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A calculator for valorizing bauxite residue in the cement industry

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ABSTRACT

A computational tool using Microsoft Excel was developed to identify opportunities to repurpose bauxite residue as a raw material in the production of Portland cement. The tool quantifies the value of utilizing BR in this manner in terms of economic and environmental factors, including on-site and off-site electricity production and carbon taxes. This enables the tool to provide an optimization of the quantity of bauxite residue to be used based on the user's specifications. The algorithm considers valorization of bauxite residue separately as both an ingredient in the raw meal and a supplementary cementitious material to maximize the opportunities to utilize the residue. The tool is designed to be used by users of both the alumina and cement industries and is compatible with the needs of each sector to consider the costs of commercialization, transportation, and cost-advantages of valorizing bauxite residue.

1. Introduction

Bauxite was defined in 2020 as a critical raw material by the European Commission due to its massive scale of consumption (Blengini et al., 2020). Bauxite residue (BR) is an industrial byproduct produced in large volumes globally but without a substantive reuse case (Evans, 2016). This has resulted in a growing global stockpile in dedicated containment systems which is expected to reach 4 billion tons by 2022 (IAI, 2021). There is a growing need to develop avenues for recycling BR. However, few applications present the opportunity to reuse the material at a scale that is relevant to its production volume. A notable exception is the potential use of BR as an additive in the synthesis of ordinary Portland cement (Liu and Zhang, 2011). Due to the massive scale of Portland cement production globally, the ability to incorporate BR in cement, even as a minor component, would mitigate the growth of the global stockpile of BR.

Moreover, the utilization of bauxite residue (BR) has received attention for its potential value as a cost-saving additive to produce cement with lower environmental footprints. Many studies have considered BR in different forms and proportions in cement mixes. BR has shown promise as both a replacement ingredient in the raw meal in cement production and as a supplementary cementitious material (SCM) (Ghalehnovi et al., 2019; Liu and Poon, 2016; Tsakiridis et al., 2004). However, the best practices for utilizing BR in cement have not been established. There are many extrinsic factors, such as transportation, power costs, and environmental taxes, which complicate the calculation of the added value of valorizing BR. These factors influence the economic incentive to utilize this material. In this study, a systematic quantification of these factors has been developed into a computational algorithm for determining the suitability of incorporating BR into cement production on a plant-by-plant basis.

Bauxite residue is a byproduct obtained during the production of alumina using the Bayer process (Power et al., 2011). Bauxite, the aluminum hydroxide bearing ore, is found in nature commingled with silicate minerals, iron oxides, titanium oxides, and many other minor or trace elements. Consequently, bauxite residue is composed of a combination of insoluble mineral oxides that are present in the extracted ore (Liu et al., 2007; Wang et al., 2021). BR may be classified as a hazardous material due to its caustic nature. This arises from the considerable content of soluble sodium phases (hydroxide and carbonates) and complicates the disposal and containment of this byproduct. Techniques have been developed to concentrate the residue through filter pressing (Angelopoulos et al., 2016). Life cycle assessments have been conducted of bauxite residue disposal to quantify its costs to the envi-

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ronment and the advantages of disposal and containment technologies (Joyce and Björklund, 2019; Rai et al., 2020). However, the substantial scale of bauxite residue production has made disposal, containment, and pacification efforts for the material a challenge.

Bauxite residue is produced on a tremendous scale. Globally, it is estimated that current aluminum consumption results in the annual production of over 150 million tons of BR (IAI, 2021). However, it is estimated that less than 3% of bauxite residue is used in conventional technology (Evans, 2016). This creates a strong imperative to develop new avenues for valorizing this material. Many studies have been conducted on different avenues for repurposing bauxite residue. As a concentrated mineral residue, BR contains minor fractions of valuable metals which can be extracted (Borra et al., 2015). The methodology has been applied to extract iron (Agrawal et al., 2018; Gu et al., 2017), gallium (Ujaczki et al., 2019), alkalis (Kaußen and Friedrich, 2016; Wang et al., 2018), scandium (Anawati and Azimi, 2020, 2019), and other rare earth metals (Borra et al., 2016; Chaikin et al., 2020). Attempts have also been made to valorize it as a raw material for sintered ceramics (Pontikes et al., 2009). However, a principal concern in the identification of a suitable end-use for BR is an application that can take advantage of the large volume of BR production and consume the byproduct at a scale that is relevant to its production scale.

