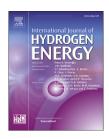


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Is iridium demand a potential bottleneck in the realization of large-scale PEM water electrolysis?



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HIGHLIGHTS

- First feasibility-study on iridium supply and demand for hydrogen economy.
- Linking iridium production and recycling with technical prospects for catalyst loading.
- Providing a technology specific iridium demand model for PEM water electrolysis.
- Scenario analysis of large-scale PEM water electrolysis future market development.

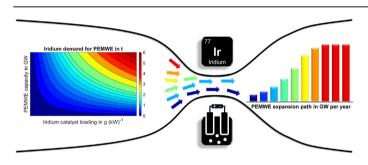
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GRAPHICAL ABSTRACT



ABSTRACT

Proton exchange membrane water electrolysis (PEMWE) is a key technology for future sustainable energy systems. Proton exchange membrane (PEM) electrolysis cells use iridium, one of the scarcest elements on earth, as catalyst for the oxygen evolution reaction. In the present study, the expected iridium demand and potential bottlenecks in the realization of PEMWE for hydrogen production in the targeted GW a⁻¹ scale are assessed in a model built on three pillars: (i) an in-depth analysis of iridium reserves and mine production, (ii) technical prospects for the optimization of PEM water electrolyzers, and (iii) PEMWE installation rates for a market ramp-up and maturation model covering 50 years. As a main result, two necessary preconditions have been identified to meet the immense future iridium demand: first, the dramatic reduction of iridium catalyst loading in PEM electrolysis cells and second, the development of a recycling infrastructure for iridium catalysts with technical end-of-life recycling rates of at least 90%.

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Introduction

As a universal energy carrier, hydrogen from water electrolysis is regarded as the key element in future sustainable energy systems. Currently, there is a rapid development towards a hydrogen economy based on large-scale water electrolysis. When electrical energy from renewable sources is used for electrolysis, the resulting green hydrogen is potentially free of greenhouse gas emissions. Three electrolysis technologies are regarded for green hydrogen generation: proton exchange membrane water electrolysis (PEMWE) and alkaline water electrolysis (AWE) in the low temperature range and solid oxide electrolysis (SOE) in the high temperature range [1].

The present study focuses on the well-established PEMWE, using iridium catalysts. While the decrease of catalyst loading for economic reasons is already under investigation, the present analysis provides the first feasibility-study published on iridium supply and demand for a large-scale PEMWE industry. The study deals with more robust data on the availability of iridium beyond the relatively meaningless scarcity. The context of primary and secondary mine production of platinum group metals is assessed with its socio-economic indications affecting the realization of large-scale PEMWE. The quantitative analysis is completed by considering iridium as a secondary raw material from an effective technical catalyst recycling.

PEMWE offers the most promising prospects for large-scale hydrogen generation due to its wide operational range of current densities, i.e. a high turndown-ratio, excellent dynamic response and the possibility to operate at significant differential pressure [2–5]. In PEM water electrolyzers, on the anode iridium serves as a catalyst for the oxygen evolution reaction due to its good trade-off between activity and stability [6,7]. On the cathode, platinum based catalysts are used for the hydrogen evolution reaction. However, iridium as a platinum group metal (PGM) belongs to the scarcest elements on earth. Considering a targeted and rapid industrialization of PEMWE in a reasonable mix with AWE and SOE raises the following questions:

- How much is the specific iridium demand of state-of-theart and future PEM water electrolyzers?
- What would reasonable installation rates of PEMWE look like?
- Does iridium demand cause potential bottlenecks in the realization of large-scale PEMWE?
- Can the iridium demand be satisfied by mining or recycling?

Before answering these questions, the reader is introduced to the context of the critical element iridium in an in-depth analysis of global iridium demand, production and recycling. The first question is addressed by the technology specific iridium demand model for PEMWE. The second question is addressed by the market model, covering market launch, ramp-up und maturation phase of industrial-scale PEMWE, proposing specific installation rates for the period of 2020—2070. In order to answer

the third question, the two models are integrated to enable the calculation of iridium demands along the temporal development of proposed PEMWE installation rates. The fourth and final question is addressed in the scenario analysis. Four scenarios are defined to evaluate the effects of a reduced catalyst loading and a closed-loop recycling of catalyst on total iridium demand for PEMWE in the market model.

Ultimately, this work is intended to provide scientists and decision-makers working along the iridium, or water electrolysis, or even hydrogen value chain with facts and perspectives that go beyond the often-used and less meaningful scarcity of iridium in order to better understand and overcome the associated challenges.

Considerations on global iridium production

First of all, a comprehensive overview of global iridium demand, production and recycling is provided in order to introduce the reader to the context of the critical element iridium.

