Optimal Purchasing of Raw Materials: A Data-Driven Approach

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An approach to the optimal purchasing of raw materials that will achieve a desired product quality at a minimum cost is presented. A PLS (Partial Least Squares) approach to formulation modeling is used to combine databases on raw material properties and on past process operations and to relate these to final product quality. These PLS latent variable models are then used in a sequential quadratic programming (SQP) or mixed integer nonlinear programming (MINLP) optimization to select those raw materials, among all those available on the market, the ratios in which to combine them and the process conditions under which they should be processed. The approach is illustrated for the optimal purchasing of metallurgical coals for coke making in the steel industry. However, it is well suited to many similar problems such as the purchasing of crude oils for refining, of ingredients for processed foods and of polymeric materials to blend into functional polymers. © 2008 American Institute of Chemical Engineers *AIChE J,* 54: 1554–1559, 2008
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Introduction

In the development and manufacture of most products an important decision is the selection and purchase of a suitable set of raw materials to be used. At the development stage for a new product, this selection of starting materials, together with the formulation (ratios) in which to combine them, and the process conditions under which to manufacture the desired product must all be decided.[1] Once the manufacturing process is operational there are still many reasons where one needs to reconsider the selection of different raw materials. These include the following:

(i) Changing prices of raw materials make alternative suppliers more attractive;

(ii) New materials become available on the market place that may offer a cost and quality advantage;

(iii) Replacement materials may be needed because currently used materials may no longer be available due to discontinuation, seasonal factors, etc.;

(iv) A change in attributes of the final products may be desired and can only be achieved with material having a different balance of raw material properties;

Some industrial examples where these issues arise include the following:

(i) The manufacture of coke in steel-making typically involves processing a blend of three or four metallurgical coals in coke ovens. The choice of suitable blends of the coals available at any given time that will yield the desired coke properties at minimum cost is important. This is the illustrative example treated later in this article.

(ii) An almost identical problem is the purchase of crude oil for refining into a slate of different products. Depending upon the attributes of the crude, the desired product slate from the refinery (time varying), and the processing capabilities of the refinery, certain crude oils may be or may not be suitable at an economical price, or may not be able to be used with blends of existing crude in storage at the refinery.

(iii) In the manufacture of functional polymer blends to have specific properties, there are wide choices of rubbers, polyolefins, and oils that can be used. On the basis of the properties of the rubbers, polyolefins and oils and the formulation ratios used, there are only certain combinations of

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these materials that will give the desired product at a reasonable cost.[1]

(iv) The processing of foods into consumer products with desired taste, texture and stability properties at the best cost requires the correct selection of appropriate ingredients from various suppliers.

In this article, we present a data-based approach to treating this problem of raw material selection based on the use of databases on (i) the properties of available raw materials, (ii) previous formulations used by the company, and (iii) processing conditions used in the past. Latent variable Partial Least Squares (PLS) regression methods are used to extract the information from these diverse databases and to provide the necessary models in an optimization framework to find an optimal set of materials. Muteki et al.[1,2] developed some of these methods for the rapid development of new products under the guise of product engineering. They also considered the design of experiments to generate the databases required for such development modeling.[3] In this article, we focus on the use of the methods for the optimal purchasing of alternative raw materials for existing processes and products, and illustrate it with a case study on the purchasing of coals for coke making in the steel industry.

Methodology

Data structure

The data structure is shown in Figure 1 for the case of blends of one class of raw materials (as is the case in the selection of coals for coke making and crude oils for refining). (The case for multiple classes of materials is discussed in Muteki et al.[1])

