Evaluation of Model Uncertainty Propagation in Mineral Process Flowsheet Designs

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Abstract: Increasing demand for critical raw materials and energy transition metals sets new targets for the mineral processing, also resulting as higher requirements for the simulation tools during process design and optimization. This study presents a framework for global uncertainty evaluation of modelled plant-wide processes, where the propagation of uncertainty sources is addressed. The uncertainties exist, for example in operational and design parameters and in material properties. The approach was demonstrated with a typical mineral processing flowsheet simulated with commercial software. First, domain knowledge was adopted to screen the parameter space and then Monte Carlo simulation was performed. After this, the generated data set was used to identify surrogate models between the uncertain inputs and process performance indicators. Finally, a global sensitivity analysis was conducted to identify the effects of uncertainties to the decision-making in process design. The results were particularly used to locate the process points where accurate information is needed for the robust process design, or where on-line measurements would be preferred to establish on-line optimization.

Keywords: Flowsheet simulation, Process design, Global sensitivity analysis, Surrogate model.

1. INTRODUCTION

As critical minerals have become more crucial for the operation of societies, the necessity to maximize the efficiency of all processes throughout the lifecycle, namely mining, refining, and recycling, is even more important than before. Increase in the demand of critical minerals opens new demand for circular economy system, in which the maximum efficiency is achieved by minimizing losses in all parts of the cycle (Whitworth et al., 2022). These developments increase the number of processes, where multiple minerals are present in the separation processes, which in turn increases the complexity of simulation models, and uncertainty of simulation and model-based decision making in process design and in process operation.

Mineral processes aim to extract valuable minerals from ore. The process usually consists of multiple stages, which all of them have their unique properties, and thus described with different mathematical models and uncertainties related to them. The uncertainties need to be attributed to their sources through simulations to facilitate the process optimization (Sepúlveda et al., 2014).

The lack of understanding that exists around inspected system creates a need to model the system, which itself holds inherent uncertainty, for example assumptions, process randomness and measurement errors (Caers, 2011a). Precisely, the definition of uncertainty is tied to the model uncertainty when it is quantified by sensitivity analysis (Sepúlveda et al., 2014, Arnst et al., 2021, Puy et al., 2022), although uncertainty is a wider concept itself. According to Campolongo et al., (2000), sensitivity analysis complements uncertainty analysis.

The goal of extracting valid information is to reduce uncertainty in an influential decision-making process. Because collecting more information does not necessarily reduce uncertainty, it is important to find the parameters that best describe uncertainty (Caers, 2011b).

Sensitivity analysis is a method that can be also applied to identify how the uncertainty in model output is divided in its inputs. There, a local sensitivity analysis provides changes one input parameter at a time. Global Sensitivity Analysis (GSA) is a more robust solution compared to local sensitivity analysis (Cisternas and Lucay, 2020). It can overcome the limitations of inspecting one variable at a time, and thus enables to find relationships between the variables that would be otherwise left undiscovered (Sepulveda et al., 2013).

GSA has been applied in mineral processing, for example, improving the milling operation by (Lucay et al., 2019) as they considered both the operational (epistemic) uncertainties and stochastic uncertainties related to feed properties. Further, a framework of deterministic process design, elimination of non-influential process variables and recognition of critical parameters through GSA was used in (Lucay et al., 2015) for a mineral concentration process. Ohenoja et al. (2023) used GSA to identify and to weight the most important process measurements in the model adaptation problem of a flotation circuit. Arancibia-Bravo et al (2022) similarly used GSA to identify critical model input parameters of copper flotation in saline systems, while (Sitorus and Brito-Parada, 2020) applied

GSA for the selection of optimal crushing equipment in multiple criteria decision-making model.

As mentioned, mineral processes are characterized by a combination of multiple processing stages making the overall flowsheet complex. The input parameter effect on the uncertainty of the global output parameters of each separation unit can be analyzed by dividing the inspected flowsheet into stages (Montenegro et al., 2015). By doing this, the propagation of the uncertainty can be analyzed. One approach to gain insight on uncertainty propagation is Monte Carlo (MC) simulation (Albert, 2020).

