17 (2023) 200137

Contents lists available at ScienceDirect

Resources, Conservation & Recycling Advances

journal homepage: www.sciencedirect.com/journal/Resources-Conservation-and-Recycling-Advances

Primary Exploration, Mining and Metal Supply Scenario (PEMMSS) model: Towards a stochastic understanding of the mineral discovery, mine development and co-product recovery requirements to meet demand in a low-carbon future

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ARTICLE INFO

Keywords:
Mining
Mineral exploration
Scenarios
Ore grade
Sustainable development
Primary Metal Supply
Mineral Resources

ABSTRACT

Existing scenario models of future material flows often exclude or place a 'black-box' around the mining industry and disregard important industry dynamics such as mineral exploration. This lack of sophistication prevents formation of knowledge required to answer key questions pertaining to future mining output, the amount of companion metals that can be supplied and the investments and lead times needed to fulfil future metal demand. To address this, we introduce the Primary Exploration, Mining and Metal Supply Scenario (PEMMSS) model, which allows for mine-by-mine modelling with full regionalisation and linkages to geological deposit types. PEMMSS allows for the assessment of required rates of mineral deposit discovery, mine development and co-product recovery overtime for a range of socio-economic and sustainable development linked primary material demand scenarios. The model can be calibrated using mineral resource grade, tonnage and density probability distribution functions for regions and deposit types to stochastically model scenarios for future greenfield discoveries and understand uncertainities. Applying PEMMSS will facilitate improved understanding of how future urbanisation across the globe and low-carbon transitions will translate into altered requirements for the exploration and primary mineral and metal supply sectors and their associated environmental impacts. A hypothetical case study is presented for a four co-product commodity system to highlight potential model behaviours and key drivers of model sensitivity.

1. Introduction

The efforts of society to improve living standards and address sustainable development challenges during the 21st century will result in increased raw material demand (Ali et al., 2017; Christmann et al., 2022; Giurco et al., 2019; OECD, 2018; IRP, 2019; 2020; IEA, 2021; Watari et al., 2020). Considerable policy efforts are emerging to begin transitioning towards a circular economy, where material demand is reduced or met by reuse or recycling wherever possible. However, the timeframes for any transition will be slow as materials can remain in the economy for long periods before becoming available for secondary production streams (Norgate, 2013) and there are limits for achievable recycling rates (IRP, 2013a). Furthermore, continuing population and economic growth may still lead to substantially rising demand, increasing requirements for primary raw material production for some time (OECD, 2018; IRP, 2019; Schandl et al., 2020). With the associated increase in metal mining, there will also be an increase in the cumulative environmental burdens associated with mining such as land transformations, greenhouse gas emissions, water use, waste generation and acid rock drainage (Elshkaki et al., 2016; 2017; Franks et al., 2021; Kuipers et al., 2018; IRP, 2013b; van der Voet et al., 2019; Watari et al., 2019). At the same time material stocks will grow, as will the flows of products that reach their end-of life. How we manage these growing stocks, secondary flows, and the ways we meet rising demand in the future will be crucial factors for efforts to decrease environmental pressures alongside meeting reduction targets for greenhouse gas emissions (Prior et al., 2012; McLellan, 2019).

Dynamic material flow analysis (MFA) has become a frequently used

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https://doi.org/10.1016/j.rcradv.2023.200137

Available online 8 March 2023
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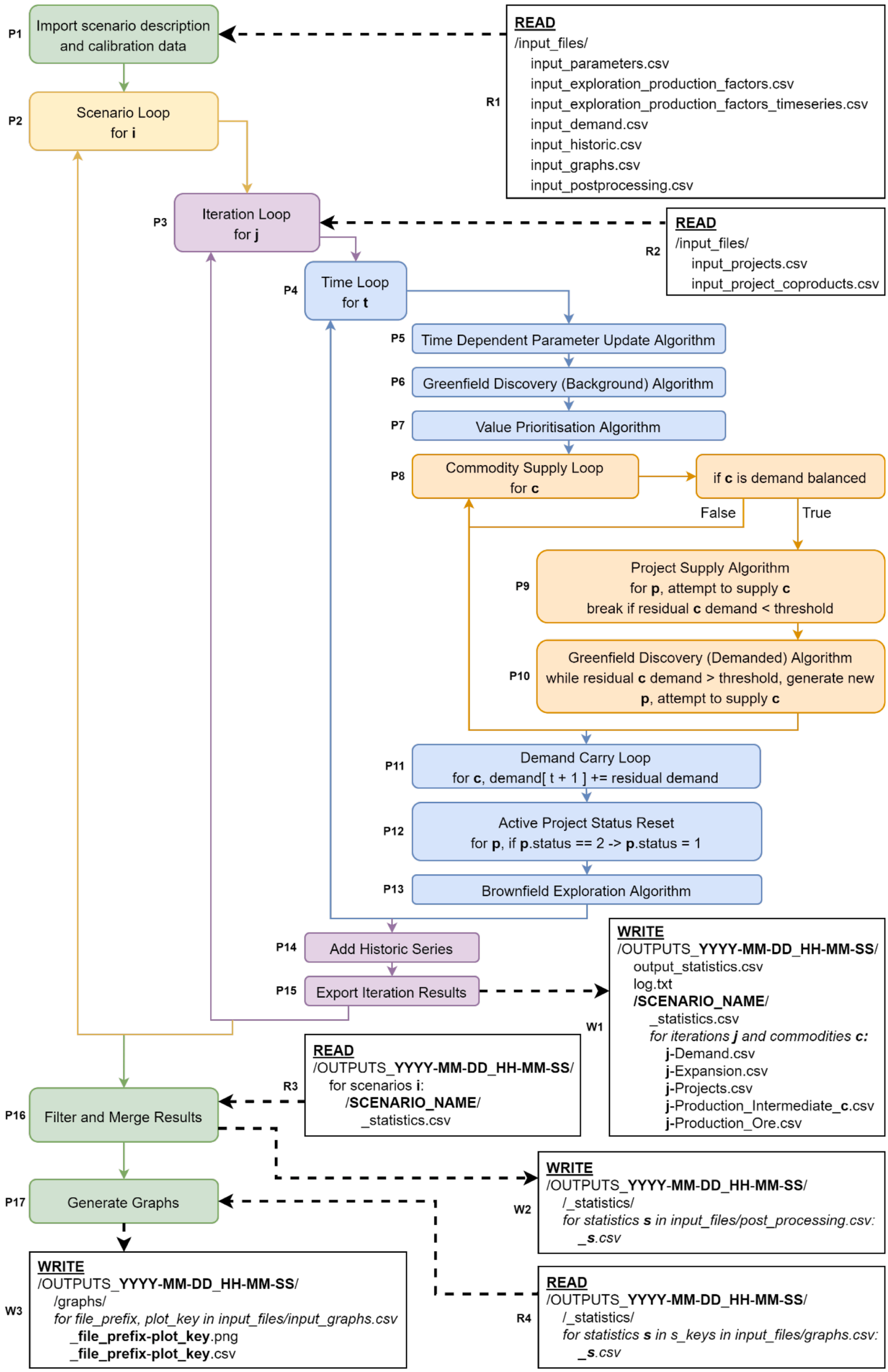

Fig. 1. PEMMSS model flowchart of key algorithms and data exchanges. Abbreviations (e.g. P13, W1, R2, etc.) are cross-references and searchable within the model's python code that is available on GitHub and Zenodo (Northey et al., 2022).

method to study the biophysical basis of society and to increase knowledge of the prospective assessment of transformation strategies by quantifying, qualifying and locating stocks and flows of different materials and products in society (Graedel, 2019; Pauliuk and Hertwich, 2016). The methodological approach varies depending on the studied objective. Some common objectives are the assessment of material demand in the future (Elshkaki et al., 2018; Schipper et al., 2018), evaluating potential supply restrictions (Gerst, 2009), evaluating recycling efficiencies (Glöser et al., 2013), the analysis of environmental impacts associated with material use (van der Voet et al., 2019) and occasionally the coupling of different metal cycles (Fu et al., 2019; Løvik et al., 2015). Some of these studies aim to offer quantitative and objective guidance for policy-makers (Haas et al., 2015; Mayer et al., 2018; IRP, 2020). The large majority, however, do not address a clear target audience (Müller et al., 2014). The majority also give limited consideration to primary supply chains and are more focused on questions of changing material use patterns or reuse within society. In addition, the current state of software programming and use in industrial ecology research faces unsolved objections regarding transparency, reproducibility, reusability and ease of collaboration. Pauliuk et al. (2015) therefore proposed a modular model approach to developing industry ecology models to increase quality and the ability for cutting-edge research.

Despite advances in dynamic MFA, existing scenario models to understand changes in material stocks and flows in the future have typically poorly conceptualised the mining industry (Northey et al., 2018a). Activities such as mining and primary metal refining are often modelled as a single, aggregated black box, and mineral exploration dynamics are often excluded. Even many of the studies focused on mineral resource depletion rarely quantitatively model future mineral exploration and generally only address it qualitatively or compare future needs with static estimates of mineral resources or reserves, which can be ill-suited for this purpose (Alonso et al., 2007; Castillo and Eggert, 2020; Northey et al., 2014; West, 2020; Wellmer, 2022). Due to these shortcomings, the required rates of brownfield (expansion of existing resources) and greenfield (discovery of new deposits) exploration, the required investment in mine development and required rates of co-/by-product metal recovery overtime are poorly understood for different scenarios of socio-economic development. This becomes important when we begin to consider the dependency of many new technologies on speciality, 'critical' mineral commodities that are often produced exclusively as by-products of bulk commodity production. In these cases, the supply potential of some speciality commodities may effectively be capped by the production rates of other commodities such as copper, zinc and nickel mineral concentrates, which may make some development scenarios infeasible. Additionally, the cumulative environmental impacts of mineral supply will differ depending upon the specific set of mineral deposits that are exploited and the economic and regulatory settings in which this occurs due to the complex relationships between the scale of individual mines, ore quality and the environmental burdens of extraction (Norgate et al., 2007; Mudd, 2010; Werner et al., 2020; Franks et al., 2021).