The data consist of raw material property databases ($\mathbf{X}_{DB}$ and $\mathbf{X}^T$) and data from manufacturing operations ($\mathbf{Z}$,$\mathbf{R}$ and $\mathbf{Y}$). The latter consists of a ($M \times N$) $\mathbf{R}$ matrix containing the ratios of all the materials (or more precisely, their mass fractions) used in the formation of blends ($0 \le r_{i,j} \le 1$, and $\sum_{j=1}^{N} r_{i,j} = 1$), the ($M \times J$) process operating conditions ($\mathbf{Z}$) used to process these formulations, and an ($M \times L$) $\mathbf{Y}$ matrix containing L properties measured on the final products. M is the number of past blends, and N is the total number of all the raw materials used in the blends. $\mathbf{X}_{DB}$ is the

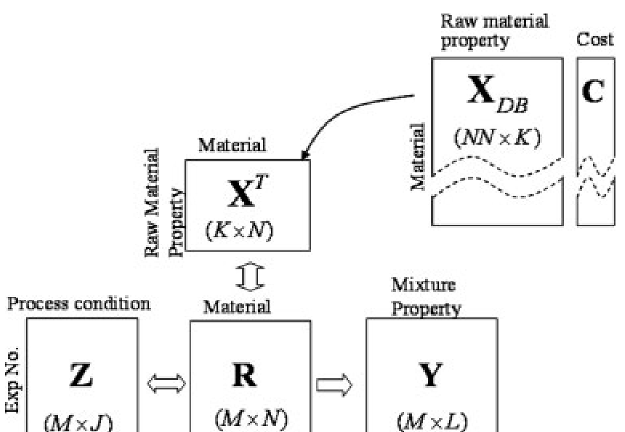

Figure 1. Structure of a typical database for a single class of raw materials (e.g. coals, crude oils).

($NN \times K$) data base matrix containing properties on all the available raw materials (including both those used and not used in the past). K is the number of raw material properties and $\boldsymbol{NN}$ is the number of the available raw materials. $\mathbf{X}^{\mathrm{T}}$ is the ($K \times N$) matrix of raw material property data for the N materials actually used in past formulations ($\mathbf{R}$) and often is a subset of the materials from $\mathbf{X}_{\mathrm{DB}}$. Some property data in the $\mathbf{X}_{\mathrm{DB}}$ matrix can be often obtained from suppliers of the raw materials, but in many cases additional measurements may have to be measured inside the company in order to more uniquely define the materials. The situation where certain raw material property measurements are not available for some of the raw materials in $\mathbf{X}_{\mathbf{DB}}$ is treated by Muteki et al.[4] where the missing data is treated via efficient missing data imputation methods. An ($NN \times 1$) matrix $\mathbf{C}$ of costs is assumed to be available for all the materials in the database.

Product formulation modeling using PLS

Mixture-property modeling based on ideal mixing rules was presented in Muteki et al.[1,3] The model is expressed as

$$\mathbf{Y} = f(\mathbf{X}_{\mathrm{mix}}) + \varepsilon \tag{1}$$

where $\mathbf{X}_{\mathbf{mis}}$ ($= \mathbf{R}\cdot\mathbf{X}$) represents the properties of the blend of materials based on ideal mixing rules. The mixture-property PLS model of Eq. 1 represents the relationship between the blend rule raw material properties ($\mathbf{X}_{\mathrm{mix}}$) and the final product blend properties ($\mathbf{Y}$). If the process operating conditions ($\mathbf{Z}$) change between process runs, then the effect of these changes is easily accounted for by incorporating $\mathbf{Z}$ into the model as follows:

$$\mathbf{Y} = f(\mathbf{X}_{\mathrm{mix}}, \mathbf{Z}) + \varepsilon. \tag{2}$$

If ideal mixing rules are not applicable then any other known rules can be used to combine the $\mathbf{X}$ and $\mathbf{R}$ matrices. Alternatively, nonlinear multiblock PLS models have been presented[2] to effectively handle nonlinearities in either the mixing rules or in the process or both. The concepts developed in this article will be unaltered by the use of either the ideal mixing PLS model or the nonlinear mixture-property PLS models, and therefore the remainder of the article is based on the simpler models based on ideal mixing (this works well in the coke making problem discussed later).

