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Estimation of Industrial Heat Balance Based on Actual Plant Data: A Case Study for Cement Plant

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Abstract. The industrial sector plays a significant role in anthropogenic effect on the environment due to greenhouse gases emissions associated with energy-intensive processes. To advance in the sustainability goals, it is essential to propose new modeling methodologies to assess the yield performance of clean technologies on industrial processes. However, due to the complexity and variety of such processes it is particularly challenging to assess the non-linear performance of industrial process in terms of heat loads, temperature, and others. The present study introduces a novel methodology to configure an estimation model of the heat released by the clinkering process in the cement industry, based only on operational data. Furthermore, a methodology is proposed to evaluate the correlation between the heat of the process and the operational parameters. The result of this methodology provides a function for the heat consumed or released by the chemical reactions of the process, based on the relevant operational parameters. The approach proposes a global specific enthalpy, parameter that represents the response of the process, only through the heat consumed or released by the chemical reactions. A methodology is proposed for evaluating the correlation of operational parameters with the proposed specific enthalpy. The methodology is validated by assessing the pyro-processes in the cement industry, renowned for its high energy intensity and pollution emissions. The proposed methodology could facilitate the evaluation of clean technologies into different industrial processes. This approach can guide industries in identifying opportunities for reducing pollution emissions while optimizing energy efficiency.

Keywords: Process Heat, Cement Industry, Heat Balance Estimation

1. Introduction

The industrial sector is responsible for 19% of the world energy demands through process heat [1] and up to 8,98 GTon of CO_2 emissions in 2022 [2]. Over 70% of these emissions come from four industrial sectors, such as iron and steel, cement, chemicals, and petrochemicals. To reduce the anthropogenic effects related to the industrial sector, it is essential to promote the energy transition in this sector to renewable energy sources [3]. One way to promote the transition is reducing the risk of adopting new technologies. Moreover, risk management assessment lies in the yield performance obtained through simulations of clean technologies on industrial processes. However, using simulations could present high uncertainties due to the different variables involved, as has been assessed for the simulations of solar heat for industrial applications [4]. Therefore, the challenge of accurately simulating the benefits of clean technologies becomes present. This industry produces around 4.158 million tonnes of cement per year and is responsible for 0,58 tonnnes of CO_2 per tonne of cement every year [5]. Efforts have been made for reducing the pollutants on the cement production, such as CO_2 capture technologies [6] or integration strategies for increasing efficiency [7].

The clinkering process represents more than half of the heat demand of the cement production in the endothermic chemical reactions [8]. Therefore, is the most relevant parameter in the heat balances of the plant. There are methodologies available to obtain the heat of reaction involved, based on chemical balances [8] an chemical exergy of the reactions [9]. The available methodologies are based only on the properties of the raw materials and the chemical reactions involved. In case the composition of the media used for the manufacturing of cement is not available, there is not an existing tool for assessing the heat of reaction in the chemical processes involved. Operational data has been used for predicting the heat of reaction for a single cement plant using machine learning [10]. Still there is a gap for extrapolating these results for plans in different operating conditions, specially due to the lack of reported operational parameters in the literature [11].

To accurately assess energy efficiency measures for the cement production, a proper estimation of the heat of reaction is mandatory. The assessment of clean technologies for reducing energy demand and pollution is especially sensible to a variation of operating parameters. Furthermore, the state of the art in the estimation of endothermic chemical reactions does not provide a modelling approach that is both correlated to the operating parameters and applicable in simple thermal balances. This lack of an easy-to-use estimation approach impairs the assessment of clean technologies in cement production.

The present study proposes a methodology for providing a correlation for the heat of reaction of the clinkering process, based on operational data reported in the literature and calculated through heat balances of the process. The heat of reaction is represented through the global specific enthalpy Δh_{cl} that reflects the heat released or consumed by the chemical reactions of the process. The methodology is based first on the creation of two data sets of cement plants: a train set composed of reported Δh_{cl} from the literature, and a test set composed of calculated Δh_{cl} through a heat balance of the process. A stepwise regression is performed on the train data set and evaluated through the test data set. Finally, a linear regression is proposed based on the features with best correlation.