MC requires a sufficiently big sample size to produce sufficient resolution for the intended purposes (Helton and Davis, 2003). Thus, complex flowsheets or detailed models may set limitations to the applicability of MC. Therefore, surrogate models are also used in uncertainty evaluation. Analytical solutions to uncertainty have been inspected utilizing surrogate models, for example in (Liu et al., 2024), where the presence of two or more uncertainty factors is the source of complexity. Lu et al. (2018) showed that generalized linear models can be used to get accurate sensitivity indices, by utilizing polynomial approximations of the data.

This study presents and demonstrates a framework for global uncertainty evaluation of plant-wide processes, where the propagation of uncertainty sources is addressed. The uncertainty propagation results in this publication give insight of the uncertainty factors and sources, that would be used during the model-based process design or in operational optimization. Thus, this work aims to extend from previous GSA studies, such as (Lucay et al., 2012), where focus was on one separation process model. The uncertainty evaluation framework is demonstrated utilizing a typical mineral processing flowsheet simulated with a commercial software.

The following sections of the paper are distributed as follows; Section 2 outlines the constructed framework, and the software and mathematical methods used. Section 3 details the selected mineral processing case study, the performance of the surrogate models identified, and the sensitivity analysis results. The evaluation of the case study results, and discussion of the proposed framework is described along Section 4. Finally, Section 5 summarizes the main findings of the research.

2. MATERIAL AND METHODS

2.1 Framework

The framework is described in Fig. 1. As a starting point, the mineral processing flowsheet model was established to a simulation software. Then, the possible input and output parameters from the software used were listed with domain knowledge and inspected through a screening step. This was performed as a local sensitivity analysis by directly inspecting the variation caused by each input to one output individually. As a result of the screening step, the number of possible input parameters for the global sensitivity analysis were reduced. This is typically necessary to facilitate the MC simulation of complex flowsheets.

The final selection of parameters, and their ranges, were confirmed from the forementioned list based on domain knowledge. After the parameters had been chosen, a MC simulation was performed in the flowsheet simulation software. The resulting data set was then utilized to train the surrogate models and to perform GSA with the identified models. To improve the performance of surrogate models, and the sensitivity analysis based on them, the flowsheet was considered as blocks, where the surrogate models of previous blocks can act as inputs for the following modelled blocks.

In the demonstration of this study, the simulation software used was USIM PAC (See Section 2.2). The screening step was analyzed using spreadsheets and interviewing the experts. The MC was conducted with the embedded MC tool in the simulation software. The MC data set was then exported to Matlab® to identify surrogate models (See Section 2.3) and to perform sensitivity analysis (See Section 2.4). The studied flowsheet is presented in Section 3.1.

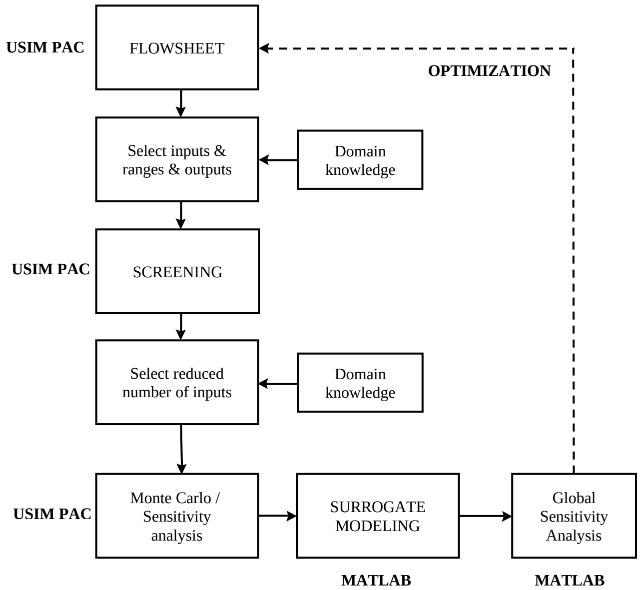


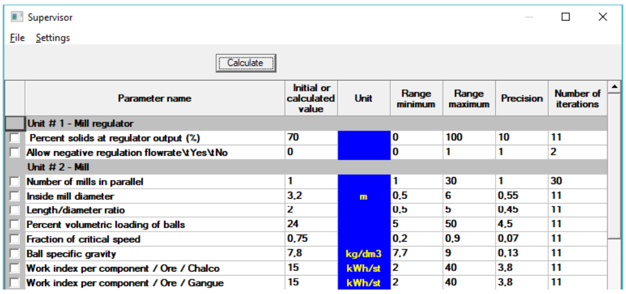
Fig. 1. Approach for estimating uncertainty propagation in flowsheet simulation.