PLS regression modeling is used in this article to model the relationships in Eqs. 1 and 2 due to the fact that the matrices $\mathbf{X}$, $\mathbf{X}_{\mathrm{DB}}$, $\mathbf{R}$, and $\mathbf{Y}$ are often quite ill-conditioned and often have many missing values.[4] PLS models[5] easily handles these two situations.[6] Prior to modeling, the matrices $\mathbf{Z}$, $\mathbf{X}_{\mathrm{mix}}$, and $\mathbf{Y}$ are usually mean centered and scaled to unit variance. The mean centering is performed since we define a model only in the vicinity of the data, and scaling is performed to account for differences in the units of measurements of the different variables. PLS regression is performed by projecting the augmented matrix $\mathbf{X}_{\mathrm{aug}} = [\mathbf{Z}, \mathbf{X}_{\mathrm{mix}}]$ and $\mathbf{Y}$ onto lower dimensional latent variable subspaces

$$\begin{aligned} \mathbf{X}_{\mathrm{aug}} &= [\mathbf{Z}\,\mathbf{X}_{\mathrm{mix}}] = \mathbf{T}\,\mathbf{P}^{\mathbf{T}} + \mathbf{E} \\ \mathbf{Y} &= \mathbf{T}\,\mathbf{Q}^{\mathbf{T}} + \mathbf{F} \end{aligned} \tag{3}$$

where the A columns of $\mathbf{T}$ are values of $A \ll (J + K)$ latent variables ($\mathbf{T} = [\mathbf{Z}\ \mathbf{X}_{\mathrm{mix}}]\mathbf{W}^*$) that capture most of the variability in the data; **W***, **P**, and **Q** are the loading matrices, and **E** and **F** are residual matrices. The PLS loading matrices are obtained by maximizing the covariance between [**Z X**$_{\text{mix}}$] and **Y**.[7,8]

For any new (1 × (*J* + *K*)) vector of J process conditions and K mixture properties $x^T_{\text{aug new}} = [z^T_{\text{new}}\ x^T_{\text{mix new}}]$ one can compute a (1 × *A*) vector of new latent variable scores as $\tau^T_{\text{new}} = [z^T_{\text{new}} \quad x^T_{\text{mix new}}]\mathbf{W}^*$ and then predict the (1 × *M*) vector of blend properties as $\hat{y}^T_{\text{new}} = \tau^T_{\text{new}}\mathbf{Q}^T$. One can also compute two distance criteria to test the validity of the model for the new conditions. The Hotelling's T^2 is expressed as

$$T^2 = \sum_{a=1}^{A} \frac{\tau^2_{\text{new}.a}}{S^2_a} \tag{4}$$

where S^2_a is the variance of the *a*-th latent variable score vector in the matrix **T**, and *A* is the selected number of latent variables in the PLS model. It provides a measure of the distance from the center point in the latent space to the projection of the new observation onto the latent variable space. The SPE (square prediction error) of the new vector of conditions and properties ($x_{\text{aug new}}$) is expressed as

$$SPE_{\text{xnew}} = \sum_{i=1}^{J+K} \left(x_{\text{aug new},i} - \hat{x}_{\text{aug new},i}\right)^2 \tag{5}$$

where $\hat{x}^T_{\text{aug new}} = x^T_{\text{aug new}}\mathbf{P}^T\mathbf{P}$ is the predicted value of $x^T_{\text{aug new}}$ estimated from the PLS model. The SPE provides a measure of the orthogonal distance (residual) of the new point from the latent variable model space. A large residual implies that the PLS model is not valid in the region of $x^T_{\text{aug new}}$.