The perspectives of different disciplines need to be integrated to study co-benefits and trade-offs across different sustainable development targets to increase the relevance of resource scenarios to decision makers. For example, adding the cost layer to material cycle models (Kram et al., 2001) is crucial for assessing the viability of different circular economy business models (Bocken et al., 2016). Interdisciplinary perspectives further need to be combined with high-resolution assessments, e.g., to understand the land-use change and impacts that may occur across regions and through time as a consequence of socioeconomic development (Sonter et al., 2018). Such interdisciplinary and high-resolution assessments of future mining supply are currently not available, but needed as a building block of realistic scenarios for future resource extraction, use, and recycling

We present the Primary Exploration, Mining and Metal Supply Scenario (PEMMSS) model that can be coupled with broader models for socio-economic metabolism assessments to provide a more target audience-orientated approach in the field of dynamic MFA. This is urgently needed to find a common basis of understanding amongst all stakeholders in order to address the challenges associated with material use now and in the future. Importantly, the PEMMSS model addresses conceptual issues and limitations associated with earlier models. For instance, the Geologic Resource Supply-Demand Model (GeRS-DeMo) (Mohr, 2010) was unable to model mineral exploration dynamics, assumed fixed characteristics of mining operations within regions, was unable to consider economic incentives for mineral extraction and did not incorporate important variables such as mineral ore grades – which required some studies to incorporate a number of exogenous assumptions and post-processing methods to address (e.g. Northey et al., 2014). Other models based on systems dynamics do address these aspects (e.g. Sverdrup et al., 2015), however often produce highly aggregated results. The complexity of model design can prohibit the calibration or validation of internal relationships, which leads to difficulty when interpreting results. In contrast, the PEMMSS model is designed to be flexible in its use and to allow mine-by-mine, deposit-by-deposit modelling of mineral supply and exploration for an arbitrary number of mineral commodities.

2. Model description

The key functionality of the Primary Exploration, Mining and Metal Supply Scenario (PEMMSS) includes:

1. Balance primary demand for multiple metal commodities with supply from a cohort of individual deposits and mining operations.
2. Model mine production, ore grades, resource recovery and depletion of individual deposits.
3. Prioritise production from individual mineral deposits according to value models specific to regions and deposit types.
4. Trigger mine development/operation and deposit discovery to meet shortfalls in demand.
5. Model greenfield exploration through stochastically generating new mineral deposits in regions based upon exploration targeting parameters and grade-tonnage distributions for defined deposit types.
6. Model brownfield exploration and ore grade dilution at existing operations.
7. Evaluate potential co-/by-product metal supply rates, including the ability to use geochemical grade inferences and mineral processing relationships.

The implementation of these features and the model's overarching framework is based upon the following guiding principles and assumptions:

1. Primary metal demand is exogenous and can be derived from external scenarios for future socioeconomic development and climate change mitigation, which may include sector-specific expectations of material requirements and end-of-life recovery from the recycling industry or urban mining.
2. Production, reserve and resource depletion should be modelled at deposit scale to enable complex resource size-throughput-value relationships and region specific conclusions to be drawn. This is important to understand the implications of deposit size distributions within total mineral resources, as well as to subsequently model regional impacts and environmental externalities of mineral supply.
3. Both brownfield (expansion) and greenfield (new) mineral exploration are to be modelled independently.
4. Supply and demand of multiple commodities should be modelled simultaneously to enable co-/by- production scenarios, interdependencies and constraints to be better understood.

Fig. 1 shows a flowchart of key model algorithms and data exchanges that are described further in the following sections. A simplified diagram

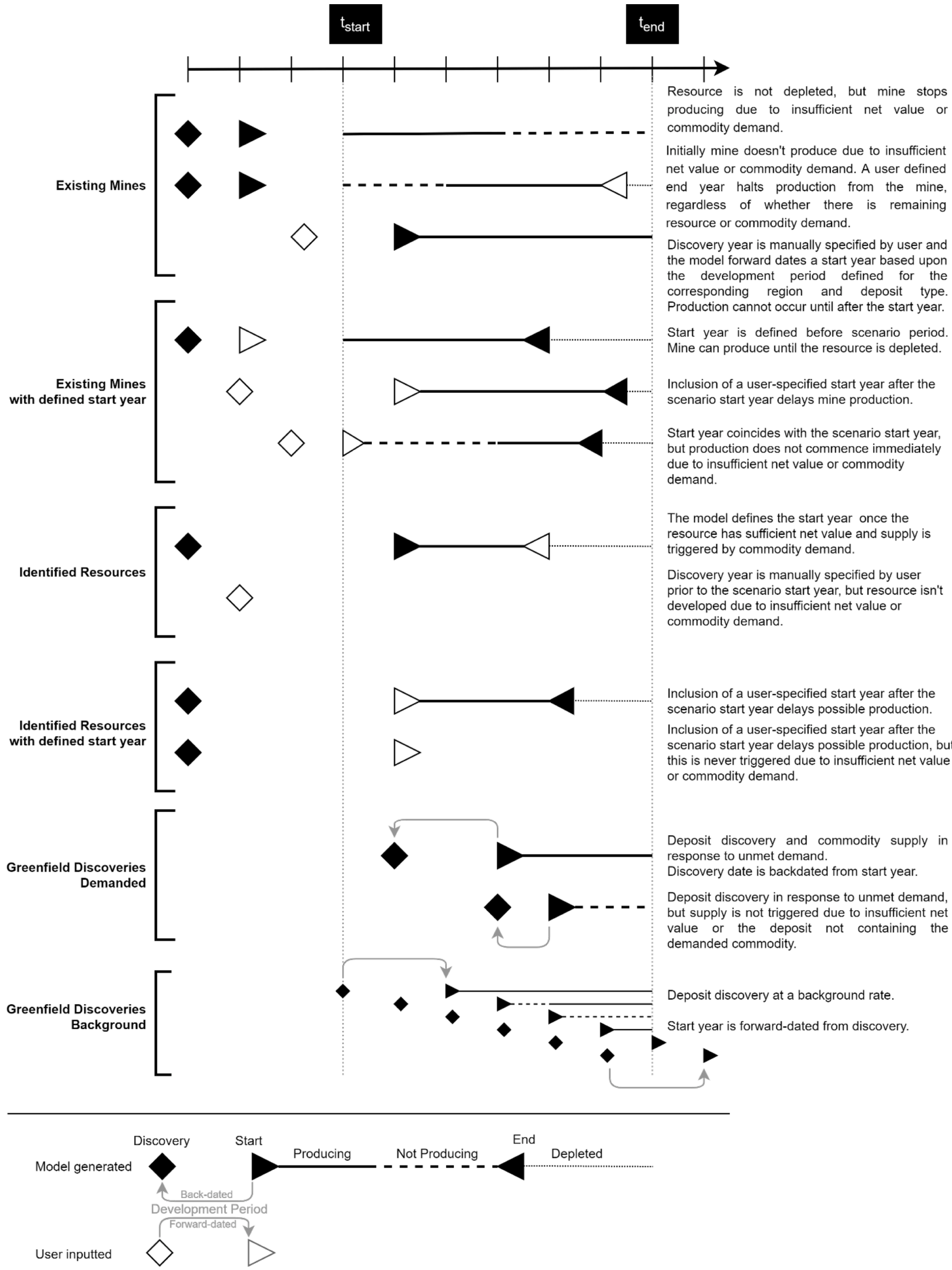

Fig. 2. Examples of possible mine behaviours and how this can be influenced by user-inputted information. The mine/resource categories on the left-hand side are referred to as 'aggregations' in model output files to enable summary statistics to be generated for specific cohorts of mines and deposits.

of model components is shown in Fig. S1 in the electronic supplementary file mmc1. The abbreviations can be cross-referenced to the comments in the Python implementation of the model that is available on GitHub and Zenodo under a BSD 3-clause licence (Northey et al., 2022).

2.1. Demand scenario descriptions and iterations

The model is driven by timeseries scenarios for primary commodity demand. As there can be stochastic elements (e.g. random generation of the size and grade of new deposits) the model will perform multiple iterations of each individual demand scenario. As part of this, the random functions can be manually seeded to enable replication of previous model runs and reproducibility of results.

2.2. Global supply-demand balance algorithm

The supply-demand algorithm balances commodity demand with mineral supply from individual mining operations. Time series of primary commodity demand (D_c) are defined exogenously for an arbitrary number of commodities (c). Commodities can be defined as either 'balanced' or 'unbalanced'. Balanced commodities are those where the model will attempt to balance supply and demand, whereas unbalanced commodities will not trigger mine supply but instead only be supplied incidentally as a co-product alongside supply of a balanced commodity. This behaviour is useful for modelling potential supply dynamics of low-value by-products. In addition, commodities can also be specified as balanced or unbalanced at the individual mine or deposit level, to provide additional flexibility when specifying the conditions under which global commodity demand will trigger commodity supply from an individual mine.

At each time-step and for each 'balanced' commodity, the primary commodity demand ($D_{c,Ex,t}$) is converted to mined commodity demand ($D_{c,M,t}$) by dividing by the global recovery factor ($Rec_{G,c}$) for each commodity (Section 2.3.1). Production from mines is ordered according to their relative net value ($V_{m,net}$) and the mine priority function (Section 2.3.2), with an increasing number (n) of additional mines (m) that meet the supply criteria (Section 2.3.3) entering into production. Each mine will produce ore ($S_{m,O,t}$) and supply mined commodities ($S_{m,c,t}$) (e.g. a mineral concentrate) that have a positive or neutral mine recovery value ($V_{m,c}$) (Section 2.3.4). This continues until Eq. (1) is satisfied for all balanced commodities, indicating that unmet demand is less than each commodity's demand threshold ($D_{c,T}$). The residual ore demand ($D_{O,m,t}$) placed on each additional mine is calculated as they are added (i.e. $n+1$) using their specific commodity recovery ($Rec_{m,C}$) and ore grade ($G_{m,c,t}$) according to Eq. (2). When supply is met from an undeveloped mine, then the status of the mine is changed to 'active' and the start time is recorded. When supply from all available mines is insufficient to meet demand of a balanced commodity, then additional mines are generated using the greenfield exploration algorithm (Section 2.4).

$$\mathbf{D}_{c,T} \geq \frac{\mathbf{D_{c,M,t}} - \sum_{\mathbf{m}}^{\mathbf{n}} \mathbf{S_{m,c,t}}}{\mathbf{Rec_{G,c}}} \tag{1}$$

$$\mathbf{D_{O,m,t}} = \frac{\mathbf{D_{C,M,t--}} - \sum_{\mathbf{m}}^{\mathbf{n-1}} \mathbf{S_{m,c,t}}}{\mathbf{Rec_{m,c}} \cdot \mathbf{G_{m,c,t}}} \tag{2}$$

Once Eq. (1), has been satisfied for all supply-demand 'balanced' commodities, any commodity under or over-supply (e.g. for 'unbalanced' or co-product commodities) will be carried forward to the next time-step according to each commodity's demand carry constant ($D_{c,Carry}$), as shown in Eq. (3). Note that when the demand carry constant is positive, unmet demand will be carried forward to subsequent time periods. When this is negative, unmet demand will suppress demand in future time periods. This provides a simplistic mechanism to simulate supply-demand elasticity.

$$\mathbf{D_{c,Carry}} \left(\mathbf{D_{c,Ex,t}} - \frac{\sum_{\mathbf{m}} \mathbf{S_{m,c,t}}}{\mathbf{Rec_{G,c}}} \right) + \mathbf{D_{c,Ex,t+1}} \rightarrow \mathbf{D_{c,Ex,t+1}} \tag{3}$$

Depending upon the characteristics of individual deposits and mines, the evolution of supply and demand through the scenario and the constraints of user-inputted variables – there are a range of potential behaviours that could be exhibited for individual mine within the model, as shown in Fig. 2.