The cement industry presents one of the strongest opportunities for matching the production of BR because of the scale of global cement consumption (Brial et al., 2021; Habert, 2014; Habert et al., 2020; Klauber et al., 2011; Pontikes and Angelopoulos, 2013). The feasibility of incorporating BR in cement production has been demonstrated by many studies (Liu and Zhang, 2011; Rathod et al., 2013; Tang et al., 2019). BR is a viable ingredient in the raw meal used to produce cement when added in controlled doses (Tsakiridis et al., 2004). In this form it acts as a supplemental source of calcium, aluminum, and iron, reducing the required clay and iron corrective that are typically added to the clinker. This offers a cost advantage of using a byproduct over virgin raw materials. Moreover, BR has been shown to act as a SCM in cement composites. It exhibits chemical reactivity in cement paste and a filler effect which can strengthen the final binder (Ghalehnovi et al., 2019; Nikbin et al., 2018). Some studies have reported a change final hydration of cement blended with BR as an SCM (Romano et al., 2018). While the compressive strength of these blended cements have been shown to be unchanged (Sapna and Aravindhraj, 2018; Venkatesh et al., 2020b), concerns have been raised about the potential impact of BR SCM on durability (Tang et al., 2019; Venkatesh et al., 2020a) and the compatibility of superplasticizers (Fujii et al., 2015). These effects may be related to the amount of soluble sodium in BR (Danner and Justnes, 2020). Nevertheless, the use of BR as an SCM presents an avenue for economic and environmental opportunities. Both avenues of utilization enable the synthesis of cementitious materials with cost and environmental advantages.

The present work is a continuation of a collaboration between aluminum producers and the cement industry to develop a more robust pathway to valorize bauxite residue in the production of ordinary Portland cement (Nattrodt Monteiro et al., 2020). This is a part of a multistep plan, proposed in the International Aluminum Institute in their Technology Roadmap (IAI, 2020), to develop technological and supply line connections between the aluminum and cement industries. The objective of the present work is to quantify the economic incentive to repurpose bauxite residue in the cement industry. However, the value of incorporating BR into cement production is dependent on many factors and constraints which are unique to regions and specific producers. For this reason, the solution to the optimal BR content in cement and its potential value to cement producers cannot be generalized. To remedy this complex situation, the present work has developed a computational tool based in Microsoft Excel, to incorporate the individual requirements of both the cement producers and the alumina suppliers. This will facilitate the future application of BR to cement production and business between the aluminum and cement industrial sectors.

2. Methodology

2.1. Definition of users

To facilitate the collaboration between the alumina and cement industries, this tool was developed to be used equally by users from both sectors. The two categories of users have different terminologies, requirements, and objectives when it comes to the use of BR. As such, the tool is designed to have separate input fields for each type of user, which can be filled in to the extent that the information is available. In the same manner, a separate results page is created for each type of user, to show the parameters and outputs that are relevant to their sector and metrics. The first category of user is a representative of the aluminum sector, labeled in this tool as the "BR Producer." For this user, the tool compiles an economic evaluation that considers storage and transport costs, potential cost and revenue flow of commercialization of BR, payback for capital expense expenditure, and local taxation. The tool requires compositional information for the BR for determining the maximal contents which can be valorized in cement.

The second category of user is a representative from the cement sector, labeled in this tool as the "Cement Industry." To satisfy the needs of this industry, the tool calculates the optimal BR content to be used and the impact of this addition on the energy consumption and carbon emissions in the cement plant. In this way, the algorithm presents an environmental and, through consideration of raw material savings, fuel costs, and carbon taxes, economic assessment of the potential value of incorporating BR into cement production. This is conducted on a plant-by-plant basis using user information about their facility's production information, raw materials used, and fuel consumption under normal operating conditions. The tool considers two different avenues for valorizing BR as either a source of alumina, calcium, and iron in the raw meal or as a supplementary cementitious material (SCM). These two computations are completed in parallel to provide a comprehensive assessment of the valorization options for adding BR to the cement production.

2.2. Summary of input parameters

To use the calculator, the user is required to supply certain metrics and information about their products and processes to inform a customized calculation of the economics. The inputs are different for each type of user and a visualization of these input categories is presented in Fig. 1. For the BR producers, inputs in the BR composition, physical characteristics, valorization expenses, expected cement production, and transportation costs are required. For the valorization expenses, the user is asked for the quantity which they seek to valorize, their operational costs for the management of conventional BR disposal, and their costs associated with packaging and preparation for transport of BR as a product. The BR composition is defined by the equivalent oxide content, in percentage, for iron oxide, aluminum oxide, silicon oxide, titanium oxide, and alkali oxides, and the loss on ignition. In the calculator, this information is presented alongside a worldwide average and the local national average, for easy comparison. The transportation and cement production inputs refer to the specific cement plant to which the BR is being sold. The transportation economics of the transportation are calculated from the combination of