Optimization based on the PLS models

In this section, we assume that the required data are available and a PLS model between $\mathbf{X}_{\text{aug}}$ = [**Z X**$_{\text{mix}}$] and the final product quality **Y** has been built. It is also assumed that the PLS model explains a sufficient percentage of the variability in **Y** to allow for adequate prediction. The objective is now to use this model to simultaneously optimize the selection of the raw materials, their blend ratios and the processing conditions in order to achieve the desired final property vector y_{des} with a minimum total raw material cost and the minimum number of raw materials. The formulation of the optimization is expressed as:

$$\begin{aligned}
&\underset{r_{\text{new}},z_{\text{new}}}{\text{Min}} \left(y_{\text{des}} - \hat{y}_{\text{PLS}}\right)^T \cdot W_1 \cdot \left(y_{\text{des}} - \hat{y}_{\text{PLS}}\right) + w_2 \cdot \sum_{j=1}^{NN} r_{\text{new},j} \cdot c_j + w_3 \cdot \sum_{j=1}^{NN} \delta_j \\
&s.t. \\
&\text{Ideal mixing rule} \quad \left\{ x^T_{\text{aug new}} = [r^T_{\text{new}} \cdot \mathbf{X}_{\text{DB}} z^T_{\text{new}}] \right. \\
&\text{Y Estimation} \quad \begin{cases} \hat{y}_{\text{PLS}} = Q \cdot \tau_{\text{new}} \\ \tau_{\text{new}} = x^T_{\text{aug new}} \cdot W^* \end{cases} \\
&\text{Hard Constraints on variables} \quad \left\{ \text{Lo}_{\text{PLS},l} \le \hat{y}_{\text{PLS},l} \le Hi_{\text{PLS},l},\ Lo_{\text{aug new},k} \le x_{\text{aug new},k} \le Hi_{\text{aug new},k} \right. \\
&\text{PLS model constraint} \quad \begin{cases} \text{SPE}_{\text{new}} = \sum_{k=1}^{k=(K+J)} \left(x_{\text{aug new}} - \hat{x}_{\text{aug new}}\right)^2 \le \varepsilon \\ T^2_{\text{new}} = \sum_{a=1}^{A} \frac{\tau^2_{\text{new},a}}{S_a} \le T^2_{\max} \end{cases} \\
&\text{Mixture constraint} \quad \left\{ \sum_{j=1}^{NN} r_{\text{new},j} = 1,\ 0 \le r_{\text{new},j} \le 1 \right. \\
&\text{Binary variable constraint} \quad \begin{cases} \delta_j = \begin{cases} 1 & r_{\text{new},j} > 0 \\ 0 & r_{\text{new},j} = 0 \end{cases} \\ r_{\text{new},j} \le M_j \delta_j \end{cases}
\end{aligned} \tag{6}$$

where r_{new} is a (*NN* × 1) vector containing the new mixture ratios of all the raw materials available on the database $\mathbf{X}_{\text{DB}}$, z_{new} is a (*J* × 1) vector of new process conditions, y_{des} is the (*L* × 1) vector of desired final product properties, c_j is the cost of raw material *j*, δ_j is the binary variable (0,1) that indicates if material *j* is used, M_j (≤ 1.0) is an upper limit on the allowable ratio for material *j* (*so-called "big*-M"),[9] W_1 is a diagonal weighting matrix providing the relative importance of each blend property, w_2 is a penalty value on the total material costs and w_3 is a penalty value on the total number of raw materials used, $Lo_{\text{PLS},l}$ and $Hi_{\text{PLS},l}$ are lower and upper limits on *y*, and $Lo_{\text{aug new},k}$ and $Hi_{\text{aug,new},k}$ are lower and upper limits on the elements of $x^T_{\text{aug new}} = [x^T_{\text{mix new}}\ z^T_{\text{new}}]$. The optimization is performed over the mixture ratio vector r_{new} and the process conditions z_{new}. The constraints on SPE_{new} and Hotelling's T^2_{new} forces the solution to lie near the space of the PLS model. The $T^2_{\max}$ value in the T^2_{new} constraint may be taken as the 95 or 99% limit on T^2 from the training data depending on how far from the training data one is willing to extrapolate. The ε value in the SPE constraint can range from zero (perfect adherence to the model) up to some larger value such as the 95% limit on the SPE values from the training data. A larger ε value may be needed when constraints are being imposed on the elements of y_{new} and $x_{aug\ new}$ to allow for the possibility of slight extrapolations of the model in order to satisfy these.