2.2 Simulation software

In active development since 1986, USIM PAC has been created by the BRGM´s (French geological survey) Process Simulation Group. Since 2004, CASPEO, a spin-off of BRGM, has been the company behind its development and distribution. Although it has been used in several industries, USIM PAC is a process simulation software primarily intended for mineral processing and hydrometallurgical operations, where it can be used for design or optimization purposes.

The Supervisor, which is one of the optimization algorithms available in USIM PAC (Guillaneau et al., 1995) was the main calculation tool used to generate the simulation results in this work. The Supervisor algorithm can be used either as a sensitivity analysis tool or for visual optimization. It calculates user-defined parameters (soft-sensors, outputs) when some input parameters (actuators) vary. The variation of the actuators can be defined using different methods: (1) Scanning, which generates a set of vectors by the combination of different values of each parameter in a given research domain; (2) Sensitivity Analysis, which evaluates each parameter using a user-defined range and step; (3) Monte-Carlo, which generates as many parameter values as required using a random procedure with the selected statistical distribution (Gauss, Uniform, or other) to constitute a point.

A screenshot of the Supervisor tool is depicted in Fig. 2. The output of the Supervisor tool is a file displaying the list of the values of the user-defined soft-sensors resulting from the simulations performed for each random value of the actuator or combination of actuators. As this file can be exported as a spreadsheet, the results can be easily exploited using statistical analysis tools.



Supervisor

File Settings

Calculate

Parameter name	Initial or calculated value	Unit	Range minimum	Range maximum	Precision	Number of iterations
Unit # 1 - Mill regulator						
Percent solids at regulator output (%)	70		0	100	10	11
Allow negative regulation flowrate\tYes\tNo	0		0	1	1	2
Unit # 2 - Mill						
Number of mills in parallel	1		1	30	1	30
Inside mill diameter	3,2	m	0,5	6	0,55	11
Length/diameter ratio	2		0,5	5	0,45	11
Percent volumetric loading of balls	24		5	50	4,5	11
Fraction of critical speed	0,75		0,2	0,9	0,07	11
Ball specific gravity	7,8	kg/dm3	7,7	9	0,13	11
Work index per component / Ore / Chalco	15	kWh/st	2	40	3,8	11
Work index per component / Ore / Gangue	15	kWh/st	2	40	3,8	11

Fig. 2. Selection of actuators in USIM PAC Supervisor.

2.3 Surrogate modeling

The data acquisition from USIM PAC to the surrogate modeling was performed using the MC simulation property in USIM PAC. The resulted *.csv was read in Matlab®, where the surrogate models were fitted using Regression Learner application. The selected modelling approach here was linear stepwise regression. The performance of the final model structure was evaluated with two different metrics: mean absolute percentage error (MAPE) and coefficient of determination (R^2).

2.4 Sensitivity analysis

According to (Campolongo et al., 2000), sensitivity analysis is an integral part of the modeling process. As a quantitative method, it can decompose the variance of output variable Y. It can be used as a tool to identify noninfluential parameters, and thus be used to simplify and/or improve the uncertainty modeling.

The total sensitivity index takes into consideration all the input parameters (X_i) and their possible combinations (X_{ij}) and displays the average effect of the inspected input variable (Lucay et al., 2019). According to (Saltelli et al., 2007), the first order sensitivity being similar in magnitude to the total effect index, means that there is no interaction between the inspected parameter and the rest of the parameters. Otherwise, the first order sensitivity index is always smaller than the total order index, if there is even a small interaction between the inspected parameter and other parameters.

The GSA approach was originally proposed in (Saltelli and Homma, 1996). The refined method in (Saltelli, 2002), gives a pathway to circumvent the curse of dimensionality when dealing with high factor count models, turning $n2^k$ into $n(2k+2)$, where k is a term of order and n is the sample size used to estimate one individual effect. They noted that the computation of the sensitivity indices is more straightforward in the higher order terms. The advantages of the method are the flexibility concerning the utilized models in the sensitivity analysis and the computational inexpensiveness. Thus, the method from (Saltelli, 2002) is more attractive tool for engineering applications, and was also selected to this study.

