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Chapter

Simulation and Optimization of an Integrated Process Flow Sheet for Cement Production

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Abstract

In this study the process flow diagram for the cement production was simulated using Aspen HYSYS 8.8 software to achieve high energy optimization and optimum cement flow rate by varying the flow rate of calcium oxide and silica in the clinker feed. Central composite Design (C.C.D) of Response Surface Methodology was used to design the ten experiments for the simulation using Design Expert 10.0.3. Energy efficiency optimization is also carried out using Aspen Energy Analyser. The optimum cement flow rate is found from the contour plot and 3D surface plot to be 47.239 tonnes/day at CaO flow rate of 152.346 tonnes/day and the SiO_2 flow rate of 56.8241 tonnes/day. The R^2 value of 0.9356 determined from the statistical analysis shows a good significance of the model. The overall utilities in terms of energy are found to be optimised by 81.4% from 6.511 x 10^7 kcal/h actual value of 1.211 x 10^7 kcal/h with 297.4 tonnes/day the carbon emission savings.

Keywords: central composite design, optimisation, response surface methodology, cement production, design expert

1. Introduction

Cement is a fine greyish or whitish inorganic, non-metallic powder commonly used as a binding agent in construction materials. It consists of pyroprocessed chemically combined hydraulic cement materials such as calcareous, siliceous, argillaceous and ferriferous [1]. Cement forms paste when mixed with water, which later becomes hard due to cement, mineral hydrate formation when solidified [2]. The various types of cement and their applications such as Portland, Siliceous fly ash, calcareous, slag and Fume silica cement differ by the amount of SiO_2, Al_2O_3, Fe_2O_3, CaO, MgO, SO_3 and other materials such as Na_2O and K_2O composition [3]. Economic growth and urbanisation have made cement one of the most consumed commodity in world with global annual production increase from 3.3 Gt in 2010 to current 4.1 Gt which is still expected to grow moderately in the next decade due to expected infrastructure development in India and other developing Asian and African countries [4, 5]. Cement production consists of three sections: fuel and raw material processing, production of clinker via pyroprocessing and grinding and

blending of cement clinker nodules with additive materials such as gypsum and anhydrite for different types of cement types [6]. Natural occurring limestone is ground and mixed in required proportion with silicon and aluminium source such as clay and sand and iron-containing compounds to form a homogenous raw mix called raw meal. The raw meal is then pyroproccessed at a high temperature of about 1450 °C in rotary kiln system where it is dried, preheated, calcined and sintered into cement clinker. The pyroprocessing can be dry, wet, semi-dry or semi-wet and their selection depends on the moisture content of the raw meal, rotary kiln configuration and energy cost. The wet process is cheaper with a high-quality product but very high energy intensity because of the high moisture content of about 36% in raw meal. The dry process is usually more compact with low operational cost and energy consumption compared with the wet process but with lesser product homogeneity [2]. The clinker produced is further grinded with about 5% gypsum which prevents pre-set and controls the hydration rate of the cement. Other types of cement are produced by blending with hydraulic, pozzolanic or inert materials [7]. Cement production processes are energy-intensive and generate huge greenhouse emissions with the clinker energy intensity of about 3.4 GJ/t in 2018 [4] generating about 4% of the global CO_2 emission [8]. Strategies identified to reduce the emissions in cement production include improving heat recovery and energy efficiency [9–11], switching to low carbon source of energy [12], feedstock and material substitute [13–15], reducing the clinker-to-cement ratio [16] and advancing technology innovations such as carbon capture and storage [17, 18]. Cement and concrete technology modelling and simulation have also been used to improve energy efficiency and usage [19–22].
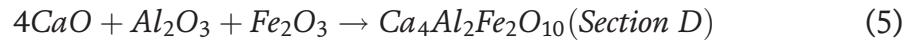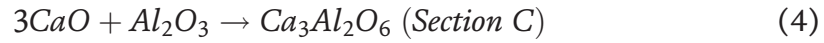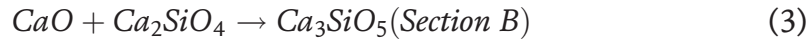
Optimization is a mathematical technique used to find the best solution to objective function (s) by maximising the desired variable and minimising the undesired variables under some set of constraints with the sole aim of improving performance and cost [23]. The optimisation technique in cement and concrete studies can be broadly classified as a meta-heuristic approach and statistical experimental design methods [24]. The meta-heuristic approach is an iterative method that intelligently exploits search space at learning strategies. It includes Genetic Algorithm (GAs), Particle swarm optimization (PSO), Harmony Search (HS), Ant Colony Optimization (ACO), Charged System Search (CSS), Big Bang-Big Crunch (BB-BC), Artificial Bee Colony algorithm (ABC), spherical interpolation of the objective function, Colliding bodies optimization (CBO), Vibrating Particles System (VPS), simulated annealing, krill herd (KH), Whale Optimization Algorithm (WOA), hybrid Harmony Search, force method and genetic algorithm, mine and improved mine blast algorithms [24–26] which are modelled from natural and social behaviours as well as physics laws.

