumstances of coal types and preparation. Therefore, it is important to consider the PSD of the coal feed and the coal composition as hard-to-control variables during normal operation.

The response surface modelling approach to robustness analysis has been advocated by Myers (1991), Myers *et al.* (1992), Myers and Montgomery (1995) and Montgomery (1999). Recently, Robinson and Wulff (2005) gave a detailed overview of response surface approaches to robustness analysis. In the response surface modelling approach a mean and variance function are constructed for each response variable. The dual response surface (DRS) approach, and correspondingly DRS optimization, has received considerable attention in the literature as a methodology to determine the optimum operating conditions for an industrial process or product (Vining and Myers, 1990; Del Castillo and Montgomery, 1993; Ding *et al.*, 2004; Tang and Xu, 2002). The DRS approach is applied to problems where the researcher can identify a primary response or quality characteristic, such as the pure gas yield production from the gasifier, which is to be optimized subject to some specified value of a secondary response or quality characteristic, such as the transmitted variance in pure gas yield from the variability in the hard-to-control variables.

In this paper we provide a case-study of the DRS approach applied to a full-scale gasification process. We derive optimum conditions for the process parameters that govern gasification performance as measured by sustainable production and stable gasifier operation. We concentrate on the pure gas yield as the performance measure alone. We consider the PSD of the coal as well as the coal properties as hard-to-control variables during normal operation. Since both these process parameters are mixture variables, which are both subject to fundamental constraints, the paper introduces a unique application to DRS optimization. We present confidence regions for the optimum mixture formulations by using the bootstrap. This is important for practical implementation since the coalmines can neither deliver a specified coal composition nor a specified coal PSD because of obvious blending, operational and mining difficulties. Furthermore, to ensure the implementation of the solutions on the gasification plant it is necessary to evaluate, for example, the feasibility of the optimum coal PSD in terms of the screen aperture sizes, and the feasibility of the optimum coal composition in terms of fundamental chemical constraints.

The paper is organized as follows. First the methodology of process robustness studies is discussed. Thereafter, the various dual response optimization formulations are presented for evaluation. The robustness analysis and results are then presented with detailed discussions. Finally, consequences for practical implementation are discussed together with future research opportunities.

2. The methodology of process robustness studies

Montgomery (1999) visualized a process as a combination of components, materials, people, equipment, processes and other resources that function collectively to transform a set of inputs into outputs that are described by one or more response variables. Montgomery (1999) argued that statistical experimental designs and modelling may be deployed to address specific objectives of the process, such as to determine which variables have the largest influence on the responses, to determine where to set the influential controllable variables so that the responses are almost always near their desired target values or to determine where to set the influential controllable variables so that the effects of the hard-to-control variables on the responses are small.

Gasification is such a process of transforming a set of inputs to outputs, such as pure gas yield and carbon utilization. Coal top size, coal bottom size, oxygen load, CO_2 in RG concentration and coal composition were investigated as the variables that can potentially influence the process. There are of course many other variables that might influence the gasification process but considerable effort was made to control those variables during the test runs. The experimental conditions of the process variables that were investigated were deliberately changed according to a planned experimental programme (Coetzer and Keyser, 2003).

Although statistical response surface models were developed previously in Coetzer and Keyser (2003, 2004) to study specific objectives of optimization and robustness, they did not consider the effect of the coal composition, and the variability thereof, on sustainable gasifier performance. The aim of this paper is to demonstrate the effect of the process variables on gasifier performance when the assumption of fully controllable variables cannot be made. We consider the PSD of the coal as well as the coal properties as hard-to-control variables during normal operation. Hard-to-control variables are sometimes also referred to as noise or environmental variables.

Myers (1991), Myers *et al.* (1992), Montgomery (1999) and Lucas (1994) discussed the development of robust processes through the use of statistically designed experiments and response surface methodology as opposed to the use of the methods of Taguchi (1986). They explained that the response surface approach involves designing an experiment with the hard-to-control variables and the controllable variables in a combined array. The experimental design should at least allow the estimation of two-order interactions between the controllable and hard-to-control variables. A response surface model is then constructed, containing one or more two-order interaction terms between the controllable and hard-to-control variables, for the performance variable of interest. The variance function is then calculated by taking the conditional variance operator across the first-order Taylor series expansion of the model over the prior distribution of the hard-to-control variables. Therefore, dual responses, i.e. a mean and variance function, are constructed for each response variable. In this paper, we perform robustness studies for mixture and normal process variables.

A response surface model in mixture and process variables was given by Cornell (1981):

$$
\begin{aligned}
Y(x,z,w) &= f(x,z,w)+\varepsilon \\
&= h(x)+\sum_{l=1}^{s} h(x)z_l+\sum_{t=1}^{v} h(x)w_t+\sum_{l=1}^{s} h(x)z_l^2+\sum_{t=1}^{v} h(x)w_t^2 \\
&\quad +\sum_{l=1}^{s}\sum_{t=1}^{v} h(x)z_l w_t+\varepsilon
\end{aligned} \tag{1}
$$

where $z_1,\ldots,z_s$ and $w_1,\ldots,w_v$ are normal process variables. The distinction between the process variables is important for the application of robustness studies to gasification performance evaluation (see Section 3.2). In model (1),

$$
h(x)=\sum_{i=1}^{q}\gamma_i x_i+\sum\sum_{i<k}^{q}\gamma_{ik}x_i x_k \tag{2}
$$

is the model in $x_1,\ldots,x_q$ mixture variables. Model (1) can be expanded to the full response surface model $f(x,z,w)$ in mixture and process variables. Cornell (1981) explained that mixture models do not contain an intercept γ_0 and squared terms $\gamma_{ii}x_i^2$ because of the constraint that the x_is sum to 1 and models containing such terms can always be reduced to those given in model (2). Model (1) can be written succinctly as

$$
Y(x,z,w)=a^{\mathrm{T}}\beta+\varepsilon \tag{3}
$$

where a is the vector containing all the terms in the response surface model and β is the vector containing all the parameters in the model. Furthermore, ε is assumed to be normally distributed with mean 0 and constant variance σ^2. Model (3) can be fitted to the data to produce the least squares estimates of β_u, namely b_u, $u=1,2,\ldots,p$.

Let the mean and variance–covariance matrix of the mixture variables x during normal operation be equal to μ_x and S_x respectively, with $E(x_i)=\mu_{x_i}$ and $\mathrm{var}(x_i)=\sigma_{x_i}^2$, $\mathrm{cov}(x_i,x_j)=\sigma_{x_i x_j}$, $i\neq j=1,\ldots,q$. Note that we are considering the covariance structure of the composition and do not assume independent variables, which is an assumption that is commonly used in the robustness literature. The response surface model for the process mean is then obtained by taking the expectation of the predicted model, $\hat{Y}(x,z,w)$ from model (1), over the prior distribution of the hard-to-control variables, i.e. $E_x\{\hat{Y}(x,z,w)\}=\hat{Y}_{\mu|x}(x,z,w)$. The response model for the process variance is approximated by applying the conditional variance operator to the first-order Taylor series expansion of model (1), i.e.

$$
\begin{aligned}
\hat{Y}_{\sigma|x}(x,z,w)^2 &= \mathrm{var}_x\{\hat{Y}(x,z,w)\} \\
&= \sum_{i=1}^{q}\sigma_{x_i}^2\left(\frac{\partial\hat{Y}}{\partial x_i}\right)^2+2\sum\sum_{i<k}^{q}\sigma_{x_i x_k}\frac{\partial\hat{Y}}{\partial x_i}\frac{\partial\hat{Y}}{\partial x_k}+\hat{\sigma}^2 \\
&= I_x(x,z,w)^{\mathrm{T}}S_x\,I_x(x,z,w)+\hat{\sigma}^2
\end{aligned} \tag{4}
$$

where $I_x(x,z,w)$ is the vector of derivatives of the model to the hard-to-control variables, and $\hat{\sigma}^2$ is the estimated residual mean square of the model fit. All the derivatives are evaluated at $b_u=\beta_u$. Model (4) describes the variability in the response as transmitted from the variability in the hard-to-control variables. Because of the interactions between the controllable and hard-to-control variables the response surface of process variance changes according to changes in the controllable variables. It is therefore possible to determine settings on the controllable variables that reduce or minimize the variability that is transmitted to the responses.