1.1 Cement pyro processing

Raw material is fed into the pyro processing tower, that contains the cyclones and preheater. The output product, called farine at this step, is then feed into the rotary kiln, and the resulting hot clinker is the discharged into the coolers, which lower the temperature of the material using air. Fuel is burned in the kiln and preheater to increase the temperature and allow chemical reactions such as calcination to occur. Several efficiency measures are implemented, such as the integration of waste heat recovery from the coolers into the rest of the processes, referred as secondary air for a stream of hot air from the coolers to the kiln, and tertiary air for a stream of hot air from the coolers to the preheater/calciner. The use of a pre-calciner before the kiln is a common practice, to reduce the fuel consumption of the rotary kiln. The outlet temperature of the kiln goes between 1200°C and 1450°C [7].

The chemical reactions in the clinkering process are known and are used to calculate the endothermic or exothermic heat flows for a specific cement mix [12]. Nevertheless, these heat flows are not correlated with operational parameters of the clinkering process, such as temperatures, mass flows, or other variables that could influence the thermal reactions.

2. Methodology

2.1 Process Heat Balance

The approach proposes a global specific enthalpy (Δh_{cl}), parameter that represents the response of the process, only through the heat consumed or released by the chemical reactions. The parameter can be obtained from the energy balance of a process:

$$\dot{Q} = \sum_{i}^{Inlet} \dot{m}_i Cp_i T_i - \sum_{o}^{Outlet} \dot{m}_o Cp_o T_o - \dot{m}_{cl} \Delta h_{cl} - \dot{Q}_{losses} + \dot{Q}_{fuel} \quad (1)$$

where $\dot{Q}$ is the heat flow entering or leaving the process, $\dot{m}$ is the mass flow, Cp is the specific heat, T is the temperature, the subindices *i* and *o* represent each process flow inlet and outlet, respectively, and $\dot{m}_{cl}$ is the clinker outlet mass flow.

To evaluate the approach for increasing the data pool for evaluating the $\Delta\square_{cl}$. Five cases were found that reported enough information for calculating the heat balance of the plant using Eq. 1. The information for each stream for the additional cases is reported in Table 1.

Table 1. *Streams for clinkering process in cement plants.*

Case	Flow Type	Media	Temperature [°C]	Mass flow [kg/s]	Heat Load [MW]
16	Inlet	Product	60	54,35	2,33
16	Inlet	Fuel	55	3,82	103,46
16	Inlet	Air	15	76,90	1,16
16	Inlet	Air	15	3,40	0,05
16	Inlet	Air	15	0,70	0,01
16	Outlet	Product	115	32,67	-3,15
16	Outlet	Exhaust	284	39,90	-12,46
16	Outlet	Exhaust	313	65,90	-22,65
16	Outlet	Losses	-	-	-9,00
17	Inlet	Product	105	25,86	2,54
17	Inlet	Fuel	55	1,78	58,71
17	Inlet	Fuel***	55	0,12	4,32
17	Inlet	Fuel***	55	0,23	8,65
17	Inlet	Air	25	38,07	0,96
17	Outlet	Product	1450	17,28	-25,78
17	Outlet	Exhaust	370	18,24	-9,80
17	Outlet	Exhaust**	90	12,50	-1,53
17	Outlet	Exhaust**	145	17,50	-3,45
17	Outlet	Air	25	27,48	-4,30
17	Outlet	Losses*	-	-	-4,90
18	Inlet	Product	950	90,28	73,26
18	Inlet	Air	38	9,24	0,02
18	Inlet	Air	1050	77,99	86,11
18	Inlet	Fuel	65	5,20	155,88
18	Outlet	Product	1350	57,78	-82,04
18	Outlet	Exhaust	950	114,54	-120,75
18	Outlet	Dust	425	10,40	-3,75
18	Outlet	Losses	-	-	-10,42
19	Inlet	Product	275	95,67	148,23
19	Inlet	Fuel+Air	275	23,92	17,29
19	Inlet	Fuel+Air	1050	5,69	38,40
19	Inlet	Air	275	119,58	9,84
19	Outlet	Product	1350	56,94	-71,98
19	Outlet	Exhaust	364	130,97	-19,50
19	Outlet	Exhaust	275	56,38	-6,49
19	Outlet	Losses	-	-	-18,73
20	Outlet	Product	112	33,15	2,65
20	Inlet	Air	810	24,70	20,13
20	Inlet	Air	17	2,77	0,05
20	Inlet	Fuel	71	2,00	66,17
20	Inlet	Electricity	-	-	9,34
20	Outlet	Product	1277	16,67	-17,88
20	Outlet	Exhaust	287	16,68	-5,74
20	Outlet	Air	437	9,36	-1,38
20	Outlet	Air	25	18,43	-4,97
20	Outlet	Losses	-	-	-36,51

