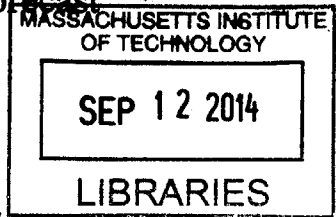


A Bottom-Up Prospective Dynamic Materials Flow Assessment  
for Platinum Group Metals (PGM) Global Demand Forecast

ARCHIVES



By

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It was a lurid afternoon, when I was holding a pot to polish a sample in a humming, lifeless machine-shop, trying to thin it down to a couple of nanometers that I decided to take arms against a sea of troubles, and by opposing – end them. Over the past two months I had finished listening to an excellent episode of 36 talks on the life of the world-renown empress – Wu Zetian (武則天). Yes, when the world was shaped by the masterful hands of an imperial maid, I was polishing tens of hopeless samples that virtually produce nothing for humanity. I asked myself – did you come to this hallowed spot to be a feeling-less technician? A voice screamed from the bottom of my heart – NO!

However, regardless of the incredible barrier of transitioning from engineering to anything related with social science, where will be a place with proper social scientific work for an engineer who knows little else than thermodynamics and kinetics? After sending out dozens of emails to almost every professor or research scientist in Harvard or MIT whose research I have interest in, I was at the verge of collapse. At this most critical moment, Angelita suggested – why don't you check out Prof. Clark's group? It seems they do a lot of work related with materials economics. I could not believe my own eyes when I saw how wonderfully the Materials Systems Lab has research that integrates what I had with who I wanted to be. I passionately sent out an email with all the enthusiasm a mortal can possibly muster, Prof. Clark and Dr. Kirchain replied me the very second day – and I knew my life would never be

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## 1. Introduction

Given the appallingly rapid consumption of exhaustible resources and an increasing awareness of the necessity of sustainable development, the study of exhaustible resources is a field that attracts more and more attention from various disciplines. It largely targets at two different but intricately correlated sets of questions. One set of the question relates with exhaustible resources in the context of long-term social welfare and sustainable development; the other set mainly deals with how exhaustible resources influence short-term industrial activities and how should manufacturers, governmental agencies, and firms in other industries adapt to uncertainties unavoidably embedded in the short-term business cycle, and respond with rationality and optimality.

The first set of questions include: what is the optimal growth path for a society that is subject to limited amount of resources and what should be the corresponding depletion and consumption rate of these resources; how are the prices of natural resources determined across the time domain, and what are the prices composed of; how to satisfy the demand of the current generation without compromising the welfare of our posterity; how should we respond to a gradually diminishing reserve of exhaustible resources, and how can we maintain a sustainable growth when the resources are depleted.

The second set of questions include: what is the price of a certain exhaustible resource likely to be in the near future; what are some of the factors that may throw the price of a certain resource off the optimal price trajectory, if there is any; what are

the most likely uncertainty contributors in a particular industrial context, and how should we deal with such uncertainties to minimize our losses, or even take advantage of such uncertainties; how will evolving market structures alter the behavior of individual players in that market, and how will such change of behavior change the dynamic equilibrium of relevant industries thereof; what technological progresses are likely to be made in the future, and if there are functionally substitutable resources of lower costs and are more accessible.

Two mainstream approaches of tackling the aforementioned problems and more broadly, the questions of resource availability, will be discussed in this work, and a detailed comparison of their strengths and weaknesses will be made. After obtaining an in-depth understanding of the state-of-the-art approaches, the author will propose a modeling approach that he believes inherits the strengths of both mainstream approaches, while at the same time ameliorates some of the current deficiencies in both approaches. Admittedly, a model is simply a way of representing the real world in a simplified and abstract way; any modeling technique has its strength and weakness, and the author's approach is not immune to this iron-clad rule. It strives to provide as clearly and accurately a picture as possible of the global demand of a set of minerals critical for emission control – platinum group metals (PGM) in the next two decades, and the author is eager to witness a most treasured evaluation made possible only by the omnipotent hands of time. The modeling method, a bottom-up prospective dynamic materials flow assessment proposed in this thesis endeavors to acquire a macroscopic prediction with a strong and robust micro-foundation, and at the same

time provides full flexibility to conduct various scenario assessments based on needs and circumstances. It largely deals with the second set of questions, namely its initial intent is to provide a roadmap to relevant firms to acquire a deeper understanding of the PGM market and to make more informed decisions when facing uncertainties. However, an extension of the time horizon and slight modifications to adapt the model to other industries may make it possible to address some of the first set questions with more specificity and accuracy.