Statistical experimental design methods are widely used to obtain desired optimise solution for a set of constraints [27]. Response Surface Methodology (RSM) is a statistical optimisation technique used to model and analyse a process to determine the effect of independent multivariable on the process response and to evaluate the relations between these variables [28]. RSM is based on understanding the topography of the response surface to determine the most appropriate response region [29]. RSM experimental design can be categorised into Box–Behnken Design (BBD), Central Composite Design (CCD), Dohlert design, Mixture response and three-level factorial design [30–32]. The BBD is created from 3 level factorial design [32] and gives quadratic response model with three minimum number of factors requiring three levels of factors (upper, centre, lower) for each factor and specific positioning of design points [33, 34]. The CCD is developed from the 2 factorial design and gives the quadratic response model with five levels for each factor. Hence it is more robust and insensitive to missing data or experimental runs [34].

In recent years, Response Surface Methodology has been applied to optimise several chemical processes such as extraction [29], adsorption [23], pharmaceutical wastewater treatment [28], leaching [35]. Studies on cement production optimisation have been carried out on clinker simulation using AspenTech [36], cement raw materials blending using a general nonlinear time-varying model [37], cement grinding using population balance model [6], clinker chemistry and kiln energy efficiency using metaheuristic optimization techniques [38], numerical and computational fluid dynamics study of cement calciner [16]. RSM has been efficient and accurate in studies on cement and concrete technology [39–43]. This study focused on the simulation of an integrated wet cement process flow sheet using Aspen HYSYS and optimisation of the cement production rate at minimum raw material feed using CCD of response surface methodology.

2. Methodology

2.1 Cement production simulation

Aspen HYSYS 8.8 was used for the steady-state simulation of the integrated process flow sheet for the cement production [44]. Within the simulation environment, topological optimization (proper arrangement of equipment) was done to enable very high energy savings or optimization. A pure component such as water, CO_2 and air are added as conventional components, while non-conventional components are added as hypothetical components to the HYSYS environment based on their physical properties (molecular weight & density). **Figure 1** shows the block diagram of the production of cement while the HYSYS process flow diagram for the cement production simulation is shown in Figure A1 in the appendix. Limestone is decomposed in the first reactor to give off CO_2 as gas, while the produced CaO is the feed to the Section A reactor to react with silicate to form Calcium disilicate. The produced Calcium disilicate reacts further with the unreacted CaO in reactor B to produce Calcium trisilicate. Calcium oxide (CaO) further reacts with Aluminium oxide to produce tricalcium aluminate, another constituent of cement, while the final product component is produced in section C, where CaO reacts with Aluminate and Ferric oxide to produce tetracalciumaluminoferrite. These separate

Figure 1.
Process flow diagram for the production of cement.

components produced at a different section of the simulated Kiln are mixed to achieve a matrix compound of the cement product, having over 70% of CaO.