Iridium scarcity and deposits

Iridium (Ir) is one of the scarcest elements on earth with a low occurrence of only 0.000003 parts per million in the earth's crust. Until today iridium is considered as a secondary mining metal, i.e. its mining production depends on the production rate of primary metals. As iridium is a PGM it is a co-product in platinum (Pt) and palladium (Pd) mine production. There is a strong geographical concentration of PGM deposits in five countries: South Africa, Russia, United States, Zimbabwe and Canada. Of these, South Africa is the dominant producer of platinum (92%) and a major producer of palladium (37%) together with Russia (40%) [8,9]. Subsequently, there is a concentration of iridium production in South Africa with 70% of the global market.

Due to the very small iridium market of below 10 t, there is no data available explicitly on iridium production before 2014, but on iridium demand. Iridium mine production before 2014 has to be derived from PGM production data. In general, available data on PGMs used here comes primarily from three sources: United States Geological Survey (USGS), Johnson Matthey and the World Platinum Investment Council (WPIC).

Iridium demand

The global iridium demand is highly volatile showing an increasing trend in the last decade as illustrated in Fig. 1(a). The significant increase in 2010 is induced by an exceptional growing demand for LED screens. Thus, a heavy stockpiling of iridium crucibles for electronic applications appeared in 2010 and 2011. At the same time the iridium demand in electrochemical applications is relatively stable at around 2 t a $^{-1}$. For detailed background information on historic market development please consider the source of data [10].

Similar to iridium, the availability and demand of platinum is an increasingly important issue. However, its increasing demand is not only, nor even mainly, driven by PEMWE, but

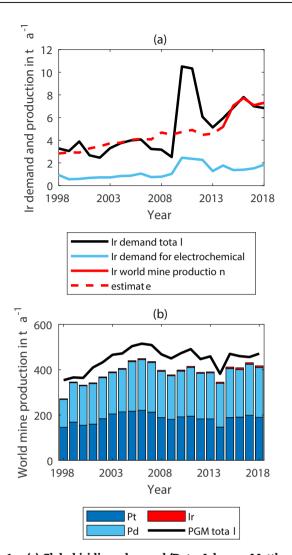


Fig. 1 - (a) Global iridium demand (Data: Johnson Matthey) and annual iridium mine production based on (b) annual mine production of PGM in total, i.e. platinum, palladium, iridium and others (Data: USGS [14]).

rather by the increasing demand for internal combustion engines and related demand for exhaust gas catalysts as well as for fuel cells and jewelry [8,9]. Iridium and platinum demands are therefore not directly coupled, but mining production is, as discussed in subsequent sections.

PGM mine production

The overall data situation on the mine production of iridium is insufficient due to the situation described above. PGM data on annual world production is provided by the USGS. They provide data on platinum and palladium world production between 1990 and 2018 in the mineral commodity summaries [11]. Aggregated data on total PGM world production is provided from 1990 to 2018 in the minerals yearbook series [12]. The USGS data from 1998 to 2018 is plotted in Fig. 1(b) showing a steady increase in PGM production until 2005 and a relatively stable level since then. The average value of around 470 t of

annual PGM production in the last 15 years corresponds to an average of about 200 t of platinum and palladium production each.

Iridium mine production

Explicit data on iridium mine production is available only from 2014 to 2018 in the recent USGS minerals yearbook [13]. In addition, a global iridium production of 4 t in 2007 is documented in literature [14]. The iridium content in PGM production varies in every mineral deposit and is on average approximately 1% [15,16]. Considering these figures, an annual iridium world production for the remaining period can be derived from the data on PGM mine production. The estimated iridium production in the period of 1990–2013 is in the range of 2.2–4.9 t. From 2014 USGS data documents a global annual iridium production of 5.2–7.7 t (Fig. 1).

Iridium recycling rate

The current global end-of-life (EOL) recycling rate of iridium can be assumed with 20-30%. However, in industrial applications including electrochemical processes a EOL recycling rate of 40-50% is already achieved [17]. Considering state of the art EOL recycling rates of platinum and palladium catalysts exceeding 90%, a target figure of R = 90% EOL recycling rate for iridium in PEMWE applications is assumed in the presented model [18]. It is reasonable to imply, that an infrastructure for a closed-loop recycling of iridium catalyst is built up in parallel within the industrialization phase of PEMWE manufacturing.

Projections on future mine production

In general, the derivation of any future scenarios for raw material mining is accompanied by a high degree of uncertainties. In the specific case of iridium, an insufficient data pool matches the current historic GOVID-19 pandemic crisis. The potential impact of socio-economic uncertainties on raw material exploration and production in South Africa is very difficult to assess.