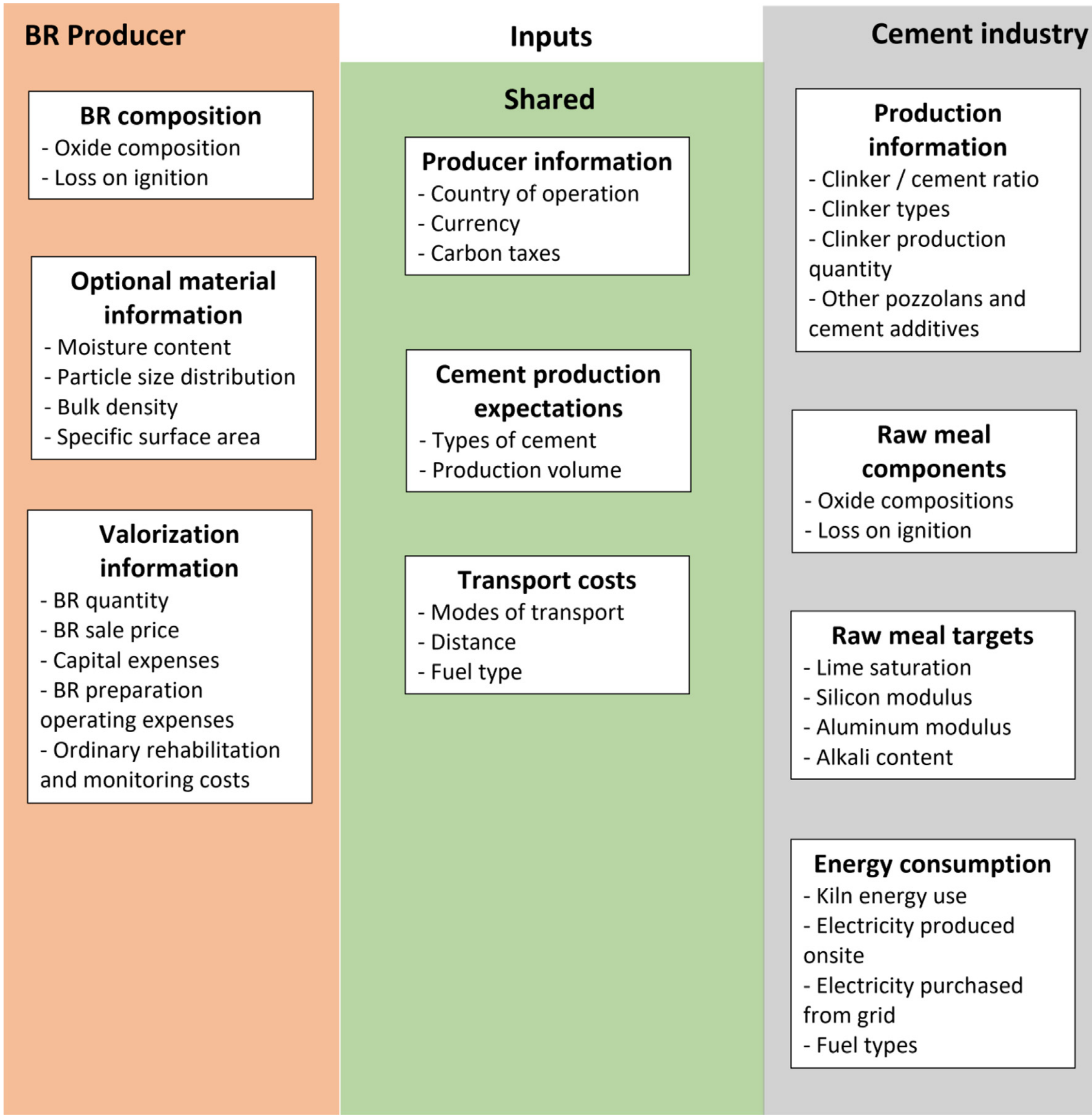


Fig. 1. Visualization of input categories for each user with examples of fields required.

transport modes required, the cost of shipment, transportation distance, and fuel type, for the calculation of transport emissions. The estimated cement production requires the quantity and type of cement produced at the end-use facility for the BR. Finally, the physical characteristics refer to the physical properties of the BR. This is, namely, the moisture content, particle size distribution, specific surface area, and bulk density. These parameters act as a signature of the BR, for comparison to other potential suppliers (Fig. 2).

For users in the cement industry, a separate input page is provided. In addition to the estimated cement to be produced and transportation costs, which are mirrored from the BR producers input page, this page requires more detailed fields of entry for the chemistry of the cement and clinker produced, onsite energy production, and total energy consumption. Input fields are provided for the chemical composition for up to four raw meal constituents, using the same equivalent oxide contents required of the BR, and targeted raw meal factors of lime saturation, silica modulus, and alumina modulus, for cement produced with BR in the raw meal. In addition, the tool calculates the economics based on the types of cement being produced and their recipe in terms of limestone, clinker, gypsum, and other pozzolans. The environmental considerations, mainly CO_2 emissions, and energy savings of utilizing BR are calculated based on the amount of onsite fuel consumed and the external electricity purchased. These values are requested from the user to produce an accurate assessment of the value of adding BR to the cement production.