To perform a heat balance of the process, it is necessary to have the energy rate of every stream going in and out of the process. Most of the studies do not report all the streams information, but it is possible to calculate all the energy rates.

Pinch analysis studies usually do not report the mass flow for each line, but instead report the amount of heat per temperature difference, or Heat Capacity Flow Rate, defined as the product of the mass flow rate times the heat capacity of the media [13]. From this information it is possible to obtain the mass flow rate for each line.

$$\dot{m} = \frac{CP}{\overline{Cp}} \tag{2}$$

where CP is the heat capacity flow rate, and $\overline{Cp}$ is the average specific heat of the stream for the temperatures in the inlet and outlet of the reported component.

For case 16, the heat loss* was calculated with the heat loss per kilogram of clinker for an European cement plant [14], and the air outlets** were added assuming that it is filtered air through the pyro tower, reported in cement plants [15], and filtered air through the kiln. The added streams to close the mass balance of the process.

For the heat input coming from the fuel, the following procedure is followed: if the combustion heat input is reported, that value is added to the heat of the fuel stream. Otherwise, the combustion heat input is calculated through the following:

$$\dot{Q}_{fuel} = \dot{m}_{fuel} LHV_{fuel} \tag{3}$$

where LHV_{fuel} is the low heating value of the fuel, and $\dot{m}_{fuel}$ is the mass flow of fuel. Cases 17 and 18 reported their combustion heat input, case 15 reported the LHV_{fuel}, and for cases 16 and 19, a LHV_{fuel} for coal of 33.000 kJ/kg_{fuel} was considered, and for case 16 a LHV_{fuel} for extra fuel*** of 37.000 kJ/kg_{fuel} was considered.

2.2 Stepwise Regression

The following methodology is proposed to perform a stepwise regression based on the reported and calculated data.

A forward stepwise linear regression was employed, implemented in Python using scikit-learn modules for linear regression and cross validation, to identify the combination of process variables that best predicts the specific enthalpy Δh_{cl}. All available cases from Table 1 (both reported and calculated) are assembled into a single dataset. Cases missing any variable under consideration are omitted from the corresponding regression.

After assembling the full dataset (features a) to k) and the target Δh_{cl}), a random partition of the data was implemented into an 80% training set and a 20% test set. On the training set, a five-fold cross-validation was performed: at each fold, the regressor is fit on 80 percent of the training data and evaluated on the remaining 20 percent.

The forward stepwise procedure begins with an empty model. In the first iteration, separate simple linear regressions using each individual feature are fit across the five folds, and the mean absolute error (MAE) is computed and averaged over the folds. The feature whose inclusion yields the lowest average MAE is selected as the first predictor. In each subsequent iteration, every feature not yet selected is added, one at a time, to the already-chosen subset, the resulting variable linear regression is re-evaluated via five-fold MAE, and the feature achieving the greatest further reduction in MAE is permanently included. This process continues until no remaining feature can lower the MAE compared to the previous model.

Finally, the regression comprising the selected subset of features is retrained on the entire 80%training set and assessed once on the untouched 20% test set; the resulting MAE and R^2 quantify the model's predictive performance. The order in which features enter the model, together with the sign and magnitude of their coefficients, provides insight into both the relative importance and the directionality of each parameter's effect on Δh_{cl}.

3. Results

3.1 Plant heat balance

The reported operational data, as well as the reported and calculated $\boldsymbol{\Delta h_{cl}}$ from cement plants is shown in Table 2.