2.3. Mine supply

The supply algorithm triggers production from mines and also any necessary greenfield exploration so that the commodity demand can be met at each time step.

2.3.1. Conversion of global primary commodity demand to mined product demand

At each time-step (t), the exogenous commodity demand ($D_{c,Ex,t}$) is converted into the demand for mined products ($D_{c,M,t}$) according to Eq. (4), by adjusting for a global recovery factor ($Rec_{G,c}$) that accounts for material losses in intermediate processing steps between the mine site boundary and the commodity market. When demand for a mined product is applied to a specific mine, this is then converted into mined ore demand based on a mine specific commodity recovery factor ($Rec_{m,c}$) and ore grade ($G_{m,c,t}$).

$$\mathbf{D_{c,M,t}} = \mathbf{D_{C,Ex,t}} \div \mathbf{Rec_{G,C}} \tag{4}$$

$$D_{O,m,t} = \frac{D_{c,M,t}}{Rec_{m,c} \cdot \mathbf{G}_{m,c,t}} \tag{5}$$

2.3.2. Mine value and prioritisation

Production from mines is prioritised according to their relative net value ($V_{m,net}$) in descending order. The model can be run in two configurations: (1) Where production from active mines is always prioritised ahead of undeveloped deposits by default; and (2) where undeveloped deposits can be prioritised ahead of active mines to enable modelling of the potential implications of competition between developed mines and undeveloped deposits.[1] The model can be configured to either update the net value of mines/deposits at each time step or instead to leave these static throughout the scenario run. The model can also be configured to only consider the marginal net value of the next ore tranche to be mined for each mine/deposit, or instead to use the total net values for the entire mine/deposit.

Eq. (6) shows a simplistic model for determining the relative net value of a mining operation ($V_{m,net}$) as consisting of the cost associated with ore mining ($V_{m,mining}$) and the sum of the net extraction value of recovering each commodity (c) from the ore ($V_{m,c,net}$). The commodity value extracted is defined in Eq. (7) simply as the difference between the revenue generated from a commodity ($V_{m,c,revenue}$) and the cost of recovery of that commodity from the mined ore ($V_{m,c,cost}$).

$$\mathbf{V_{m,net}} = -\mathbf{V_{m,mining}} + \sum_{\mathbf{c}} \mathbf{V_{m,c,net}} \tag{6}$$

$$\mathbf{V_{m,c,net}} = \mathbf{V_{m,c,revenue}} - \mathbf{V_{m,c,cost}} \tag{7}$$

The relative value of mining operations does not necessarily need to

[1] This is achieved by setting the 'priority_active' parameter as false ('0') in the model input files. This will only affect prioritisation of undeveloped mines/deposits that are specified in the model input files and will not influence greenfield exploration/new deposit discovery that has been triggered by a supply shortfall. 'Background' greenfield deposit discovery occurs before mine prioritisation, so if the development period for a new discovery is '0' then it is possible that new background discoveries in that time period could also produce during the same time period of discovery.

Table 1
Value models implemented in the PEMMSS model v1.1.0, where 'a' is a user-defined calibration parameter.

Value Model	Relationship
fixed	a
size	$R_{m,t}$
grade	$G_{m,c,t}$
grade_recoverable	$G_{m,c,t}*Rec_{m,c}$
contained	$R_{m,t}*G_{m,c,t}$
contained_recoverable	$R_{m,t}*G_{m,c,t}*Rec_{m,c}$
size_value	$R_{m,t}*a$
grade_value	$G_{m,c,t}*a$
grade_recoverable_value	$G_{m,c,t}*Rec_{m,c}*a$
contained_value	$R_{m,t}*G_{m,c,t}*a$
contained_recoverable_value	$R_{m,t}*G_{m,c,t}*Rec_{m,c}*a$

use monetary units and could instead use other more accessible parameters as a proxy for value. A simple approach to determining a cost or value of used for mine prioritisation is by making this equivalent to a known characteristic of the mineral deposit, such as the initial reserve or resource size, the ore grade, the contained product (i.e. target mineral / metal) or the contained recoverable product. To provide flexibility for users a number of generic cost/value models are shown in Table 1, which can be used to interchangeably determine mining, extraction and recovery values of individual mines/deposits or for specific regions or deposit types. This provides flexibility when investigating different approaches to ordering or scheduling the extraction of mineral deposits within the model. Although the structure of the value functions may limit the ability to capture some types of economic relationships and behaviours. We note that the python implementation is easy to modify should the user wish to implement more complex user-defined value functions as necessary,[2] for instance, of the type outlined by Camm & Stebbins (2020) or Walsh et al. (2020).

2.3.3. Mine supply criteria

When commodity demand is placed on a mine, a number of criteria must be satisfied to trigger ore production:

- The mine's net value ($V_{m,net}$) must be positive.
- The mine must be able to supply the demanded commodity and also consider it a 'balanced' (i.e. trigger) commodity.
- If a start time for the mine exists then this must have passed.
- The mine must not have already produced during the current time-step.
- For an undeveloped deposit, it must also pass a random test of its' development probability ($P_{dev,m}$).

2.3.4. Mine supply

The ore supply rate ($S_{m,o,t}$) for a mine (m) at timestep (t) is determined according to Eq. (8), a function of the mine's recovery factor ($Rec_{m,c}$) and ore grade ($G_{m,c,t}$) for the demanded commodity (c), subject to the constraints of the mine's remaining ore reserves or resources ($R_{m,t}$), ore supply capacity ($S_{m,cap}$) and the residual ore demand ($D_{O,m,t}$; Eq. (2)). All commodities with a positive extraction value ($V_{m,c}$) are then supplied by the mine according to Eq. (9). The model code can also handle deposits being defined in multiple ore tranches that are mined sequentially. Each ore tranche can have independent remaining reserve or resource tonnages ($R_{m,t}$), ore grades ($G_{m,c,t}$) and value estimates. When one ore tranche is depleted, supply from the next ore tranche will first be attempted according to Eq. (8) and Eq. (9), before the model attempts to supply from another mine. This enables more complex modelling of mine production profiles. For instance a user could specify multiple ore tranches based on CRISCRO (2019) definitions for proven reserves, probable reserves, measured resources, indicated resources and inferred resources for each deposit and model these ore tranches as being mined sequentially.

$$S_{m,o,t} = \begin{cases} D_{O,m,t} \text{ for } D_{O,m,t} \le R_{m,t} \text{ and } D_{O,m,t} \le S_{m,cap} \\ S_{m,cap} \text{ for } D_{O,m},t \le R_{m,t} \text{ and } S_{m,cap} < D_{O,m,t} \\ R_{m,t} \text{ for } R_{m,t} < D_{O,m,t} \text{ and } R_{m,t} \le S_{m,c} \\ S_{m,cap} \text{ for } R_{m,t} < D_{O,m,t} \text{ and } S_{m,c} < R_{m,t} \end{cases} \tag{8}$$

$$S_{m,c,t} = Rec_{m,c} \cdot G_{m,c,t} \cdot S_{m,o,t}, \text{ when } V_{m,c} \ge 0 \tag{9}$$

The ore supply capacity ($S_{m,cap}$) of each mine (m) represents the maximum allowable ore extraction at each time period. This can be predefined for individual mines or mineral deposits in the model input files. Otherwise, the production capacity of a mine or deposit will be approximated at the point of model initialisation or when a new deposit is generated. The ores supply capacity ($S_{m,cap}$) of each mine (m) can be approximated based upon the initial reserve or resource size (R_m) of the deposit using a power law, except where this would result in a mine life that is outside the bounds of the minimum (L_{min}) and maximum (L_{max}) allowable generated mine life as defined in the scenario input parameters. This power law relationship between resource size and production capacity is sometimes referred to as Taylor's Law in the mining industry. The calibration parameters 'a' and 'b' are available from literature sources (e.g. Long, 2009) or can be determined empirically for different mining methods or deposit types based upon regression using resource size and production data for existing mines. This will still give estimates with significant uncertainty. So within the model code the power law estimate ($a.R_m^b$) is treated as producing the mean of a normal distribution for which the user can define a standard deviation. For very small standard deviations the model produces an ore supply capacity ($S_{m,cap}$) approximating Eq. (10). Otherwise, the ore supply capacity ($S_{m,cap}$) is stochastic but still bounded by the minimum (L_{min}) and maximum (L_{max}) allowable generated mine life.

$$S_{m,cap} = \begin{cases} R_m \big/ L_{min} \ \mathit{for} \ \dfrac{R_m}{a \cdot R_m{}^b} < L_{min} \\ a \cdot R_m{}^b \ \mathit{for} \ L_{min} < \dfrac{R_m}{a \cdot R_m{}^b} < L_{max} \\ \dfrac{R_m}{L_{max}} \ \mathit{for} \ L_{max} < \dfrac{R_m}{a \cdot R_m{}^b} \end{cases} \tag{10}$$

2.4. Resource discovery (Greenfield)

The PEMMSS model will simulate the discovery of new mineral deposits (i.e. greenfield exploration). This can occur at a fixed background rate of discovery in each time-step and can also be triggered when supply from available mines is insufficient to meet a balanced commodities demand. At the point of resource discovery:

- A region and deposit type are stochastically assigned based upon their relative discovery probability factors ($P_{disc,r,d}$) (Section 2.4.1).
- A resource size and commodity ore grades are stochastically assigned based upon probability distributions (Section 2.4.2).
- For demand-triggered discovery, the current time-step is assigned as the start time and then the discovery time is backdated by an assumed development period (Section 2.4.3 and Fig. 2).
- For background discoveries, the current time-step is assigned as the discovery time and the start time is forward-dated by the assumed development period (Section 2.4.3 and Fig. 2).

2.4.1. Region and deposit type selection

A region and deposit type are randomly assigned to new resources

[2] Custom cost models could be manually added to the value_model() function in modules/deposits.py, which would enable these to be specified in the input . csv files.