In preparation for the likely scenario that certain quantitative metrics may be unavailable to a specific user, a variety of national averages have been compiled for various BR properties and cement production parameters which are important to the valorization of BR in cement. The database includes national averages from Australia, Brazil, Canada, France, Germany, Greece, India, Ireland, Jamaica, Romania, Spain, and the USA. This enables the tool to progress and make reasonable estimates even in the case of incomplete information. This methodology has been applied for supply and production factors, such as the composition of the BR, the clinker production carbon emissions, and fuel composition by type, and for external market factors such as the purchased electricity carbon emissions and transportation fuel efficiency. To correctly select which national averages to utilize, the tool asks each user to enter geographical information for their aluminum or cement production facility. This information is used to estimate local taxation, relevant carbon taxes, and compose the economic figures in the output in the local currency to facilitate value assess-

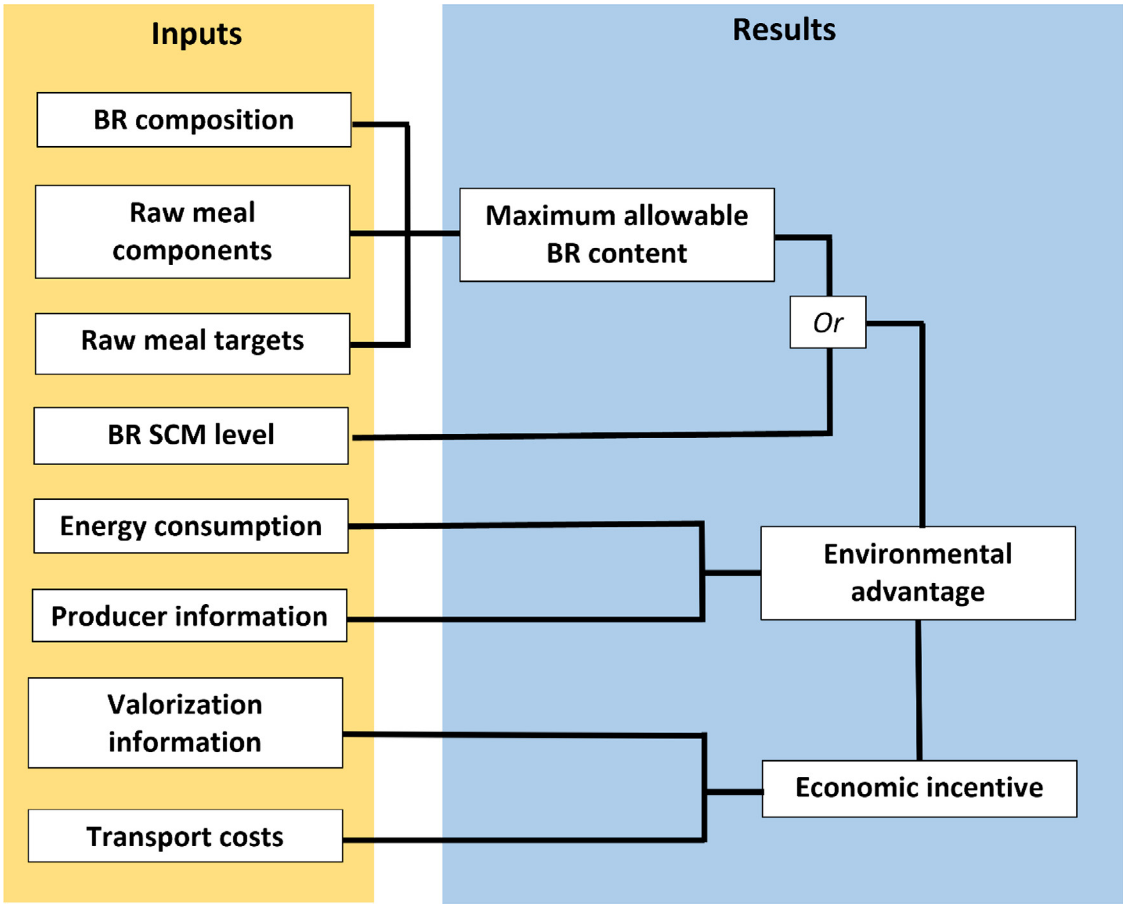


Fig. 2. Process flow diagram for computing the calculator results from the categories of user inputs. Refer to Fig. 1 for details on each category of input.

ment. With the help of the national average database, the two user input pages can be used separately or concurrently to improve the accuracy of the calculations with more detailed composition information from both the BR and the cement raw meal.