Table 2. *Operating data reported for cement plants.*

$\boldsymbol{\Delta h_{cl}}$	a)	b)	c)	d)	e)	f)	g)	h)	i)	j)	k)	Case	Source
1764,8	53,3	101,1	-	-	67	-	-	0,16	2,12	0,11	-	1	Rep
1835,4	49,8	111,5	-	-	83	-	-	0,17	2,27	0,12	-	2	Rep
1723,0	39,4	197,7	1190	-	77	-	1267	1,65	1,22	0,06	608,8	3	Rep
1781,3	41,0	153,9	-	-	60	900	-	1,74	1,88	0,07	227,0	4	Rep
1795,0	6,9	25,6	1250	992	50	308	1300	1,67	2,09	0,12	517,0	5	Rep
1850,0	31,0	117,1	1050	200	50	900	1100	1,56	2,27	0,15	600,0	6	Rep
1772,4	37,1	118,8	972	-	359	-	1331	-	-	0,11	-	7	Rep
1784,9	36,7	118,1	977	-	364	-	1341	-	-	0,11	-	8	Rep
1719,4	64,3	214,9	-	-	110	-	-	-	-	-	365,3	9	Rep
1818,9	21,9	181,0	-	-	-	-	-	1,65	1,14	0,14	2687,8	10	Rep
1740,0	-	-	1340	630	110	820	1450	-	-	-	303,0	11	Rep
1750,0	-	-	-	-	-	-	-	-	1,50	-	310,0	12	Rep
1764,8	49,4	161,7	-	1350	71	-	1350	1,71	2,11	0,14	443,2	13	Rep
1781,6	23,9	94,0	-	355	-	845	1200	1,09	1,06	0,65	1422,0	14	Rep
1792,3	38,1	183,6	1203	167	77	1113	1280	1,05	1,26	0,09	900,4	15	Rep
1828,3	32,7	109,1	1077	277	60	860	1137	1,66	2,02	0,12	275,6	16	Calc
1726,9	17,9	75,2	1345	640	105	810	1450	1,50	1,06	0,12	275,6*	17	Calc
1701,5	57,8	315,3	-	400	-	950	1350	1,56	1,98	0,09	180,3	18	Calc
1704,5	56,9	213,8	1075	496	275	854	1350	1,68	2,30	0,00	329,0	19	Calc
1740,7	16,7	101,7	1165	539	112	738	1277	1,99	1,00	0,12	2190,3	20	Calc

The studies selected are those that reported the Δh_{cl} value, usually considering a chemical assessment of the heat balance. Operational parameters a) to k) for each case are also reported, and the description of each is reported in Table 3. The source of each case is reported in annexes in Table 4.

Table 3. *Name and unit of reported parameters.*

Point	Name	Units
Δh_{cl}	Clinkering specific enthalpy	[kJ/kg]
a)	Clinker mass flow	[kg/s]
b)	Plant heat input	[MW]
c)	Pyro temperature difference	[°C]
d)	Kiln temperature difference	[°C]
e)	Cyclone temperature inlet	[°C]
f)	Kiln inlet temperature	[°C]
g)	Kiln outlet temperature	[°C]
h)	Farine mass flow / Clinker mass flow	[-]
i)	Kiln exhaust mass flow / Clinker mass flow	[-]
j)	Fuel mass flow / Clinker mass flow	[-]
k)	Heat losses / Clinker mass flow	[kJ/kg]

Table 4. *Reference for each case.*

Case	1	2	3	4	5	6	7	8	9	10
Reference	[16]	[16]	[17]	[18]	[19]	[20]	[21]	[21]	[12]	[22]
Case	11	12	13	14	15	16	17	18	19	20
Reference	[7]	[8]	[23]	[24]	[9]	[14]	[25]	[26]	[27]	[15]

With these results, the linear regression can be calculated using the reported and calculated $\boldsymbol{\Delta h_{cl}}$. The results are shown in Figure 1.