DRS optimization can now be performed to obtain specific engineering objectives. For example, Montgomery (1999) demonstrated that the objective of minimizing the process variability around a target can be achieved through the following optimization formulation:

$$\min_{(x,z,w)}\{\hat{Y}_{\sigma|x}(x,z,w)^2\} \qquad \text{subject to } \hat{Y}_{\mu|x}(x,z,w)=T \tag{5}$$

where T is a desired target value for the mean response. The optimization scheme in problem (5) was first proposed by Vining and Myers (1990) as a methodology to determine the optimum operating conditions for simultaneously optimizing the process mean and variance. Since then many alternatives to problem (5) have been proposed (Del Castillo and Montgomery, 1993; Ding *et al.*, 2004; Tang and Xu, 2002; Kim and Lin, 1998, 2006). In particular, Lin and Tu (1995) proposed the use of the mean-square error criterion for simultaneously optimizing the mean and variance response surface models. In Section 4 we present different dual response surface optimization strategies which are evaluated in this paper.

Myers and Montgomery (1995) provided a confidence region for the variable conditions which minimizes the process variance (4). Let $c_0=(x_0,z_0,w_0)$ denote the optimum conditions for minimum process variance. Let $I(c_0)=I_0$, the vector of derivatives of the model to the hard-to-control variables at c_0. Assuming normally distributed errors around the response surface model (1) then all the conditions of (x,z,w) which satisfy the inequality

$$(I_x-I_0)^{\mathrm{T}}\,\mathrm{var}(I_x)^{-1}(I_x-I_0)\leqslant r_x F_{\alpha,r_x,\mathrm{df}_\mathrm{e}} \tag{6}$$

provides a $100(1-\alpha)\%$ confidence region for the optimum variable conditions c_0, where $\mathrm{var}(I_x)$ is the variance–covariance matrix of I_x and df_e are the error degrees of freedom for the estimate of the mean-square error MSE of the model fit. Here, r_x is the number of hard-to-control variables that interact with control variables, and $F_{\alpha,r_x,\mathrm{df}_\mathrm{e}}$ is the upper percentage point of $F_{r_x,\mathrm{df}_\mathrm{e}}$. Applying inequality (6) resulted in some difficulties for the current application.

Firstly, mixture variables are subject to multiple constraints, i.e. $\Sigma_i x_i=1$, and $L_i\leqslant x_i\leqslant U_i$, where L_i and U_i are the lower and upper bounds of the ith component. Therefore, if the optimal solution lies on the edge of the constraint region, as for the pure gas yield variance, then I_0 will contain elements which are not equal to 0 for those variables which enforce the constraint. However, this is true in general for optimizing response surface models where the variables are subject to an experimental range, specifically when the ranges are narrow.

Secondly, the form of the response surface model that is discussed in this paper included interaction terms between the mixture and process variables, as well as interaction terms between the mixture variables and quadratic terms for the process variables. Therefore, the vector $I_x(x,z,w)$ in model (4) contains quadratic terms and the variance model is a fourth-degree polynomial in the mixture and process variables, which makes it a very difficult computational problem to solve for the roots of 11 variables simultaneously. Therefore, condition (6) was not suitable for the current application.

Instead, we generated confidence regions of the optimum conditions by using the bootstrap. Efron and Tibshirani (1993), chapter 13, pointed out that the bootstrap is a computational technique for obtaining good approximations to the standard errors and confidence regions of statistics. Furthermore, the bootstrap is independent of the complexity of the estimation procedure. This is particularly important in the current application because there are no analytical expressions for the confidence region for the optimum conditions minimizing the DRS optimization formulations as will be discussed in Section 4. We shall therefore generate confidence regions of the optimum conditions minimizing the DRS optimization formulations by using the bootstrap.

3. The hard-to-control variables

3.1. Particle size distribution as a hard-to-control variable

The crusher opening determined the coal top size and the screen aperture size determined the coal bottom size. Between the top and bottom size, the PSD follows a typical Rosin–Rammler distribution (Rosin and Rammler, 1933). For each combination of top and bottom sizes prepared, the actual PSD of the coal was obtained through a full sieve analysis. Sieve analyses were done according to the American Society for Testing and Materials (ASTM) aperture sizes, and comprised 13 screen sizes from 0.5 mm to 75 mm. Therefore, the PSD of the coal is not uniquely determined by the planned top and bottom sizes. Instead, three aperture sizes from the ASTM sieve analysis were selected to define the coal PSD and, for purposes of this paper, will be referred to as the coarse, medium and fine fractions, and were denoted x_1, x_2 and x_3 respectively. Since the three size fractions have to add up to 100% of the coal feed, the three variables describing coal PSD can be regarded as mixture variables (Cornell, 1981). The source data are proprietary and confidential to the operator and are thus not reported. Notwithstanding the confidentiality obligations, the exact values and ranges of the coarse, medium and fine fractions are of lesser importance to this paper, since the data are only applicable to the particular South African coal that was tested. Optimum size distributions are likely to differ for different coal sources.

Manipulation and control of the coal PSD, i.e. coal top and bottom sizes, can be achieved to some extent at a marginal cost by effective screening of the run-of-mine coal before feeding to the gasification process (Coetzer and Keyser, 2003). However, operational conditions of varying PSD can occur under certain circumstances, e.g. if coal is mined which has a high tendency of break-up during handling and if the coal screening plant is overloaded or experiences operational upsets. The mechanical operations of crushing and screening also introduce variability into the final prepared PSD. Therefore, it is important to consider the PSD of the coal feed as a hard-to-control variable during normal operation and the other variables as controllable. We perform robustness studies to evaluate conditions of coal composition, oxygen load and CO_2 in RG concentration, as well as the PSD fractions that reduce or minimize the effect of variability or instability of the PSD fractions on gasifier performance.

The measured values were recorded during each test run for all the gasification process variables and were used in the statistical modelling and robustness studies. This is because the top and bottom size fractions of the coal PSD were replaced by three size fractions from the sieve analysis, the coal composition was analysed for its properties, and the oxygen load and CO_2 in RG levels varied slightly from the planned conditions. Table 1 depicts the summary statistics for the process variables. The coal PSD is a constrained region in mixture variables and, in particular, the range of the fine fraction is very small, i.e. 0.195. Note that the values for the oxygen loads and the CO_2 in RG levels are given in coded design units, i.e. $(x-\bar{x})/\{\frac{1}{2}(x_{\max}-x_{\min})\}$ where x is the process variable.

For purposes of the robustness studies, the variance–covariance matrix needs to be defined for the PSD fractions. The first 10 tests were performed according to a full 2^3 factorial design with a duplicated centre point. Therefore, the measured values at the middle point were used for the variance–covariance matrix of the PSD fractions. It is assumed that the variability at the middle point is representative of the variability at all the other test conditions. Montgomery (1999) and Myers and Montgomery (1995) also recommended that known or measured

Table 1. Summary statistics for the gasification process variables

Variable	*Units*	*Minimum*	*Mean*	*Maximum*	*Standard deviation*	*Range*
Oxygen load	Coded	−1.00	−0.07	1.00		
CO_2 in RG	Coded	−1.00	−0.21	1.00		
PSD						
Coarse coal	Fraction	0.106	0.287	0.540	0.094	0.434
Medium coal	Fraction	0.393	0.646	0.882	0.100	0.489
Fine coal	Fraction	0.011	0.067	0.206	0.046	0.195
Coal properties (air-dried basis)						
Water†	%	2.800	4.316	5.700	0.594	2.900
Ash	%	18.900	23.285	30.900	2.943	12.000
Carbon	%	50.350	58.121	62.850	2.864	12.500
Hydrogen	%	1.090	2.958	3.550	0.625	2.460
Nitrogen	%	1.303	1.538	1.730	0.096	0.428
Sulphur	%	0.510	0.997	1.610	0.218	1.100
Oxygen	%	7.180	8.784	11.230	0.829	4.050

†Inherent moisture.

variability of the hard-to-control variables should be used in the modelling of the process variance. The variance–covariance matrix that was used in the robustness studies in equation (4) for the three PSD fractions in Table 1 is

$$S_x = \begin{pmatrix} 8.40 \times 10^{-4} & -6.44 \times 10^{-4} & -1.97 \times 10^{-4} \\ -6.44 \times 10^{-4} & 5.53 \times 10^{-4} & 9.09 \times 10^{-5} \\ -1.97 \times 10^{-4} & 9.09 \times 10^{-5} & 1.06 \times 10^{-4} \end{pmatrix}. \tag{7}$$

3.2. *Coal properties as hard-to-control variables*

In practice the run-of-mine coal can be highly variable in certain coal seams, e.g. the stone content or the ash content in the coal, and in such cases it can be controlled by removing part or all of the stone in a beneficiation plant, which adds additional cost to the feedstock preparation and should therefore preferably be avoided. Furthermore, coal composition is subject to the type of coal that is mined, the source of coal and efficiency of the blending plant as well as sampling analysis errors. Controlling coal composition can result in significant capital investments for the coal-to-gas facility. It is therefore important to evaluate the effect of coal composition as a hard-to-control variable during normal operation.