2.3. Calculations employed

2.3.1. Bauxite residue in the raw meal

The calculator takes the inputs and expectations provided by the users and computes options for the valorization of BR within the cement production. An illustration of the way in which each user input category is utilized to The utilization of BR in the raw meal is evaluated through the calculation of the maximum BR which can be added to clinker. This computation uses the chemical composition of the BR, provided by the producer, the composition of the raw meal under normal operating conditions, and the targeted raw meal factors if desired to be changed with the addition of BR. To calculate the quantity of BR which can be valorized in the raw meal, a Bogue calculation is applied using the lime saturation factor, silica modulus, and alumina modulus. This standard calculation assumes the oxides of calcium, silicon, aluminum, and iron within a cement are distributed stoichiometrically among four phases: alite (tricalcium silicate), belite (dicalcium silicate), tricalcium aluminate, and tetracalcium aluminoferrite (Swain, 1995; Taylor, 1989). This analysis, in conjunction with the chemical compositions of the raw meal components, enables the calculation of the impact of BR addition into the clinker in terms of the chemistry of the cement. Using the lime saturation, silica modulus, and alumina modulus factors, a maximum allowable BR content can be established, to present the optimal composition for the valorization of BR in the raw meal.

Reductions in energy consumption are calculated to quantify the economic value of the addition of BR. Each production step is analyzed separately to enable the independent assessment of savings from each processing stage. The use of BR, as an industrial byproduct, in the raw meal can reduce energy consumption related to extraction, homogenization, and grinding of the raw materials (Banyasz et al., 2003; Madlool et al., 2011). The list of processing equipment and the type and quantity of fuel required to operate it, provided by the cement user as inputs or drawn from the national average database, are used to calculate the energy consumption for each process using standard conversion factors (Canada, 2018; US EPA, 2015). Fuel consumption due to BR transportation is also accounted for, in the same manner, using the inputs of transportation modes and distances provided by the user.

The calculated reductions in energy consumption are also used to compute the anticipated reductions in greenhouse gas emissions from the use of BR in the raw meal. For BR with high calcium levels, the reduction in limestone required to meet the targeted calcium levels results in a reduced emission from decarbonation. BR also acts as a source of alumina and iron, reducing the quantity of clay and iron corrective required to meet the raw meal specifications and effectively reducing the energy and emissions required for the processing of these raw materials at each processing step. This is converted to a total reduction in carbon dioxide equivalent emissions using standard conversion factors (IPCC, 2006). These carbon reductions are subsequently used with the local carbon taxes supplied by the user or from the national database, to incorporate this factor into the economic analysis.

2.3.2. Bauxite residue as a supplementary cementitious material

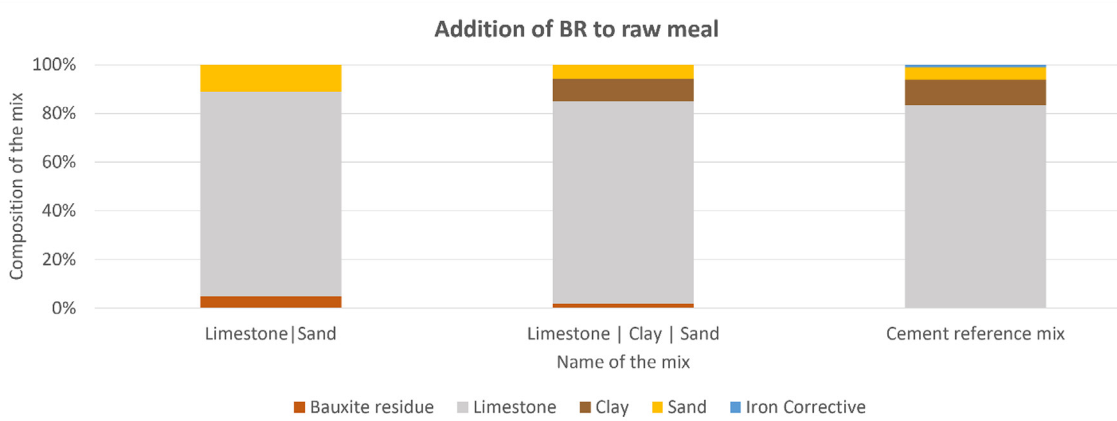
In the utilization of BR as a SCM, BR replaces a portion of the clinker. This can reduce the energy costs of cement production by reducing the volume of material requiring heat treatment per ton of product. This effect is directly proportional to the quantity of BR incorporated as an SCM. The cost savings are calculated based on the cost avoidance of the clinker production less the raw material cost and grinding costs of the BR. The energy savings can be computed directly as a proportional reduction in the amount of clinker required per ton of cement products, plus the energy to grind, filter, and dry the BR, as necessary. These energy savings can be translated directly into emissions reductions using the process described in Section 2.3.1 and the user inputs for fuel types and consumption using standard conversion factors. The replacement of clinker with BR as an SCM results in a reduction in the equivalent carbon dioxide emissions which translates to further economic incentives for production facilities in regions with carbon taxes.