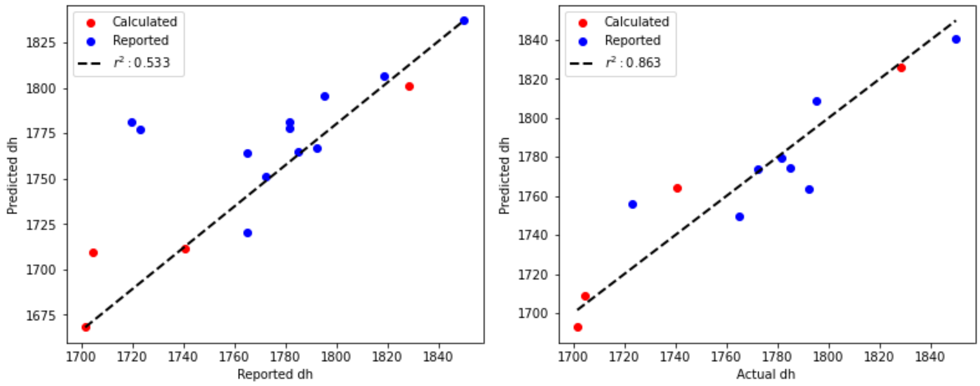

Figure 1. *Linear regression incorporating calculated data.*

3.2 Heat of Reaction from Composition

The heat of reaction for the clinker formation is usually obtained through a linear function depending of the composition of the clinker [8], showed in Eq. (4).

$$H_R = 3200\ CaO + 2710\ MgO - 2140\ SiO_2 - 250\ Fe_2O_3 + 1720\ Al_2O_3 \quad (4)$$

Furthermore, a regression is performed adding the outlet temperature of the kiln to the composition, shown in Eq. (5).

$$\Delta h_{cl} = 4645{,}3 - 9{,}02\, T_{out,Kiln} - 2770{,}1\, CaO + 1020{,}7\, MgO - 214{,}2\, SiO_2$$
$$-2807{,}8\, Fe_2O_3 + 4232{,}3\, Al_2O_3 \quad (5)$$

The composition for each plant is shown in Table 5.

Table 5. *Composition of clinker for reported cases.*

Case	CaO	MgO	SiO2	Fe2O3	Al2O3	Calculated	reported	error
1	66,55%	1,33%	22,54%	3,11%	5,15%	1764,07	1764,8	0,04%
2	-	-	-	-	-	-	1835,4	-
3	66,30%	1,60%	21,45%	3,84%	4,70%	1777,17	1723,00	3,14%
4	65,60%	2,90%	21,70%	3,80%	4,50%	1781,31	1781,32	0,00%
5	64,58%	2,81%	20,55%	4,08%	5,98%	1795,59	1795,00	0,03%
6	67,00%	3,00%	21,00%	3,00%	4,00%	1837,2	1850,00	0,69%
7	64,13%	1,10%	20,26%	4,24%	6,59%	1751,15	1772,37	1,20%
8	64,50%	1,30%	20,34%	4,24%	6,48%	1764,81	1784,86	1,12%
9	67,07%	1,14%	22,28%	3,36%	5,20%	1781,38	1719,37	3,61%
10	66,05%	1,88%	20,44%	3,89%	5,19%	1806,67	1818,85	0,67%
11	-	-	-	-	-	-	1740,00	-
12	-	-	-	-	-	-	1750,00	-
13	63,86%	1,87%	21,68%	3,60%	5,76%	1720,31	1764,81	2,52%
14	66,95%	0,00%	21,15%	3,40%	5,61%	1777,82	1781,55	0,21%
15	65,40%	1,30%	20,55%	3,24%	5,04%	1766,84	1792,30	1,42%
16	67,14%	1,10%	21,83%	3,15%	5,71%	1801,50	1892,59	4,81%
17	-	-	-	-	-	-	1726,89	-
18	63,04%	1,44%	21,50%	5,62%	5,01%	1668,13	1701,51	1,96%
19	65,41%	0,00%	21,84%	2,63%	5,26%	1709,57	1704,49	0,30%
20	63,38%	1,20%	20,42%	3,42%	5,62%	1711,79	1844,60	7,20%

In Figure 2 is shown how these functions correlate with the predicted $\boldsymbol{\Delta h_{cl}}$.