The first term of the objective function is a weighted measure of the estimation error between the desired product properties and the estimated properties through the mixture PLS model. The new raw material properties $x_{mix\ new}$ are estimated based on the ideal mixing rule between r_{new} and $\mathbf{X}_{DB}$. The second term in the objective function refers to the total raw material cost of the mixture. The third term in the objective function penalizes the total number of raw materials used to obtain the blend, since it is usually desirable to use a minimum number of materials. Since the binary variable δ_j is involved, this is a mixed integer quadratic optimization.

Solutions to these MINLP problems were obtained using the branch and bound algorithm[10,11] in GAMS/SBB.[9] This approach was found to work much better than the GAMS/DICOPT[9] on this problem. If the total number of raw materials is not penalized (last term in the objective function of Eq. 6), a solution can be obtained by a much easier sequential quadratic programming (SQP) approach[12] (MATLAB and GAMS/MINOS were used). If the cost term in the objective function of Eq. 6 is also omitted then this SQP approach will give unacceptable solutions having small amounts of a large number of raw materials. However, it was found that due to different material costs, when this cost term was included, the simpler SQP approach almost always resulted in solutions with only a small number of raw materials. In this study, solutions were found using both SQP and MINLP approaches.

Optimal Purchasing of Coals for Coke Making

Cokes are manufactured from blends of several different types of metallurgical coals (usually 3–5) processed in coke ovens. The objective is to make cokes with a set of desired final properties (y_{des}), at minimum cost, and satisfying certain safety conditions while using any combination of the available coals on the market. The question is which combinations of available coals should be purchased, given the current inventories available at the purchasing company and the current costs of the coals. In general, the ratios in which the coals are blended (r) and the coke oven operating conditions (z) will also affect the final coke properties (y) and so as shown in Eq. 6, the optimization is performed simultaneously over the ratios for all possible coals and the coke oven conditions. The optimization may need to be run frequently because

(i) Coal prices fluctuate frequently due to supply and demand.

(ii) All coals are not always available for various reasons. For example some coals are not available in the winter months due to shipping limitations, and so replacement coal blends have to be found.

(iii) New coals become available as new mines open and it is of interest to see if these can be used in achieving good blends.

(iv) The desired coke properties, or their constraints, or the safety limits on the coal mixtures may change.

Data bases and mixture-property PLS model

The industrial data (supplied by Dofasco, Hamilton, ON) consisted of (refer to Figure 1) a (54×20) coal property data base $\mathbf{X}_{DB}$ with 20 measured properties on 54 available coals, a cost vector **c** of costs for each of these coals at a given snap-shot in time, a (54 × 17) coal property matrix **X** on 17 coals that had actually been used by the company in the past, a (63 × 17) corresponding blend ratio matrix **R** containing the ratios in which the 17 coals had been blended during 63 coke oven runs in the past, and a (63 × 3) coke property matrix **Y** containing 3 critical coke and coke oven properties measured on the 63 coke runs. A (63 × J) matrix of coke oven operating conditions **Z** was also available for the 63 runs, but these conditions were almost constant and so are not treated in this study.

A mixture-property PLS model of the form of Eq. 3 were built from these databases based on ideal mixing rules. The fraction of the sum of squares of the three response variables explained by the fitted model was $R^2 = 0.71$ using 4 PLS latent variables. The resulting PLS model revealed relationships between $\mathbf{X}_{mix}$ and **Y** that were quite consistent with the experienced scientists knowledge. Score (t_1 vs. t_2) and loadings (w_1^* vs. w_2^*) plots for the first two dimensions of the model are shown in Figure 2. The score plot (b) clearly