3. Results and discussion

The calculation algorithm developed in this work was prepared in Microsoft Excel for ease of use, wide useability, and the capacity to efficiently visualize the results in tables and figures. From the input parameters provided by the user, the tool calculates the results and composes figures to quantify and visualize the options for adding bauxite residue (BR) as a component in cement production. The tool presents the proposed formulations based on the compositional data available, the cost savings, and the reduction in carbon emissions for cement production with BR in comparison to normal operations. These results are presented in a number of subsections dedicated to each topic and subsequently summarized with printer-friendly reports for each type of user. For the BR producers, the tool calculates revenue based on the operational and capital expenses of commercializing BR and the cost avoidance from conventional disposal of the volume of bauxite residue which is being valorized. For cement industry users, the tool presents the options for the use of BR as a component in the raw meal or as a supplementary cementitious material (SCM). For each, there is a numerical display of the proposed recipe and the projected impact of its use on energy consumption and carbon emissions. The raw material, energy, and carbon tax savings are presented separately and in summary to quantify the economic advantage to valorizing BR as a raw meal component and a SCM in cement production. In this section, the results will be explained, and a worked example is shown to display the format and high level of accessibility of the results achieved in this calculation tool. This example calculates the value of BR addition to a hypothetical cement plant in Germany which produces 1 M ton of cement per year, produced in a petroleum coke burning kiln, and assumes national averages for bauxite residue composition and other factors.

3.1. Bauxite residue as a component of the raw meal

The first results which are presented pursue the option of BR as a component of the raw meal in cement clinker. Using the compositional information provided by the user and the targeted clinker moduli, the calculator proposes a maximum content of BR which can be valorized in the cement production based on the targeted values and inputs provided by the user. In Fig. 3, the worked example shows two clinker recipes that have been calculated that include bauxite residue and a comparison to reference cement produced under normal operating



Bogue calculation applied to calculated clinker

Component name	C3S	C2S	C3A	C4AF
Limestone|Sand	72%	6%	2%	15%
Limestone | Clay | Sand	66%	10%	8%	11%
Cement reference mix	67%	9%	8%	11%

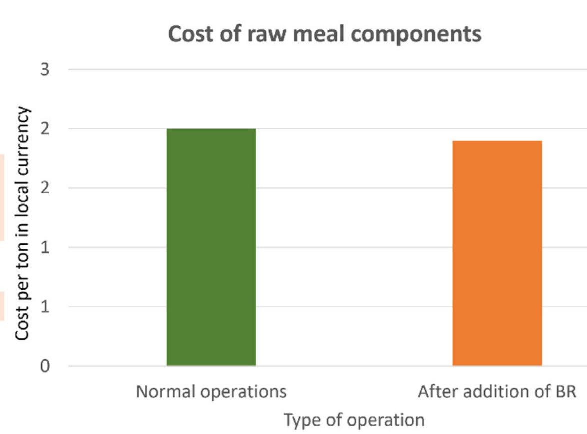


Fig. 3. Example of compositions of proposed BR as a component in the raw meal using German national averages. Acronyms in bogue calculation section follow cement chemist notation. (C3S = tricalcium silicate, C2S = dicalcium silicate, C3A = tricalcium aluminate, C4AF = tetracalcium aluminoferrite).

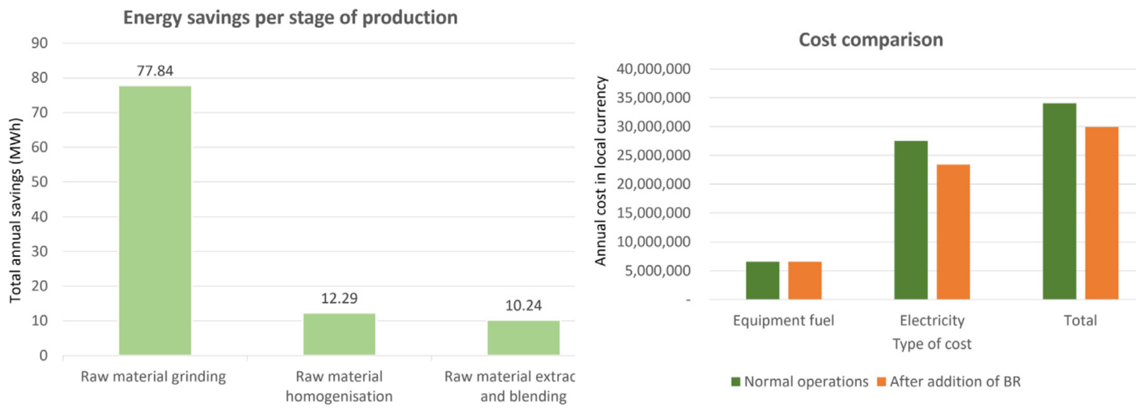


Fig. 4. The energy savings with the addition of BR in the raw meal in each production step and the corresponding cost savings due to reduced fuel and electricity consumption for the worked example simulating a 1 M ton annual cement production.

conditions. The tool provides a numerical presentation of the proposed BR addition levels and raw meal constituents, as well as a Bogue analysis of the phase composition, as shown below. Finally, the raw material costs of the limestone, clay, sand, iron corrective, and bauxite residue used to form the raw meal are calculated compared to normal operating conditions. This value is used as a part of subsequent calculations of the economics of BR addition in the raw meal.