Table 1 depicts the summary of the seven coal properties from the ultimate analysis of the coal on an air-dried basis. The coal properties are mixture variables which constitute the coal composition. The properties are denoted by z_1, z_2, z_3, z_4, z_5, z_6 and z_7. However, since the PSD fractions are also mixture variables, and it had been shown previously to be the most important predictors of gasifier performance (Coetzer and Keyser, 2003, 2004), it was decided to treat the coal properties as process variables and to use only six of them in the statistical model for pure gas yield. Furthermore, this was necessary to reduce the number of terms in the statistical model, which contains mixture and normal process variables. After rigorous evaluations, it was decided to omit sulphur content from the model. As for the PSD fractions, the variability of the coal properties at the middle point was considered to be representative of the variability at all the other test conditions. The variance–covariance matrix that was used in the robustness studies for the six coal properties is

$$S_z = \begin{pmatrix} 0.330 & 0.046 & -0.267 & 0.013 & -0.017 & -0.128 \\ 0.046 & 0.422 & -0.438 & -0.003 & -0.019 & -0.047 \\ -0.267 & -0.438 & 0.635 & -0.008 & 0.025 & 0.109 \\ 0.013 & -0.003 & -0.008 & 0.002 & -0.001 & -0.005 \\ -0.017 & -0.019 & 0.025 & -0.001 & 0.007 & 0.008 \\ -0.128 & -0.047 & 0.109 & -0.005 & 0.008 & 0.079 \end{pmatrix}. \tag{8}$$

4. Dual response optimization formulations

The DRS approach requires an overall optimization, i.e. a simultaneous satisfaction in terms of two performance characteristics. In this case the performance characteristics are the mean and standard deviation of the performance variable. Since the simultaneous optimization of gasifier throughput and variance is a function of mixture components, which are subject to fundamental constraints, it introduces a unique application to DRS optimization.

Lin and Tu (1995) proposed the use of the mean-square error criterion for simultaneously optimizing the mean and standard deviation response surface models. To improve on this, Ding *et al.* (2004) proposed the following weighted mean-square error optimization scheme. Two functions, i.e. $\hat{Y}_{\sigma|x}(x, z, w)$ and $\hat{Y}_{\mu|x}(x, z, w)$, can be simultaneously optimized by combining them into a single objective function by taking the convex combination of them:

$$\min_{(x,z,w)} (\text{WMSE}) = \lambda\{\hat{Y}_{\mu|x}(x, z, w) - T\}^2 + (1-\lambda)\, \hat{Y}_{\sigma|x}(x, z, w)^2$$
$$\text{subject to } (x, z, w) \in (\Omega_x, \Omega_z, \Omega_w) \quad \text{with } \lambda \in [0, 1] \tag{9}$$

where Ω_x is the experimental range for the coal PSD, Ω_z is the experimental range for the coal properties and Ω_w the experimental range for the other two process variables, i.e. oxygen load and CO_2 in the RG concentration. The experimental ranges Ω_x and Ω_z are constrained mixture spaces, which introduce a significant number of constraints into the optimization algorithm. For example, in addition to the general mixture constraints $\Sigma_i x_i = 1$, and $L_i \leqslant x_i \leqslant U_i$, where L_i and U_i are the lower and upper bounds of the ith component, it was also necessary to introduce binary constraints on the components, i.e. $L_{ij} \leqslant x_i + x_j \leqslant U_{ij}$, $\forall i \neq j$. For the coal PSD, these type of constraints were required to conform to the PSD distribution between the top and bottom sizes. For the coal composition, the additional constraints were required to capture the fundamental relationships between the coal properties.

In the weighted mean-square error optimization scheme a weight λ is assigned for the squared deviation of the mean response from the target value T and a weight $1-\lambda$ for the variance of the performance variable. Using scheme (9) one can choose different values for the weight λ according to the relative importance of the two responses. When $\lambda = 0$ or $\lambda = 1$, marginal optimizations are obtained. The dual optimum solutions for the mean and standard deviation from the marginal optimizations, i.e. $\hat{Y}^{o}_{\mu|x}$ and $\hat{Y}^{o}_{\sigma|x}$ respectively, are referred to as the ideal solution. However, this solution is not generally achievable in industry. The optimal solution (x^*, z^*, w^*) is a function of the weight λ. For a specified λ, one can plot the value $\hat{Y}_{\mu|x}(x^*, z^*, w^*)$ against $\hat{Y}_{\sigma|x}(x^*, z^*, w^*)$, which is called an efficient point. If λ is varied from 0 to 1 then a plot of the optimum solutions $(\hat{Y}_{\mu|x}(x^*, z^*, w^*), \hat{Y}_{\sigma|x}(x^*, z^*, w^*))$ is referred to as the efficiency curve in the optimization literature. The point on the efficiency curve which is closest to the ideal solution is the optimal solution for scheme (9). Ding *et al.* (2004) demonstrated that this is a data-driven method which provides a balance between two quality characteristics, i.e. the mean and standard deviation of the performance variable. However, all the solutions on the efficiency curve with different weights are considered to be equally feasible in some sense. For example, the decision maker may decide to put more weight on the squared deviation from the target value than on minimizing the variance. Coetzer *et al.* (2006) also developed a weighted criterion for estimation of the start of accelerated auto-ignition of fuels in spark ignition engines.

Derringer and Suich (1980) introduced the transformation of the response or quality characteristic to one aggregate measure of performance known as a desirability function. In the current problem, the target $T=\hat{Y}^{\max}_{\mu|x}$, since we are interested in maximizing the pure gas yield of the gasifier. This is known as the larger-the-better problem (Montgomery, 1999). The desirability function approach is probably one of the most frequently used multiresponse optimization techniques. Kim and Lin (1998) introduced a non-linear membership function as an alternative to the Derringer and Suich (1980) method. The degree of satisfaction of the experimenter with respect to the mean response is maximized when $\hat{Y}_{\mu|x}=T$ and decreases as $\hat{Y}_{\mu|x}$ moves away from T. The experimenter does not accept any solution for which $\hat{Y}_{\mu|x}\leqslant\hat{Y}^{\min}_{\mu|x}$. Thus the satisfaction level with respect to the mean response can be modelled by a function which increases monotonically from 0, at $\hat{Y}_{\mu|x}=\hat{Y}^{\min}_{\mu|x}$, to 1, at $\hat{Y}_{\mu|x}=T$. The membership function value of the mean response, which is denoted as $m(\hat{Y}_{\mu|x})$, is interpreted as the degree to which $\hat{Y}_{\mu|x}$ satisfies the target on the mean and is a value between 0 and 1.

If the marginal rate of change of membership values of the response is not constant, a non-linear membership function should be employed. Kim and Lin (1998) proposed the following exponential membership function:

$$m(g)=\begin{cases}\dfrac{\exp(d)-\exp(d|g|)}{\exp(d)-1} & \text{if } d\neq 0,\\ 1-|g| & \text{if } d=0\end{cases} \tag{10}$$

where d is a constant and $(-\infty\leqslant d\leqslant\infty)$, called the exponential constant, and g is a standardized parameter representing the distance of the response from its target in units of the maximum allowable deviation. Note that, when $d=0$, $m(g)$ is a linear function. For the larger-the-better case,

$$g_{\mu|x}=\frac{\hat{Y}^{\max}_{\mu|x}-\hat{Y}_{\mu|x}}{\hat{Y}^{\max}_{\mu|x}-\hat{Y}^{\min}_{\mu|x}} \tag{11}$$

for $\hat{Y}^{\min}_{\mu|x}\leqslant\hat{Y}_{\mu|x}\leqslant\hat{Y}^{\max}_{\mu|x}$. Similarly, for the standard deviation, which is the smaller-the-better case,

$$g_{\sigma|x}=\frac{\hat{Y}_{\sigma|x}-\hat{Y}^{\min}_{\sigma|x}}{\hat{Y}^{\max}_{\sigma|x}-\hat{Y}^{\min}_{\sigma|x}}. \tag{12}$$

Both $g_{\mu|x}$ and $g_{\sigma|x}$ range between 0 and 1. In both cases the membership function attains its maximum value of 1 when $g=0$, i.e. when $\hat{Y}_{\mu|x}=\hat{Y}^{\max}_{\mu|x}$ and $\hat{Y}_{\sigma|x}=\hat{Y}^{\min}_{\sigma|x}$. Kim and Lin (1998) demonstrated that the function $m(g)$ can have many different shapes by adjustment of its parameters. Specifically, the degree of satisfaction changes faster as $\hat{Y}$ moves away from the target when $d<0$, and changes slower when $d>0$. Therefore, the membership function is flexible to the preferences of the experimenter.