The general structure of the thesis can be divided into five segments. Chapter two provides a detailed assessment and comparison of two mainstream approaches, namely the resource economics approach and the materials flow assessment. Chapter three lays out the methodology of the model that the author has constructed, and provides some concrete examples at places where the author believes might be somewhat abstract. Chapter four exhibits the results generated by utilizing the said model, and provide a holistic evaluation and discussion of the results. Apart from the Base Case, it showcases a large set of scenario analyses that demonstrates the flexibility and complexity of the model. Among the scenario analyses are: five cases of different Pt/Pd price ratios, one case of increasingly tightening emission regulation that cannot be entirely offset by increasing the efficiency of the PGM, the High Diesel Case (where the diesel vehicle annual sales is assumed to increase at the expense of gasoline vehicle sales), and the Alternative Technology Vehicle Case (where first the electric vehicle, and then the fuel cell vehicle annual sale is assumed to increase at the expense of the sales of conventional vehicle). Chapter five summarizes the previous



chapters, recaptures the most prevailing methodologies in analysis of exhaustible natural resources and their respective strengths and weaknesses, reiterates the significance of the modeling approach proposed in this thesis along with some key results provided by the model, and attempts to offer insights regarding future work that may be undertaken to build on and perfect the modeling approach described in this thesis.

## 2. Existing Approaches to the Study of Natural Resources

### 2.1. Introduction

The unprecedentedly rapid growth of consumption of non-renewable resources over the past two centuries has taxed every fiber of firms whose business relies heavily on these resources, and individuals whose daily life rely on the utilization of products containing these resources. The intellectual arena has spared little effort to resolve, or at least understand this conundrum. In this chapter, I will examine the two main-stream approaches to the study of natural resources, namely resource economics and materials flow assessment (MFA). I will discuss their individual disciplinary goals, and their respective strengths and deficiencies. This discussion will serve as a jumping board to transition into my own study, which, though broadly falls into the category of dynamic materials flow assessment (DMFA), takes into consideration of the deficiencies from both camps, and strives to overcome some of the principal weaknesses of both modeling approaches.

In the long run, going far enough into the future, if one assumes renewable resources and recycling of scrap will not be able to completely replace our profligate consumption of non-renewable resources and the humans fail to reach another planet with a new host of such non-renewable resources, then the physics of limited non-renewable resources seems to be all too clear – these resources are going to be asymptotically depleted someday in the future.[2, 3] This fact is particularly alarming, for it implicates that given the assumptions mentioned above are accepted, the growth economics of our society is not sustainable.[4] Someday in the future, we may not be

able to produce items essential to our daily life. The limited supply of natural resources in the long run has been extensively studied by resource economists.[4-7]

In the short run, the need to carefully plan for the procurement of the necessary materials and to match the resources at hand with anticipated demand in a timely manner while keeping inventory as low as possible but without supply disruption has been a persistent challenge for many manufacturers. The intrinsic volatility in commodity prices, the ever-changing demand pivoted on technological necessity and progress, the potentiality of constrained supply due to limited amount of resources, geopolitical uncertainty, and functionality constraints all contribute to the difficulties of planning. These factors may wreck the well-being of domestic firms and have further impact on the economy as a whole, and the US has spent much effort in providing a better understanding of minerals scarcity to prevent its economy from the risk brought by resource scarcity.[8] Firms whose businesses are at the mercy of varying supply and demand of these exhaustible resources want to know the future supply and demand of the resources of their interest, and materials flow assessment has demonstrated its capability of providing such valuable predictive information.[9, 10]

## **2.2. The Resource Economists' Approach**

### **2.2.1. Pre-modern Period (18~19<sup>th</sup> century)**

The first approach to the resources limitation was undertaken by economists in the 18<sup>th</sup> and 19<sup>th</sup> centuries. Among the most often cited is Thomas R. Malthus. He

investigates the contemporary population boom, and argues such a boom cannot be sustained by a limited amount of arable land, thus predicting a gloomy future with a decrease in food per person, a pessimistic certainty only to be relieved by a prevalent disease or a bloody war.[2] Although Malthus has been criticized for his omission of the technology augmentation factor in his model (methinks unjustly for an individual without supernatural power to foresee the unfolding industrial revolution), his concept of limited resources and its potential implication on human development are nonetheless valuable. A latter economist, David Ricardo, refines the notion of geophysical constraints based on the observation that resources, especially minerals, occur in different levels of quality.[11] In simple terms, Ricardo rightly points out that all ores are not created equal. Ores with the easiest accessibility and best quality are to be first extracted, and ores with lesser grade are accessed after the former resource has been depleted, until the marginal cost of extraction exceeds that of the gain from the extracted resources. The economic analysis of the pre-modern period has been largely quantitatively, and in terms of methodology it does not have too much relevance with modern economic studies. But many of the elucidations of that period has guided renewed interest in resource economics in the 20<sup>th</sup> century; concepts such as limited resources, unsustainable growth, materials scarcity, and Ricardian metrics prove to be foundational in the field of resource economics.