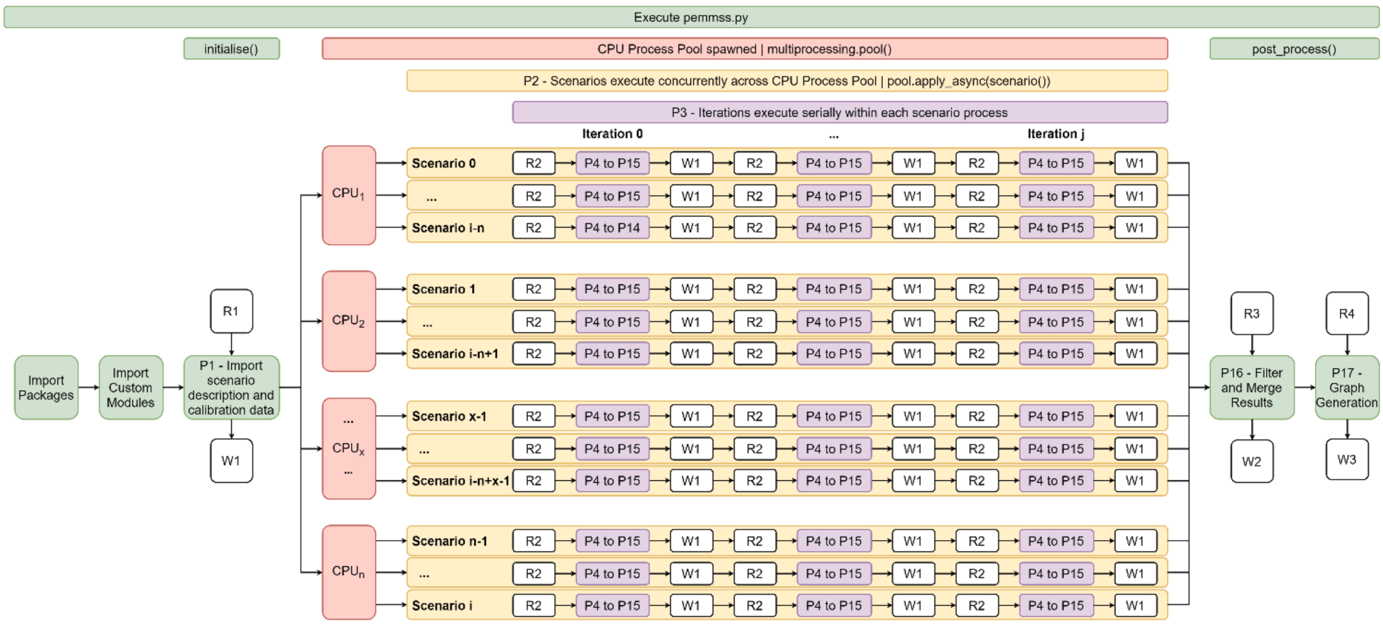

Fig. 3. Model execution flowchart as implemented in python (PEMMSS v1.0.0), showing concurrent processing through the assignment of individual scenarios to a pool of (n) CPU processes. Iterations (j) execute sequentially within each scenario (i) to preserve random seeds and ensure reproducibility of results. Unit process abbreviations and colours correspond to those presented in Fig. 1.

based upon user-defined discovery probability factors ($P_{disc,r,d}$). An arbitrary number of region and deposit type combinations can be specified which then are used to define the key characteristics of new resources, including:

- Resource tonnage models (Section 2.4.2)
- Ore grade models (Section 2.4.2)
- Production capacity variables (for Eq. (10))
- Brownfield tonnage and grade factors (Section 3.5)
- Factors for the mining cost and commodity recovery value models (Section 2.3.2)

To enable evaluation of the influence of exploration targeting strategies on generated scenarios, a deposit type and a region are randomly assigned to a new discovery based upon weightings specified in the model input file. Weightings can be specified for an arbitrary number of regions and deposit types using the model input files. This approach provides a high degree of flexibility as the weightings could be assigned based upon understanding of geological factors or on an investment risk adjusted basis across regions and deposit types. An arbitrary number of regions and deposit types can be defined, so for instance regions could be specified for each cell in a spatial grid to enable detailed regionalisation. This functionality could also be used to simulate discovery of resource at different depths (with corresponding variations to grade/tonnage definitions and extraction cost models). Or instead more coarse aggregations at national or continental scales could be used to better align with the basis of cost and price data informing the value models.

2.4.2. Reserve or resource tonnage and grade generation

Deposit ore tonnages and grade relationships and probability distributions can be defined for each region and deposit type for use when generating new greenfield deposits. There is flexibility in how these are defined. For instance, it is possible to have static assumptions, where all new deposit discoveries are assigned the same characteristics and fixed values. As the characteristics of future mineral discoveries is uncertain, it is also possible to calibrate grade and tonnage probability distributions based upon the distributions observed in known deposits. These can be defined for each region and deposit type.

The resource size, resource grade and contained resources of deposits has been observed to commonly follow lognormal distributions for many major deposit types (Gerst, 2008; Singer, 2013). If resource grade and size are both assumed to be independently log-normally distributed, then their values can be generated using the probability density function shown in Eq. (11), where x is the resource grade or size, σ is the geometric mean of x and μ is the geometric variance of x.

$$\mathbf{f}(\mathbf{x}) = \frac{1}{\mathbf{x}\sigma\sqrt{2\pi}}\mathbf{exp}\left(\frac{-(\mathbf{log}(\mathbf{x}) - \mu)^2}{2\sigma^2}\right) \tag{11}$$

2.4.3. Required development period

Mineral projects can be thought of as having several defined stages in their life cycle, which may include: initial resource discovery, exploration and delineation of a mineral resource or reserve, technical and mining feasibility studies, regulatory permitting processes, funding, mine and processing infrastructure development, active mining and mineral production, mine closure, rehabilitation and decommissioning. Development periods between initial resource discovery and actual mining can be considerable, meaning that exploration to discover new resources needs to be conducted far in advance of commencement of supply from a mine. To enable evaluation of the required magnitude and timing of investment in greenfield exploration, a time of discovery will be assigned at the point of new deposit generation by backdating the current time period by a user inputted development period ($t_{dev,r,d}$)(e.g. 20 years). These development periods are generally highly variable, however some literature describing these is available that may be used as a guide for assigning an appropriate development period (e.g. Kharatinova et al., 2013; Ali et al., 2017).

For a demand-triggered greenfield discovery, the discovery date ($t_{m,disc}$) will be backdated by the development period (Eq. (12)). Whereas, for 'background' greenfield discovery, the start date ($t_{m,start}$) will be forward-dated by the development period (Eq. (13)).

$$t_{m,disc} = t_{m--start} - t_{dev,r,d}, \ where \ t_{m,start} = t \tag{12}$$

$$t_{m,start} = t_{m,disc} + t_{dev,r,d}, \ where \ t_{m,disc} = t \tag{13}$$

2.5. Resource expansion (Brownfield)

Commonly mining operations will continue to explore and increase the size of their defined mineral resource throughout their mine life. This process is commonly known as brownfield resource exploration and can encompass activities such as inclusion of additional peripheral and often lower grade ore, lowering cut-off grades to reclassify additional material as economic, or even inclusion of near-field satellite deposits into the resource estimate and mine plan. In order to simulate this, at the end of a time-step (t), each 'active' mine undergoes brownfield resource expansion by modifying the remaining resource size and ore grades. Each mine has a constant brownfield resource factor ($B_{m,R}$), defined as the ratio of additional brownfield ore resource discovered at each time-step (ΔR) to the remaining ore resource ($R_{m,t}$), as shown in Eq. (14). This creates an additional tranche of brownfield ore that expands the remaining resource according to Eq. (15). Each mine also has a defined brownfield grade factor for each commodity ($B_{m,G,c}$), which is the ratio of the grade of added brownfield ore ($G_{C,\Delta R}$) to the grade of the remaining resource ($G_{m,c,t}$)(Eq. (16)). These are used to determine the grade of the additional ore tranche and to update the overall resource grade for the following time-step according to Eq. (17).

$$B_{m,R} = \frac{\Delta R}{R_{m,t}} \tag{14}$$

$$R_{m,t+1} = R_{m,t}\left(1 + B_{m,R}\right) = R_{m,t} + \Delta R \tag{15}$$

$$B_{m,G,c} = \frac{G_{c,\Delta R}}{G_{m,c,t}} \tag{16}$$

$$G_{m,c,t+1} = \frac{G_{m,c,t} \cdot R_{m,t} + G_{m,c,t} \cdot B_{m,G,c} \cdot \Delta R}{R_{m,t+1}} \tag{17}$$

2.6. Python implementation

An implementation of the PEMMSS model was developed and tested in Python. The model code and example data input files are provided in a GitHub repository (https://github.com/sanorthey/pemmss/). Version releases are archived on Zenodo, with PEMMSS v1.1.0 being the version described by this article (Northey et al., 2022). The structure of the code implementation includes a number of optimisations, such as concurrent processing of major demand scenarios by spreading these across pooled CPU processes as shown in Fig. 3. The python implementation of the model relies only on core python (v3.10) packages, with the exception of the automated graph generation module using matplotlib (v3.5.2), imageio (v2.19.3) and dependant packages.

Model setup and calibration data is passed to the model via a series of .csv files. Multiple scenario runs can be defined so as to generate multiple, stochastic iterations of each scenario. To ensure reproducibility of results, random functions are initially seeded and all input files are saved alongside model outputs.

2.6.1. Model inputs and outputs

The required data inputs and resulting outputs of the primary scenario model are summarised in electronic supplementary file mmc 1. Data inputs are entered into the model through 10 comma separated value (CSV) files, each containing a row of column headers and then rows of values. The expected column headers and acceptable input values for the various fields are described in the associated file import functions in the code repository (modules/file_import.py) (Northey et al., 2022).

There are a range of required data entries. Some data inputs can be infilled where data is unavailable and so these aren't considered mandatory. The nomenclature table (Table 3) also shows which input files are associated with the variables described in this article.

Following a model run, a range of statistics are generated across a

Table 2
Hypothetical test scenario parameter definitions for new deposit discoveries.