The economics of the proposed raw meal recipe with BR is then calculated in terms of energy savings. This analysis builds upon the user input information as to the energy consumption in each processing stage under normal operating conditions. The addition of BR to the raw meal formulation reduces the required raw material processing which manifests as projected reduced energy consumption in the grinding, homogenization, and blending steps (Banyasz et al., 2003; Madlool et al., 2011). The energy savings for these processing steps are presented in the results numerically and in a visualization such as in Fig. 4. This step-by-step analysis presents a more in-depth rationalization of the total energy savings projected by the tool for the addition of BR to the raw meal. It also enables the breakdown of the energy savings by fuel consumption type, using the input information provided by the user. This allows cost comparison by fuel type consumption, as shown in Fig. 4. The total cost savings contribute to the economics of the addition of BR in the raw meal.

Finally, the reduced energy consumption, analyzed by fuel type, is used to calculate the projected emissions reductions due to the addition of BR in the raw meal. Using standard EPA guidelines for greenhouse gas conversions (US EPA, 2015) and typical fuel compositions based on established fuel types (Canada, 2018), the carbon dioxide equivalent emissions can be estimated for the proposed BR-modified production and under normal operating conditions of cement production. A comparison of these values, such as those shown in Fig. 5, is presented to the user of the calculation tool to quantify the environmental benefits of incorporating BR into cement production. Based on the local carbon tax information provided by the user, this environmental advantage can be directly translated into the projected cost avoidance by reduced taxation. This value completes the economic analysis of the proposed BR addition to raw meal. All of the results, including numerical descriptions of the proposed raw meal formulation, energy savings, and emission reductions, are presented along with a cumulative analysis of the total economic value of the use of BR in the raw meal. This comprehensive report is structured in a printer-friendly format for the user alongside the same analysis for the use of SCM, which is explained in the following section.

3.2. Bauxite residue as a supplementary cementitious material

The potential use of BR as a SCM is considered as a parallel use-case for the addition of BR to cement production. In this case, BR is being utilized only as a replacement for clinker in the final product. This simplifies the calculation of the economic and environmental impact of BR on cement production because it requires no changes to the clinker formulation or kiln operation. However, the impact of BR as an SCM must be validated with laboratory testing to confirm that the proposed cementitious material meets local standards. A warning about this is presented in the calculation tool. As mentioned previously, concerns have been raised in the literature about the impact of BR as an SCM

Type of emissions	Total CO2-e (kg/t of clinker) avoided
From cement production	10.9
From electricity	0.1
Total	**11.0**

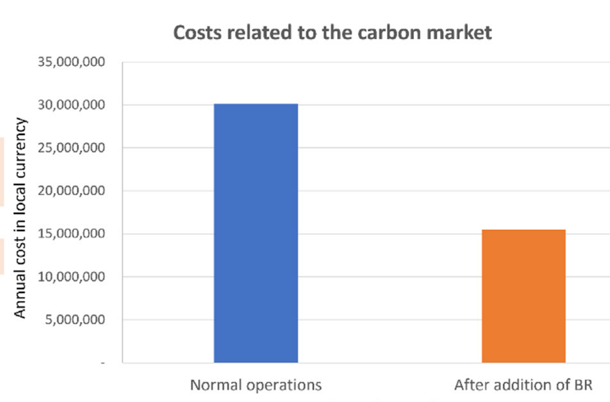


Fig. 5. Carbon dioxide equivalent emission reductions caused by the addition of BR to the raw meal and the corresponding reduction in carbon market taxes for the worked example of a 1 M ton per year cement production in a coke-fired kiln, subject to German carbon taxes.

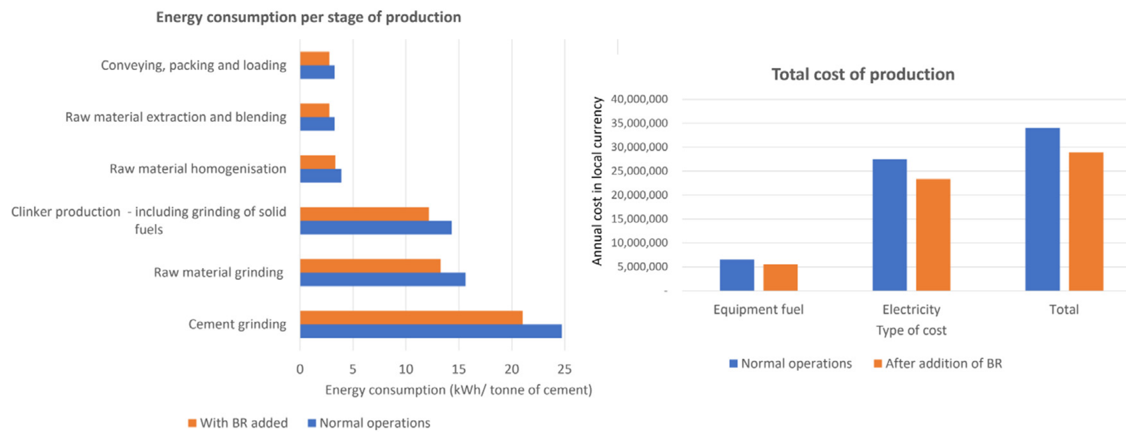


Fig. 6. The energy savings, distinguished by stage of production, and the corresponding cost reductions, analyzed by fuel types, for BR as a SCM in the example of a 1 M ton annual production in a coke-fired kiln.