### **2.2.2. Modern Period (20<sup>th</sup> century ~ now)**

Shantayanan Devarajan, an economist from the University of California, Berkeley, has once made a remark on the field of resource economics: there are only a few

fields in economics whose antecedents can be traced to a single, seminal article. One such field is natural resource economics, and the author of that seminal paper, the economics of exhaustible resources, is Harold Hotelling.[12] There is no exaggeration in this remark. Hotelling is the first economist to make a serious endeavor into the field, and the first to successfully formulate a rigorous mathematical model based on the calculus of variation to study some of the most essential features of resource economics, and his paper paves the ground and leads all the economists thereafter.[3] Therefore, I believe a systematic reflection on modern resource economics following the branches laid out by Hotelling will prove to be fruitful.

The modern resource economists' approach can be roughly described in the following framework: from the perspective of the supplier, a group (or a single, in the monopoly case) of profit maximizing agents under a certain set of interest rate projected into the future trying to maximize their individual profits in the present value terms, subject to budget constraint and resource constraint; from the perspective of the society, their total utility is also calculated in the present value terms (in Hotelling's context, utility is defined as an integration of price over quantity), and the optimal path maximizes the total utility of the society. In this way, the model is transformed into solving a dynamic general equilibrium model, and a general equilibrium is reached when the utility increase by extracting an additional unit of resource should be uniform at any point in time.

The questions that the economists have been trying to answer can be generally divided into four categories.

- I. If the market is imperfect, or more specifically, if free competition does not exist, and in the extreme case if there is a monopolist, what will be the rate of depletion? [3, 13]
- II. What is the “net price” of irreplaceable resources, and what is the effect of cumulative production on it? [14]
- III. What are the uncertainties associated with the exhaustible resources market? [15, 16]
- IV. Last but not least, what is the optimal economic growth path given that the resources essential to production are physically limited? [17]

Before summarizing the results the economists have put forward for these questions, one may notice that the questions posed by the economists are in general associated with the market structure, the welfare of the society, and optimal growth. These questions are less concentrated on a particular industry, therefore are intrinsically abstracted and more macroscopic, and necessarily have to forgo some characteristics related with particular resource industries.

- I. Monopolists in the irreplaceable resource industries will have a general tendency to retard production. Production is significantly less than in the perfect competition case, and this is expected, since monopolist will attempt to put a quota on production to jack up the price way above the marginal cost of production, and seek to find the combination of price and demand which will maximize their profit. This has been pointed out by Hotelling in his original work, and has been confirmed and observed over the years by other

economists.

Further, if demand is becoming more elastic, or in other words, demand is relatively more inelastic at the present, then the monopolist is likely to take advantage of the relatively inelastic demand in the early periods by restricting output then.[18] The hypothesis that demand is becoming more elastic is quite plausible, considering agents may find functional substitutes for the resource with the development of technology in the future. A good example will be mercury, which was widely used but ultimately replaced by the mid-20<sup>th</sup> century, and has been addressed in detail by Meadows Donella.[4] Another example is platinum in three way catalytic converter. Platinum used to be the predominant catalyst used in three way catalytic converter, but recent technologically progress has replaced platinum with palladium, which is a functional substitute, but can be purchased at a lower price. This substitution is critical for the techno-economic model we have constructed, and will be addressed in much more detail in the latter chapters.

Lastly, it is interesting to note a paradox mentioned in Hotelling's original paper. The conservation movement of the 30s has criticized the over-exploitation of natural resources, whereas the monopolists, as I have mentioned in part I, will in general retard production. Therefore, in order to "pacify" the former and regulate the latter, "a Scylla and Charybdis between which public policy must be steered". [3]

II. The mine owner's profit depends not only on the current rate of production but

also on the amount of cumulative production, or the stock remaining in the ground. Hotelling offers two explanations. Firstly, the extraction cost increases over time “as the mine goes deeper”, or, in Ricardian term, the lower grade ores have to be accessed when the higher grade ores which are more accessible and have a lower extraction cost get depleted. The famous “Hotelling rule” states the price of an exhaustible resource must grow at a rate equal to the rate of interest, both along an efficient extraction path and in competitive resource industry equilibrium. Robert Solow has lucidly described the Hotelling rule: net price is a function of the sum of extraction cost and scarcity rent. The scarcity rent increases at the rate of the market interest rate, therefore any price deviation from the optimal price will lead to potential arbitrage. However, Solow also notes that in order for the future spot prices to follow this formulation, it is advisable that the government agency provide as much accurate and complete information as possible on reserve, exploration, and the mining industry in general;[14] this point has been strongly echoed by other more recent resource economists.[15, 19, 20] It is also crucial that a functioning futures market be put in place, so that arbitrage will push the spot prices of the present and the future onto the path described by the Hotelling’s rule.