The total order index, S_{Ti}, is formed by following formula (Saltelli et al., 2007, p.164):

$$S_{Ti} = 1 - \frac{V[E(Y|X_{\sim i})]}{V(Y)}, \qquad (1)$$

where i refers to the input parameter, $V(Y)$ is the variance of the inspected output Y, and $E[Y|X_{\sim i}]$ is the estimated conditional mean of output Y in relation to input $X_{\sim i}$. $V(E[Y|X_{\sim i}])$ is the conditional variance of output Y in relation to input $X_{\sim i}$.

The sensitivity analysis was done in Matlab® utilizing Latin hypercube (LHS) sampled data based on the utilized parameter ranges. The used functions for the sensitivity analysis can be found in (Vandy, 2016).

3. RESULTS

3.1 Input screening and the studied flowsheet

The flowsheet used in simulations is presented in Fig. 3. The grinding circuit (GC) comprises a ball mill and a hydrocyclone classification with one recycle stream. The flotation circuit (FC) includes four flotation stages (Rougher, Scavenger, Cleaner 1, Cleaner 2) with two recycle streams.

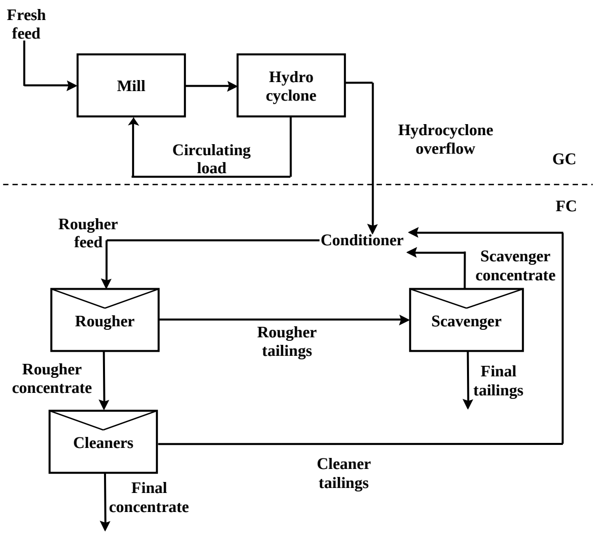


Fig 3. Studied flowsheet.

In the studied flowsheet, the streams under interest were:

- GC product,
- Circulating load to the mill (hydrocyclone underflow),
- Rougher feed,
- Final tailings, and
- Final concentrate.

From these streams, several properties were monitored as outputs, namely:

- Ore concentration,
- Particle size,
- Ore mass flowrate,
- Total volumetric flowrate,
- Solids concentration, and
- Grade.

These represent the outputs *Y*, that are modeled and subjected to GSA.

For the screening step, a large number of input parameters were reduced to a smaller group of important input parameters with domain knowledge and simulations using the Scanning feature of USIM PAC. Table 1 presents the selected input parameters after the screening. For the grinding circuit, mill rotation speed and grinding media loading represent operational variables, whereas grindability is a material property. Similarly in flotation circuit, the pulp level and water content can be manipulated in an operational environment. The floatabilities can be considered either material properties (liberation, mineral properties) or operational variables (addition of flotation chemicals). The different flotation cells in the flowsheet, namely rougher, scavenger, and two cleaners, have unique parameters. As mentioned in Section 2.1., the surrogate model outputs from the grinding circuit also act as inputs for the flotation circuit surrogate models.

Table 1. Selected process parameters for MC simulation and surrogate modeling.

Grinding circuit	*Flotation circuit*
Grinding media loading	Pulp level in cell
Mill speed	Pulp water content in cell
Ore grindability	Ore floatability in cell
Gangue grindability	Gangue floatability in cell
Hydrocyclone feed diameter	Surrogate model outputs from the grinding circuit
Hydrocyclone overflow diameter	
Hydrocyclone underflow diameter	

3.2 Monte Carlo simulation

MC simulation was performed utilizing uniform distribution for the input parameters. The used range of the input parameters varied from ±5% to ±10% in USIM PAC supervisor. The variation amplitude was based on domain knowledge. The number of MC simulations done in USIM PAC was 10,000. The generated data was used to fit surrogate models for the GSA. In GSA, MC was used in generating sample inputs for the surrogate models utilizing LHS design. The input range was extrapolated to ±10% for all inputs. The sample data consisted of 10,000,000 points.