on the properties of the cement. Calcination of the BR is a common method for improving the reactivity in the blended cement and minimizing negative impacts on the properties (Liu et al., 2011; Wu and Liu, 2012). Since the purpose of this tool is to calculate and compile the economic and environmental advantages of the use of BR, the option of calcination is presented to the user to estimate the impact of this process on the cost and environmental savings of BR addition. Moreover, to facilitate the investigation of BR as an SCM at different potential dosages, the user is provided with the option to select the percentage of BR to be incorporated in the binder as an SCM, in the range of 1% and 30%. For the worked example presented below, 15% BR was selected to generate the figures.

The selected content of BR as an SCM is used to calculate the energy and cost savings in terms of the production volume. This is a proportional reduction for all factors, based on the process information input by the user (Banyasz et al., 2003; Madlool et al., 2011). A worked example of the figures generated to visualize these results is presented in Fig. 6. In the same manner as was calculated for the use of BR in the raw meal, these energy savings are converted into cost savings, categorized by fuel types. In turn, this analysis is used to calculate the total carbon dioxide equivalent emissions for BR-SCM and normal operations cement production to quantify the emission avoidance enabled by the addition of BR. The tool presents these results to the user and calculates the projected value in terms of cost avoidance due to reduced carbon taxation, based on the provided local carbon market information. Examples of these figures are displayed in Fig. 7. The tool compiles the total energy savings, emissions reductions, and economic incentive of apply BR as an SCM in a printer-friendly report presented alongside the options for BR as a raw meal component.

4. Conclusion

The present work has developed a new tool to support collaboration between the aluminum and cement industries in the valorization of bauxite residue. The large volume storage of bauxite residue globally creates an opportunity for the use of this material in cement production to the benefit of both industries. The calculation tool is designed to be used by representatives of each industry, separately or jointly, to accurately calculate the value proposition to both industrial sectors. The tool considers two parallel methods for utilizing bauxite residue in cement production, as a raw meal component or as a supplementary cementitious material. The tool incorporates factors that are unique to each bauxite residue producer and cement production facility, including the bauxite residue composition and equipment-specific energy consumption, improve the accuracy of projections for the energy consumption and carbon emissions reductions on a plant-by-plant basis. In the case of missing data, a database of national averages from countries on four continents has been assembled to provide an avenue for reasonable estimation and allows cement producers to compare their processes to typical productions in their locality. This has created a robust and versatile compositional

Total emissions - (kg CO2-e/ton of cement)

Type of emissions	Emission avoided
From clinker production - raw meal calcination	124.10
From electricity	0.01
Total	**124.11**

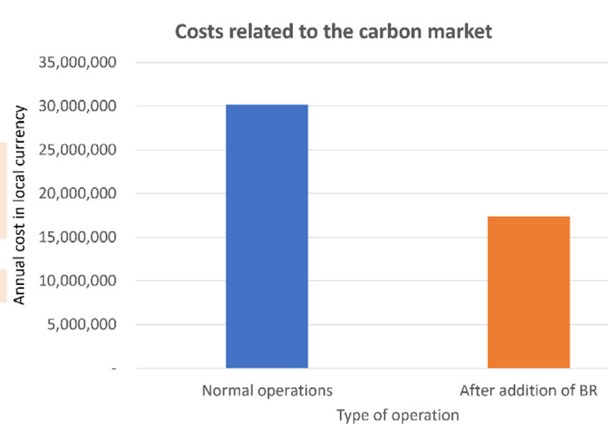


Fig. 7. The carbon dioxide equivalent emissions reduction projected for the use of BR as an SCM at a level of 15% and the corresponding reduction in carbon taxes for the worked example of a 1 M ton annual production of cement at a carbon tax of 24€/ton of carbon dioxide equivalent emitted.

tool that will be useful for continued collaborations between the aluminum and cement industries to develop economically and environmentally conscious processes for utilizing bauxite residue.

Declaration of Competing Interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Sébastien Fortin is employed by Rio Tinto, a producer of bauxite residue. Katy Tsesmelis is employed by the International Aluminum Institute, an advocate for technological improvements in the production of aluminum and the treatment of its wastes. Marcelo Montini is employed by Norsk Hydro Brasil, a cement and concrete producer. Diego Rosani is employed by RosCon, a consulting firm for the cement industry.

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