Any projections on iridium production are primarily derived from considerations on the economically important PGM platinum, as described above. In a most recent statement, WPIC describe a significant fall in platinum production and demand dominated by impacts of the COVID-19 pandemic. Accordingly, for 2020 the demand is expected to be 10% below the average of the last five years and the production in analogy 10% below [19]. Currently, there is no indication on when the market will recover and grow again.

Considering PGM reserves in the earth's crust of 69,000 t in total and 63,000 t of those in South Africa, the security of supply is primarily a question of mining activities [11]. Material reserves refers to the quantity to be extracted economically at present. On the other hand, material resources, however, means currently known deposits. Usually both values grow over time (neglecting mining) as new deposits are explored and resources are converted into reserves due to cheaper mining production technologies and/or increased raw material prices. The static range of PGM is 172 years based

on the reserves and annual world production in 2019. However, potential increasing efforts to explore new mines in South Africa would require an escalation exceeding 20–25% in platinum prices [20]. According to expert opinion, the exploration of a new mine would take six to ten years in this context

In the presented model, an iridium production according to the average level of the last five years is assumed for projections on 2020 to 2070. Considering the great uncertainties and the long period, all subsequent considerations are based on a constant annual world production rate of 7 t a $^{-1}$ iridium.

Modeling iridium demand for large-scale PEM water electrolysis

The present study is structured in three modeling steps. First, the specific iridium demand model for PEMWE is provided. It is based on technical assumptions for the PEM water electrolyzer. Second, the market model with projected installation rates for industrial-scale PEMWE covering a period of 50 years is described. Third, in order to be able to discuss results in a balanced way, four scenarios are defined: two conservative scenarios with and without iridium recycling and two innovative scenarios with and without iridium recycling.

Technology specific iridium demand model for PEMWE

The technology specific iridium demand model for PEMWE is based on technical assumptions for the PEM water electrolyzer aggregated in Table 1. Data is structured in three data sets: '2020 status', '2020 target' and '2035 target' figures.

System energy efficiency

In accordance with technical targets for hydrogen production from electrolysis by the United States Department of Energy (DOE), system energy efficiency is based on a lower heating value (LHV) basis (Eq. (1)) [21].

$$\eta_{\text{LHV}} = \text{LHV}_{\text{H2}} \cdot e_{\text{el}}^{-1} \tag{1}$$

Therein, $\eta_{\rm LHV}$ is the PEMWE system energy efficiency and $e_{\rm el}$ is the specific electric energy input for the production of 1 kg H_2 .

Considering a relatively high specific energy demand of $47.7 \text{ kWh} (kg_{H2})^{-1}$ results in an overall energy efficiency of 70% (2020 status). A lower specific energy demand of 44.7 kWh

Table 1 $-$ Technical data for PEM water electrolyzers.				
Parameter	Unit	2020 status	2020 target	2035 target
System energy efficiency	_	0.70	0.75 ^a	0.75 ^a
·	$kWh (kg_{H2})^{-1}$	47.7	44.7 ^{a,b}	44.7 ^{a,b}
Ir loading	mg cm ⁻²	2.00 ^{c,d}	1.00 ^c	$0.40^{ m d,e}$
Ir loading	$\mathrm{g}\ \mathrm{kW}^{-1}$	0.67 ^d	0.33	0.05 ^d
Power density	${ m W~cm^{-2}}$	3^{d}	3^{d}	8^{d}
Current density	${\rm A~cm^{-2}}$	2^{d}	2 ^d	$3^{\rm d}$
References: ^a [21]; ^b [22]; ^c [23]; ^d [24]; ^e [25].				

 $(kg_{H2})^{-1}$ results to an increased energy efficiency of 75%, which is the target figure for the years 2020 and 2035, respectively (Table 1).

Iridium catalyst loading

Current state of the art iridium loading is about $1-2 \text{ mg cm}^{-2}$, normalized to the geometrical (active) area [4,23], but there are already several research efforts to reduce this value significantly by more than one order of magnitude [25–29]. In order to correlate iridium catalyst loading and PEMWE installation rates in the present study, the catalyst loading L is expressed in grams per kilowatt of nominal power of the electrolyzer. Basic assumptions listed in Table 1 are cited from literature [23–25].

The '2020 status' figure is a catalyst loading of 0.67 g kW $^{-1}$ based on a loading of 2 mg cm $^{-2}$ at a power density of 3 W cm $^{-2}$ and a current density of 2 A cm $^{-2}$. The '2020 target' assumption is an iridium catalyst loading of 0.33 g kW $^{-1}$ based on a loading of 1 mg cm $^{-2}$ at a power density of 3 W cm $^{-2}$ and a current density of 2 A cm $^{-2}$. The '2035 target' figures comprise a reduction of the iridium loading to 0.4 mg cm $^{-2}$ at an increased power density of 8 W cm $^{-2}$ and current density of 3 A cm $^{-2}$. This leads to a power specific iridium loading of 0.05 g kW $^{-1}$.