Discovery Probability %	**Deposit Type** Region	**Reserve Tonnage (kilotonnes)** Commodity Grade (ratio) Note: Lognormal distribution parameters shown (mean, stdev, max)	**Recovery** (ratio)	**Value Models** Net Value = sum (Revenue – Recovery Cost) – Mining Cost
	Type 1	**Reserve Tonnage (8.75, 0.27, 10,000)**		**Revenue** | $A = R*G*1500$, $D = R*G*Rec*300$ **Recovery Cost** | $A = R*G*500$, $D = R*G*Rec*100$
20	Region 1	A(-3.91, 0.2, 0.05), D(-3.94, 0.2, 0.05)	A(0.9), D (0.5)	**Mining Cost** | 100
5	Region 2	A(-3.9, 0.2, 0.05), D(-3.94, 0.15, 0.05)	A(0.85),D (0.5)	**Mining Cost** | 80
5	Region 3	A(-3.92, 0.2, 0.05), D(-3.94, 0.15, 0.05)	A(0.8), D (0.5)	**Mining Cost** |100
	Type 2	**Reserve Tonnage (8.638, 0.36, 8000)**		**Revenue** | $A = R*G*1500$, $B = R*G*Rec*400$ **Recovery Cost** | $A = R*G*400$, $B = R*G*Rec*100$
5	Region 1	A(-3.95, 0.2, 0.05), B(-3.93, 0.15, 0.05)	A(0.9), B (0.8)	**Mining Cost** | 100
20	Region 2	A(-3.93, 0.2, 0.05), B(-3.92, 0.15, 0.05)	A(0.85),B (0.8)	**Mining Cost** | 80
5	Region 3	A(-3.91, 0.2, 0.05), B(-3.94, 0.15, 0.05)	A(0.8), B (0.8)	**Mining Cost** | 100
	Type 3	**Reserve Tonnage (7.47, 0.73, 4000)**		**Revenue** |$A = R*G*1500$, $B = R*G*Rec*600$, C = R*G*Rec*575 **Recovery Cost** | $A = R*G*300$, $B = R*G*Rec*100$, C = R*G*Rec*100
10	Region 1	A(-3.92, 0.2, 0.05), B(-3.95, 0.25, 0.03), C (-3.8, 0.1, 0.03)	A(0.9), B (0.9), C (0.95)	**Mining Cost** | 100
10	Region 2	A(-3.92, 0.2, 0.05), B(-3.94, 0.25, 0.03), C (-3.85, 0.1, 0.03)	A(0.85),B (0.9), C (0.95)	**Mining Cost** | 80
20	Region 3	A(-3.95, 0.2, 0.05), B(-3.93, 0.25, 0.03), C (-3.9, 0.1, 0.03)	A(0.8), B (0.9), C (0.95)	**Mining Cost** | 100

All Deposit Types and Regions – Other Parameters.
Brownfield Grade Factors | A (0.0001), B(Type 2 0.99, Type 3 0.97), C(1), D(1).
Brownfield Tonnage Factor = 0.01.
Development Period = 15.
Development Probability = 0.9.
Production Capacity = $R/5 < 0.2R^{0.85} < R/500$, Standard Deviation = 0.0001.
Time Altered Parameters.
Region 2 (all deposit types) between 2 and 15 and 2025 - Development Period increases from 15 to 20.
Type 1 deposits (all regions) between 2000 and 2050 – Recovery of Commodity D increases from 0.5 to 0.82.

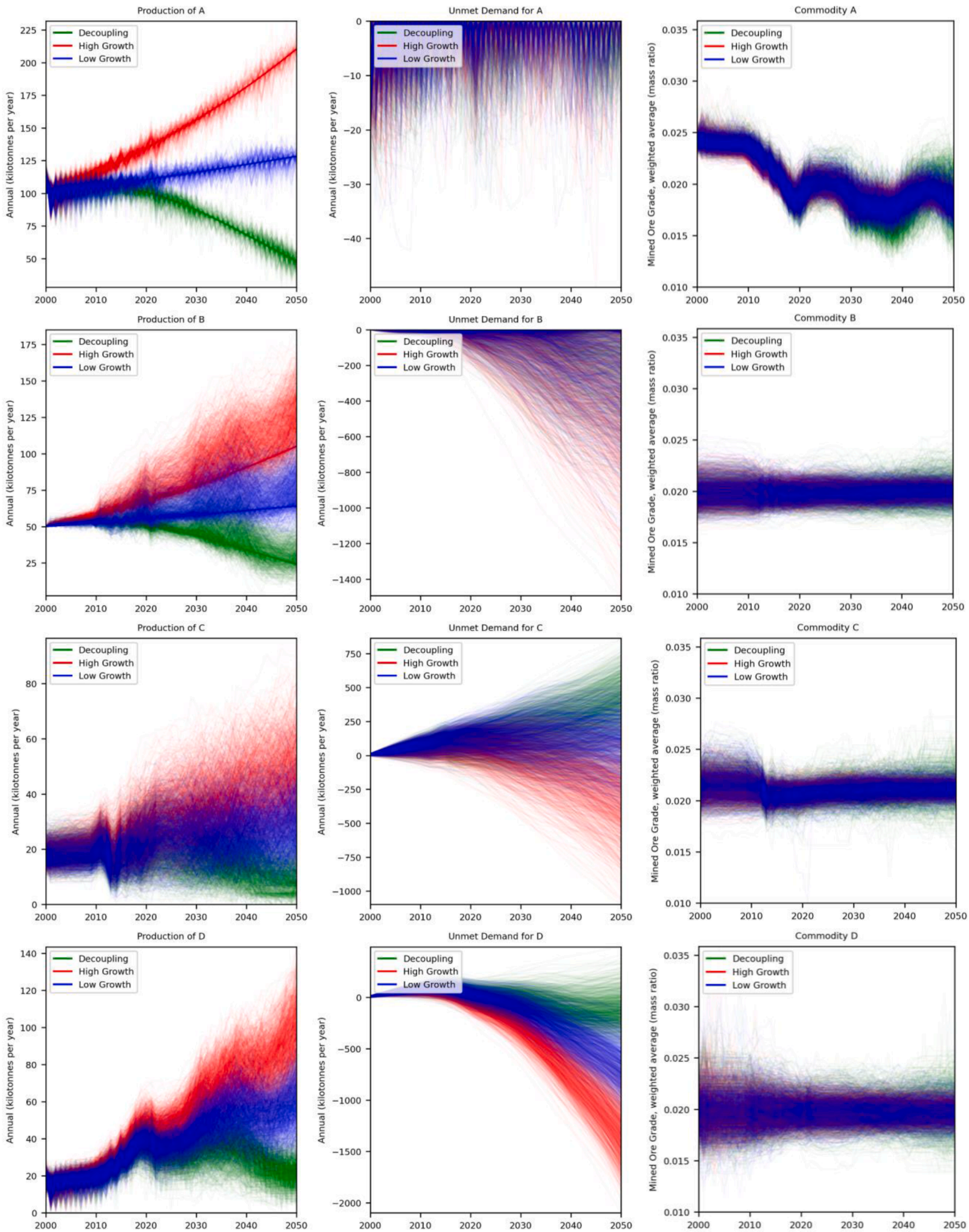

Fig. 4. Total primary commodity supply, unmet demand and average mined ore grades for a 4 hypothetical co-product commodity system (A, B, C & D), where demand for A and B must always be met. Results for three demand scenarios are shown, with 1000 iterations of the model run. The range of results for each scenario is primarily due to differing deposit discovery and mine development outcomes for each model run.

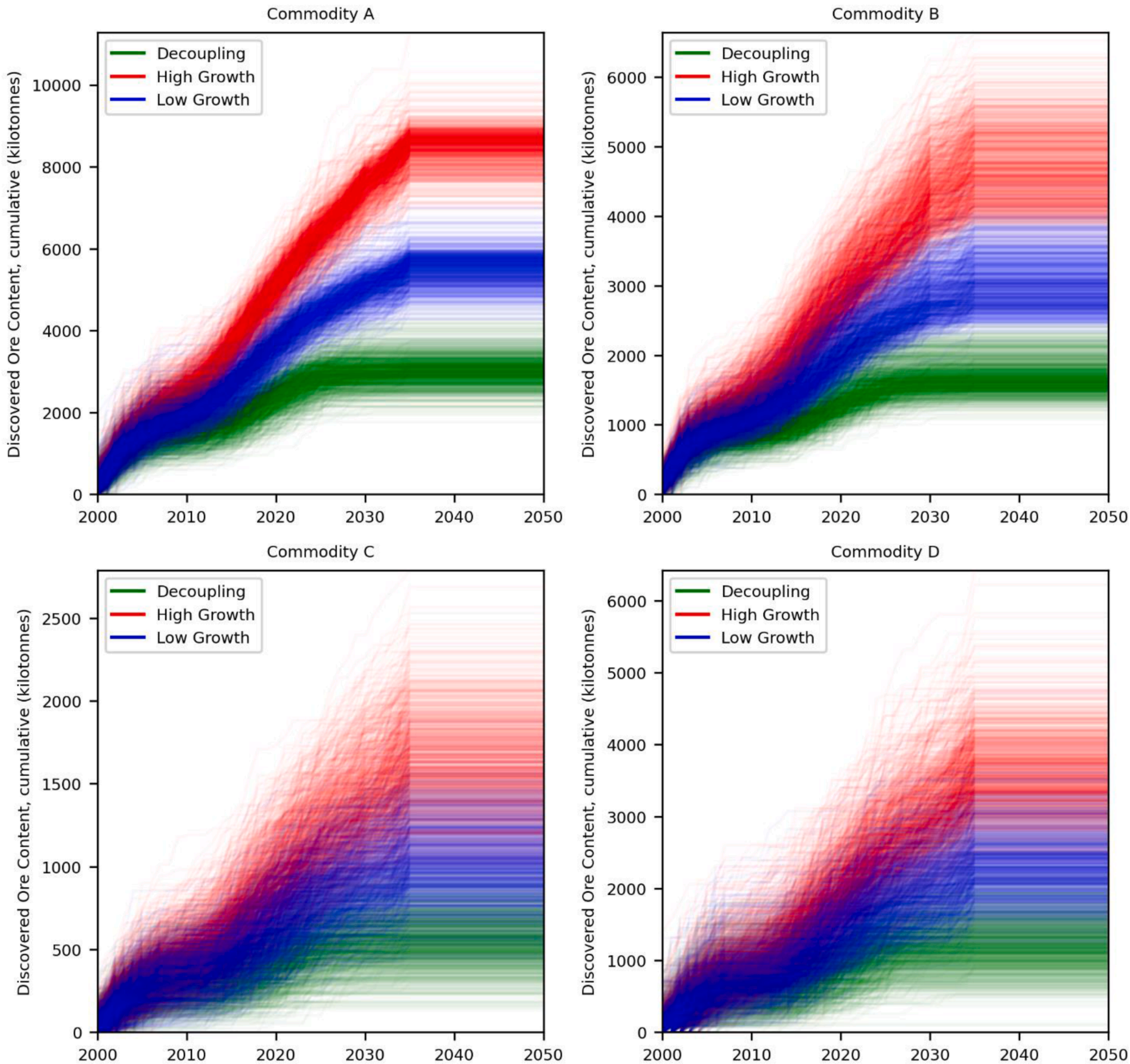

Fig. 5. Cumulative discovered ore content for a hypothetical 4 co-product commodity system (A, B, C & D), where demand for A and B must always be met. Results for three demand scenarios are shown, with 1000 iterations of the model run.

range of different aggregations to aide with data analysis and interpretation. This includes output CSV files containing mine level data, as well as aggregated statistics for regions, deposit types and commodity groups. The model can also be configured using the input files to auto-generate and format graphs and GIFs of model results.