3.3 Surrogate modeling

In total, 30 surrogate models, representing the outputs *Y*, were identified using the MC data set from USIM PAC. The model performance, in terms of MAPE, for the GC outputs and FC outputs are presented in Fig. 4 and Fig. 5, respectively. Overall, the low MAPE values (< 1.8%) indicate that the GC stream properties from the flowsheet simulation can be accurately described with surrogate models. The solids concentration in Fig. 5 lacks modeling error values for Final concentrate or Rougher feed streams, as the MC data set indicated constant output values.

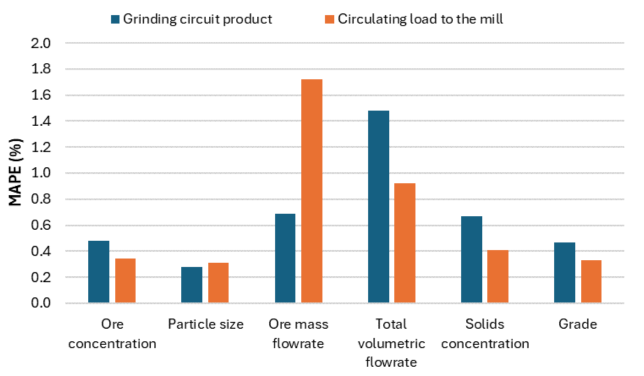


Fig. 4. Model performance (MAPE) of the identified surrogate models for GC.

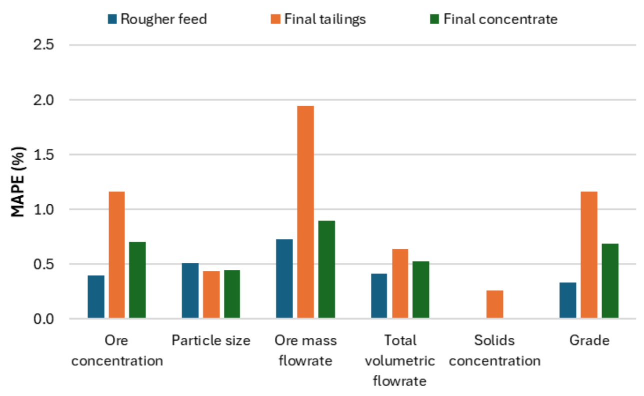


Fig. 5. Model performance (MAPE) of the identified surrogate modes for FC.

The scatter plots of the worst performing surrogate models (Circulating load to the mill and ore mass flowrate in final tailings) are presented in Fig. 6 and Fig. 7, respectively. The MAPE values inspected together with R^2 give a more comprehensive understanding of the model performance. The figure shows that the R^2 values are also at acceptable levels (greater than 0.70) in this case. For the ore mass flowrate in Fig. 6, the surrogate model seems to systemically underestimate some of the values above 11.8 t/h. Thus, for this variable, another model structure could be studied to improve the modeling performance further.

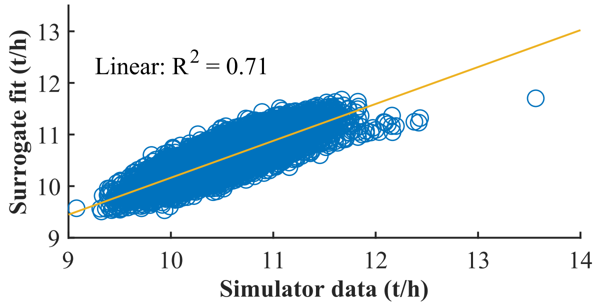


Fig. 6. Scatter plot of ore mass flowrate in the Circulating load to the mill. The scale in both axes begins at 9.

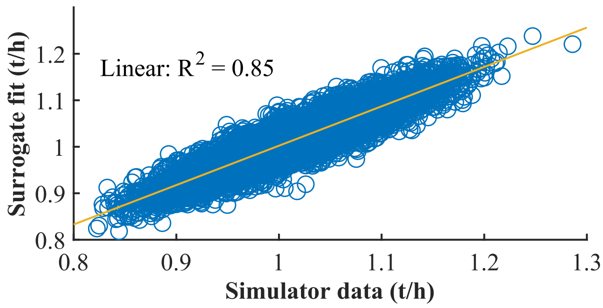


Fig. 7. Scatter plot of ore mass flowrate in the Final tailings. The scale in both axes begins at 0.8.