2.2 Aspen Hysys simulation

Aspen Hysys was used for the steady-state simulation of the integrated process flow sheet for the cement production. Within the simulation environment, topological optimization (proper arrangement of equipment) was done to enable very high energy savings or optimization. A pure component such as water, CO_2 and air are added as conventional components, while non-conventional components are added as hypothetical components to the HYSYS environment based on their physical properties (molecular weight and density). Based on the process description, the different reactions taking place in each simulated reactor, as presented in the flowchart are:

$$CaCO_3 \rightarrow CaO + CO_2 (Limestone\ decomposition) \tag{1}$$

$$2CaO + SiO_2 \rightarrow Ca_2SiO_4\ (Section\ A) \tag{2}$$

$$CaO + Ca_2SiO_4 \rightarrow Ca_3SiO_5 (Section\ B) \tag{3}$$

$$3CaO + Al_2O_3 \rightarrow Ca_3Al_2O_6\ (Section\ C) \tag{4}$$

$$4CaO + Al_2O_3 + Fe_2O_3 \rightarrow Ca_4Al_2Fe_2O_{10} (Section\ D) \tag{5}$$

The various products in the various sections of the process reactors are; Tricalcium silicate (Ca_2SiO_4) which is responsible for early strength and the initial set of the cement; Dicalcium silicate (Ca_3SiO_5) which increases the strength as it age; Tricalcium aluminate ($Ca_3Al_2O_6$) which contributes to the concrete strength development in the first few days but least desirable due to its reactiveness with sulphate containing soils and water; Tetracaliumaluminoferrite ($Ca_4Al_2Fe_2O_{10}$) which reduces clinkering temperature. The equipment design parameters employed in this work are provided in **Table 1**.

The flow rate of the major raw materials for the production of cement in the clinkering reactor as depicted by Eqns. (6–12) are carefully chosen based on the standard provided by Winter N. B. [45]. The Chemical parameters based on the oxide composition are very useful in describing clinker characteristics. The following parameters are widely used.

a. *Lime Saturation Factor (LSF):* is the measure of the ratio of alite to belite in the clinker. It is estimated by the ratio of CaO to the sum of other three main oxides SiO_2, Fe_2O_3 and Al_2O_3. The equation is given by:

$$LSF = \frac{CaO}{2.8SiO_2 + 1.2Al_2O_3 + 0.65Fe_2O_3} \tag{6}$$

$$LSF = \frac{190}{2.8(60) + 1.2(15) + 0.65(10)} = 0.98 \tag{7}$$

LSF values in clinkers range between 0.92–0.98. The LSF value of 0.98 falls within an acceptable range.

b. *Silica Ratio (SR):* This is also known as Silica Modulus. The expression of SR is given as:

$$SR = \frac{SiO_2}{Al_2O_3 + Fe_2O_3} \tag{8}$$

Simple separator	Delta P	Stream fractions			
	0.000	Solids in vapour	0.0100		
		Solids in liquid	0.0100		
		Liquid in bottoms	0.0100		
Exchanger	Delta P (bar)	Delta T (°C)	Duty (kcal/h)		
Cooler	0.000	655	2.691 x0 10^7		
Component Splitter	Top Temp. (°C)	Bottom Temp. (°C)	Top Pressure (bar)	Bottom Pressure (bar)	Duty
Splitter 1	30	30	1	1	2.054 x 10^5
Splitter 2	1252	1252	1	1	1.825 x 10^4
Splitter 3	1252	1252	1	1	1.923 x 10^4
Reactors	Delta P	Vessel volume (m^3)	Liquid level (%)	Liquid volume (m^3)	Duty (kcal/h)
CaCO$_3$ decomp reactor	0.0000	0.0000	50.00	25.00	2.6764 x 10^7
Section A reactor	0.0000	50.00	50.00	25.00	7.6209 x 10^6
Section B reactor	0.0000	50.00	50.00	25.00	2.6131 x 10^6
Section C reactor	0.0000	50.00	50.00	25.00	4.5634 x 10^5
Section D reactor	0.0000	50.00	50.00	25.00	7.4721 x 10^5

Table 1.
Equipment design parameter.