3. Testing model functionality and behaviour

The model's behaviour was tested to understand the response and sensitivity to different input parameters and potential model behaviours. A series of hypothetical scenarios were modelled with differing settings and inputs to test key aspects of the model behaviour, including:

- Capability of the model to handle multiple supply-demand balanced and unbalanced commodities.
- Model behaviour when greenfield and brownfield exploration was turned on or off.
- Behaviour of the model during rising and declining commodity demand.
- Behaviour of the stochastic deposit generation algorithms for grade and tonnage generation.
- Handling of competing deposit types, with differing coproducts and supply trigger commodities.

3.1. *Hypothetical test scenario descriptions*

The hypothetical test scenarios considered four different commodities (A, B, C and D) produced as products or coproducts from the mining of three different deposit types (Type 1, Type 2, Type 3) in three regions

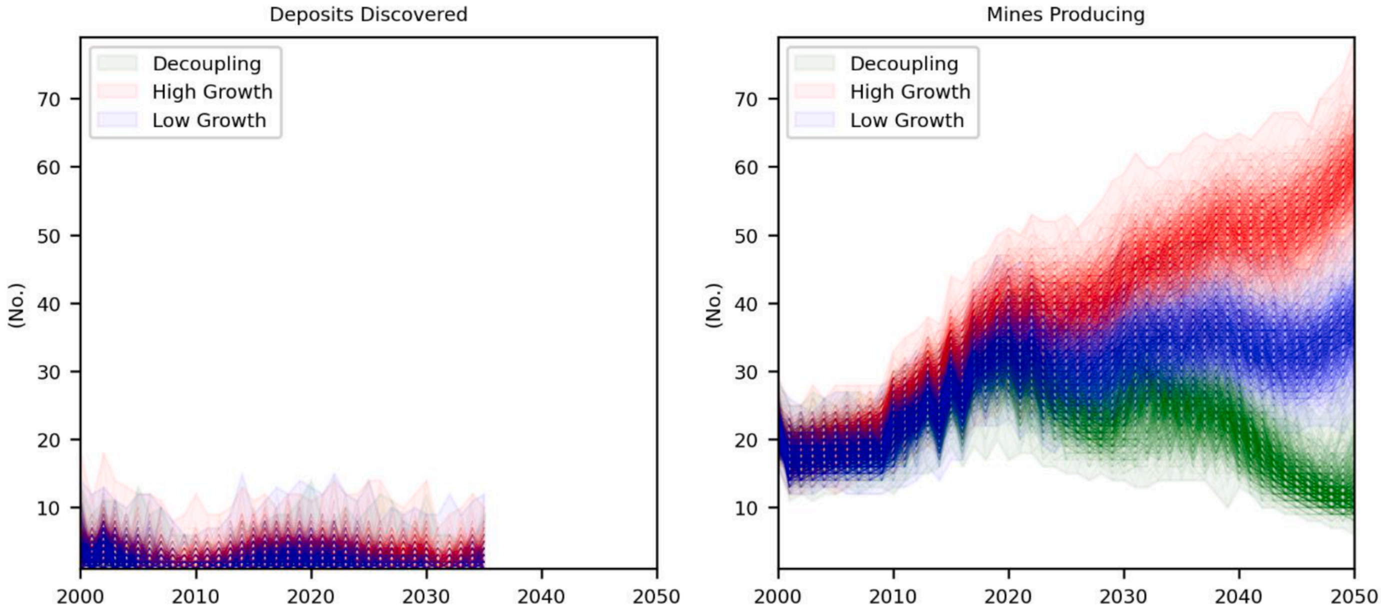

Fig. 6. Annual deposit discoveries and mines producing for a hypothetical 4 co-product commodity system. Results for three demand scenarios are shown, with 1000 iterations of the model run.

(Region 1, Region 2 and Region 3). All deposits contain commodity A. However, each deposit type has a differing mix of recoverable co-product commodities, grade and tonnage probability distributions, and value models. Each region was seeded with one Type 3, two Type 1 and two Type 2 mining projects in each region, plus an additional six undeveloped deposits.

Commodity supply from the seeded mines and undeveloped deposits are insufficient to meet demand in all hypothetical scenarios and so new deposits are discovered stochastically and assigned attributes according to the parameters defined in Table 2. As part of this, the deposit type and region of each deposit is randomly assigned based upon the discovery probability factors. Then the reserve tonnage and ore grade of each new deposit is assigned based upon a set of lognormal probability distributions. The revenue and recovery cost models vary between deposit types, but are a function of the *contained reserve* for commodity A and the *contained recoverable reserve* for other commodities. Deposits discovered in Region 2 have slightly lower fixed mining costs compared to Region 1 and Region 3. The development period of all deposits is 15 years, except for in Region 2 where this increases to 20 years by 2025. There is a 90% development probability for an undeveloped deposits in a given time period in response to demand. Recovery rates of commodity D from new Type 1 deposits were also set to increase substantially from 50% to 82% by the end of the scenario period.

Three demand scenarios (high growth, low growth and decoupling) were constructed for the period 2000 to 2050. A range of global parameters were set to control the model behaviour. Demand for commodities A and B must always be balanced by supply. However, demand for C and D does not trigger additional mine supply or new deposit discovery and so extreme shortfalls of C and D are potentially possible. Brownfield reserve expansion at active mines and greenfield exploration for new deposits in response to demand were both set to on. However, the rate of constant background greenfield discovery was set to zero. Supply from active mines was prioritised above undeveloped deposits. The value of mines and deposits are not updated through time. The global recovery rate of all commodities was set to 90%. Any unmet demand or oversupply fully rolls over and modifies demand in the subsequent year. A basic sensitivity analysis of each of these global parameters was also constructed using the high growth scenario.

The input files for the test case scenario description are located in the "input_files_examples" folder of the PEMMSS model v1.1.0 code repository (Northey et al., 2022). These include specifications for automated graph generation that will reproduce the figures in this article and the electronic supplementary files. For testing purposes, it is suggested to alter the number of iterations to 100 or less in the "input_parameters.csv" file to reduce execution time.

3.2. Hypothetical test scenario results

Supply scenarios to meet the three demand scenarios were modelled iteratively 1000 times using the PEMMSS model to understand how uncertain and stochastic exploration and mine development outcomes can lead to large variance and divergence in long-term co-product commodity supply-demand profiles. Figs. 4, 5 and 6 are the result of highly customisable, automated graph generation by the PEMMSS model.

Fig. 4 shows that supply of commodity A and B was able to meet demand in all scenarios and that in-fact periods of oversupply of C and D can occur for these commodities due to their co-production. However, for commodity C there is a potential for either long-term oversupply or under-supply depending on the demand scenario due to supply being governed by the production of commodities A and B. Only in the high growth scenario is potential supply of commodity C sufficient to meet demand, indicating the presence of a structural supply constraint if the low growth or decoupling scenarios were pursued. This can be compared with the long-term tendency for over-supply of commodity D under all scenarios. Another interesting aspect is the gradual decline in mined ore grades for commodity A due to a combination of very low A grades in brownfield ore, new deposit discoveries tending to be lower grade than the initially seeded mine sites and undeveloped deposits and the cyclical nature of new developments caused by marginal tranche valuation for brownfield ore and the development period.

Fig. 4 also demonstrates that there is a very high variability in potential supply outcomes for commodity C and D (and to a lesser extent B), even when considering the same major demand scenario. As we turn our attention to Fig. 5, we can see that this variability is largely associated with uncertain outcomes associated with new deposit discovery. As commodity C and D are only produced from specific deposit the supply of these commodities is dependant on these specific deposit types being discovered and brought into production. This also means that a scenario where high supply of commodity C is achieved may also be

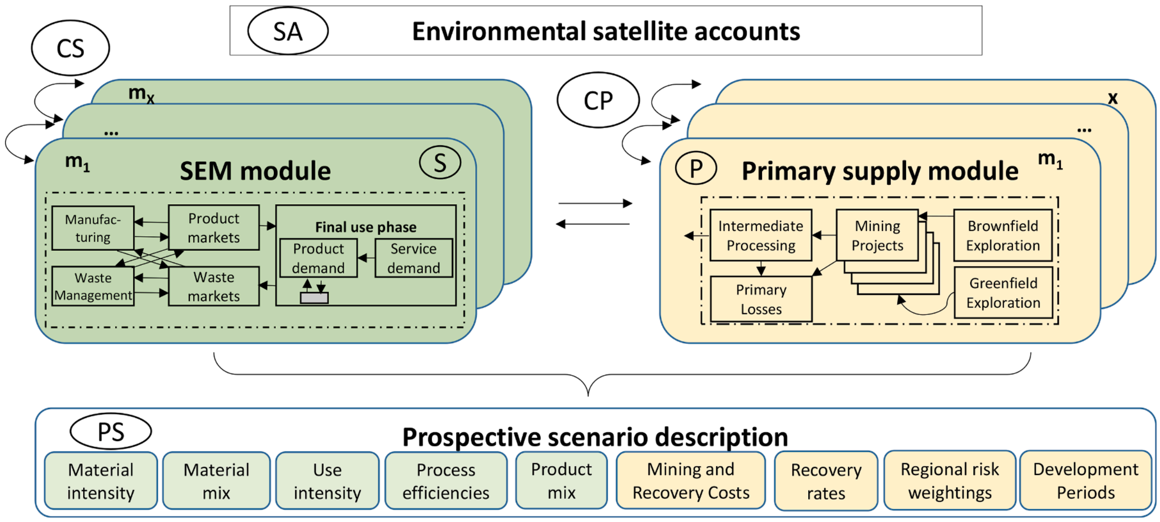

Fig. 7. This system definition shows a modular approach to prospective material flow assessment (MFA). We propose an approach for MFA to address stakeholder specific research questions by explicitly thinking about the needed detail and extensions. S: Socio-economic metabolism (SEM) module, P: primary supply module, CS: Coupling of material cycles in the SEM, CP: coupling of primary material cycles in the mining industry, SA: Environmental satellite accounts, PS: Prospective scenario description. Some research questions also are addressed with more rough estimates for the supply and demand of materials in the future. The system definition within the dotted lines, therefore, is often seen as black box (in case of the supply module) or described by a less flexible top-down approach (for the SEM module).

associated with a lower supply potential for commodity D, as these two commodities are not produced from the same deposit type. An additional component of uncertainty contributing to the variability shown in Figs. 4 and 5 is the random assignment of ore grades for new deposits in accordance with the defined log-normal probability distributions.

