

# Chapter 33

## Predictive Geometallurgy: An Interdisciplinary Key Challenge for Mathematical Geosciences



K. G. van den Boogaart and R. Tolosana-Delgado

**Abstract** Predictive geometallurgy tries to optimize the mineral value chain based on a precise and quantitative understanding of: the geology and mineralogy of the ores, the minerals processing, and the economics of mineral commodities. This chapter describes the state of the art and the mathematical building blocks of a possible solution to this problem. This solution heavily relies on all classical fields of mathematical geosciences and geoinformatics, but requires new mathematical and computational developments. Geometallurgy can thus become a new defining challenge for mathematical geosciences, in the same fashion as geostatistics has been in the first 50 years of the IAMG.

**Keywords** Geostatistics · Statistical scales · Microstructure · Computational geometry · Processing optimisation · Value of information · Mineral liberation analyser · QUEMSCAN

### 33.1 Introduction

*Geometallurgy*, from the Greek words for earth (geia), metal (metallo) and work (ergon), can be understood as the exploitation of a metallic ore based on a precise understanding of its geoscientific characteristics. Geometallurgy is hence a cooperation field for geoscientists and mineral processing engineers, something which has occurred in virtually all mining operations. A modern understanding of geometallurgy, what we could call *predictive geometallurgy*, proposes a quantitative approach to the subject. In rough terms, that requires optimizing the ore processing based on automated mineralogy and microstructure characterisation of the ore, coupled with geometallurgical tests. These are tests conducted at several scales (from lab to plant) along which the actual ore is processed in realistic conditions in order to study the differential behaviour of the several ore and waste mineral phases, and thus the enriching potential of the ore through the processes considered.

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As a subject, mathematical geosciences has always had a wide application in mining. Nowadays typical topics of the area are geostatistics, the analysis of data from special scales (such as compositional data or spherical data), numerical analysis of flow models, remote sensing, (mineral) potential modelling (for instance with weights of evidence), fractals, geodata standards, 3D geomodelling, or data integration techniques. The aim of this chapter is to show the deep link between geometallurgical problems and techniques from the main fields of mathematical geosciences.

Geometallurgy distinguishes primary and secondary properties of the ore (Coward et al. 2009). Primary properties are intrinsic to the ore and do not depend on the process. Secondary or response properties describe the behaviour of the ore during processing. The primary properties are observed by chemical assays, automated mineralogy (like with QUEMSCAN or Mineral Liberation Analyser—MLA—), X-ray methods, and other analytical instrumentation. Secondary properties are measured with geometallurgical tests, such as blasting tests, Bond mill test, flotation tests, magnetic separation, density separation and so on. These can even be conducted using the operation itself, that is, on the real plant. The secondary properties are used to predict the outcome and costs of the processing.

To the authors' knowledge, all studies conducted on predictive geometallurgy by mathematical geoscientists (Bye 2011; Boisvert et al. 2013; Rossi and Deutsch 2014; Hosseini and Asghari 2015; Tolosana-Delgado et al. 2015; Ortiz et al. 2015; Deutsch et al. 2016) consisted on appropriately predicting the secondary properties at each block of a mining block model, and proposing the mining and processing engineers to conduct their mine planning and plant scheduling based on those properties instead of on metal grades. The first step (Vann et al. 2011) is the geometallurgical analysis of the ore body with respect to its primary properties. Samples of similar primary properties or geology are often said to belong to the same *geometallurgical domain*. Conventional descriptive exploratory analysis like k-means clustering, PCA (Caciagli Warman 2015) or machine learning methods are nowadays used for this task. Moreover, primary properties are also interpolated to the block model, ideally with geostatistics.

The second step is a geometallurgical testwork, i.e. the characterisation of secondary properties of material from different geometallurgical domains. Often the goal of these tests is to define a mapping from the primary properties to the secondary properties, e.g. via more or less complex regression models (Keeney et al. 2011; Everett and Howard 2011; Sepulveda et al. 2017). Having it makes possible to populate the block model with estimated secondary geometallurgical properties and to infer the expected income and costs of each block. Such interpolation of secondary variables is often done on additive proxies (Ortiz et al. 2015; Deutsch et al. 2016). The result is typically called a *geometallurgical (block) model*.