Based on the experimental design for the simulated cement production process. The flow rate of Al2O3 and Fe$_2$O$_3$ are 15 tonnes/day and 10 tonnes/day respectively. The low level and high levels of SiO$_2$ are found to be 50 tonnes/day and 60 tonnes/day respectively. Hence, the SR values are the high and low value of the SiO2 flow rate are calculated as follows:

$$SR = \frac{50}{15 + 10} = 2.0 \tag{9}$$

$$SR = \frac{60}{15 + 10} = 2.4 \tag{10}$$

A high silicate ratio means that more calcium silicates are present in the clinker and less aluminate and ferrite. SR is typical, between 2.0 and 3.0. The SR values of 2.0 and 2.4 fall within an acceptable range of 2.0 and 3.0.

c. *Aluminate Ratio (AR):* This is the ratio of aluminate and ferrite phases in the clinker. AR value ranges between 1–4 in Portland clinkers. The flow rate of Al$_2$O$_3$ and Fe$_2$O$_3$ used in the process simulation are 15 tonnes/day and 10 tonnes/day respectively. The equation governing the AR of the oxide is given by

$$AR = \frac{Al_2O_3}{Fe_2O_3} \tag{11}$$

$$AR = \frac{15}{10} = 1.5 \qquad (12)$$

The mass flow and corresponding clinker quality parameters are presented in **Table 2**.

2.3 Multivariate design of experiment

The central composite design of response surface methodology was used to analyse the effect of CaO and SiO_2 on cement production rate. The total number of experimental runs (N) required for n independent variables and n_c number of replica centre points is given by Eq. 13

$$N = 2^n + 2n + n_c \qquad (13)$$

Design Expert 10.0.3 software was used to generate the experimental design from the ten experimental runs to study the combined effect of two variables on the response. For two variables factor in the experiments; four factorial points (2^n), four axial points ($2n$) and two replicates at the central points (n_c) at distance $\alpha = 1.414$ from the centre were used for the CCD design. A polynomial empirical model was developed from the ten experimental runs to correlate the response with the independent variables. The mathematical expression can be expressed as:

$$Y = \beta_o + \sum_{i=1}^{n} \beta_i X_i + \sum_{i=1}^{n} \beta_{ii} X_i^2 + \sum_{1 \le i \le j}^{n} \beta_{ij} X_i X_j + \varepsilon \qquad (14)$$

Where Y = Predicted response, β_o = constant coefficient, β_i = Linear coefficient, β_{ii} = Quadratic, β_{ij} = Interaction coefficients and ε = model random error, n the number of variable factors, X_i and X_j are the coded values of the variable parameters [35].

The response generated function distance from the centre $\alpha = 2^{n/4}$. The codes are calculated as a function of the range the factors as shown in **Table 3**.

The central composite experimental design for the synthesis of cement via simulation is depicted in **Table 4**. The mass flow rate of CaO and SiO_2 measured in tonnes/day are the independent variables or predictors which are studied for their effect on the response variable (cement flow rate) at a constant Al_2O_3 and Fe_2O_3 flow rates.

2.4 Model fitting and statistical analysis

The interaction between the variables and the response data as well as the statistical parameters were analysed graphically by analysis of variance (ANOVA) in the Design-Expert software. Regression analysis, significance, F-test, surface and contour plots of the response were also generated from the software. A probability

	Mass flow (tonnes/day)				Clinker quality parameter		
	CaO	SiO₂	Al₂O₃	Fe₂O₃	LSF	SR	AR
High level	190	60	15	10	0.98	2.4	1.5
Low level	135	50	15	10	0.82	2.0	1.5

Table 2.
Raw material mass flow and clinker quality parameter.

	Code	Mathematical relationship
Lower axial point	- α	X_{min}
Lower level	- 1	$[(X_{max} + X_{min})/2] - [\alpha(X_{max} - X_{min})/2]$
Centre point	0	$(X_{max} + X_{min})/2$
Upper level	1	$[(X_{max} + X_{min})/2] + [\alpha(X_{max} - X_{min})/2]$
Upper axial point	α	X_{max}

Table 3.
Relationship between the variable values and their assigned codes.

Factor	Name	Units	Low	High	-α	+α
A	Flow rate of CaO	tonnes/day	135	190	123.609	201.391
B	Flow rate of SiO_2	tonnes/day	50	60	47.9289	62.0711

Table 4.
Design of Experiment using central composite (C.C.D) Design of Response Surface Methodology (R.S.M).

value of 95% confidence level was used to evaluate the significance of the model terms and coefficients.

3. Results and discussion

3.1 Simulation and optimisation of cement flow

All simulations were done in duplicate and the experimental design were generated by the Central Composite Design (C.C.D) of the Design-Expert Software, which resulted in a total of 10 experimental (simulation) runs and the results of the experiments (simulations) are shown in **Table 5**.