Variability in deposit supply potential and co-production dynamics also translates into variability in both the number of deposit discoveries and the number of simultaneously operating mines required to meet long-term demand (Fig. 6). Due to the 15 year development period, the deposits required to meet demand in 2050 must be discovered by 2035 at the latest to avoid supply shortfalls. Except for region 2 where the development period increases to 20 years, requiring discovery by 2030 to contribute to supply in 2050. In addition, the set of existing mines and undeveloped deposits manually inputted into the model is slightly insufficient to meet demand at model commencement (see Fig. S6 and mmc2 in the electronic supplementary files). This could be interpreted to indicate that insufficient exploration success prior to the modelled period is creating a supply bottleneck or that there may be additional existing mines and deposits missing from the input files.

Additional examples of model results, including sensitivity analysis, are shown in Supplementary Figs. S1 to S16 in electronic supplementary file mmc1 run (e.g. commodity losses, production by region and deposit type, rates of mine commencement or closure, etc.). These provide a sense of the flexibility of automated statistic and graph generation by the model. The model can also be configured to automatically generate GIFs of model results. Examples of these are shown in electronic supplementary files mmc2, mmc3 and mmc4, where each frame of the GIF is a different iteration of the scenario run.

4. Potential model applications

4.1. Integration with broader material cycle scenario models

The mining supply model presented here needs an exogenously determined primary demand for different mineral or metal commodities. This integration may allow for studying the resource implications of macro-level scenarios for sustainable development, such as the widely established Shared Socioeconomic Pathways (SSP) that form the basis for climate policy assessment (O'Neill et al., 2014; Riahi et al., 2017). Material demand scenarios for the SSP, energy transition and net-zero carbon scenarios have already been generated (Schandl et al., 2020; Pedneault et al., 2022; IEA, 2021; Watari et al., 2020; Marscheider-Weidemann et al., 2021; Hund et al., 2020) Integration with these would enable researchers to study the implications of different resource efficiency strategies, not only on primary metal demand at an aggregate level, but also to more formally interrogate potential outcomes in the mining sector and the associated energy demand and environmental impacts in more detail. Developing a more coherent description of anthropogenic metal cycles across all stages of the cycle allows for policy-relevant assessment of consequences associated with prospective metal supply and demand, as well as the potential for material bottlenecks to be assessed.

Fig. 7 shows a modular framework for constructing prospective material flow assessments. Modular software development allows unit testing of model behaviour. Combined with open data and model transparency this facilitates reproducibility of results and the ability to extend or modify code without limitations. The PEMMSS model is designed to function as the primary supply module shown in Fig. 7. It could be coupled to a socio-economic metabolism module that models material use, stocks and flows in society and outputs the demand for primary mining and supply of different metals. Modules for the socio-economic metabolism are not described here but a number of suitable examples exist (Hatayama et al., 2010; Pauliuk et al., 2013). Notably the ODYM-RECC model developed as part of the UN International Resource Panel's Resource Efficiency and Climate Change (RECC) mitigation project (Pauliuk, 2020). The key to the use of this type of modular framework is to have well-defined interfaces (e.g. primary material demand) between modules. Multi-metal assessments can be conducted to consider the coupling between different metals across all stages of the cycle, from mining (co-product metals), to material production (including alloys), to use (alloys combined into products), and recycling (alloys mixed into scrap groups). Extensions of these models with environmental satellite accounts allow detailed prospective assessments of how different climate change mitigation strategies affect the global mining sector, and how environmental impacts associated with material supply and demand may affect the feasibility of climate change mitigation strategies. Such applications have profound relevance as they allow us to quantify trade-offs when pursuing sustainable development goals related to raw material supply.

4.2. Understanding supply interdependencies of co-/by-product commodity systems

Many critical metal commodities are produced as co-products or by-products from the production of other mineral and metal resources (Nassar et al., 2015; Fu et al., 2019). For instance, elements with high geochemical affinity and co-production potential have also been referred to as belonging to the same 'geological family' by studies that have used criticality assessment to assess material supply risks, for instance Zn-Pb-Ge-Cd-In-Sn (Harper et al., 2015) and Cu-As-Se-Ag-Te-Au (Nassar et al., 2012). Nassar et al. (2015) and Reuter and Verhoef (2004) provide useful diagrams showing grouping of host minerals and metals and their potential co-product elements.

Some elementary groupings that may well suited to initial application of the PEMMSS model to understand supply-demand dynamics interdependencies during sustainability transitions include Cu-Ni-Co, as these are important for electrification and battery production, and also Cu-Zn-Ge-In, as these can be important for infrastructure, renewable energy, electronics and optical technology deployment. The authors view these two commodity groupings as low-hanging fruit because global service-based demand projections already exist, as well as detailed production and mineral reserve and resource datasets (Mudd et al., 2013; Mudd and Jowitt, 2014, 2017; Mudd and Jowitt, 2018), and specific methodologies for estimating In and Ge ore grades and resources within Cu and Zn deposits (Werner et al., 2017; Yellishetty et al., 2017). Although we note that significant uncertainties exist with all these data sources and methods, especially for minor elements, due to conceptual and practical limitations in industry data collection, reporting practices and transparency. This may make calibration of the model exceedingly difficult for some minor by-product elements. In these cases, the general approach taken to developing the hypothetical case study could also be used to test assumptions and understand possible by-production dynamics for generic sets of commodities. We also note that there has also been scenario based studies for many of these elements using other modelling approaches, which would provide a basis for comparison and assessment of the relative strengths and weaknesses of the PEMMSS model.

As part of this, one hypothesis that the authors are working towards testing is that exploration and mine development strategies targeting specific deposit types for major commodities may be highly influential in dictating long-term supply potential of by-product commodities due to differences in ore grades of these by-products between deposit types. An open question is whether the strategies pursued in mineral exploration may render some sustainable development trajectories infeasible due to potential co-/by-product supply imbalances? And also, can any challenges of this type potentially be overcome simply through efforts to further increase recovery rates or by introducing incentive schemes related to by-product supply?

A limitation of the PEMMSS model is that primary commodity demand and additional parameters that could be useful for the mine value model, such as commodity prices, are defined exogenously to the model. So although there are published long-term demand scenarios for many commodities that the PEMMSS model could be coupled to, often these do not include specific commodity price scenarios or assumptions that would be useful for model calibration. Further modification of the PEMMSS model to incorporate endogenous price formation was considered, but ultimately viewed as too conceptually difficult to implement as commodity prices are influenced by secondary material supply, which is outside the model's system boundary. Due to these forms of limitations, we strongly encourage systematic sensitivity analysis of input parameters when using the model. Particularly for multi-commodity systems, where the relative value of deposits may change substantially depending upon alteration to assumed prices for each commodity.

4.3. Understanding the long-term supply implications of differing models of geological understanding

Although mineral deposits have diverse characteristics, they can be classified into a set of mineral systems using temporal and genetic relationships, the tectonic setting and the chemical characteristics of their hosts. The most widely adopted system for some time, especially for resource assessments, was the mineral deposit models classification of Cox and Singer (1986), which included grade and tonnage models. Although considerable advancements to these systems have been made in recent years (e.g. Dill, 2009). As an example of the application of these systems, assessments exist for Australian major mineral systems, deposit-types, and their potential to contain major and companion metal (s) (Skirrow et al., 2013, Jaques et al., 2010). There is still considerable uncertainty inherent in these forms of assessment– especially when applied to regions where there has been limited prior systematic geological study and mineral exploration.

The PEMMSS model provides functionality to understand the long-term implications of different models of understanding for mineral resources. For instance, it could be used to test whether different models of resource size and grade distributions would meaningfully alter long-term outcomes in the mining sector. As an example, Gerst (2009) postulated that if resource size and grade are instead correlated[3] and that the contained resource of deposits (i.e. the product of resource size and grade) is also log-normally distributed, then resource size as a function of resource grade can be approximated according to Eq. (18). The parameters σ_w^2 and μ_w are the weighted geometric mean and the weighted geometric variance of the grade(G)–tonnage(T) density function. These can be determined based upon mineral resource datasets using Eq. (19) and Eq. (20), respectively, where n is the total number of deposits, i is a deposit index, T is the resource ore tonnage (T) and G is the resource ore grade (G) of each deposit. The parameter θ is a scaling factor equal to the sum of all contained resources (Eq. (21)).

$$G_i \cdot T_i = \frac{\theta}{G\sigma_w\sqrt{2\pi}} exp\left(\frac{-(log(G) - \mu_w)^2}{2\sigma_w{}^2}\right) \quad (18)$$

$$\mu_w = \frac{\sum_{i=1}^{n} log(G_i)T_i}{\sum_{i=1}^{n} T_i} \quad (19)$$

$$\sigma_w{}^2 = \frac{\sum_{i=1}^{n} log(G_i)^2 T_i}{\sum_{i=1}^{n} T_i} - \mu_w{}^2 \quad (20)$$

$$\theta = \sum_{i=1}^{n} (G_i \cdot T_i) \quad (21)$$

This approach would assume that future resource discoveries have the same grade-size distribution of historic discoveries and that these relationships hold across all deposit scales. However as a counterpoint, it has been hypothesised that very large deposits, which often form the bulk of global commodity production, may have alternative size-grade distributions (e.g. hyperbolic; Agterberg, 1995). Additionally, a multi-modal distribution of ore grades may plausibly be expected for some commodities due to the mineralogical barrier hypothesis (Skinner, 1976). It is relatively straightforward to modify the PEMMSS model code to incorporate these different forms of probability distributions to enable testing of the long-term implications of these distributions on resource supply. However, we note that reserve and resource definition is also dependant upon prevailing economic, technological and other factors that influence important factors such as cut-off grades. These complexities introduce considerable methodological and data uncertainties and biases that may not always be captured in uncertainty

[3] Anecdotally, some economic geologists that the authors have interacted with dispute this correlation.

distributions derived from empirical data. So we emphasize the need to appreciate the considerable the uncertainty associated with this type of long-term scenario modelling.