This can be used in at least three different ways by an operation, to inform both in short- and long-term actions (McKay et al. 2016). First, the prediction of costs and recovery allows to assign monetary values to each block. These values can be used instead of grade as better proxy of cashflow in further calculations, like the mentioned ultimate pit or mine scheduling. Value is generated by minimizing capital costs, due to early exploitation of highly valuable parts of the deposit, and by

an improved distinction between ore and waste (Bye 2011). Second, the predicted properties can be used as well to find matching ore partners in blending to reduce feed variability in the plant, and ensure constant plant operation conditions. Value is generated by lower risk of plant failure, optimal use capacity of all parts of the plant, and lower controlling efforts by the ability to find the optimal operation conditions empirically (Shaw et al. 2013). The third option is to use that knowledge to actively adapt the processing conditions to each portion of the varying feed. The value lies in higher recovery, lower operation costs, more extensive exploitation (Powell 2013; Tolosana-Delgado et al. 2015) and ultimately lower ecological footprint.

### 33.2 Process Modelling

With the exhaustion of simple-texture, single-commodity, easy-to-reach deposits, the mining industry has been confronted with the need to study a broad range of ore properties, beyond the classical grade. As mentioned in the introduction, predictive geometallurgy proposes to obtain a wealth of primary and secondary properties at each mining block in order to reproduce its behaviour through the processing chain and, ultimately, to predict its monetary value. This section focuses on such process modelling.

A couple of steps along the value chain after extraction and crushing, ores are treated with a variety of processes, mostly physical and physico-chemical, in order to liberate the several mineral grains and separate them in different streams. Later on, streams enriched in ore minerals are sent through metallurgical processes, mostly chemical and physical changes of state processes devised to break the crystal structure of the ore minerals and produce the final value metals. All these steps can be studied with two approaches. In the first one, each operation unit is considered as a black box, and data from both the conditions of operations and the properties of input and output streams are obtained in order to build empirical rules to predict the output streams (Matos Camacho et al. 2015). In the second strategy, these prediction laws are built in accordance with thermodynamical, chemical and physical first principles. These strategies are not mutually exclusive, as one can derive the form of a parametric predicting equation by first principles and fit the parameters with the empirical approach.

The first kind of processes mentioned, those mostly keeping the crystal structure of the minerals involved, include many different processes. Grinding and milling aim at splitting particles in order to produce single mineral, or *liberated*, particles. Sizing, magnetic separation, density separation and many other separation processes aim at splitting a *feed* stream into two or more streams with particles primarily classified according to one particular bulk volumetric property, like size, magnetic susceptibility or density. Finally, froth flotation aims at separating particles according to the hydrophobicity of its surface minerals as they fall through a bubble-rich 2- or 3-fluid medium (including water, gas, nonpolar liquids, oils). This is one of the most complex yet barely understood processes in minerals processing, including effects

from fluid dynamics, surface physics, organic and anorganic chemistry. In processing plants, several of these processes might be combined so that the output streams of each processing unit is fed into other units, thus building serial or parallel chains, trees and even complex networks, with feed-back loops.

Particle based models (Lamberg 2011) are a particular simple and promising modelling strategy, primarily of use for such networks of minerals processing processes. Here, each particle of the general feed is given a probability of going to each one of the output streams of each processing unit, according to its singular properties and certain characteristics of the bulk material within the unit. As long as these probabilities can be considered constant in time, the transient behaviour of the system can be modelled with a simple system of first order differential equations with constant coefficients (Tolosana-Delgado et al. 2015). Other more complex settings, in particular, milling steps within loops, pose a much more complex challenge and remain yet unexplored to the authors' knowledge.

The second kind of processes typically destroy the ore mineral structure into a fluid state: a water solution (hydrometallurgy, electrometallurgy) or a melt (pyrometallurgy). All these processes can be modelled with relatively well-known thermo-electro-chemical reactions. Lack of space and a certain distance from the classical fields of mathematical geosciences made us leave the subject out of this contribution.