Run No.	Factors				Response	
	Coded levels		Actual values		The flow rate of cement	
	A	B	A	B	HYSYS Simulation	C.C.D Model
1	1.000	1.000	190	60	46.6	45.6674
2	−1.000	−1.000	135	50	30.74	31.9851
3	0.000	0.000	162.5	55	46.04	46.04
4	0.000	−1.414	162.5	47.9289	30.57	31.271
5	1.000	−1.000	190	50	44.3	42.1551
6	−1.414	0.000	123.609	55	46.04	43.4867
7	0.000	0.000	162.5	55	46.04	46.04
8	−1.000	1.000	135	60	46.6	49.0574
9	1.414	0.000	201.391	55	46.04	48.2808
10	0.000	1.414	162.5	62.0711	46.84	45.8265

Table 5.
Simulation and predicted results from central composite design (C.C.D).

The change in mean response in cement flow per unit increase in variable occurs when other predictors area kept constant and is estimated by the coefficient of estimation and is presented **Table 6**.

The empirical quadratic equation for the optimal cement product rate as a function of CaO and SiO$_2$ mass flow in coded form as derived from **Table 7** was obtained according to the CCD and is given in Eq. 15

$$C = 46.04 + 1.70A + 5.15B - 3.39AB - 0.078A^2 - 3.75B^2 \qquad (15)$$

The test of the significance and the adequacy of the model and its coefficients lack fitness which was based on F-value or P-value at 95% confidence level was tested from analysis of variance (ANOVA) and the result is presented in **Table 7**. The result shows that the model at an F value of 20.35 and a very low P-value of 0.0005 indicates that the statistical regression model was significant. The result also shows that A, B, AB and B^2 are significant terms.

The regression statistical analysis is summarised in **Table 8**. The R squared value of 0.9356 is in good agreement with the adjusted R-square value of 0.8896, showing a good fit of the model, as the closer the R squared value to 1.00, the more significant the model. The adequate precision of 13.55 indicates the low noise level and a

Factor	Coefficient Estimate	df	Standard Error	95% CI Low	95% CI High	VIF
Intercept	46.04	1	0.86	44.00	48.08	
A-Flowrate of CaO	1.70	1	0.68	0.080	3.31	1.00
B-Flow rate of Silica	5.15	1	0.68	3.53	6.76	1.00
AB	−3.39	1	0.97	−5.67	−1.11	1.00
A^2	−0.078	1	0.73	−1.81	1.65	1.02
B^2	−3.75	1	0.73	−5.48	−2.01	1.02

Table 6.
Coefficient estimation for cement flow rate in terms of coded factors.

Source	Sum of squares	df	Mean	F value	p-value (Prob > F)
Model	379.61	5	75.92	20.35	0.0005
A	22.98	1	22.98	6.16	0.0421
B	211.86	1	211.86	56.78	0.0001
AB	45.97	1	45.97	12.32	0.0099
A²	0.042	1	0.042	0.011	0.9180
B²	97.60	1	97.60	26.16	0.0014
Residual	26.12	7	3.73		
Lack of Fit	26.12	3	8.71		
Pure Error	0.000	4	0.000		
Cor. Total	405.73	12			

Table 7.
ANOVA results for the statistical model for cement flow rate.

Parameter	Values
R-Squared	0.9356
Adj R-Squared	0.8896
Pred R-Squared	0.5422
Mean	43.69
Std. Dev.	1.93
C.V. %	4.42
Adeq Precision	13.554

Table 8.
Statistical information for the statistical model for cement flow rate.

strong signal for optimisation. Hence, this indicates the two predictors (flow rate of CaO and flow rate of SiO_2) could predict the flow rate of cement, thus the model equation, contour plot and 3D surface plot could be used to predict the response (flow rate of the cement).

3.2 Surface plots

The contour plot which shows the possible relationship between the CaO, SiO_2 and cement product mass flow is presented in **Figure 2**. The darker red regions indicate higher C (response) values. Here, the optimum flow rate of cement is found from the isolines to be 47.748 tonnes/day at a flow rate of 152.346 tonnes/day of CaO and 56.8241 tonnes/day SiO_2.