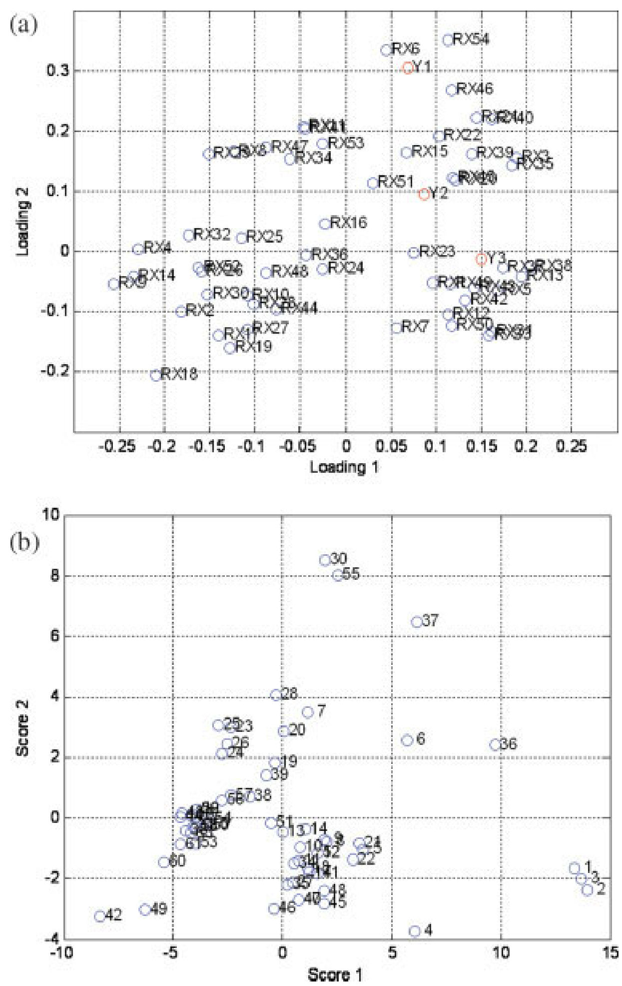

Figure 2. Plots of (a) the loadings (w_1^* vs. w_2^*) and (b) the scores (t_1 vs. t_2) for the first two latent variable dimensions of the PLS mixture model.

[Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

Table 1. Two Existing Coal Formulations Used for Coke Production

	Existing Coals and Ratios				Cost	Mixture Constraint	Final Coke Properties		
1	Coal1	Coal2	Coal4	Coal14		RX54	*Y*1	*Y*2	*Y*3
	30	25	25	20	7550	−12	1.2	61.9	59.7
2	Coal1	Coal4	Coal6	Coal14					
	30	30	20	20	7560	−9.3	0.88	60.6	61.7

Shown are the coal type, ratios in which they are blended (as weight percents), total cost of the formulation, and final coke properties and safety condition on the mixture.

shows which coal mixtures and their resulting cokes were very similar or very different (cokes with score values close together in the plot will be very similar, while those with score values far apart will be quite different). For example cokes 1, 2, and 3 are very similar as are cokes 30 and 55, and cokes 42 and 49. However, these grouping of cokes have properties quite different from each other. The loadings plot in (a) reveals why these coke grouping are different. For example, cokes 30 and 55 (with high t_2 values) are mainly different from other cokes due to having high values of Y_1 and being made from coal blends with high values of coal mixture properties such as RX_6 and RX_{54}.

Optimization results

Several examples of the optimal selection of coals for manufacturing coke to satisfy final coke property constraints and to satisfy coke oven safety constraints and do so at minimum cost are presented to illustrate the methodology. The general optimization problem was posed in Eq. 6. However, here not all the terms in that general formulation are necessary. In this problem there is no desired target value for the 3 *Y* properties, only inequality constraints:

$$Y1 < 1.5, \quad Y2 > 60, \quad Y3 > 60. \tag{7}$$

Therefore the first quadratic term in the objective function (6) drops out. There is also a safety constraint related to the coke oven operation that could be expressed in terms of property number 54 for the final mixture of coals as

$$r_{\text{new}}^{T} \, x_{\text{DB},54} \leq -7.0. \tag{8}$$

The constraint ε on the SPE was taken as zero, and the $T^2_{\max}$ limit on Hotelling's T^2 as the 95% limit from the training data set. This forces a solution to exactly satisfy the PLS model ($\varepsilon = 0$) and to lie within the latent variable region of the training data.