Whichever strategy of modelling is followed, it is necessary to characterise the frequency distribution of certain properties on the particle streams. The most obvious are the size and mineralogical composition of the particles, in exposed surface, mass and even in volume proportions. Derived from these, elemental deportment and liberation distribution are also relevant. Elemental deportment is the proportion of a given element mass apportioned by each mineral. The liberation distribution gives the volume (or mass) of particles containing a certain mineral in a (volume, mass or surface) proportion equal or larger than a threshold, as a function of that threshold. This is a cumulative distribution in the fashion of the better known recovery and tonnage curves in classical Geostatistics. Finally, more complex mineral association or paragenesis indicators do also matter, as often concentration processes do not target the value minerals themselves, but some accompanying, more abundant minerals. Next section discusses which instruments are used to measure these properties and which are the challenges brought with them to mathematical geoscientists.

### 33.3 Ore Characterisation

In the past, one-commodity grade was considered the sole and sufficient variable to characterize a mining block or a deposit. This variable could be more or less safely considered as a positive variable yet with an interval scale, according to the definition by Stevens (1946). This explains why Geostatistics was originally concerned with univariate properties following the properties of Gaussian or lognormal random fields (Journel and Huijbregts 1978).

However, the present and the future evaluation of a mining operation will require many more variables, kinds of scales and new geostatistical models. Multi-commodity grades, geochemistry and mineralogy, being vectors of positive or relative components (Pawłowsky-Glahn 2003; Boogaart and Tolosana-Delgado 2013), have already brought the need of considering multivariate ratio scales and compositional scales (Caciagli Warman 2015). The routine analysis of mineral and chemical properties by techniques like X-ray Fluorescence (XRF) or Instrumental Neutron Activation Analysis (INAA) for bulk geochemistry, X-ray Diffraction (XRD) for bulk mineralogy, or Electron Probe Microanalysis (EPMA), Proton-Induced X-ray emission (PIXE), Laser Ablation Inductively Coupled Mass Spectrometry (LA-ICP-MS) or Raman spectroscopy for single grain or locally resolved chemistry and mineralogy will ensure a continuous growth of compositional and multivariate positive data in predictive geometallurgy. The generalisation of microstructural analysis, with machines like QUEMSCAN, MLA or X-ray tomography (Bam et al. 2016; Becker et al. 2016), will make further primary properties easy to obtain: particle size curves (showing a distributional scale (Delicado 2008; Menafoglio et al. 2016a)), interphase mean contact length composition (a sort of two-way composition (Caracciolo et al. 2012)), grain size curves of each mineral phase (a discrete set of parallel distributions), deportment (a composition informing of the proportion of mass of a certain element contributed by each of its bearing minerals), and many more properties. Even the application of EBSD (electron backscatter diffraction) will make it possible to characterise the distribution of crystal orientations (spherical distributions) or its modal values (spherical directions). Spectral information is also produced by many instruments, and although spectra are nowadays preferably interpreted in terms of chemical elements, minerals or paragenesis (Chlingaryan et al. 2015) before treatment, one might think of future applications in which core scanning or airborne spectral data are considered as informative on their own in a 3D geomodel. Consider that spectral information is easy and fast to obtain in the operation and thus could help to guide the extraction process and identify ore types during mining and further processing (Nguyen 2013).

Many of these characterisation techniques can be ordered in a chain of methods, where the more advanced techniques provide more and more detail but at the price of lower precision, higher costs, and longer acquisition or turnaround times. For instance, XRD, though primarily measuring modal mineralogy, can be used to infer bulk geochemical composition, though with higher uncertainty than directly using XRF. Also, MLA, though primarily measuring grain and particle structures, can provide a modal mineralogy, but at higher costs than XRD. Finally, EBSD allows to characterize crystallites and defects, but can also be used to infer the mineralogical microfabric, albeit at longer measurement times than MLA for a fixed precision.

The other way around, inferring more advanced characteristics of the ore indirectly from cheaper measurements, is in general an inverse problem. Inverse problems are much more difficult to handle and often do not have a unique solution. For instance, inferring modal mineralogy from XRF is an *endmember problem*, and delivers at most equivalence classes of solutions (Tolosana-Delgado et al. 2011; Berry et al. 2011). Interpreting spectra into chemical and mineral compositions often

requires as well unmixing the signal obtained as a linear mixture of known endmember spectra. Finally, inferring processing properties from primary properties might require statistical models or machine learning methods to approximate the inverse problem solution (e.g. Matos Camacho et al. (2015) for magnetic susceptibility from MLA data). In summary, each analytical method has a specific role to play, and several methods will be required to appropriately characterise all relevant aspects of the ores.