The three-dimensional (3D) response surface plots obtained from the model equation using Design Expert 10.03 is depicted in **Figure 3**. This depicts the effect
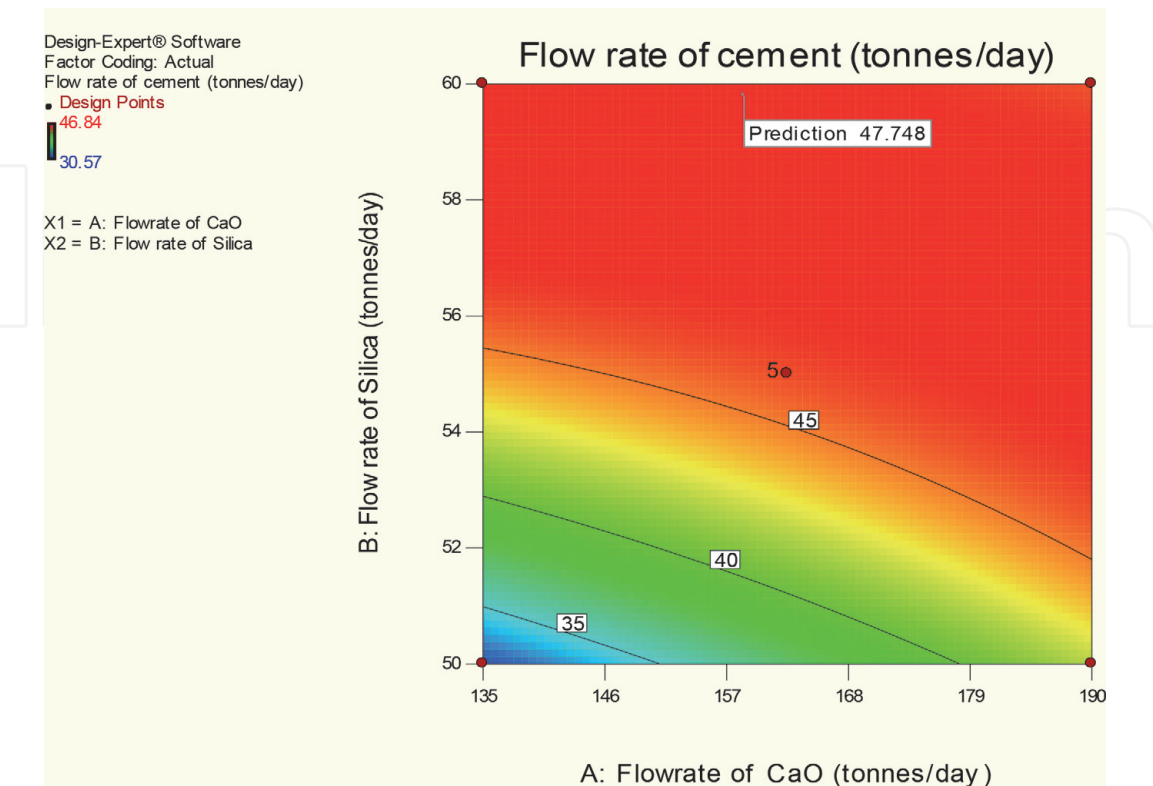
Figure 2.
Contour surface plot showing the effects of the flow rate of CaO and flow rate of SiO_2 on the flow rate of cement.
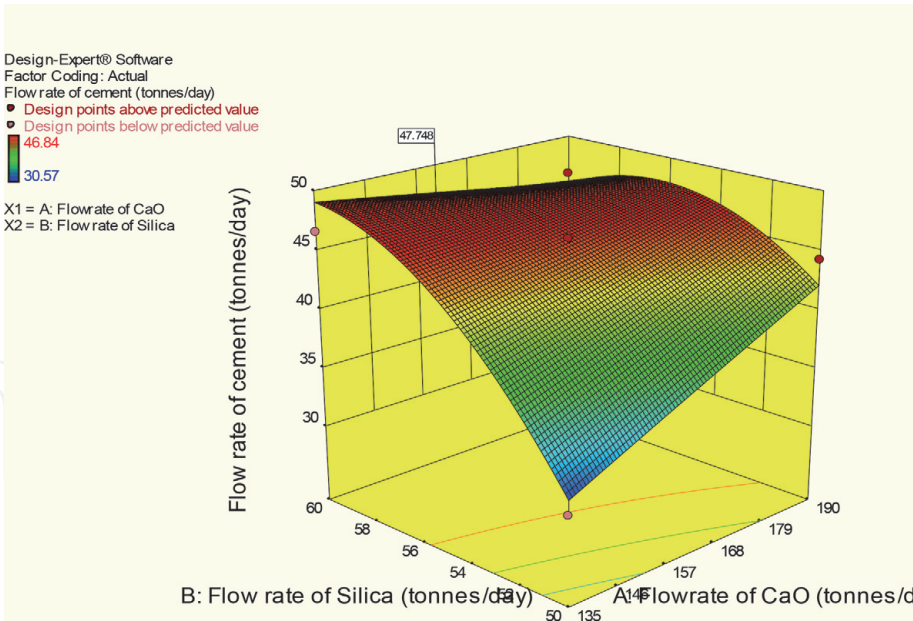
Figure 3.
Response surface plot of the effects of CaO and SiO$_2$ mass flow on cement production.