Using expression (10), we evaluate the following weighted optimization problem:

$$\max_{(x,z,w)}\{W(g)\}=\lambda\, m(g_{\mu|x})+(1-\lambda)\, m(g_{\sigma|x})$$
$$\text{subject to } (x,z,w)\in(\Omega_x,\Omega_z,\Omega_w) \quad \text{with } \lambda\in[0,1]. \tag{13}$$

As for the WMSE-optimization (9), the optimal solution for the weighted membership function (13) can be found as the point on the efficiency curve which is closest to the ideal solution, i.e. $(m(g^{o}_{\mu|x}), m(g^{o}_{\sigma|x}))$. The formulation (13) finds the optimum conditions (x^*, z^*, w^*) which simultaneously maximize the degree of satisfaction on both the mean and the standard deviation criteria. Formulation (13) achieves an optimal balance between the mean and standard deviation of the performance variable. In addition to specifying the rate of satisfaction by adjusting the parameter d for the mean and standard deviation separately, the experimenter also has control over the relative importance of the mean to the standard deviation by specifying the weight λ in problem (13). Kim and Lin (2006) also evaluated formulation (13) for multiresponse optimization but did not utilize the efficiency curve.

Kim and Lin (1998) introduced a 'maximin' operator for aggregating the two objectives, i.e.

$$\max_{(x,z,w)} (\xi) \qquad \text{subject to } m(g_{\mu|x}) \geqslant \xi, \quad m(g_{\sigma|x}) \geqslant \xi, \quad (x, z, w) \in (\Omega_x, \Omega_z, \Omega_w). \tag{14}$$

This formulation aims to maximize the minimum degree of satisfaction, ξ, with respect to the two membership functions, i.e. to maximize the minimum of $m(g_{\mu|x})$ and $m(g_{\sigma|x})$, for $(x, z, w) \in (\Omega_x, \Omega_z, \Omega_w)$. Formulation (14) achieves a good balance in the sense that the contributions of both the mean and the variance are reflected in the optimization. In addition, scheme (14) ensures that the solution is not dominated by one of the objectives, which might happen with the weighted approach of formulations (9) and (13). Formulation (14) also provides a basis for a meaningful comparison between different design points. For example, a design point (x_1, z_1, w_1) is preferred to a different point (x_2, z_2, w_2) if $\xi(x_1, z_1, w_1) > \xi(x_2, z_2, w_2)$.

Kim and Lin (2006) also pointed out that approach (14) has some possible disadvantages. Specifically, the above approach is only concerned with the lowest degree of satisfaction. Therefore, it would not be known whether the degree of satisfaction for the other objective could be improved. To avoid this outcome, Kim and Lin (2006) proposed the introduction of slack parameters as follows:

$$\max_{(x,z,w)} \{\xi + \alpha(\xi_\mu + \xi_\sigma)\} \qquad \text{subject to } m(g_{\mu|x}) - \xi_\mu = \xi, \quad m(g_{\sigma|x}) - \xi_\sigma = \xi, \quad (x, z, w) \in (\Omega_x, \Omega_z, \Omega_w) \tag{15}$$

where ξ_μ and ξ_σ are positive slack parameters that are associated with the two sets of original constraints in scheme (14), and α is a positive scaling constant. If $\alpha = 0$, formulation (15) reduces to scheme (14). As the value of α increases, formulation (15) places more weight on the sum of the slack parameters, and therefore tends to maximize the total sum of individual degrees of satisfaction as opposed to the 'maximin' approach of scheme (14). Kim and Lin (2006) noted that there is no fixed rule for choosing the value of α. Therefore, we evaluated formulation (15) for values of α from 0 to 1 with increments of 0.1.

Finally, we investigate the formulation of Derringer and Suich (1980):

$$\max_{(x,z,w)} \{D(g)\} = \{m(g_{\mu|x})\, m(g_{\sigma|x})\}^{1/2} \qquad \text{subject to } (x, z, w) \in (\Omega_x, \Omega_z, \Omega_w). \tag{16}$$

Formulation (16) aims to maximize the overall desirability of the degree of satisfaction in terms of the product of the individual degrees of satisfaction. If one of the objectives is not met with associated degree of satisfaction equal to 0, then the overall desirability is zero. Formulation (16) is probably one of the most frequently used multiresponse optimization techniques and is commonly available in software packages, such as Design-Expert (Stat-Ease, 2002).

5. Robustness studies on gasifier performance variables: particle size distributions as hard-to-control variables

The aim is to determine the optimum mixture and process conditions which maximize the pure gas yield production (m^3 n ton^{-1} dry ash-free coal, which is the volume of pure gas produced per mass of dry ash-free coal), and simultaneously minimize its variance due to the variability that is transmitted through the coal PSD size fractions. A response surface model of the form (1) was constructed in the mixture and process variables for pure gas yield. The form of the predicted model was obtained as

$$\begin{aligned}\hat{Y}(x,z,w) = {} & b_1x_1 + b_2x_2 + b_3x_3 + b_{12}x_1x_2 + b_{1w_1}x_1w_1 + b_{3w_1}x_3w_1 + b_{1w_2}x_1w_2 + b_{2w_2}x_2w_2 \\ & + b_{3w_{11}}x_3w_1^2 + b_{1w_{22}}x_1w_2^2 + b_{2w_{22}}x_2w_2^2 + b_{2z_1}x_2z_1 + b_{3z_1}x_3z_1 + b_{1z_2}x_1z_2 \\ & + b_{3z_2}x_3z_2 + b_{1z_3}x_1z_3 + b_{3z_3}x_3z_3 + b_{1z_4}x_1z_4 + b_{2z_4}x_2z_4 + b_{3z_4}x_3z_4 \\ & + b_{2z_5}x_2z_5 + b_{2z_6}x_2z_6 + b_{3z_6}x_3z_6 \end{aligned} \qquad (17)$$

where x_1 is the coarse fraction, x_2 is the medium fraction and x_3 is the fine fraction of the PSD, w_1 is the oxygen load (km^3 n h^{-1}), w_2 is the CO_2 in RG concentration (volume per cent), z_1 is the percentage water, z_2 is the percentage ash, z_3 is the percentage carbon, z_4 is the percentage hydrogen, z_5 is the percentage nitrogen and z_6 is the percentage oxygen in the coal. Note that water refers to inherent moisture. The parameter values b are obtained from least squares estimation. An adjusted R^2-value of 0.8 was obtained for the model. The response surface model (17) yielded the same trends in the PSD, loads and CO_2 in RG that were reported previously (Coetzer and Keyser, 2003, 2004).

The model for the process variance is calculated from model (4) where $I_x(x,z,w)$ is a vector consisting of the derivatives of model (17) to the three PSD size fractions, x_1, x_2 and x_3. The variance–covariance matrix S_x is given in equation (7). The residual standard error of the model was obtained as $\hat{\sigma} = 18.95$. From model (17), $\hat{Y}_{\mu|x}(x,z,w)$ can be calculated for given process conditions, such as for PSD size fractions according to specific ASTM sieve sizes. Correspondingly, the process variance $\hat{Y}_{\sigma|x}(x,z,w)$ can be calculated from model (17) by using model (4). Note that $\hat{Y}_{\sigma|x}(x,z,w)$ is a function of all the variables in the model. Therefore, it is possible to determine conditions of the PSD, the coal properties and the loads and CO_2 in RG that achieve maximum pure gas yield and minimum process variance simultaneously.

Table 2 depicts the solutions that were obtained with the squared deviation of the mean response from the target $((\hat{Y}_{\mu|x} - T)^2)$, variance $\hat{Y}^2_{\sigma|x}$ and mean-square error criteria (9) respectively. The second column in Table 2 provides the optimum conditions for minimizing the variance in pure gas yield alone. The minimum variance was achieved as indicated by the standard deviation row $\hat{Y}_{\sigma|x}$, which is equal to the residual standard error of the model. The criterion value row indicates the value of the objective function, i.e. $\hat{Y}_{\sigma|x}$. The optimum coal PSD is obtained as 0.493, 0.497 and 0.011 for the coarse, medium and fine fractions respectively. This PSD is similar to the average size fractions of a 100×6 mm PSD, which is the current base case for gasification performance evaluation. Although the transmitted variance is minimized the pure gas yield is very low, which is indicated by the absolute deviation from the target, i.e. $|\hat{Y}_{\mu|x} - T|$, where $T = 1630$.

The third column gives the optimum conditions for minimizing the squared deviation from the target alone. In this case the target has been achieved and the deviation is zero. The standard deviation of pure gas yield is higher compared with the variance criterion alone. The optimum coal PSD is obtained as 0.106, 0.882 and 0.012 for the coarse, medium and fine fractions respectively. This PSD is significantly different from that for the variance criterion, and it is similar to the average size fractions of a 35×4 mm PSD. This is a narrower size fraction and entails maximizing the middle fraction and minimizing the fine fraction, within their respective experimental ranges.