System lifetime

The system lifetime of a PEM water electrolyzer is assumed to be T=20 years, based on expert interviews, in accordance with the detailed analysis on cycle and calendrical lifetime provided in a recent study [24].

Calculation of technology specific iridium demand

The technology specific iridium demand for PEMWE *m* can be calculated from the above described data basis as the product of the nominal power of the PEM water electrolyzer *P* and the catalyst loading *L* (Eq. (2)).

$$m = P \cdot L$$
 (2)

Market model for PEMWE

The market model describes a temporal development path with projected installation rates for industrial-scale PEMWE from 2020 to 2070. Data and basic assumptions are cited from a recent national study on industrialization of water electrolysis in Germany providing projections for the period of 2020-2050 [24]. That study is based on a comprehensive model for the transformation of the German energy system (Energy system model REMod-D by Fraunhofer ISE) [30]. The installation figures for water electrolysis are based on a target of 85% CO2 reduction by 2050. One basic assumption of the model is a technology mix of 40% PEMWE, 40% AWE and 20% SOE. These data and assumptions are generalized to a global, location-independent market model applicable to hydrogen economy in general. In the context of the present work, the period under consideration was also extended to 50 years (2020-2070) in order to be able to cover the topic of EOL and recycling.

The model, illustrated in Fig. 2, covers three market phases for large-scale PEMWE: market launch (2020), ramp-up (2020–2040) and maturation (2041–2070). The annual gross

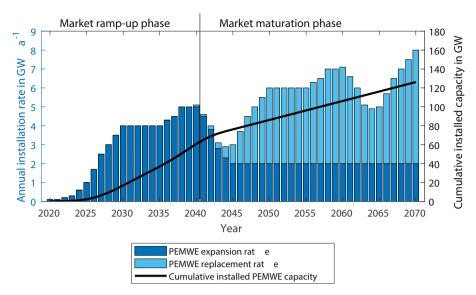


Fig. 2 — Market model with installation rates for PEMWE (bar chart) and cumulative installed capacity (line chart) considering 20 years of system lifetime (Data [24]).

installation rates in GW $\rm a^{-1}$ consist of expansion rates (or net additional installation rates, blue bars) and replacement rates (cyan bars) for PEMWE capacity reaching EOL after 20 years of system lifetime. The cumulative installed capacity is 61 GW by 2045 and 126 GW by 2070, showing a linear growth from 2045 (Eq. (5)). The projected development of PEMWE installed capacity is plotted in Fig. 2 (line chart).

Definition of PEMWE expansion rate

From the detailed scenario analysis in the study cited [24] the following figures are extracted in the present study for projections of annual target expansion rates of PEMWE: 0.1 GW a^{-1} in 2020, 1 GW a^{-1} in 2025, 4 GW a^{-1} in 2030 and a peak with 5 GW a^{-1} in 2040 followed by a decrease to 2 GW a^{-1} in 2045. In the present study a constant expansion rate of 2 GW a^{-1} is considered from 2045 to 2070 as no further external forecasts are available for this period yet. The expansion rate $\dot{P}_{ad,k}$ in GW a^{-1} is defined as the annual net additional installation (Fig. 2, blue bars). Therein, index k stands for any year in the considered period of 2020–2070.

Definition of PEMWE installation rate

Installation rates for PEMWE \dot{P}_k are modeled for a period from 2020 to 2070. A system lifetime of T=20 years is considered. Thus, some of the summarized installed capacity is dismantled from 2040 onwards. This amount is rebuilt in order to maintain the overall capacity. The corresponding annual replacement rate $\dot{P}_{re,k}$ in GW a⁻¹ for considered years k and lifetime T=20 years is defined by Eq. (3) (Fig. 2, cyan bars).

$$\dot{P}_{re,k} = \dot{P}_{(k-T)}$$
 for $k - T \ge 2020$ (3)

In total, the annual gross installation rate \dot{P}_k in GW a^{-1} is defined as the sum of annual expansion rate (or net installation

rate) and annual replacement rate (Eq. (4) and Fig. 2, stacked bars).

$$\dot{P}_k = \dot{P}_{ad,k} + \dot{P}_{re,k} \tag{4}$$

The above described market model and input data result in a cumulative installed PEMWE capacity P_n in GW for a considered period of years (Fig. 2, line chart):

$$P_n = \sum_{k=2020}^{n} \dot{P}_k \text{ for } 2020 \le n \le 2070$$
 (5)

Scenario analysis

In the final step, four scenarios are defined in order to integrate the above described technology specific iridium demand model and the market model for PEMWE. This method enables the calculation of annual iridium demands according to varying annual installation rates, as well as cumulative iridium demands for specific market phases.