of the flow rate of CaO, the flow rate of SiO$_2$ on the flow rate of cement. The flow rate of cement was observed to increase with an increase in the flow rate of CaO. Conversely, increasing the flow rate of SiO$_2$ did not increase the flow rate of cement. Hence, the major predictor in cement production in the clinkering section is the flow rate of CaO.

The optimization plot of the cement output is shown in **Figure 4**. The optimum cement flow rate of 47.239 tonnes/day is found to be at CaO flow rate of 152.346 tonnes/day and SiO$_2$ flow rate of 56.8241 tonnes/day.

3.3 Energy optimization

Aspen Energy Analyser was used to determine the percentage of energy savings based on converged steady-state simulation of the process flow sheet in **Figure 1**. The total energy savings as a function of process utilities and carbon emissions are present in **Figure 5**.

The overall utilities in terms of energy are found to be optimised from the actual value of 6.511 x 10^7 kcal/h to 1.211 x 10^7 kcal/h and indicating available energy savings of 5.3 x 10^7 kcal/h, with overall energy savings of 81.40% which also correspond to 297.4 tonnes/day carbon emission reduction.
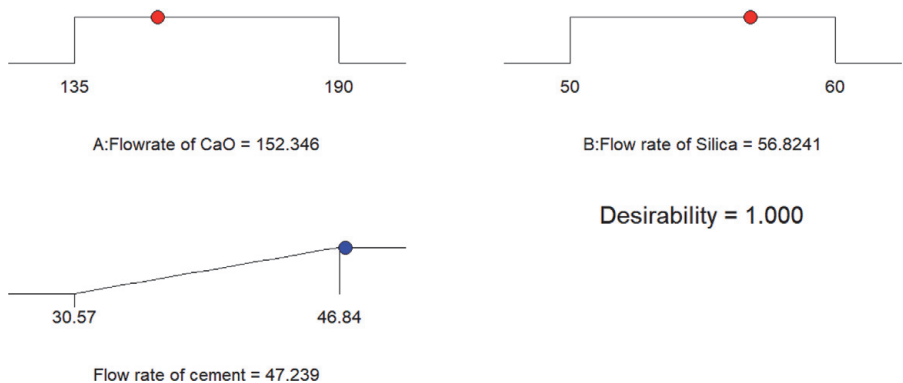
Figure 4.
Optimization plot showing the effects of the flow rate of CaO and flow rate of SiO$_2$ on the flow rate of cement.
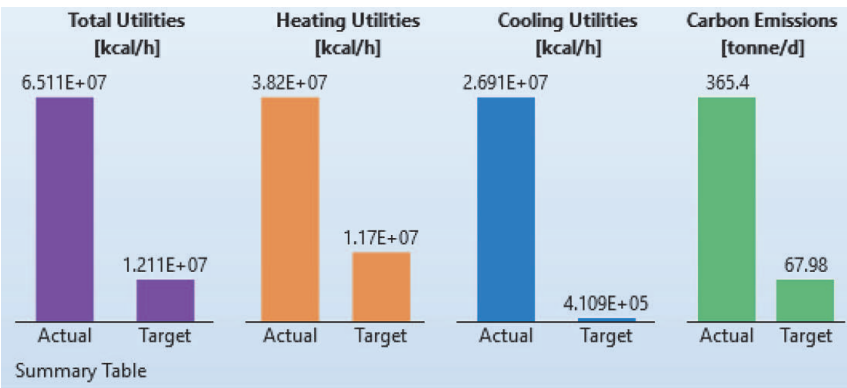
Figure 5.
Energy savings at optimum feed (CaO and SiO₂) rate and product (cement) flow rate.