Another classical class of metrological problems appearing in ore characterisation is *instrumental calibration*, namely the inference of the composition of bulk samples or spots by comparing their signals with the signal obtained from a reference material or *standard* where the property is known, as well as the corresponding uncertainty. The specific challenges for geometallurgy are the high variability of natural materials, difficult to reflect in standards with comparable compositional and physical characteristics (called *matrix matched*), and to measure in a single method. This concerns many of the techniques mentioned before, like XRF, INAA, ICP-MS, PIXE and EPMA.

From the point of view of mathematical geosciences, these problems imply calibration problems, data fusion and consensus building. Data has often been collected during different periods with different instruments at different labs. Seldom all methods were applied to all locations. Different batches need to be made compatible and calibrated against each other. In the authors' opinion, solutions for such problems will require existing concepts and tools and new developments from geodata management, geo-ontology and geoinformatics.

Additionally, local analytics techniques (MLA, QUEMSCAN, X-ray tomography, PIXE, EPMA, Raman) bring their own problems to be solved with mathematical geosciences techniques. It is often very challenging or impossible to acquire standard material homogeneous at micron scale and matrix-matched to the ore samples. Geostatistical models have been proposed for supporting such local calibration efforts (Tolosana-Delgado et al. 2013).

Imaging techniques are also becoming more and more popular, at all spatial scales. More and more methods (hyperspectral satellite- and air-borne, drone-borne imaging, mine face imaging, core scanning, EBSD, MLA, X-Ray-CT, PIXE, ...) acquire images rather than only univariate or compositional information. On large scales, from the drill core to deposit scale, imaging gets a rising importance for the characterisation of the meso- to megastructure of the deposit, because selectivity of ore zones from barren zones during exploration, mining, extraction and waste pre-screening is highly dependent on such structures. If we focus on sub-millimeter scales, processing methods and processing costs react very sensitively to analogous microstructural properties: for instance, the type of intergrowth of minerals strongly conditions the necessary milling to achieve sufficient liberation (Perez-Barnuevo et al. 2013), and milling is one of the most cost intensive processing steps. Many of these methods measure spectral information at each pixel. Various supervised and unsupervised machine learning techniques have been used for mapping spectral information to geometallurgically relevant quantities (Decamp et al. 2015;

Harraden et al. 2016; Nguyen et al. 2016). Image processing analysing structure will thus become more and more relevant in geometallurgy.

Moreover surface imaging techniques like MLA or QUEMSCAN suffer of stereologic degradation: these instruments are devised to characterise geometric properties of 3D bodies, but only observe them on 2D sections. It is well-known that only some 3D properties can be estimated unbiasedly by averaging over their 2D counterparts. This allows e.g. to have certain confidence in properties like volumetric modal mineralogy (estimated from the proportions of pixels of the several minerals on the measured surface), mineral association as the proportion of surface of a mineral in contact with all other minerals (estimated from the proportion of contact lengths on the measured surface) or specific surfaces. But other highly relevant properties, like liberation distribution, grade curves, tonnage curves or particle and grain size distributions suffer significant stereological degradation (Perez-Barnuevo et al. 2012).

Open problems for the next generation of mathematical geoscientists will include, to mention a few, the development of widely accepted local analytics calibration procedures; the propagation of uncertainties through image analysis methods; or the integration of several analytical techniques through consensus-building, e.g. to deliver mutually consistent measurements of bulk mineral and chemical compositions as well as elemental department together with their uncertainties out of XRD, XRF, EPMA and MLA measurements of the same sample. Correcting stereological degradation is as well an open issue.