The four scenarios are defined in a 2×2 matrix approach (Table 2): the scenarios differ either in the technical data set for the PEM water electrolyzer (conservative or innovative), or in the source of iridium supply. The iridium demand may be covered by mining production only, or partly by additional closed-loop recycling of iridium catalyst.

First, the conservative and innovative data sets are defined. Then, formulas for the calculation of iridium demand for PEMWE without and with consideration of closed-loop recycling are provided.

Definition of the conservative scenarios

The conservative scenarios are based on the technical dataset for the PEM water electrolyzer labeled '2020 target' figures provided in Table 1. These data are applied for the entire modeled

Table 2 — Definition of scenarios.					
	Primary Ir from mining production	Primary Ir from mining production and secondary Ir from closed-loop catalyst recycling			
Ir catalyst loading of $0.33 \ g \ kW^{-1}$ from 2020 to 2070	Conservative scenario	Conservative scenario with recycling			
Ir catalyst loading of 0.33 g kW^{-1} from 2020 reduced to 0.05 g kW^{-1} by 2035	Innovative scenario	Innovative scenario with recycling			

period from 2020 to 2070. In particular, a constant iridium catalyst loading of $L_k = 0.33 \text{ g kW}^{-1}$ is assumed.

Definition of the innovative scenarios

For the innovative scenarios, the '2020 target' figures on PEM water electrolyzers from Table 1 are applied for the period from 2020 to 2034. A technological leap is assumed for 2035 leading to a dramatically reduced catalyst demand. Thus, '2035 target' data from Table 1 are applied for the subsequent period from 2035 to 2070. In particular, the iridium catalyst loading L_k is reduced from 0.33 g kW⁻¹ to 0.05 g kW⁻¹ by k = 2035.

Calculation of annual iridium demand for PEMWE

In the scenario analysis, the technology specific iridium demand model (Eq. (2)) is applied in the market model. For every year k in the considered period from 2020 to 2070 there is a fix assigned PEMWE installation rate \dot{P}_k in GW a^{-1} (Eq. (4)). The corresponding iridium demand \dot{m}_k in t a^{-1} varies dependent on the installation rate. The resulting iridium demand for PEMWE in the year k is defined as the product of the annual installation rate \dot{P}_k and the iridium catalyst loading L_k :

$$\dot{m}_k = \dot{P}_k \cdot L_k \tag{6}$$

Calculation of cumulative iridium demand for PEMWE The cumulative iridium demand for the modeled PEMWE market m_n is the sum of annual iridium demands from 2020 to considered year n:

$$m_n = \sum_{k=2020}^n \dot{m}_k$$
 for $2020 \le n \le 2070$ (7)

Calculation of annual amount of iridium recycling material The annual amount of secondary iridium material from closed-loop recycling of iridium catalyst is a function of system lifetime T and recycling rate R. At the end of system lifetime in year k the same mass flow of iridium that went into the PEM water electrolyzer becomes available for the recycling process $(\dot{m}_{(k-T)})$. For the year k the resulting amount of iridium recycling material $\dot{m}_{\rm rec,k}$ in t a⁻¹ is calculated using Eq. (8).

$$\dot{m}_{\text{rec},k} = \dot{m}_{(k-T)} \cdot R \quad \text{for } k-T \ge 2020$$
 (8)

In accordance with the general idea of the closed-loop recycling approach, this annual mass flow of iridium from recycling $\dot{m}_{\rm rec,k}$ is available to the PEMWE market. In addition to iridium from mining production, this represents a second

material source contributing to meet the iridium demand calculated in Eq. (6).

Calculation of cumulative iridium demand with catalyst recycling

In the presented approach, the closed-loop recycling of iridium catalyst leads to a decreased demand for iridium from external sources (mining production) for the considered PEMWE market. Thus, the resulting cumulative iridium demand considering closed-loop recycling m_n from 2020 to considered year n is calculated using Eq. (9).

$$m_n = \sum_{k=2020}^{n} \left(\dot{m}_k - \dot{m}_{\text{rec},k} \right)$$
 for empty stock (9)

Results and discussion

Technology specific iridium demand for PEMWE

The technology specific iridium demand model for PEMWE is based on technical assumptions for the PEM water electrolyzer: system energy efficiency, iridium catalyst loading, power density and system lifetime. Literature data and estimates are aggregated in Table 1 structured in three data sets: '2020 status', '2020 target' and '2035 target' figures.