Table 2. Comparison of optimum results for the squared deviation from the target, variance and mean-square error criteria (9)

Variable	*Results for the following criteria:*			
	$\hat{Y}^2_{\sigma\mid x}$	$(\hat{Y}_{\mu\mid x}-T)^2$	MSE	$WMSE$
Weight (λ)	0	1	0.500	0.254
Coarse coal	0.493	0.106	0.107	0.107
Medium coal	0.497	0.882	0.882	0.882
Fine coal	0.011	0.012	0.011	0.011
Load (coded)	0.609	−0.115	−0.999	−0.999
CO_2 in RG (coded)	1.00	−1.00	−1.00	−1.00
Water (%)	4.273	4.700	4.873	5.073
Ash (%)	27.425	27.700	27.700	27.700
Carbon (%)	53.123	53.550	53.550	53.550
Hydrogen (%)	1.848	3.550	3.377	3.177
Nitrogen (%)	1.730	1.303	1.303	1.303
Oxygen (%)	10.602	8.198	8.198	8.198
$\hat{Y}_{\mu\mid x}$ (m^3 n ton^{-1})	1313.541	1630.000	1626.777	1621.309
$\hat{Y}_{\sigma\mid x}$ (m^3 n ton^{-1})	18.950	26.388	24.802	24.111
$\mid\hat{Y}_{\mu\mid x}-T\mid$	316.459	0.000	3.223	8.691
$\sqrt{\text{MSE}}$			25.011	25.629
Criterion value	359.104	0.000	312.764	452.862

The oxygen load changes from a relatively high load to a medium load, and CO_2 in RG changes from a high level to a low level, for the squared deviation criterion compared with the variance criterion. The percentage ash is slightly higher, which indicates that more ash can be tolerated in the gasifier for a finer PSD. The percentage carbon is also higher, which is sensible because the finer fraction with a higher middle fraction releases more carbon, which can be converted to RG and as a consequence improves the pure gas yield. Contributions from the other properties are very small.

For the MSE-criterion (9), where the squared deviation from the target and variance have the same weight, i.e. they are equally important, the optimal coal PSD is the same as for the squared deviation criterion. However, the optimal pure gas yield is very close to the target value, which indicates that the squared deviation is minimized more easily than the variance. For the WMSE-criterion (9), the optimal weight is obtained as 0.254 from the efficiency curve. Again, since more weight is assigned to the variance criterion it indicates that the squared deviation is minimized more easily. However, the root-mean-square error is greater compared with the equal importance case owing to a larger deviation of the mean response from the target. The optimal PSD is also the same as for the previous criteria. This shows that the PSD shifts from a broad PSD, for minimizing the variance alone, to a narrower PSD for minimizing the squared deviation from the target and mean-square error criteria. Since PSD can only be prepared according to ASTM sieve sizes it is recommended that the narrower size fraction is optimal for maximizing the pure gas yield and minimizing the variance simultaneously.

Although optimum results were obtained with the criteria that are presented in Table 2, it is an additional objective of this paper to evaluate various DRS optimization strategies for application to sustainable gasifier performance. Table 3 depicts the optimum solutions for the linear membership function type criteria (13)–(16), i.e. for d_μ and d_σ in expression (10) both equal to 0. The optimal PSD for all the solutions are similar to the average size fractions of a

Table 3. Comparison of optimum results for the linear membership function type criteria (16), (13), (14) and (15), i.e. for d_μ and d_σ in expression (10) both equal to 0

Variable	*D(g) (16)*	*W(g) (13)*	*Maximin (14)*	*Maximin (15) for the following values of α:*		
				0.500	*0.800*	*1.000*
Weight (λ)		0.574				
Coarse coal	0.201	0.107	0.107	0.214	0.253	0.493
Medium coal	0.789	0.882	0.882	0.775	0.737	0.497
Fine coal	0.011	0.011	0.011	0.011	0.011	0.011
Load (coded)	−0.031	−0.999	−0.999	−0.762	−0.179	0.609
CO_2 (coded)	−1.000	−1.000	−1.000	−1.000	−1.000	1.000
Water (%)	4.659	5.128	5.128	5.128	5.128	4.273
Ash (%)	28.087	28.128	28.128	28.128	28.128	27.425
Carbon (%)	53.937	53.978	53.978	53.978	53.978	53.123
Hydrogen (%)	1.556	2.346	2.476	2.207	1.937	1.848
Nitrogen (%)	1.343	1.303	1.303	1.303	1.303	1.730
Oxygen (%)	9.417	8.119	7.989	8.258	8.528	10.602
$\hat{Y}_{\mu\|x}$ (m^3 n ton^{-1})	1480.622	1557.465	1565.137	1523.552	1508.603	1313.541
$\hat{Y}_{\sigma\|x}$ (m^3 n ton^{-1})	18.969	20.387	20.676	19.319	19.044	18.950
$\|\hat{Y}_{\mu\|x} - T\|$	149.378	72.535	64.863	106.448	121.397	316.459
$\sqrt{\text{MSE}}$	150.578	75.345	68.079	108.187	122.882	317.025
$m(g_{\mu\|x})$	0.547	0.780	0.803	0.677	0.632	0.041
$m(g_{\sigma\|x})$	0.998	0.836	0.803	0.958	0.989	1.000
Criterion value	0.739	0.804	0.803	0.818	0.918	1.000

35×4 mm PSD, except for the maximin criterion (14) where the slack parameter is equal to 1. In this case the desirability for the variance becomes the slack parameter because of the assigned importance and forces the variance to be minimized while sacrificing the deviation from the target, and as a consequence results in a broader PSD as being optimal.

Among all the solutions the weighted membership function criterion (13) and the maximin criterion (14) gave the best overall results with high desirability for both the deviation from the target and the variance. The optimal weight is equal to 0.574 for the $W(g)$ criterion obtained from the efficiency curve. The efficiency curve for the $W(g)$ criterion is depicted in Fig. 1, indicating the ideal solution and the optimal solution at $\lambda = 0.574$. The weighted membership function provides a smooth curve of possible solutions depending on the relative importance of the squared deviation from the target and the variance. The optimal solution for the $W(g)$ criterion in Table 3 is a much better solution compared with that of the WMSE criterion in Table 2. The optimal solution from the $W(g)$ criterion provides small variance and squared deviation, together with a slightly higher percentage ash, which is closer to the current operating conditions of the plant.

Table 4 depicts the solutions of the $W(g)$ criterion for various values of the exponential parameters d_μ and d_σ, i.e. for the non-linear membership function. Although the optimum weights, which were obtained with the efficiency curve, differ slightly from that of the linear membership function, the optimum solutions are very similar. Note that the desirability for both the deviation from the target and the variance, as well as for the overall desirability, increases with an increase in the exponential parameters because the desirability function becomes increasingly concave (Kim and Lin, 1998). Fig. 2 depicts the efficiency curve for $d_\mu = 5$ and $d_\sigma = 5$, which shows that the optimal solution is much closer to the ideal solution compared with the solution for the linear membership function in Fig. 1. However, the best solution is obtained for $d_\mu = 2.5$ and

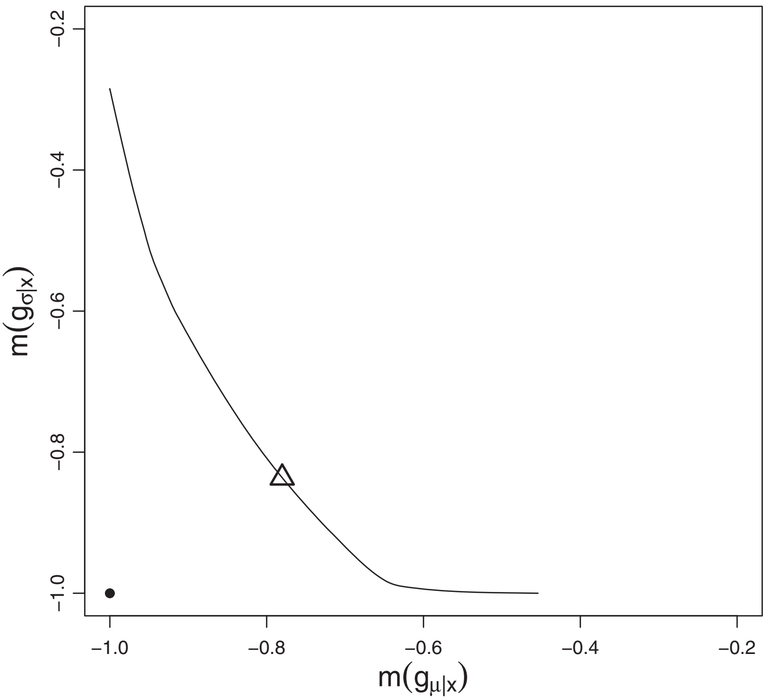

Fig. 1. Efficiency curve for the $W(g)$ criterion with $(d_\mu, d_\sigma) = (0, 0)$ and $\lambda = 0.574$ (●, ideal solution; △, optimal solution)

$d_\sigma = 5$ among all the membership functions, giving the smallest root-mean-squared error. This corresponds to our earlier findings that more weight should be placed on the variance criterion, or that the criterion should be relaxed, for obtaining higher pure gas yield at sustainable rates.