### 33.4 Orebody Modelling

The generation of large scale 3D models of the ore bodies is the classical key contribution of Mathematical Geosciences to the mining business. Nowadays, point and block kriging or simulation for grade variables and indicator-based techniques (indicator kriging, sequential indicator simulation, plurigaussian simulation) for categorical variables are accepted standard techniques. Beyond the framework of Gaussian random fields, cumulant based (Dimitrakopoulos et al. 2010; Minniakhmetov and Dimitrakopoulos 2017) and Copula based (Musafer et al. 2013, 2017) proposals, as well as multiple point geostatistics (MPS) can be found in scientific papers, though their penetration and acceptance in the industry is yet negligible. Multivariate issues are also seldom considered, though compositions (mineral or chemical) are geometallurgically relevant primary variables, and techniques do exist to predict or simulate them at both point (Pawłowsky 1989; Pawłowsky-Glahn and Burger 1992; Pawłowsky-Glahn and Olea 2004; Tolosana-Delgado 2006; Tolosana-Delgado et al. 2011; Mueller et al. 2014) and block support (Tolosana-Delgado et al. 2013) in a fashion consistent with their scale, namely delivering positive and constant-sum predictions/simulations abiding to a relative scale.

The geostatistical treatment of other geometallurgically relevant multivariate scales has received limited to no attention so far by the mathematical geosciences community. The challenges are multiple (Boogaart et al. 2013). Geometallurgical

data from EBSD are known to exhibit spherical scales, for which a kriging approach is readily available (Boogaart and Schaeben 2002a, b). One-dimensional distributions are much more abundant, and methodological developments for kriging, cokriging and conditional simulation exist via functional analysis (Menafoglio et al. 2016a, b). Nevertheless, application to the many geometallurgical data with distributional scale still requires theoretical and practical developments. Upscaling of these geometallurgical properties present counter-intuitive characteristics: for instance, a categorical variable at point support gives rise to a compositional variable at block support, and while block kriging is generally thought to reduce uncertainty, block “estimates” of distributional and of categorical variables may very well exhibit higher entropy themselves. With a few exceptions based on geostatistical simulation (Deutsch et al. 2015), downscaling has not yet been systematically considered, but it may become a necessary tool to populate block models with smaller scale granularity, for instance for incorporating information from blast-hole analysis on the 3D models. Finally, the joint consistent modelling of several variables from different scales (for instance modal mineralogy, geochemistry, hardness and lithology) has received limited attention (see Maleki and Emery 2015 for a two-point case study with one continuous and one categorical variable), and only seminal ideas about the combination of Bayesian spaces (Boogaart et al. 2014), multigrid Markov Mesh Models (Stien and Kolbjornsen 2011; Kolbjornsen et al. 2014), generalized linear models and MPS have been presented for discussion (Boogaart et al. 2014).

It has been shown that the conditional distribution of the geostatistical simulation is highly relevant for optimal processing choices (Boogaart et al. 2013). Gaussian geostatistics only delivers that correctly in a Gaussian random field setting. Like with strategic mine planning (Dimitrakopoulos 2011; Goodfellow and Dimitrakopoulos 2017), non-linear simulation methods better reproducing the conditional distributions would thus be more appropriate for geometallurgical optimisation. However so far (April 2017), beyond single categorical variables, no case studies could show the added value of MPS methods in the context of geometallurgy. The fundamental difficulty appears to be producing sufficiently large, stochastically representative training images (Emery and Lantuejoul 2014), a problem made even worse by the many relevant variables, some with multivariate, compositional or distributional scales.

Besides the geometric modelling of the large-scale structure of a deposit, 3D Geomodelling offer also a tool for modelling and simulation of microstructure and texture of the ores. Stochastic simulation of such 3D geomodels of ores might be necessary to appropriately simulate breakage of microstructure by crushing, grinding and milling, as well as to offer an approach to stereological reconstruction. This is so because all these problems require an appropriate description of the geometric spatial relations between the mineral grains, and not just summaries of their composition. However, new concepts, models and techniques have to be developed to link the macroscale described by geostatistics and the microscale, possibly described by stochastic geometry.

Another challenge posed by such multi-scale (in the sense of spatial granularity), multi-scale (in the sense of statistical kinds of data), multi-step (data is added to the models at different times), multi-dimensional geometric modelling of ore bodies is



the structuring, management and exploitation of the necessary data to appropriately provide input for the methods used. A more intimate link between geostatistical and geodatabases will be required for that, as flexible and sequential conditioning methods able to incorporate into the conditional distributions data on batches, as they become available. Sequential data assimilation techniques have been successfully used for this task in the assessment of univariate quantities (Wambeke and Benndorf 2017).