The technology specific iridium demand for PEMWE is the product of iridium catalyst loading (x-axis) and PEMWE power capacity (y-axis), represented as a colormap in Fig. 3. The contour lines represent levels of resulting iridium demand in tons. The selected value range corresponds to the figures for the market model, which is discussed in subsequent sections.

Results for specific catalyst loadings from Table 1 are highlighted in Fig. 3 with white dashed lines: $0.67~\rm g~kW^{-1}$ (2020 status), $0.33~\rm g~kW^{-1}$ (2020 target) and $0.05~\rm g~kW^{-1}$ (2035 target). Results illustrate clearly, that a significant reduction of catalyst loading is required in order to enable large-scale industrial PEMWE capacity. The '2020 status' and '2020 target' assumptions result in material requirements of tons of iridium for some gigawatts of PEMWE capacity.

Iridium demand in the PEMWE market model

The results from integrating the technology specific demand model (Eq. (2)) in the market model (Eq. (6)) can also be discussed in Fig. 3. The subsequent theoretical considerations are based on a fix iridium catalyst loading represented by the

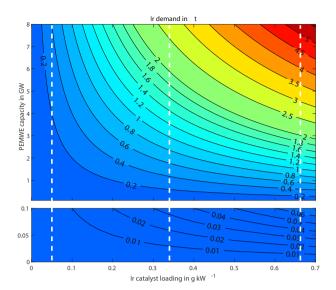


Fig. 3 – Results of technology specific demand model. Iridium demand (contour lines in colormap) resulting from catalyst loading and PEMWE capacity on a small industrial scale (0–0.1 GW on interrupted y-axis) and a large industrial scale (0.1–8 GW on interrupted y-axis). Indicated catalyst loadings of 0.67 g kW $^{-1}$ (2020 status), 0.33 g kW $^{-1}$ (2020 target) and 0.05 g kW $^{-1}$ (2035 target).

white dashed lines. Then, each pair of values for PEMWE capacity and iridium demand in the colormap is identified for one specific year following the temporal development of installation rates.

The calculated iridium demand for the market launch of industrial-scale is based on the assumption of a necessary annual production volume of 20–50 MW a⁻¹ per manufacturer in 2020 [24]. An iridium catalyst loading of 0.67 g kW^{-1} (2020) status, Table 1) is assumed. Consequently, the initial total installation rate of 100 MW in 2020 requires an amount of 67 kg of iridium (Fig. 3). The iridium demand for the market launch is equivalent to 1% of the global annual mine production. In the market ramp-up phase, installation rates increase to 5 GW a⁻¹ within 20 years. Thus, the annual iridium demand increases to 3.35 t a⁻¹, which is about half of the estimated global annual iridium mining production for this single market. In the subsequent phase of market maturation, gross installation rates reach up to 8 GW a⁻¹. The corresponding required iridium catalyst demand is 5.36 t a⁻¹. These results emphasize the need for a significant reduction of iridium catalyst loading in PEM water electrolyzers.

The PEMWE market model can reasonably be evaluated on the basis of the '2020 target' figure of 0.33 g kW $^{-1}$ (Table 1). Thus, a market launch with 100 MW of PEMWE capacity requires 33 kg of iridium (Fig. 3). The maximum PEMWE installation rate of 5 GW a-1 in the market ramp-up phase requires 1.65 t a $^{-1}$ of iridium catalyst, representing about 24% of the estimated global annual iridium mining production. Considering the analysis of iridium production provided in previous sections, meeting this demand seems hardly feasible. Finally, gross installation rates for PEMWE grow further in the market

maturation phase after 2040. The peak rate of 8 GW a^{-1} results in an immense iridium demand of 2.64 t a^{-1} .

The '2035 target' figure for iridium catalyst loading in PEMWE is 0.05 g kW $^{-1}$ (Table 1). The effects of a significantly reduced catalyst loading may be analyzed in a simulation of the market model using this value. In Fig. 3 the results are illustrated in form of the white dashed line at 0.05 g kW $^{-1}$. It is obvious that the value of 0.4 t a $^{-1}$ of iridium demand for a maximum PEMWE installation rate of 8 GW a $^{-1}$ is not exceeded. This represents less than 6% of the estimated global annual iridium mining production, which is still a significant proportion for the proposed PEMWE market alone.

Scenario analysis

The effects of a reduced iridium catalyst loading and a closed-loop recycling of catalyst on total iridium demand for PEMWE in the presented market model are evaluated in four scenarios. Results are plotted and discussed in Fig. 4.