III. The uncertainty of the exhaustible resource industry is three-folded.

Firstly, there is uncertainty in exploration. Whoever finds a mineral deposit can, by filing a claim, exclude competitors from access. Presumably this leads



to socially excessive levels of exploratory activity. At the same time, due to knowledge spillover of geological information, or in other words, the exploration undertaken by the others provide valuable information as guidance for my behavior, may lead to socially deficient levels of exploratory effort: everyone waits around hoping his neighbor will drill first. The combined effect is unclear. [12]

Secondly, there is uncertainty in the supply side. The behavior of the owner when facing “uncertain in estimation” of the content of a mine, and there is also uncertainty associated with exploration with varying costs. [21]

Lastly, uncertainty finds its presence in the demand side as well, for there is uncertainty in price which may lead to speculative behavior of the buyers, and there is also the potential for substitution.[16]

- IV. Ultimately, the limited supply of exhaustible resources will impact production, and therefore the long-term economic growth of nation-states. Economists have typically extended the traditional Cobb-Douglass production function to incorporate the rate of depletion of exhaustible resource. The study is complicated, for there are two state variables – the capital stock and the stock of natural resources, and makes a complete quantitative analysis of optimal control problems a lot more difficult.[17] Such a model nonetheless finds that paths which involve high rates of natural resource utilization (i.e. a high ratio of resource use per unit of time to stock) have permanently lower long run rates of growth. In addition, a higher discount rate (alternatively, the more

impatient the people are), the faster the depletion rate of the natural resources. Lastly, a higher rate of technical change leads to a higher or lower rate of extraction as the elasticity of marginal utility is greater or less than unity and a higher elasticity of marginal utility leads to a higher or lower rate of extraction as the rate of resource-augmenting technical progress is larger or smaller than the rate of discount.

## **2.3. Materials Flow Assessment**

### **2.3.1. A Critique of the Resource Economists' Approach**

One weakness of the economists' approach is its vagueness and overly abstracted treatment of the technological influence on resource economics. The influence comes first from the fact that materials are not perfectly fungible factors of production – specific materials are employed to achieve specific functionality, and this functionality is otherwise difficult, if not impossible, to achieve. Therefore, substitutability is not smooth among potential factors of production, and a production function of the Cobb-Douglas form is certainly far from ideal. Compounding the first factor is technological progress – we learn new ways to achieve the same functions, under the impetus of economic pressures. The “new ways” may be using renewable resources to replace exhaustible ones, to use cheaper materials to functionally substitute for the more expensive ones, and to use less resource to achieve the same performance. [22] In addition, as has been previously mentioned, the abstraction intrinsic in economic modeling techniques overlooks industry-particular traits and characteristics. The demand for these materials is a derived demand (i.e., consumers

do not purchase materials or resources, but the functionality that the resource and materials enable). Changes in market desires for functionality, as well as changes in the technologies for achieving functionality can lead to unexpected changes in derived demand. Each industry has its individual traits, and a simplification can lead to erroneous results and interpretations. [23]

Last but not least, it is clear from our previous exhibition that the economists' approach has a central theme – the optimal and efficient path of consumption, price, and growth. This extremely forward-looking formulation makes some of them intentionally or unintentionally dismisses short-term volatility of the resource availability and prices, and at the same time renders some of the models largely theoretically appealing, but comparatively less industrially applicable and instructive. Firms and manufacturers yearn to understand the potential price pattern of the near future, with uncertainties burgeoning from exploration, geopolitical factors, and rapid technological advancement. The wild swing of prices of exhaustible resources cannot be explained away by abstract economic models. Although recently economist has argued Hotelling's rule has seen its impact, particularly on the oil spot price in the market, it is also acknowledged in their own profession that Hotelling's rule is largely absent for most commodities of interest. [19]

### **2.3.2. A Case Study of Palladium**

To substantiate these critiques, it is instructive to consider a case related with palladium (Pd), a central element to be discussed in much detail in this thesis.