4.4. Regionalised scenarios of mineral supply and exploration

Previous scenario models incorporate limited regionalisation of future supply. This is difficult to incorporate into scenario modelling that includes greenfield exploration, as the exact location of future mineral discoveries is unknown. However, through the process of *permissive tract assessment*, deposit density models can be used to estimate the number of undiscovered mineral deposits of specific types that may exist in different regions based upon regional geology (Singer 2018; Kesler and Wilkinson, 2008; Johnson et al., 2013). This could provide an indication of where future discoveries may occur and gives some basis to give a probabilistic weighting for the relative likelihood of deposit discovery across regions when using the PEMMSS model. When developing deposit density models and grade-tonnage distributions, consideration should be given to the methodological controls placed on their development. For instance, consistent spatial aggregation and the inclusion of only maturely explored deposits in the datasets may be preferred when calibrating deposit density, grade and tonnage models for certain purposes– as described by Singer (2018). Other aspects of importance, such as likely depth of deposits could be incorporated to place further bounds on deposit discovery and the economics of extraction. Which in turn could be linked to resource valuation models that can incorporate this type of regional and geological data, such as the Bluecap model (Walsh et al., 2020)

In the literature, there also exists the notion of differentiated 'geological maturity' of regions. The basic idea being that the 'geologic maturity' of a region increases as exploration is undertaken and a region's geology is more fully understood. Of particular relevance, it is posited that mineral deposit discoveries have potential to cause information spill overs that may make subsequent discoveries more likely or easier (Castillo et al., 2021). This is counterbalanced by the fact that only a fixed number of mineral deposits truly exist within a region and that a deposit discovery depletes the remaining exploration potential of the region. Wellmer (2022) argues that exploration spill overs are still positive for most commodities and that we are not facing any immediate risk of depletion of mineral deposits to mine (although we would posit that there may be growing restrictions or constraints on exploration and developing new mine sites due to changing socio-political conditions). Incorporation of geologic maturity information could be implemented in the PEMMSS model through modification of the development probability factors used for assigning regions and deposit types to new discoveries. If required by a study, the PEMMSS model could be further modified to allow recursive relationships between deposit discovery and the likelihood of further discovery in the region. This would allow evaluation of the potential influence of geologic maturity on long-term scenario results, and the ability to test to see whether self-reinforcing regional discovery and supply may become apparent (i.e. will 'mature' regions disproportionately contribute to future supply despite other regions potentially being more prospective in an absolute sense?).

4.5. Adding environmental extensions

Environmental impacts and stressors of mining are substantial and potential limiting factors to continued or expanding operations in certain regions. A range of recent studies have sought to assess the environmental impacts of mineral or metal supply overtime through analysis of demand scenarios with parametrised estimates of environmental impacts of supply (e.g. Elshkaki et al., 2016; 2017; Kuipers et al., 2018; van der Voet et al., 2019; van der Meide et al., 2022). Several of these have also considered feedbacks between metal supply life cycle inventories and broader inventory databases (Harpprecht et al., 2021). These types of studies generally take a fairly top-down approach with high levels of regional aggregation, and so do not fully capture the diversity of impacts observed across the mining industry and the relationship of these impacts to site-specific factors.

Recently, more disaggregated life cycle inventories and datasets for mineral production are gradually emerging that could be incorporated into an extended PEMMSS model to undertake prospective life cycle assessments of mineral production on a site-by-site basis. For instance, datasets have been developed for energy use and greenhouse gas emissions of mining operations (Koppelaar and Koppelaar, 2016; Mudd, 2010; Northey et al., 2013), water use of mining operations (Northey et al., 2019), land-use changes associated with mine development and mine-site infrastructure (Maus et al., 2020; Werner et al., 2020), as well as life cycle inventory data for mine tailings management (Adrianto et al., 2022). A particular strength of the PEMMSS model is the ability to stochastically produce regionalised results for mineral supply. This functionality could be used as a basis to add a scenario or time dimension to existing studies that consider potential land-use change and biodiversity impacts of mining (Murguía et al., 2016; Sonter et al., 2018), or even assessments of industry exposure to climate risks (Northey et al., 2017). There is also potential to develop more informed scenarios of water consumption and contributions to water scarcity associated with mineral production, which previous research has identified should be conducted using watershed rather than national regional boundaries – as this would avoid biases associated with the regional averaging schemes used to derive national life cycle impact characterisation factors for water use (Northey et al., 2018b). Pursuing this line of modelling and research would provide a mechanism to more comprehensively evaluate the future natural resource implications and environmental burdens associated with metal production as we pursue the United Nations' sustainable development goals, which have complex inter-relationships with extractives sectors (Yakovleva et al., 2017; Yakovleva and Nickless, 2022).

5. Conclusions

A range of plausible and divergent futures for material supply chains are possible due to the combination of economic growth, changing standards of living, technology development and population increases combined with growing societal ambitions to decarbonise and transition towards a circular economy. Alongside this, the rapid adoption of new technologies is driving substantial growth in minor, speciality metals and there is also speculation that demand for some metals produced in large quantities (e.g. copper or zinc) may plateau as the material intensity of developed economies approach saturation levels. This is contrasted by persistent concerns regarding material scarcity or depletion of mineral resources.

Existing research to understand society's uncertain material future has been focused on how demand and supply may evolve, as well as the opportunities for increasing secondary production or economic dematerialisation. As a contrast, the PEMMSS model takes a bottom-up approach, which has been designed to allow the results of demand-side scenario modelling to be translated into a more nuanced understanding of their implications for primary mineral and metal supply chains. In doing so, the application of the PEMMSS model may help to identify material supply bottlenecks that could hinder long-term technology deployment and sustainable development. Or more optimistically, application of the PEMMSS model may reveal potential policy, investment or industry responses in mineral exploration, mining and metal production, which if implemented could assist in the transition towards a sustainable, decarbonised economy.

Electronic Supplementary Files

Readers are encouraged to review the contents of electronic supplementary files mmc1, mmc2, mmc3 and mmc4 that provide additional examples of the potential use and outputs of the PEMMSS model. A code

Table 3
Description of nomenclature used in the equations and cross-reference to relevant PEMMSS model input files.

Symbol	Equation	Description	Input File
a	10	Supply capacity calibration parameter	E, ET*
b	10	Supply capacity calibration parameter	E, ET*
$B_{m,G,c}$	16, 17	Brownfield grade factor of commodity (c) for mine (m)	E, P*, PC*, ET*
$B_{m,R}$	14, 15	Brownfield resource factor for mine (m)	E, P*, ET*
$D_{c,T}$	1	Demand threshold of commodity (c)	D
$D_{c,carry}$	3	Demand carry constant for commodity (c)	D
$D_{c,Ex,t}$	3, 4	External commodity (c) demand at time (t)	D
$D_{c,M,t}$	1, 2, 4, 5	Mined commodity (c) demand at time (t)	–
$D_{O,m,t}$	2, 5, 8	Residual ore demand placed on mine (m) at time (t)	–
G	18, 19, 20, 21	Reserve or resource ore grade	–
$G_{c,\Delta R}$	16	Ore grade of commodity (c) in a unit of discovered brownfield ore	–
$G_{m,c,t}$	2, 5, 9, 16, 17	Ore grade of commodity (c) in mine (m) at time period (t)	E, ET*, P*, PC*
L_{min}	10	Minimum allowable mine life	E, ET*
L_{max}	10	Maximum allowable mine life	E, ET*
$P_{dev,m}$	–	Probability/likelihood of mine (m) development due to demand	E, P*
$P_{disc,r,d}$	–	Probability/likelihood of a deposit discovery being assigned a specific region (r) and deposit type (d)	E, ET*
R_m	10	Initial ore reserve or resource of mine (m)	E, ET*, P*
$R_{m,t}$	8, 14, 15, 17	Remaining ore reserve or resource of mine (m) at time (t)	ET*
$Rec_{m,c}$	2, 5, 9	Recovery factor of commodity (c) from ore at mine (m)	E, ET*, P*, PC*
$Rec_{G,c}$	1, 3, 4	Global recovery factor of commodity (c) for processes between mine boundaries and external commodity demand (e.g. refining)	D
$S_{m,cap}$	8, 10	Ore supply capacity of mine (m)	E, ET*, P*
$S_{m,O,t}$	8, 9	Supply of ore by mine (m) during time period (t)	–
$S_{m,c,t}$	1, 2, 3, 9	Supply of commodity (c) by mine (m) during time period (t)	–
$t_{dev,r,d}$	12, 13	Development time period for region (r) and deposit type (d)	E, ET*
$t_{m,disc}$	12, 13	Discovery time of mine/deposit (m)	ET*, P*
$t_{m,start}$	12, 13	Start time of mine (m)	ET*, P*
T	18, 19, 20, 21	Resource tonnage	–
$V_{m,c,cost}$	7	Cost of extracting commodity (c) from ore at mine (m)	E, ET*, P*, PC*
$V_{m,c,net}$	6, 7	Net value of extracting commodity (c) from ore at mine (m)	E, ET*, P*, PC*
$V_{m,c,revenue}$	7	Revenue from extracting commodity (c) from ore at mine (m)	E, ET*, P*, PC*
$V_{m,mining}$	6	Cost of mining ore at mine (m)	E, ET*, P*
$V_{m,net}$	6	Net value of mining ore and extracting all commodities at mine (m)	P*
x	11	Reserve or resource size or grade	–
ΔR	14, 15, 17	Additional unit of brownfield ore discovered	–
μ	11	Geometric variance	E, ET*
μ_w	18, 19, 20	Weighted geometric variance	–
σ	11	Geometric mean	E, ET*
σ_w^2	18, 20	Weighted geometric mean	–
Θ	21	Scaling factor	–

Input File Abbreviations:.
E – input–exploration_production_factors.csv, ET - input_exploration_production_factors_timeseries.csv, D – input_demand.csv, P – input_projects.csv, PC – input_project_coproducts.csv.
Notes:* Indicates that specification of this variable or associated estimation parameters is optional in this input file.

repository for PEMMSS v1.1.0 is archived on Zenodo (Northey et al., 2022). Latest releases and development versions can also be viewed on GitHub (https://github.com/sanorthey/pemmss/).

CRediT authorship contribution statement

S.A. Northey: Conceptualization, Methodology, Software, Validation, Data curation, Visualization, Writing – original draft, Writing – review & editing. **S. Klose:** Conceptualization, Methodology, Writing – review & editing. **S. Pauliuk:** Conceptualization, Methodology, Writing – original draft, Writing – review & editing. **M. Yellishetty:** Conceptualization, Methodology, Writing – original draft, Writing – review & editing. **D. Giurco:** Conceptualization, Writing – review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

The model code and input data used to generate all figures in the article has been archived on Zenodo - https://doi.org/10.5281/zenodo.7495966

Acknowledgements

The authors gratefully acknowledge the support of several funders for this research. Initial model conceptualisation and development was conducted as part of a researcher exchange between Monash University and the University of Freiburg funded through the Australia-Germany Joint Research Co-operation Scheme 2018 and the German Academic Exchange Service (DAAD). As part of this, Stephen Northey and Mohan Yellishetty received a travel grant from Universities Australia, whilst Stefanie Klose and Stefan Pauliuk received a travel grant from DAAD. Further model development has occurred as part of a UTS Chancellor's Postdoctoral Research Fellowship project being undertaken by Stephen Northey. Aspects of the model design have been inspired by discussions over the years with Gavin Mudd (RMIT University).

Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.rcradv.2023.200137.

Appendix A – nomenclature

Table 3

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