PSD size fractions can only be prepared according to the ASTM aperture sizes for specifying the top and bottom sizes of the coal feed. Therefore, the optimum solutions for the PSD that are provided in Tables 1–4 cannot be prepared precisely for the gasification plant. Furthermore, it is desired to determine confidence regions for the optimum PSD solutions. This is necessary to determine whether any size fraction is captured in the confidence region for the optimal PSD. It is also desired to discriminate between different size fractions, such as a broad *versus* a narrow size PSD. For this we employed the bootstrap for generating the confidence region of the optimum process conditions (Efron and Tibshirani, 1993). The bootstrap is especially useful in the current study because there are no analytical expressions for the confidence region for the optimum conditions from the weighted mean-square error and membership type criteria.

We generated bootstrap least squares estimates for β in equation (3) by randomly selecting a sample of size n from the estimated residuals $\hat{\varepsilon} = Y(x, z, w) - a^{\mathrm{T}} b$, where b is the vector of least squares estimates from the original data (Efron and Tibshirani, 1993). Denote the random sample by ε^*; then the bootstrap responses are generated from $Y^*(x, z, w) = a^{\mathrm{T}} b + \varepsilon^*$. The bootstrap least squares estimates b^* are obtained by minimizing the residual squared error:

$$\sum_{i=1}^{n} \{Y_i^*(x, z, w) - a_i^{\mathrm{T}} b^*\}^2. \tag{18}$$

The bootstrap estimates are then used to specify the bootstrap mean response model $\hat{Y}^*_{\mu|x}$ and the bootstrap variance response model $\hat{Y}^{*2}_{\sigma|x}$. These bootstrap estimates of the mean and

Table 4. Comparison of optimum results for the non-linear weighted membership function criterion (13) for various values of d_μ and d_σ in expression (10)

Variable	*$W(g)$ for the following values of (d_μ, d_σ):*			
	(2.5, 2.5)	*(2.5, 5)*	*(5, 2.5)*	*(5, 5)*
Weight (λ)	0.560	0.525	0.639	0.554
Coarse coal	0.107	0.107	0.192	0.107
Medium coal	0.882	0.882	0.797	0.882
Fine coal	0.011	0.011	0.011	0.011
Load (coded)	−0.999	−0.999	−0.867	−0.999
CO_2 (coded)	−1.000	−1.000	−1.000	−1.000
Water (%)	5.128	5.128	5.128	5.128
Ash (%)	28.128	28.128	28.128	28.128
Carbon (%)	53.978	53.978	53.978	53.978
Hydrogen (%)	2.391	2.906	2.230	2.415
Nitrogen (%)	1.303	1.303	1.303	1.303
Oxygen (%)	8.074	7.559	8.235	8.050
$\hat{Y}_{\mu\|x}$ (m^3 n ton^{-1})	1560.133	1590.689	1528.657	1561.517
$\hat{Y}_{\sigma\|x}$ (m^3 n ton^{-1})	20.484	21.832	19.460	20.536
$\|\hat{Y}_{\mu\|x} - T\|$	69.867	39.311	101.343	68.483
$\sqrt{\text{MSE}}$	72.808	44.966	103.194	71.496
$m(g_{\mu\|x})$	0.938	0.969	0.975	0.988
$m(g_{\sigma\|x})$	0.951	0.972	0.986	0.990
Criterion value	0.944	0.970	0.979	0.989

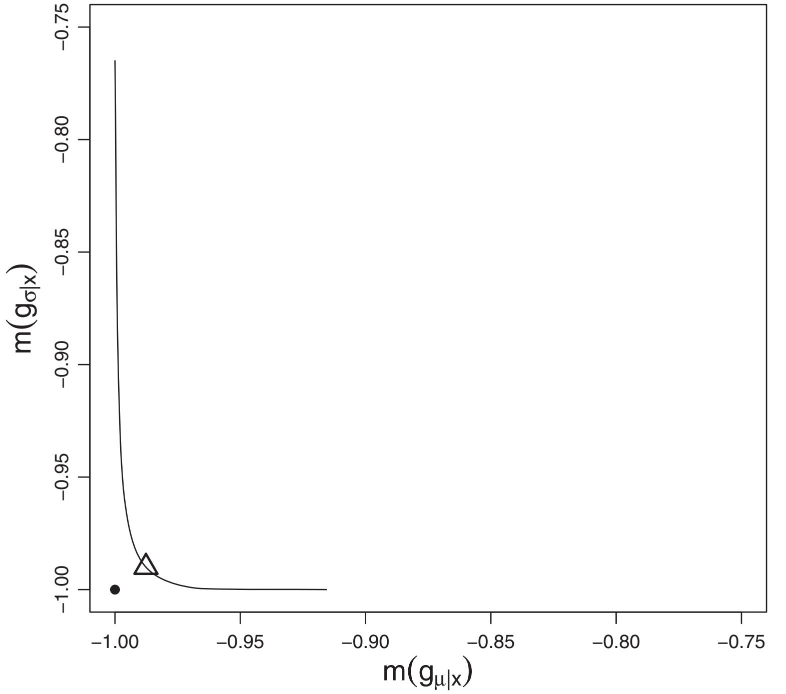

Fig. 2. Efficiency curve for the $W(g)$ criterion with $(d_\mu, d_\sigma) = (5, 5)$ and $\lambda = 0.554$ (●, ideal solution; △, optimal solution)

variance response models are used in the DRS optimization criteria to obtain bootstrap estimates of the optimum conditions minimizing the criterion. 1000 bootstrap replicates were performed. The percentile method was used to specify the 90% confidence interval for the criterion, i.e. the confidence interval was obtained as the values falling in the interval $[C^*_{0.05B}, C^*_{0.95B}]$, where C^*_v is the vth smallest value on the criterion distribution from B bootstrap replicates. The 90% confidence region for the optimum conditions was specified as those solutions corresponding to the 90% confidence interval of the criterion.

Fig. 3 depicts the 90% confidence region for the optimal coal PSD in Table 3 for the $W(g)$ criterion with $(d_\mu, d_\sigma) = (0, 0)$. In comparison, Fig. 4 depicts the 90% confidence region for the optimal coal PSD in Table 4 for the $W(g)$ criterion with $(d_\mu, d_\sigma) = (5, 5)$ and optimal weight $\lambda = 0.554$. The confidence region for the linear membership function is wider compared with that for the larger exponential parameter because the linear membership function is more strict in satisfying the target and therefore more variability is introduced. For both criteria, the confidence region specifies a range for the coarse and medium fractions but restricts the fine fraction to its minimum value. Furthermore, the confidence region confirms the importance of maximizing the middle fraction of the PSD that was reported earlier (Coetzer and Keyser, 2004). Therefore, the 35 × 4 mm PSD is contained in the 90% confidence region for maximizing pure gas yield and minimizing its variance simultaneously, confirming the narrower fraction to be the optimal PSD for the coal feed. Note that the broader 70 × 4 mm PSD is very remote from the 90% confidence region, indicating its suboptimality according to the criterion.