3.4 Global sensitivity analysis

The GSA was performed using identified surrogate models. In GSA, the results are interpreted individually to different flowsheet sections in order to understand the propagation routes of the uncertainties.

Grinding circuit

The utilized input parameters for GC were listed in Table 1. From the GSA results, some essential outputs, such as in PSD (Particle size distribution), ore concentration and grade were inspected in detail and are discussed below.

PSD is usually the key process quality parameter in grinding circuits. According to the results, PSD of the Grinding circuit product is mainly affected by the hydrocyclone parameters (S_{Ti} from 0.51 to 0.06), whilst mill and ore parameters had very small sensitivity (S_{Ti} <0.04) to the PSD. However, for Circulating load to the mill, the gangue grindability (0.41), mill speed (0.32) and the grinding media loading (0.25) explain the PSD variation according to the GSA.

Grinding circuit product concentration variation is best explained by gangue grindability (1st, 0.55), ore grindability (2nd, 0.45) and hydro cyclone underflow (3rd, 0.11). The same finding applies to the concentration in Circulating load to the mill, and to the grade variation in both streams.

Overall, the operational variables show only moderate sensitivity to the studied outputs in GC; Grinding media loading affects the total volumetric flowrate of GC product and PSD of circulating load. Mill speed affects the GC product solids concentration and PSD of circulating load. One explanation could be that the selected ranges of the other input parameters mask the effect of mill operational parameters in most of the studied outputs. One way to overcome this problem in sensitivity analysis would be to narrow down the parameter ranges of feed characteristics, or to sample the parameter values from different types of probability distributions as done in (Lucay et al. 2019).

Flotation circuit

The utilized input parameters for FC are listed in Table 1. In addition to these parameters, the outputs from the GC surrogate models are used as surrogate model inputs, and thus, in GSA. Three of those were identified to be very significant inputs parameters for all FC outputs.

In all three FC streams, the concentration in the GC product stream shows significant sensitivity to the ore concentration (or grade), and particle size (S_{Ti} between 0.47 and 0.29). This is an expected result, as variation in flotation fresh feed properties determine the flotation performance. According to the GSA results, the gangue floatability in rougher and pulp water content in cleaner 1 are also sensitive parameters (S_{Ti} between 0.10 and 0.16) to the rougher feed and final concentrate concentrations, respectively.

Interestingly, the ore concentration and particle size in Circulating load to the mill seems to explain some variation in flotation streams' properties (S_{Ti} up to 0.30 and 0.32, respectively). This might be contributed by the fact that the circulating load affects the water addition rates in the flowsheet model, which then propagates into a variation in flotation circuit. Another explanation could be that the mentioned circulating load properties are affected by mill speed, grinding media loading, and hydrocyclone parameters, which were also seen in the GSA results for the grinding circuit.

Regarding the solids concentration in final concentrate, the GSA shows that the total pulp water content in cleaner 2 is the most influencing variable (S_{Ti} 0.85). This is natural, as the higher water content in the final flotation cell corresponds to the lower solids concentration of the product. Otherwise, the flotation circuit operational parameters are not among the most sensitive parameters in the simulated data set, again highlighting the need to carefully determine the input's probability distributions for the sensitivity study. Another observation from these results is that there can be limited possibilities for the operational parameters to mitigate the effect of the disturbances entering to the FC from upstream process steps.

Summary of GSA results

The GC circulating load parameters have a high effect (S_{Ti} >0.10) to the flotation circuit variation. This is due to the mill being unable to process the feed (and recycle) fast enough, thus increasing the amount of water and decreasing the solids concentration in the feed to the FC. This is observable from the parameters with influential S_{Ti} in the circulating load being ore grindability, mill speed and mill grinding media loading.

In Fig. 8, the occurrence of the most sensitive inputs for the rougher feed properties is depicted. The frequency corresponds how often the input parameter was among the three most significant input parameters based on GSA. Similarly, Figure 9 shows the result for final tailings properties and Figure 10 for the final concentrate properties.