### 33.5 Decision Making

Geometallurgy touches on all levels of optimization of the mining operation, from exploration, investment, and strategic mine planning towards the daily operation. Each optimization task can be stated as a *w*-question, and delimits a certain scope of the decision to be taken.

Blending ores from different localities to ensure a stable feed properties for the plant presents the smallest decision scope, as it only changes *where* to mine and not *when* or *how to process*. Having the ability to predict mining and processing behaviour for different feed materials allows to better predict block values or machine time and maintenance requirements. Such better block values can be used in classical strategic mine planning tools for an optimal exploitation of the deposit, that is answering the *when* and *where* issues related to pushbacks and ultimate pit calculations. For this task a statistic model relating the primary geometallurgical properties, with secondary ones is typically enough (Vann et al. 2011). If the processing model is good enough to predict the value as a function of the processing choices, it can be used in conjunction with a geostatistical description of the geometallurgical ore properties to optimize the processing itself either for the whole deposit or each block (optimal adaptive processing) (Turner-Saad 2011; Tolosana-Delgado et al. 2015). Goodfellow and Dimitrakopoulos (2017) shows how blending, strategic mine planning and routing can be optimized together. The optimizability, i.e. the optimal achievable productivity, depends on very basic decisions like the size of selective mining units, available equipment and available data. The overall value of the mine and thus the decision to mine itself depends on all details. Boogaart et al. (2015) shows the relevance of the selective mining unit and the decision strategy for the value of the mine (*how to model*). Boogaart et al. (2016) shows how to quantify these values and the value of the available equipment, determining costs and available processing choices, before the actual mining operation starts. Such calculations are based on geostatistical simulation, and thus allow to optimize the geometallurgical approach (*how to optimize*) and the investment (*what to build*). Boogaart et al. (2016) show the substantial influence of the exploration plan and the data acquisition strategy (e.g. the influence of processing data) on the overall value of the operation and how quantifying the value of information can be used to optimize the geometallurgical exploration strategy. This offers a way to economically justify and timely plan extensive geometallurgical data acquisition campaigns (*what and when to measure*).

All these approaches rely on stochastic optimisation in a geostatistical framework for geometallurgical data combined with a geometallurgical processing model, both based on quantitative ore characterisations. That is, they rely on the mathematical tools described in the preceding three sections. Applying these techniques is still a major geoinformational challenge including big data management, data fusion, massive parallel computing and real time data management (Jones and Moorhead 2013; Lopez et al. 2016).

### 33.6 Conclusions

Geometallurgy requires substantial geomathematical developments in all the classical fields of mathematical geosciences and geoinformatics. The challenges are beyond the classical solutions, e.g. a truly multivariate, multi-scale Geostatistics honoring non-Gaussian relationships is required; statistical analysis for various scales beyond positive data and compositions is required, in particular distributional data; a full space-time 3D data fusion and fast automated updating of models will be required; there are new challenges to the mathematical background of metrology including issues of local analytics, compositional calibration, and varying material matrices; structural characterisation on several scales from the ore body to the microfabric are needed on a quantitative level from limited 2D stereological data and supportive conditioning information (bulk mineralogy and geochemistry, accessory information on mineral stoichiometry, crystallographic defects, etc.); geostatistical models of the spatial variation of the microstructure throughout the deposits (i.e. a structure Geostatistics) needs to be developed; and so on.

The mathematical challenges of integrating characterisation, stochastic modelling, process simulation and optimisation, and data reconciliation, will extend to manmade and secondary resources (tailing dams, recycling, urban mining) and to the optimisation of other geosystems (water management, ecosystem management, urban ecosystems, the trisystem of energy-minerals-water), hence the lessons learnt from primary ores geometallurgy will be relevant for many fields beyond ore geology and mining. Beyond the classical fields of mathematical geosciences, geometallurgical questions will as well require solutions from mathematical disciplines uncommon at the IAMG, like optimisation, operations research and numerical process modelling. Thus, geometallurgy extends the scope of the IAMG towards these fields. In this way geometallurgy can become the scientific and economic driving force for the next generation of mathematical geosciences and geoinformatics.

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