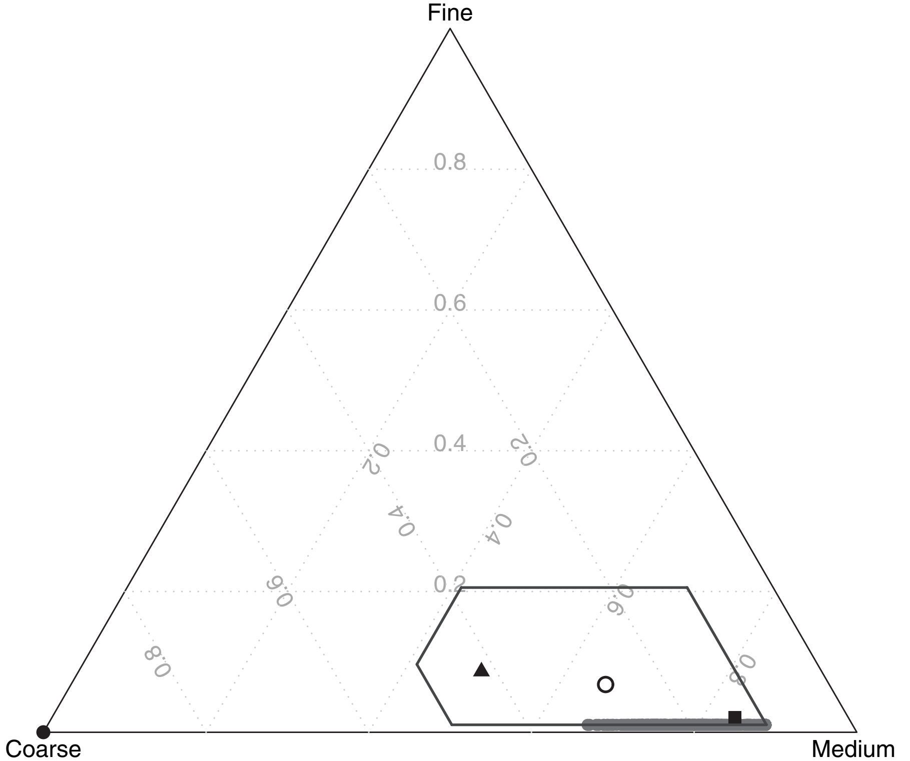

Fig. 3. Confidence region in the coal PSD for the $W(g)$ criterion with $(d_\mu, d_\sigma) = (0, 0)$ and $\lambda = 0.574$ (●, 90% confidence region; ■, 35 × 4 mm PSD; ▲, 70 × 4 mm PSD; ○, 50 × 5 mm PSD)

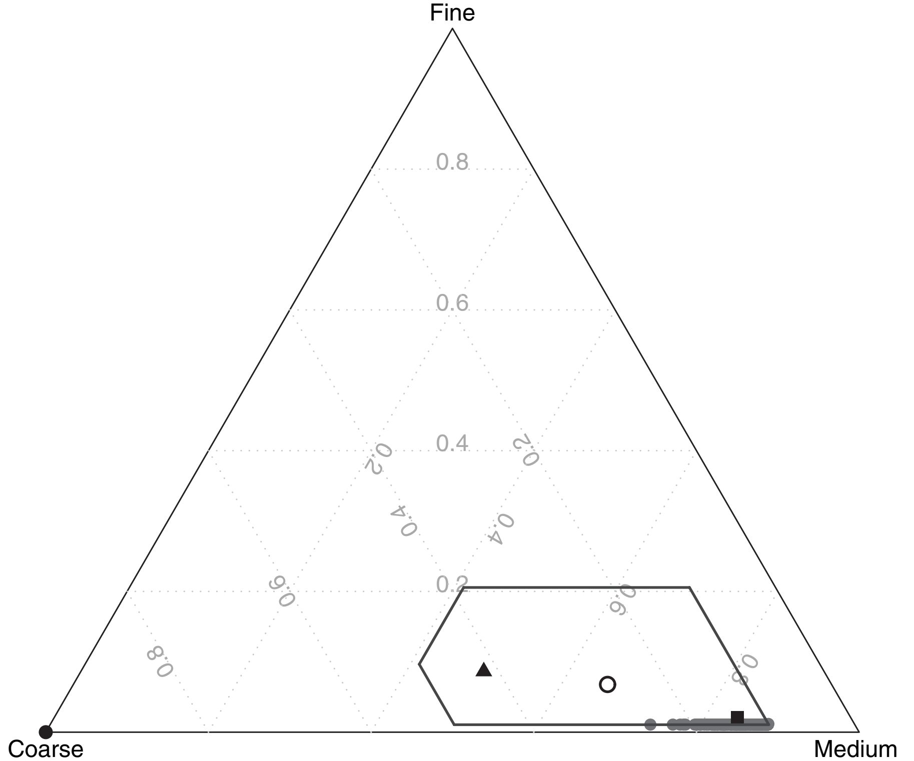

Fig. 4. Confidence region in the coal PSD for the $W(g)$ criterion with $(d_\mu, d_\sigma) = (5, 5)$ and $\lambda = 0.554$ (●, 90% confidence region; ■, 35 × 4 mm PSD; ▲, 70 × 4 mm PSD; ○, 50 × 5 mm PSD)

6. Robustness studies on gasifier performance variables: coal properties as hard-to-control variables

In Section 5 we discussed the results for maximizing gasifier performance given the variability or uncertainty in the coal PSD. The results in Tables 2–4 indicate that there are very little differences between the optimum solutions for the coal properties. In other words, the coal composition does not vary much under different DRS optimizations and it should be possible to recommend an optimal coal composition. However, seven coalmines service the factory, and because of mining, operational and coal preparation difficulties it is impossible to blend coal from seven sources according to an exact coal composition. Consequently, variability is evident in any prepared coal composition. Therefore, since the coal composition is hard to control or impossible to control during normal operation, it is very important to conduct robustness studies to evaluate the effect of the variability in the coal properties on gasifier performance. The aim here is to determine the optimum conditions which maximize the pure gas yield production and simultaneously minimize its variance due to the variability that is transmitted through the coal properties.

The model for the process variance is calculated from model (4) where $I_z(x, z, w)$ is a vector consisting of the derivatives of model (17) to the six coal properties, $z_i, i = 1, \ldots, 6$. The variance–covariance matrix S_z is given in equation (8). From model (17), $\hat{Y}_{\mu|z}(x, z, w)$ can be calculated for given process conditions, such as the composition from a specific coal source. Correspondingly, the process variance $\hat{Y}_{\sigma|z}(x, z, w)$ can be calculated from model (17) by using model (4). Note that $\hat{Y}_{\sigma|z}(x, z, w)$ is a function of the PSD size fractions alone since model (17) does not contain interactions between the coal properties and the loads and CO_2 in RG. Therefore, it is possible to determine conditions of the coal PSD that yield maximum pure gas yield production and minimum process variance simultaneously, given the variability in the coal properties.

Since it was shown in Section 5 that the weighted membership function gave the best results with high desirability for both the variance and the deviation from the target, we shall discuss only criterion (13) in this section. Table 5 depicts the results for the weighted membership function criterion (13) for various values of d_μ and d_σ in expression (10), using the variance of the coal properties. The optimum weights were determined from the efficiency curve. The optimal standard deviation of the pure gas yield $\hat{Y}_{\sigma|x}$ is much higher compared with those in Section 4 because of the much higher variance of the coal properties. However, the optimal pure gas yield is also much lower than those in Table 4. Therefore, the desirability for the various criteria is much lower compared with those in Table 4, indicating that it is much more difficult to satisfy the targets for the pure gas yield and its variance.

The optimal coal PSD in Table 5 is also very different from the results in Table 4 for all the exponential parameters of the membership function. In this case, the optimal PSD is typical of a 50×5 mm PSD. This is again a narrow PSD with an approximate ratio of 10:1 for top:bottom size, but with a slightly higher bottom size and top size compared with the 35×4 mm PSD. This is a very important result for the factory because it specifies the optimal PSD for obtaining high pure gas yield which is robust against the variability in the coal composition. However, it must be noted that the optimal pure gas yield is lower for the 50×5 mm PSD compared with the finer 35×4 mm PSD.

Table 5. Comparison of optimum results for the weighted membership function criterion (13) for various values of d_μ and d_σ in expression (10), using the variance of the coal properties

Variable	*W(g) for the following values of* (d_μ, d_σ)*:*				
	(0, 0)	*(2.5, 2.5)*	*(2.5, 5)*	*(5, 2.5)*	*(5, 5)*
Weight (λ)	0.582	0.678	0.745	0.43	0.607
Coarse coal	0.298	0.302	0.321	0.287	0.297
Medium coal	0.638	0.635	0.618	0.648	0.639
Fine coal	0.064	0.063	0.061	0.064	0.064
Load (coded)	−0.362	−0.393	−0.487	0.064	−0.342
CO_2 (coded)	−1.000	−1.000	−1.000	−1.000	−1.000
Water (%)	5.128	5.128	5.128	5.128	5.128
Ash (%)	28.128	28.128	28.128	28.128	28.128
Carbon (%)	53.978	53.978	53.978	53.978	53.978
Hydrogen (%)	1.193	1.193	1.193	3.123	1.193
Nitrogen (%)	1.303	1.303	1.303	1.303	1.303
Oxygen (%)	9.273	9.273	9.273	7.343	9.273
$\hat{Y}_{\mu\|x}$ (m^3 n ton^{-1})	1499.460	1500.367	1505.963	1493.618	1499.047
$\hat{Y}_{\sigma\|x}$ (m^3 n ton^{-1})	29.793	29.899	31.112	29.541	29.753
$\|\hat{Y}_{\mu\|x} - T\|$	130.540	129.633	124.037	136.382	130.953
$\sqrt{}$MSE	133.896	133.037	127.879	139.545	134.291
$m(g_{\mu\|x})$	0.604	0.851	0.861	0.953	0.957
$m(g_{\sigma\|x})$	0.551	0.812	0.923	0.822	0.943
Criterion value	0.582	0.838	0.876	0.878	0.952