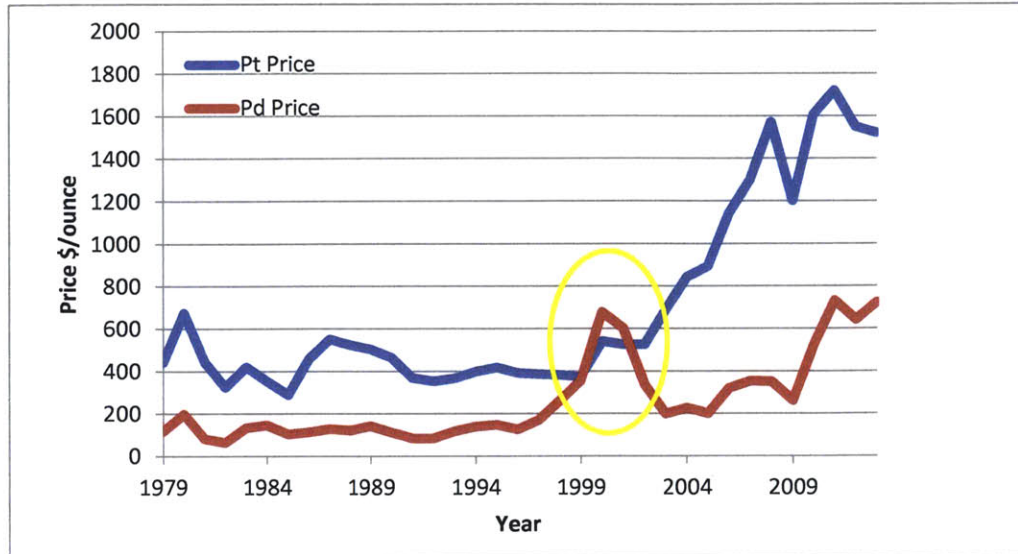


Figure 1: Spot nominal prices of Platinum (Pt) and Palladium (Pd) from 1979 to 2011.[1]

Noticing historically Pd price has been lower than that of Pt, auto-manufacturers have been progressively substituting Pd for Pt, investing on research and development especially for three way catalytic converters (TWC). By the late 90s, more than half of Pd demand was from the auto-industry. Moreover, around 1997, more stringent emission standard was imposed, and auto-manufacturers decided to rely more heavily on Pd.

The geopolitical risk underlying the Pd supply did not have enough attention as it should have. More than 40% of the global supply of Pd is from Russia alone, a country recovering from the collapse of communism, undergoing dramatic structural change and institutional consolidation. The quickly emerging oligopolistic corporations coupled with a Duma (the lower parliament of Russia) questing for more political voice resulted in a stern standoff between President Boris Yeltsin and acting Prime Minister Sergei Kiriyenko, and President Yeltsin was unable to timely discontinue the embargo of palladium enacted by the Duma. A supply disruption

developed, and investors betted on continuing political instability in Russia will keep delaying shipment of the materials to Japan.[24] The upward price spiral is further worsened by an unknown Russia palladium strategic stockpile. The lack of information and transparency from Russia encouraged more speculation. Holders of palladium were unwilling to let go of the materials expecting for higher prices, limited supply was unable to cater the already dramatically significant momentum of increasing palladium demand especially from the auto-industry, and the price of palladium quadrupled in a matter of several quarters.

More interestingly, after President Vladimir Putin came into power shortly after, and with his capable but (sometimes unsettling) hands, he was able to dispel dissenting voices from the Duma, and with some industries switching away from palladium to designs that were proved to be more costly, the price of palladium dropped abruptly.

This utterly unexpected price excursion of palladium has been a combined result of increasing demand due to regulatory pressure in the West, a decrease of supply due to Russia geopolitical instability, and information asymmetry.[25] Though most traditional resource economists, whose models are deficient in even providing a scenario assessment of such unlikely events, may dismiss short-run business cycle as all too common a phenomenon and has no bearing on long-run economic growth, such a drastic excursion proved extremely costly for the industries that rely on palladium. To give a sense of the magnitude of the losses, one major US auto-manufacturer we have interviewed lost over one billion dollars during the

palladium crisis, despite the fact that less than one ounce of palladium is used in a car.