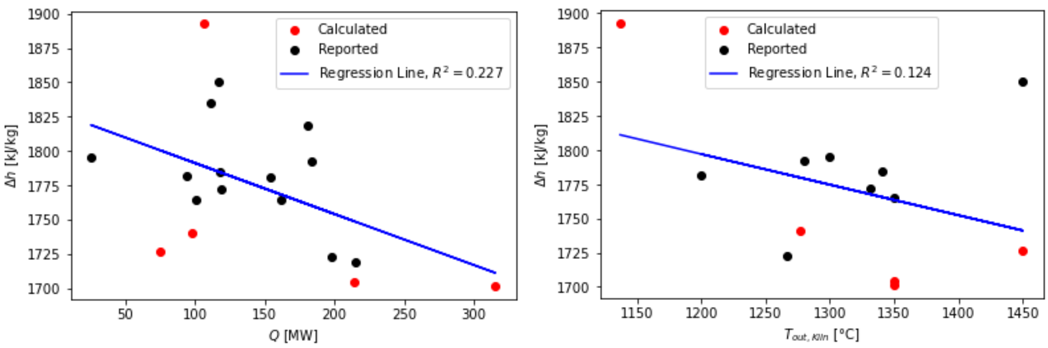

Figure 2. *Stepwise regression using composition from Table A2 (Left) and from Table A2 and the outlet temperature of the kiln.*

3.3 Stepwise Regression

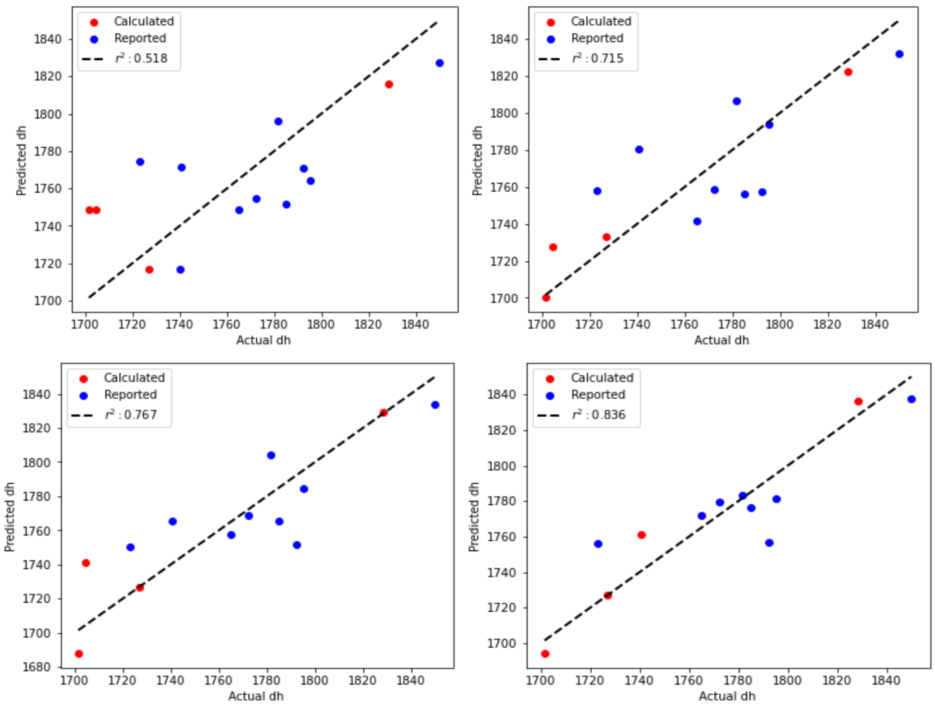

Figure 3. *Stepwise regressions for features g), b), j) and a).*

For each selected regression, the R^2 value is calculated between the regression and the test data. The data points are shown for four regressions in Figure 3. The features selected are g), b), j) and a), in that order.