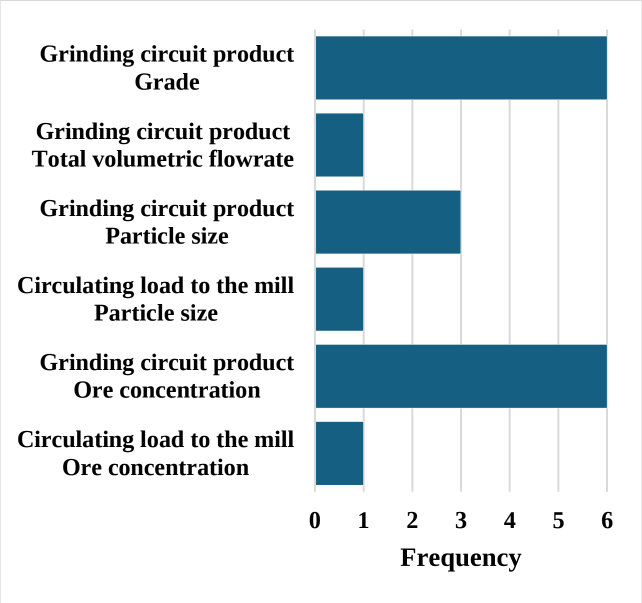


Fig. 8. Occurrence of the most sensitive inputs for rougher feed properties.

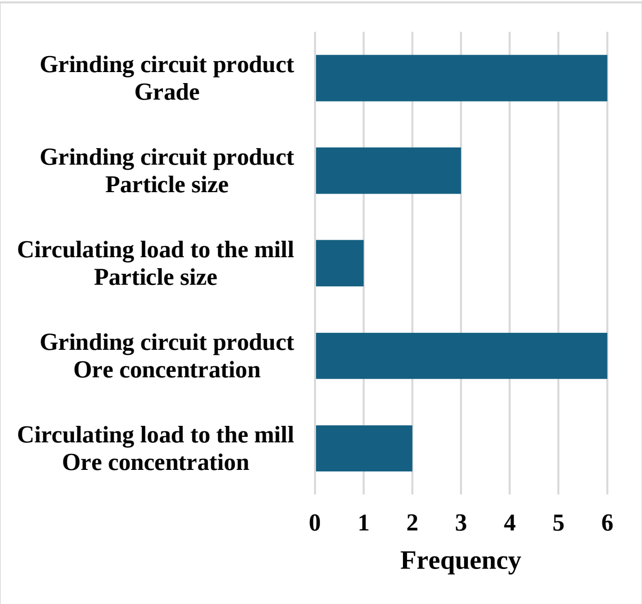


Fig. 9. Occurrence of the most sensitive inputs for FC final tailings properties.

From Fig. 8, it can be observed that the rougher feed properties are naturally sensitive to the parameters in GC product. According to the results, the input parameters that describe the ore concentration, grade and particle size thus describe the flotation circuit performance and the final concentrate variation.

The ore feed characteristics and the ability of the GC to categorize the feed into set particle size similarly most describe the variation in the final concentrate and final tailings (See Fig. 9 and Fig. 10), which is an expected result after the rougher feed results. An outlier to this statement is the Pulp water content in cleaner 2, which is an operational input parameter in FC. As the fresh feed characteristics can't be affected by the operation of the GC, the only thing left to do is to minimize the variation in the ore size distribution by GC operation.

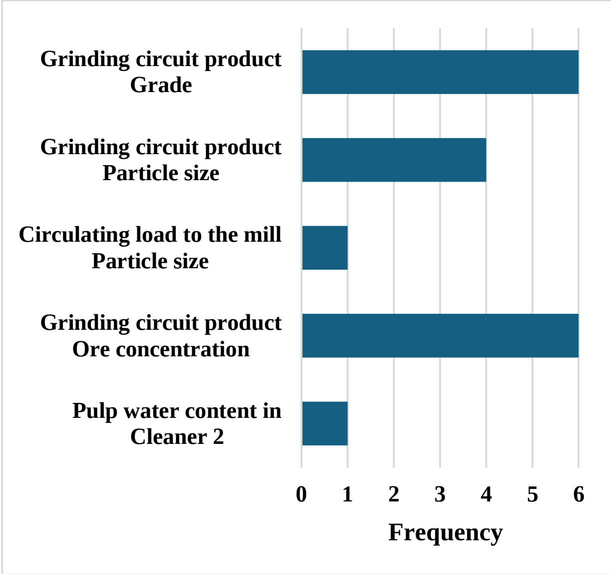


Fig. 10. Occurrence of the most sensitive inputs for FC final concentrate properties.