### **2.3.3. An Introduction of Materials Flow Assessment (MFA)**

Some of the weakness of the economists' approach, especially of analysis on materials, can be well compensated for by a more system-dynamics approach – materials flow assessment (MFA). Generally speaking, MFA can be defined as an analytical method of quantifying flows and stocks of materials or substances in a well-defined system. It is an important tool to assess the physical consequences of human activities and needs in the field of industrial ecology. MFA typically defines a system boundary, and limit its scope on one or several particular materials. It is composed of an anthropogenic cycle, tracking the entire flow of the material from the ore stock to production, fabrication & manufacturing, usage, and lastly wastes.[9] It also enables the researcher to focus his/her attention on certain steps of the process if necessary, and allows for integration of technological factors into the model. Scenario assessments that take into consideration of potential technological or geopolitical disruptions are also frequently conducted to test for the robustness of the model. A graphic representation is reproduced below based on Wei-Qiang Chen and T. E. Gradel's work on anthropogenic cycles of the elements.[9]

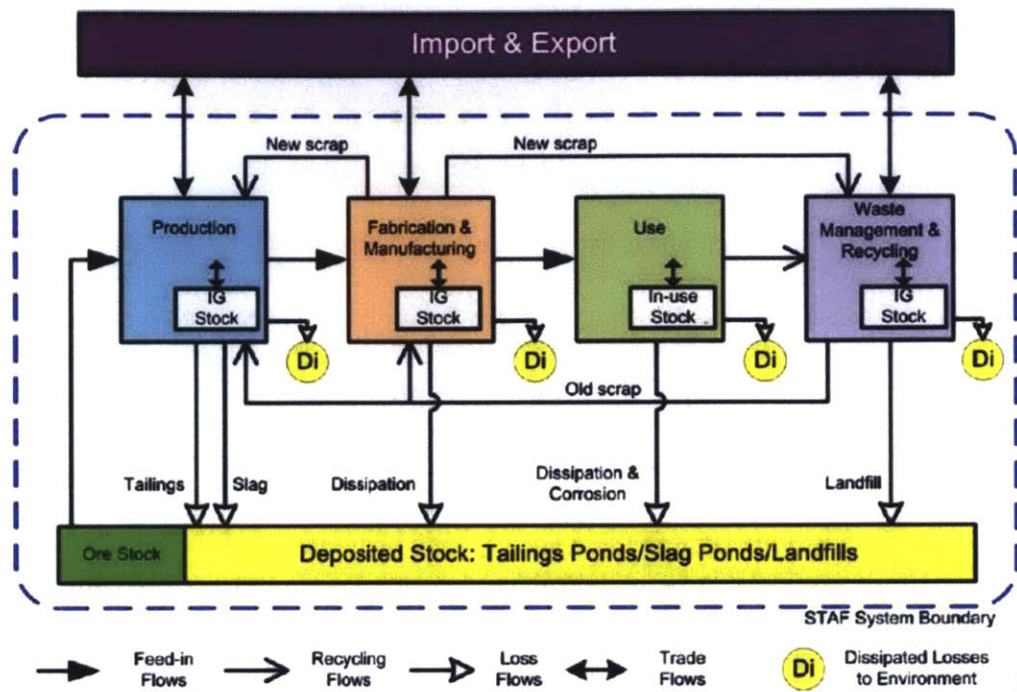


Figure 2: Schematic diagram of generic elemental cycle with life processes depicted from left to right. IG Stock = industrial, commercial, and governmental stock. Cycles not derived from ores, such as carbon, will vary somewhat from this general framework.

The author believes the central distinction between resource economics approach and MFA is, resource economists attempt to understand the dynamics and values of materials exchange and consumption and its implication for social welfare and development mostly in the context of varying economic forces, where MFA directly addresses the topic of its ultimate interest – materials. MFA analyzes its subject of interest – the dynamics of materials flow itself by considering both physical substance flow analysis and the impact from social or economic forces. In short, MFA incorporates some basic elements of resource economics but it's most interested in the physical flows themselves, whereas the resource economists are more intrigued by the value of materials exchange, consumption, and growth economics that has bearing on resource utilization.

MFA can be broadly divided into static materials flow assessment (SMFA) and dynamic materials flow assessment (DMFA).[10] SMFA depicts the flow of a certain material during a particular, typically one year period. DMFA, however, usually involve an assessment across the horizon of time for as short as several years to as long as over a hundred. DMFA can be roughly divided into two sub-categories: those tracking stocks and flows in the past (retrospective DMFA), and those conducting scenario predictions for future stocks and flows under the concept of “stock drive flows” (prospective DMFA).

This thesis, given the duty to understand future global demand of PGM, is a prospective dynamic materials flow assessment. It is slightly different from most existing prospective DMFA for its focus on techno-economic analysis and a relentless endeavor to integrate the economics and technological spheres with as much information as is currently available. Before the modeling methodology I have employed is discussed, it is possibly beneficial to summarize and reflect on existing approaches with prospective DMFA, identify their pros and cons, and think of ways to mitigate the deficiencies. This will be the content of the last section of this chapter.