Finally, in equation (6) and (7) is presented a regression for obtaining the $\Delta\square_{cl}$ using only the first two main features. The features used are the sum of the heat rates going into the process Q_{in}, and the temperature out of the process $T_{out,Kiln}$.

$$\Delta h_{cl} = -0{,}316\, T_{out,Kiln} + 2174{,}701 \tag{6}$$

$$\Delta h_{cl} = -0{,}314\, T_{out,Kiln} - 0{,}269\, \dot{Q}_{in} + 2208{,}346 \tag{7}$$

3.4 Parametric Analysis

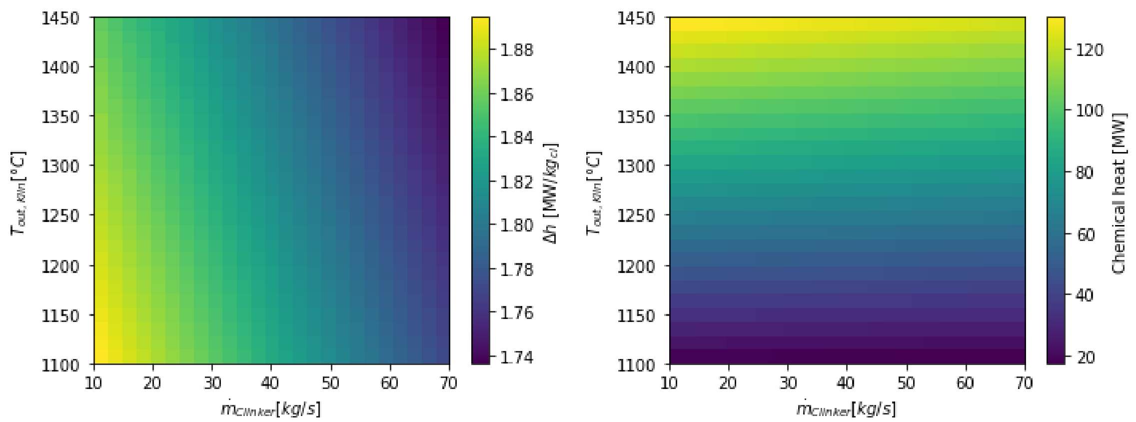

Figure 4. *Parametric analysis of specific enthalpy for operating conditions.*

Finally, a parametric analysis of the regression using equation (1) and (7), for a range of kiln temperature and clinker mass flow is shown in Figure 4. The ranges are defined using actual cement plant data [25].

4. Conclusions

From the collection of studies reported in this article, it is possible to conclude that studies in the literature report the heat related to the chemical reactions of the clinkerizarion process in cement plants. The value of the heat released Δh_{cl} is usually calculated based only on the chemical composition of the raw materials and chemical balances, but without considering the operating conditions of the thermal processes involved.

The operational parameters of the process can be used to build a regression for the heat released by the chemical reactions clinkering process. Measures must be considered for the lack of reported operational data to build the regression. A heat balance of the process through the reported streams can be performed to obtain the heat released $\Delta \square_{cl}$ and increase the data pool of cement plants.

The regression for $\Delta \square_{cl}$ is built using a stepwise approach, by adding features to the regression that reduces the error and increases the similarity of the regression to the data. A test and train data set are built using random points and cross validation. Nevertheless, the stepwise procedure could lead to overfitting of the regression and should be used with caution. The least number of features possible should be used to build the regression.

A comparison of the reported $\Delta \square_{cl}$ values with the standard procedure for calculating the "heat of reaction", based on the clinker composition, shows a R^2 value of 0,533. The regression is enhanced by adding the outlet temperature of the kiln as an extra feature, reaching a R^2 value of 0,833. It is possible to evaluate the regressions just using operational parameters as features, providing a R^2 of 0,518 for the outlet temperature of the kiln as a feature, and a R^2 of 0,715 for the outlet temperature of the kiln and heat input as features.

The parametric analysis performed, show how the provided regression could be used to assess an actual process response to a variation in the operational parameters. Finally, the proposed regressions could be used for modeling the clinkering process in different operational scenarios, thus reassuring that scaling the process will lead to an accurate response. The presented methodology could be tested in other industrial sectors and help promote the evaluation of efficiency measures such as the integration of renewable energy, thermal storage, or waste heat recovery.

Data availability statement

All data is available in the article.

Author contributions

IW: Conceptualization, Data curation, Formal Analysis, Investigation, Methodology, Validation, Visualization, Writing – original draft, Writing – review & editing. AS: Methodology, Supervision, Validation, Visualization, Writing – original draft, Writing – review & editing. AKS: Supervision, Writing – review & editing. JMC: Methodology, Supervision, Writing – review & editing.

Competing interests

The authors declare that they have no competing interests.

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