The resulting iridium demand in the market model for PEMWE is primarily dependent on the development of research on iridium catalyst loading which is expressed in the conservative and innovative scenarios. Results from the conservative scenarios are illustrated in Fig. 4(a), those of the innovative scenarios in Fig. 4(b).

Iridium demand and recycling in conservative scenarios Fig. 4(a) illustrates the annual iridium demand (Eq. (6)) considering the '2020 target' iridium loading of 0.33 g kW $^{-1}$ for the whole period of 2020–2070. In the market ramp-up phase (2020–2040) a maximum of 1.7 t a $^{-1}$ is reached in 2040 (blue bars). In the subsequent market maturation, the volatile, but increasing iridium demand is between 1.0 t a $^{-1}$ and 2.6 t a $^{-1}$. These figures result in the depicted cumulative iridium demand (Eq. (7)) for PEMWE industry of 20 t by 2040 and more than 75 t by 2070 (solid black line).

Two strategies to reduce this immense iridium demand from primary sources, which are very limited due to the above described situation, are outlined as follows:

- the installation of an effective recycling industry for iridium catalysts
- and a significant reduction of the iridium catalyst loading in PEMWE cells.

System lifetime and EOL recycling rate of iridium catalyst affect the production rate of iridium from primary and secondary sources for this application. In further considerations, secondary material is iridium from a closed-loop recycling of PEMWE cells. With an assumed EOL recycling rate of 90% the iridium purchased for this application can be re-used with low material losses (Eq. (8)). Assuming a system lifetime of 20 years makes secondary iridium available from 2040 onwards. However, little material will initially be available for recycling, as reasonable low installation rates are assumed for the market launch. By 2045 the annual amount of secondary iridium has the potential to flatten the curve for iridium demand from external sources significantly. The availability of closed-loop recycling material is illustrated in Fig. 4(a) in cyan bars.

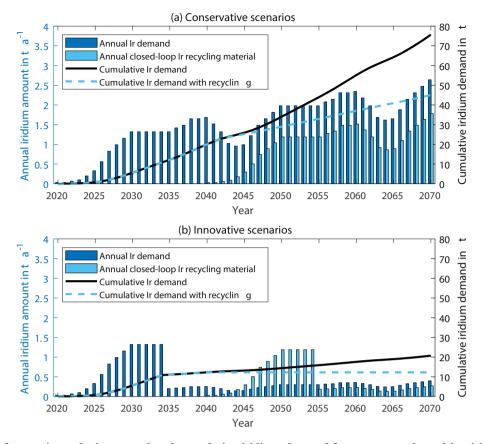


Fig. 4 – Results of scenario analysis. Annual and cumulative iridium demand for PEMWE and resulting iridium demand from external sources when considering the use of available closed-loop recycling material: (a) conservative scenarios with iridium catalyst loading of 0.33 g kW $^{-1}$; (b) innovative scenarios with initial iridium catalyst loading of 0.33 g kW $^{-1}$ reduced to 0.05 g kW $^{-1}$ by 2035.

The resulting total iridium demand on the basis of a functional PEMWE recycling industry (Eq. (9)) can be reduced to 45 t by 2070 (dashed cyan line). Thus, recycling leads to a reduction in iridium demand of -40% compared to the initial calculation. Nevertheless, this scenario still reveals an immense amount of iridium combined with a clear increase in material requirements.

Iridium demand and recycling in innovative scenarios. The need for a reduction of iridium catalyst loading in PEMWE has been emphasized in previous sections. In the innovative scenarios a significantly reduced catalyst loading of 0.05 g kW $^{-1}$ by 2035 is assumed. Resulting iridium demand with and without considering recycling are illustrated in Fig. 4(b). The maximum annual iridium demand (Eq. (6)) is 1.3 t a $^{-1}$ in the period of 2030–2034 (blue bars). After the technological leap to a lower iridium loading, a volatile annual demand with a moderate increase is expected in a range of 0.25–0.40 t a $^{-1}$.

The resulting total iridium demand (Eq. (7)) in order to realize a PEMWE industry according to the market model would be 21 t by 2070 (solid black line). In the innovative scenarios, the final cumulative iridium demand for PEMWE is reduced by -72% compared to the conservative scenario with

iridium mine production only as an effect of significantly decreased catalyst loading.

Nevertheless, the results imply that it would be difficult to meet even this demand from primary sources. Therefore, the closed-loop recycling approach introduced above is applied to the second innovative scenario, analogously. The annual amounts of recycling material (Eq. (8)) exceed the annual iridium demands in the period of 2044–2054 significantly, following the curve of the ambitious market ramp-up phase. From 2055, the annual amount of recycling material covers on average 64% of the iridium demand in each subsequent year (cyan bars).