#### **2.3.4. DMFA as a Forecast Method**

DMFA is a frequently used method to assess past, present, and future stocks and flows of exhaustible resources (especially metals) in the anthroposphere. Over the past fifteen years, DMFA has contributed to increased knowledge about the quantities, qualities, and locations of metal-containing goods. Muller et al. has written an extremely helpful review paper that summarizes most of DMFA work that has been



done. They have noticed that most of the reviewed studies (43 of 60) aim at understanding the pathways of metals, the magnitudes of their stocks and flows, and how they evolve as a function of time. The studies involve quantifying and visualizing the dynamics of relevant stocks and flows of metals and their use in specific product groups or end-use sectors. Additional purposes of these studies include: to examine in detail the recycling potential of certain metals,[26, 27] including recycling efficiency and future recycling flows[28]; to evaluate scenarios of future resource availability; to assess the changing environmental impacts related to changing material flows[29], and to compare different methodological approaches.[30, 31]

Any DMFA or MFA in general may be described as an integrated treatment of stocks and flows, but what truly defines MFA as a systems approach are the feedback loops continuously influence previous stocks and flows. In the rest of this section, we will examine in-use stocks, inflows and outflows, and ultimately, physical and socio-economic feedback loops.

The in-use stocks can be modeled in two ways – either top down or bottom up. The top-down approach derives the in-use stock  $S$  from the net flow by using the following equations:

$$dS(t) = (\text{inflow}(t) - \text{outflow}(t)) \times dt = \text{net flow}(t) \times dt \quad (1)$$

$$S[n] = (\text{inflow}[n] - \text{outflow}[n]) \times T + S[n-1] \quad (2)$$

$$S[N] = S[0] + T \sum_{n=1}^N (\text{inflow}[n] - \text{outflow}[n]) \quad (3)$$

Note that (2) and (3) are simply two equivalent representation of the same concept.

The bottom-up method derives the in-use stock  $S[n]$  at a time  $n$  by summing all the

metals contents  $c_i$  in their respective products or end-use sectors  $P_i$  according to the following equation:

$$S[n] = \sum_{i=1}^I P_i[n] c_i[n] \quad (4)$$

where  $I$  is the total number of products or end-use sectors considered.

Approximately 90% of the reviewed literature applies the top-down approach and 10% the bottom-up approach.[10] The author has used the bottom-up approach and believes the bottom-up approach is more robust, accurate, and flexible despite its sometimes much more costly requirements for the quality and amount of data for reasons to be discussed in the methodology chapter.

The inflows are typically constructed using historical data (e.g., on long-term consumption), whereas outflows, which are rarely measured, are modeled by assigning lifetime distribution functions to specific products or end-use sectors, with the relationship between inflows and outflows corresponding to a convolution (the residence time model or population balance model). The convolution, being difficult to be solved analytically, is typically numerically integrated.

$$\text{outflow}(t) = (\text{inflow} * f)(t) = \int_{-\infty}^{\infty} \text{inflow}(t - u)f(u)du \quad (5)$$

Lastly, the feedback loop has been modeled either physically or with a combination of physics and economics. Physical feedback typically involves recycling of old scrap and new scrap, landfill, incineration, materials dissipation, and discovery of new reserve of resources; potential socio-economic feedback includes the impact of changing GDP, GDP/capita, price of the resource, and population on stocks and flows.[28, 30-35]

It is instructive to provide some concrete examples to substantiate the theories. Yamaguchi and Ueta used substance flow analysis where the inflow is a function of socio-economic indicators and outflow modeled as a Weibull distribution, and consequently constructed a dynamic model with physical feedback considering mineral resource stock, stock in the economy, and stock in the environment [34]; Kapur's study on copper models copper in use as a product of population, GDP/capita, and intensity of use, further dividing intensity of use into three stages (incline stage, turning point, and decline stage), and constructed three scenarios with recycling corresponding to fast economic growth (tech world), medium economic growth (green world), and low economic growth (trend world) [33]; Elshkaki's study on platinum models inflow with economic response such as GDP, GDP/capita, population, and cost, and physical response such as Pt loading and vehicle production – by considering both primary production and secondary production (physical response – recycling), provides a model for forecasting Pt stocks and flows [32]; Alonso's study on the auto-industry's demand impact on platinum mostly focuses on physical response and the other industries are modeled using an autoregressive integrated moving average model with a first order in p and zeroth order in q and d, and conducted various scenario tests of varying patterns of auto-industry behaviors to examine the global demand for platinum under each scenario. [36]

Other authors have studied a plethora of other minerals using a variety of methods.[28, 30, 37-42] As a burgeoning field of research, the boundary of DMFA is vague. Although it makes any generalization or categorization of the methodologies

somewhat challenging, it nonetheless provides a wide window for researchers from different backgrounds to integrate their expertise into this methodology to improve the performance of their models. A summary table of different modeling parameters of DMFA based on the modeling approach is provided below as a roadmap. Note the difference retrospective and prospective is that the prospective models, using the data supply from the retrospective ones, typically also needs forecasts of certain physical or socio-economic variables. Since the distinction is straightforward, they are not included in the table.