4. Conclusion

Process flow diagram for the cement production was simulated to achieve high energy optimization and optimum cement flow rate by minimising the flow rate of the feed (CaO and SiO$_2$). Central composite Design (C.C.D) of Response Surface Methodology used to design the experiment for the simulation using Design Expert 10.0.3. The optimum cement flow rate is found from surface and contour plots to be 47.239 tonnes/day at CaO flow rate of 152.346 tonnes/day and SiO$_2$ flow rate of 56.8241 tonnes/day. The R squared value of 0.9356 determined from the statistical analysis shows a very high significance of the model. Energy efficiency optimization is also carried out using Aspen Energy Analyser. The overall utilities in terms of energy are found to be optimised by 81.4 % from 6.511 x 10^7 kcal/hactual value to 1.211 x 10^7 kcal/h with 297.4 tonnes/day the carbon emission savings.

Further work could be performed on fault identification and diagnosis of the process plant. Incorporated with an automated plant to guarantee the safety of workers, reduce environmental problems and increase yield to sustain production improvement.

5. Recommendations

This research work sought to recommend the following concerns in which cement production could be improved:

1. Research and development (R&D) in the cement production, processing and utilisation should be encouraged. This will play a vital role in the construction industry, operation and maintenance of efficient road network and effective transportation system.

2. Automation of cement and kiln sections of the cement production is recommended

3. Optimization of the cement production can be tailored into the fabrication of high tech cement equipment and parts.

4. Optimization of the limestone crusher to quantify the amount of crushed limestone is needed.

5. Looking into future the results obtained in this research will open up several important possibilities in the cement production at optimum conditions. This will have a multiplier effect on infrastructural amenities development.

Conflict of interest

There is no conflict of interest associated with this work.

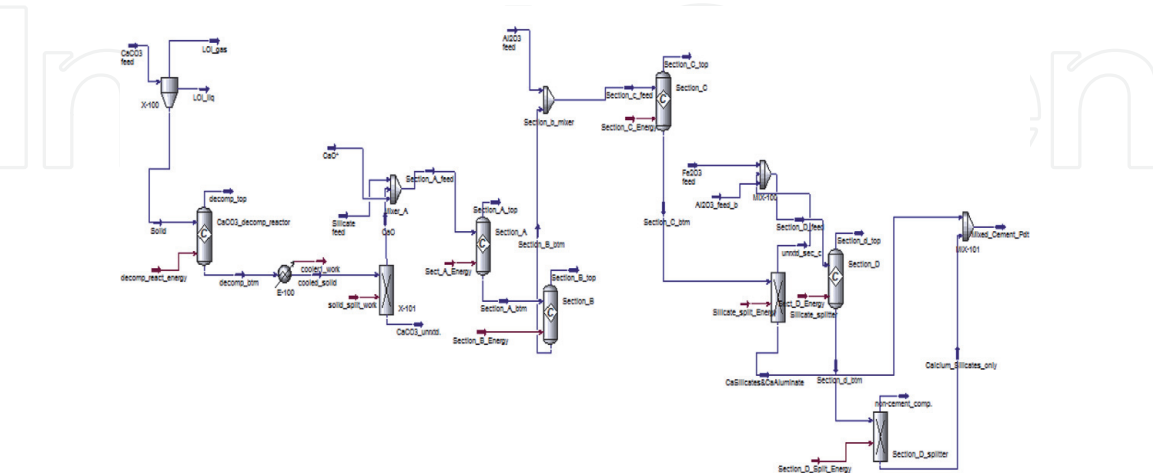## Appendix

Figure A1.
HYSYS process flow simulation diagram for the production of cement.

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