Table 1 shows two of the existing coal formulations used by the company for manufacturing the coke. Shown in the table are the specific coals used, the formulation ratios used, the total cost of that formulation, the final coke properties (y_1, y_2, y_3) and the coal mixture safety property achieved.

Table 2 shows the results of running the optimization over all available coals in $\mathbf{X}_{\text{DB}}$, including both those coals that had been used by the company in the past as well as those that had never been used before by the company. Four alternative optimal formulations are shown in Table 2 each using a different number of coals and having a different final cost. These alternative solutions were obtained by altering the ratio of weight w_2/w_3 in the objective function (6), thereby trading off cost against the desire for a smaller number of coals. Each of the new coal formulations is predicted not only to achieve the required product quality and satisfy the safety requirement, and to do so at a lower cost than the two existing formulations shown in Table 1. By providing these alternative solutions the company personnel could select their preference, taking into account other intangibles such as the reliability of suppliers. Also, from a business viewpoint, it is very important for the company to know such alternative solutions in advance, because their business situation can often change suddenly.

A major problem in Canada is that certain coals that are readily available in the summer are not available in the winter. This is the case with coals 1, 3, 6, 14. Solution C in Table 2 already provides a solution that does not use these coals. However, another optimization was performed with these four coals excluded from the database. The result, with a lower cost (but more coals) than solution C, is shown in Table 3. Note that, due to the unavailability of coals 1 and 14, the total formulation cost has increased over most of those in Table 2 (which use coal 14), but is still projected to be lower that the two existing formulations in Table 1 (which use coal 1 and 14).

Table 2. Optimal Solutions for Coal Blending in the Manufacture of Coke

	Selected Coals & Ratios				Cost	Mixture Constraint	Final Coke Properties		
A	Coal2	Coal4	Coal14			RX54	*Y*1	*Y*2	*Y*3
	32.68	56.74	10.58		7206.67	−11.288	0.786	63.912	60
B	Coal2	Coal4	Coal10	Coal14					
	30.011	58.24	3.365	8.385	7207.4	−10.796	0.932	63.689	60.312
C	Coal2	Coal4							
	32.33	67.67			7364.66	−11.151	0.837	64.293	61.449
E	Coal2	Coal4	Coal8	Coal14					
	28.354	57.233	10.768	3.645	7269.73	−9.424	1.032	62.437	60.097

Optimization is over all available coals. Different solutions are obtained by changes in the weight functions w_2 and w_3 in the objective function (6).

Table 3. Optimal Solution for Coal Blending in the Manufacture of Coke

	Selected Coals & Ratios					Cost	Mixture Constraint	Final Coke Properties		
G	Coal2	Coal4	Coal8	Coal19	Coal20		RX54	*Y*1	*Y*2	*Y*3
	22.278	49.747	11.431	14.231	2.313	7350.29	−8.728	1.5	61.741	61.722

Optimization excludes coals 1, 3, 6 and 14 that are not available in the winter.

Conclusions

A data-driven approach based on property-mixture PLS models is presented for the optimal purchasing of raw materials to achieve a desired product quality at minimum cost. The models are built on databases of the properties of raw materials currently available in the market, and on databases of formulation and manufacturing conditions used in the company's manufacture of past products. These PLS models are then used in an optimization framework to select the best combination of raw materials, the optimal ratios in which to combine them and the process conditions under which to manufacture them.

The methods are illustrated on the industrial problem of the purchase of metallurgical coals for the manufacture of cokes used in steel making. However, they are well suited to many similar problems such as the purchase of crude oils for refining, the purchase of ingredients for the formulation of processed foods, and the purchase of materials for formulating functional polymer blends.

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