How much iridium is thus required in total in this scenario? Following the idea of closed-loop recycling, it is reasonable to assume that the surplus recycling material of the decade 2044 to 2054 is kept in stock for later use. The cumulative iridium demand on the basis of a functional PEMWE recycling industry (Eq. (9)) results to a maximum of 12.7 t by 2043 (dashed cyan line). This advanced scenario leads to a dramatic reduction in iridium demand of –83% compared to the initial calculation of the conservative scenario without recycling. Moreover, the summarized iridium amount is already purchased by 2043 and kept in the system. Please note, that this is a simplified approach towards consideration

of a closed material cycle for the critical element iridium in PEMWE. Detailed socio-economic aspects, e.g. business models, go beyond the scope of the present technical feasibility study.

To conclude, two effects are illustrated in the scenario analysis: the implementation of an effective closed-loop recycling system leads to a significant decrease of the gradient of iridium demand over time, while a reduction of the catalyst loading in PEMWE cells lowers the overall level of material demand. Only the combination of both effects may lead to a feasible market entry and maturation scenario for PEMWE.

Conclusions

The present study covers the iridium demand and potential bottlenecks in the realization of PEM water electrolysis for large-scale hydrogen production. The initial questions raised in the introduction are answered as follows:

- A technology specific iridium demand model is provided for PEMWE. Graphical model results clearly illustrate the impact of catalyst loading on the iridium demand for PEMWE.
- A detailed model of a market launch, ramp-up and maturation phase in a near future period of 50 years starting in 2020 is provided on the basis of literature data [24]. PEMWE installation rates are defined as the sum of expansion rates and replacement rates. Thus, after 25 years an installed capacity of 61 GW is realized with subsequent linear growth of 2 GW a⁻¹ installed capacity.
- Considering the historic and current market development
 of PGMs indicates that the iridium demand for PEMWE cells
 is a bottleneck in the realization of a mature market. The
 analysis reveals that a significant proportion of global
 iridium mine production would be required to meet the
 demand for the PEMWE market alone.
- The bottleneck is clearly not induced by the static range of this critical metal, which is 172 years for PGMs, but by the geographical and socio-economic preconditions in exploration and mining.
- The iridium demand for a mature PEMWE market cannot be covered from mine production with current production rates of approximately 7 t a⁻¹. This is due to the scarcity of the element, its geographical concentration in South Africa and coupling of its production rate to the primary PGMs, e. g. platinum and palladium.
- The iridium catalyst loading in PEMWE cells has to be reduced significantly within the next 15 years to e.g. a target loading of 0.05 g kW^{-1} by 2035.
- Two preconditions are necessary to cover the immense future iridium demand for a large-scale PEMWE industry: first, the dramatic reduction of iridium catalyst loading in PEMWE cells and second, the development of an effective recycling infrastructure for iridium catalysts with technical EOL recycling rates of minimum 90% in parallel with the realization of industrial scale PEMWE manufacturing.

 Following these recommendations leads to an ambitious, but feasible scenario with a summarized iridium demand of 13 t, to be provided within 24 years, covering the whole considered market ramp-up and maturation phase of 50 years.

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.

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Nomenclature

Acronyms

AWE Alkaline water electrolysis

DOE United States Department of Energy

EOL End-of-life Ir Iridium

LHV Lower heating value

PEM Proton exchange membrane

PEMWE Proton exchange membrane water electrolysis

PGM Platinum group metal

Pt Platinum Pd Palladium

SOE Solid oxide electrolysis
USGS Unites States Geological Survey
WPIC World Platinum Investment Council

Symbols

 $e_{\rm el}$ Specific electric energy input for the production of 1 kg H₂, kWh (kg_{H2})⁻¹

L Power specific iridium catalyst loading, g kW^{-1}

L_k Power specific iridium catalyst loading in year k, g

 kW^{-1}

m Mass of iridium required, t

 m_n Cumulative mass of iridium required in year n, t m_n Cumulative mass of iridium required in year n

considering closed-loop recycling, t \dot{m}_k Mass flow of iridium required in year k, t a⁻¹

 $\dot{m}_{\mathrm{rec},k}$ Mass flow of recycled iridium material available in

year k, $t a^{-1}$

P Nominal power of PEM water electrolyzer(s), GW P_n Cumulative installed PEMWE capacity in year n, GW

 \dot{P}_k PEMWE gross installation rate in year k, GW a⁻¹

 $\dot{P}_{ad,k}$ PEMWE expansion rate (or net additional installation

rate) in year k, GW a^{-1}

 $\dot{P}_{re,k}$ PEMWE replacement rate in year k, GW a⁻¹

R Recycling rate for iridium catalyst

- T PEMWE system lifetime, a
- η PEMWE system energy efficiency

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