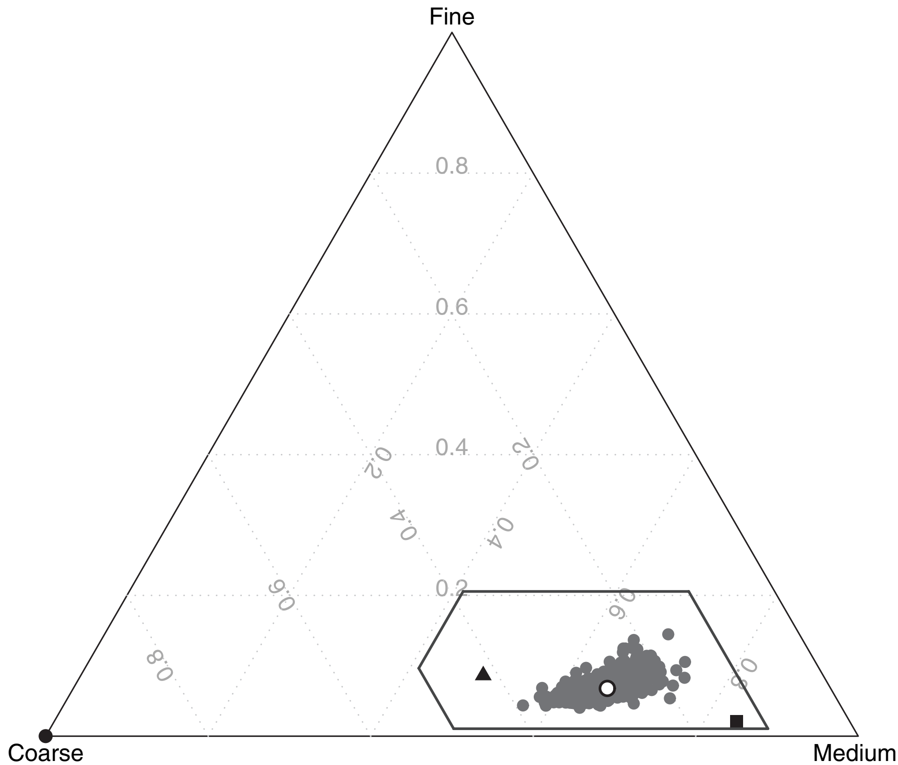

Fig. 5. Confidence region in the coal PSD for the $W(g)$ criterion with $(d_\mu, d_\sigma) = (0, 0)$ and $\lambda = 0.582$, using the variance of the coal properties (●, 90% confidence region; ■, 35 × 4 mm PSD; ▲, 70 × 4 mm PSD; **o**, 50 × 5 mm PSD)

Fig. 5 depicts the 90% confidence region for the coal PSD for the $W(g)$ criterion with $(d_\mu, d_\sigma) = (0, 0)$ and $\lambda = 0.582$, obtained from 1000 bootstrap replications. The shift in the optimal PSD is clearly demonstrated compared with Fig. 3. The average 50 × 5 mm PSD is also indicated in Fig. 5 and is contained in the 90% confidence region, which confirms that it is the optimal PSD for high pure gas yield which is robust against the variability in coal composition. For the coal PSD as the hard-to-control variables, the 50 × 5 mm PSD is remote from the 90% confidence region in Figs 3 and 4. Fig. 6 depicts the 90% confidence region for the coal PSD for the $W(g)$ criterion with $(d_\mu, d_\sigma) = (5, 5)$ and $\lambda = 0.607$. The 90% confidence region is basically the same as in Table 5.

7. Conclusions

DRS optimization was performed to determine the optimum operating conditions for maximizing gasifier performance. Gasification performance was studied in terms of the pure gas yield and its variance. The response surface method was employed to construct a response surface model for the pure gas yield and to calculate its variance propagated through the model due to the variability in the hard-to-control variables. Two types of evaluations were performed, i.e. coal PSD was considered as hard to control and coal composition as controllable, and coal composition as hard to control and PSD as controllable. Several DRS strategies were evaluated for determining the optimum coal PSD, coal composition, oxygen load and CO_2 in RG levels which maximize the pure gas yield and simultaneously minimize its variance.

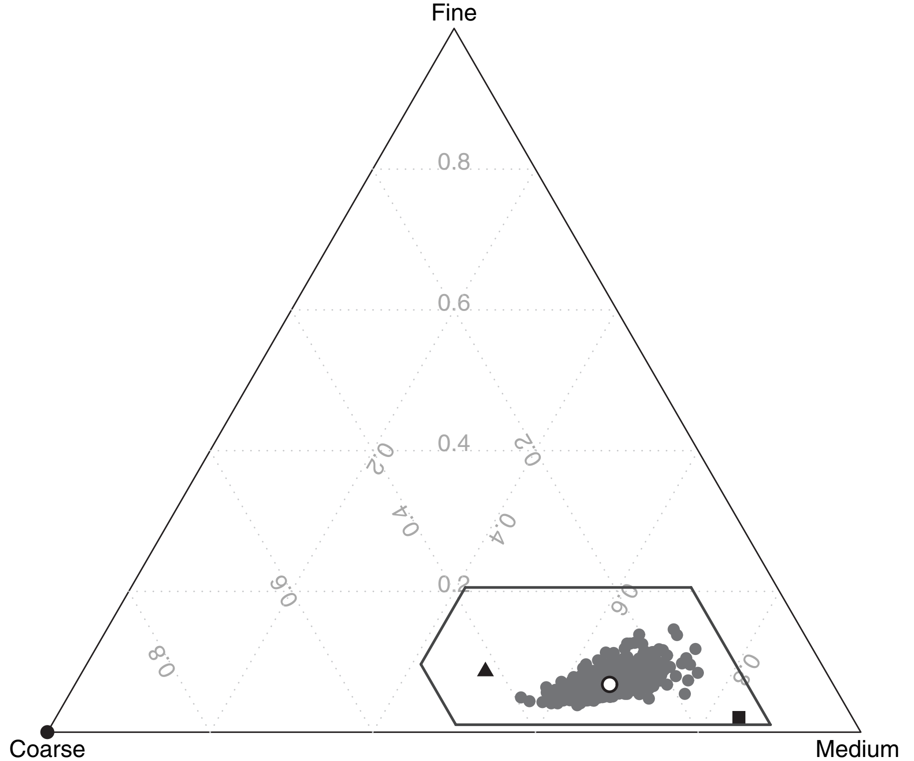

Fig. 6. Confidence region in the coal PSD for the $W(g)$ criterion with $(d_\mu, d_\sigma) = (5, 5)$ and $\lambda = 0.607$, using the variance of the coal properties (●, 90% confidence region; ■, 35 × 4 mm PSD; ▲, 70 × 4 mm PSD; o, 50 × 5 mm PSD)

For the PSD as hard-to-control variables, it was shown that a 35×4 mm PSD is optimal for maximizing gasifier performance. This is in agreement with previous reports (Coetzer and Keyser, 2004; Keyser *et al.*, 2005). Keyser *et al.* (2005) claimed that a 2.5–3% increase in pure gas yield is expected from running the Sasol–Lurgi fixed bed dry bottom gasification process on split feed sizes, i.e. the maximum number of gasifiers on a 35×4 mm PSD and the remainder on a 70×35 mm PSD. Controlling the PSD can be accomplished at a marginal cost with efficient screening of the run-of-mine coal. However, controlling coal composition and accurate blending from seven coal sources are very difficult and can only be achieved marginally at considerable costs to the business. For coal composition as hard-to-control variables, it was shown that a 50×5 mm PSD is optimal for maximizing the pure gas yield and simultaneously minimizing its variance. Therefore, controlling the PSD with a 50×5 mm fraction predicts maximum gasification throughput which is robust against the variability in coal composition. Therefore, the feasibility and performance of the 50×5 mm PSD will be tested on commercial scale.

It was shown that the weighted membership function approach, where the optimal weight is determined from the efficiency curve, gives the best overall results with high desirability for both the pure gas yield and its variance. This study emphasizes the importance of statistical experimental design and response surface modelling on a full-scale production plant for process and product improvement and optimization. The methods and results that are presented in this paper provide practical evidence that the DRS approach is a powerful method for performing robustness studies.

Future work includes the evaluation and optimization of the Sasol–Lurgi fixed bed dry bottom gasification process in terms of additional performance indicators, such as utilities and RG composition. Specifically, the gasification process must be optimized to be robust against the variability in coal composition for all the performance indicators.

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