4. DISCUSSION

In addition to the surrogate models presented, the FC outputs were also modelled using only the MC data without GC surrogates. The performance of the FC surrogates, in this case, was slightly worse (>0.05 lower R^2). This alternative would also make it more difficult to inspect the propagation of uncertainties as GC models do not act as inputs for the FC.

Production of outliers by the GSA method, or volatility, is due to its non-additive nature. Non-additivity in this context means, that the generated S_{Ti} value is not equal to the sum of the values of the component parts. This is a cost caused by the computational and straightforward nature of the used Saltelli's approach over the original Sobol's method (Saltelli et al., 2007). This limits the interpretation of the lower magnitude S_{Ti}. Thus, mainly the three most significant S_{Ti} were discussed in this study. Naturally, a more thorough GSA interpretation could involve inputs with lower influences into the analysis of uncertainty, if the volatility issue can be solved.

Like (Puy et al., 2022) concludes in their publication, Saltelli's total order method becomes inaccurate with higher dimensionality (k>10). The exponential growth in input parameters of more complex flowsheets is an issue that needs to be addressed thoroughly, utilizing similar design of experiments and domain knowledge methods that were shown in this study. Domain knowledge gives insight on what parameters are influential based on previous experiences and the local sensitivity analyses on the possible unknown sensitivities in the analyzed setup.

The proposed approach for the uncertainty analysis with surrogate models resulted in a lower computational load and made it possible to use large sample size in GSA. This decreases the inherent volatility of Saltelli's method. The accuracy of Saltelli's method for the most important parameters can be improved by repeating the GSA with multiple LHS designs (Puy et al., 2022). Alternative methods for calculating total order sensitivity indices, such as Jansen, Razavi and Gupta, Janon/Monod and Azzini and Rosati, suggested by (Puy et al., 2022) could also be considered.

The results in this study suggested that the most influential S_{Ti} are related to the feed characteristics and the mill performance. Thus, for more robust operational decisions, the focus could be shifted to better measure the feed properties in on-line to minimize the effect of stochastic (inherent) uncertainty. For process design purposes, the results highlight the emphasis needed for GC design and its flexibility to tackle and decrease the uncertainties, that will otherwise strongly propagate downstream to FC streams. If stochastic uncertainties remain, only the epistemic uncertainties can be affected, and thus the focus needs to be on lesser magnitude, operational sensitive indices. To achieve the best design and operational reduction of uncertainty, maximum range of uncertainties (all $S_{Ti} > 0.10$) need to be considered.

The proposed framework could benefit from the development of software interfaces establishing more automated data transfer. Dividing the process into parts is beneficial for understanding the propagation of uncertainty through the different parts of the process. At the same time, more data is generated that needs to be handled efficiently between the different software tools. Further, the interface between the sensitivity analysis results and decision-making in process design or on-line operation requires further development.

5. CONCLUSIONS

In this work, an uncertainty propagation evaluation framework was established to be used in model-based decision making. The proposed methods were chosen to enable rapid inspection of complex systems typically seen in flowsheet simulators. The results in this paper demonstrated that this framework can be used to identify the most influential parameters throughout the whole inspected process chain. This allows to focus further analyses to the propagation of uncertainty attributed to these identified parameters.

Regarding the case study, the propagation of uncertainty within the studied flowsheet was observed through dividing the flowsheet into the grinding circuit (GC) and to the flotation circuit (FC). By doing this, the changes in the GC were seen to have strong influence on the flotation circuit model output variation. The GC inputs were the top three most influential inputs for all observed output parameters in the FC. The most sensitive operational FC input parameters were not found among the top three most influential input parameters but were still considered influential (total sensitivity index values >0.10). Those parameters were gangue floatability in rougher and pulp level in cleaner.

Final sensitivity indices indicating the most sensitive parameters in the whole process were found in the fresh feed characteristics (ore concentration/grade and particle size distribution), and the ability of the mill to reduce the particle size distribution to the desired range. The operational input parameters had a lower influence in general, but that result might be due to the small range of changes applied in simulation, so further studies are required.

ACKNOWLEDGEMENTS

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