	Top-down	Bottom-up
Physical Feedback	Mineral resource stock; Stock in the economy; Stock in the environment;	Stock in each industrial sector; Scrap in each industrial sector; Size of usage unit (e.g., fleet size)
Socioeconomic Feedback	GDP & GDP growth; Price and cost; Technological progress;	GDP/capita & population; GDP/capita growth; Population growth;

Table 1: Modeling parameters based on different modeling DMFA modeling schemes. Many studies have used either a combination of top-down & bottom-up methods, or have considered both physical and socioeconomic feedbacks, and some have adopted a mix of modeling parameters of all four quarters. The distinction between the quarters is supposedly less important than constructing a robust and illustrative model.

Although the modeling methodology proposed in this thesis will be discussed in detail in the following chapter, it is perhaps instructive to provide a brief summary of it at this stage so as to compare and contrast with existing literatures.

The model in this thesis can be generally categorized as a prospective bottom-up

dynamic materials flow assessment model. It aims to forecast for the global demand of three important minerals widely used in automobiles as catalysts – platinum, palladium, and rhodium. It is bottom-up because the global demand is reached by summing the product of usage of each mineral in each type of automotive in five different regions in the world with the number of sales of each type of automotive in each region. It is distinctive from any previous studies because of three reasons: firstly it is the first study that investigates the global demand of palladium and rhodium; secondly it is the first study that conducts an involved meta-analysis of the functional substitution relationship between palladium and platinum and how does the recipe of the mix respond to technological progress, geopolitical risk, or price variation; lastly, it is among the first attempts to explicitly model the price of these minerals as an exogenous variable, for the intrinsic volatility of the supply and demand of these minerals coupled with the exponentially growing liquidity provided by the financial market (options and futures markets) makes any endogenous treatment of price variable deficient of predictive power. A set of scenario tests has been conducted to infer demand relationship under varying price ratios as a result of supply disruption or speculation, changing technological progresses and regulations, and different fleet characteristics of the next two decades.

### 3. Methodologies

#### 3.1. An Introduction to the Overall Model Framework

Platinum group metals (PGM) are essential for the auto-industry as powerful catalysts that enable the auto-manufacturers to conform to stringent emission regulations and reduce environmental pressure caused by emissions. PGMs, specifically platinum, palladium, and rhodium, are a set of excellent catalysts that can be used at relatively high temperatures and are stable in many aggressive chemical environments.<sup>1</sup>[43, 44] In fact, in 2011, the automotive industry used approximately 48%, 82% and 93% of the global supply of platinum, palladium, and rhodium, respectively.[45] Such figures clearly indicate that given the current technology, the markets for vehicles and PGM are inextricably linked. As one would expect, in facing stricter emission regulation standards and rising global automotive sales with a growth rate of 3.4% for the past thirty years, the demand for PGM has been increasing in an unprecedented way.[46, 47] This economically important role coupled with the limited geographically accessible PGM resources has led to PGMs being labeled as “critical” resources. [48] Several studies have projected that the world fleet could approach two billion vehicles by 2030. Reaching that level would represent the production of more than one billion new vehicles (and new catalytic converters) over that time period. Future growth in the automobile industry (especially the developing world), technological innovations such as new PGM mixes and alternative drive trains, and changing emissions regulations in different parts of the world could significantly

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<sup>1</sup> Note technically PGM refer to Pt, Pd, Rh, Os (osmium), Ir (iridium), and Ru (ruthenium). Ru, Ir, and Os form volatile oxides so these elements are unsuitable. In this thesis, PGM is narrowly defined to include only Pt, Pd, and Rh.

alter the patterns of PGM use.[49-51] It is important to understand the potential evolution of global demand for these critical minerals.

The model proposed in this thesis will take on a broader view on the global demand of all three major PGM, namely, Platinum, Palladium, and Rhodium using a bottom-up prospective DMFA approach. We believe a bottom-up approach that takes into account of the deep parameters that govern the behaviors of the microeconomic decision-makers is more robust against structural uncertainties (policy change, geopolitical risks, and technological innovations), and an aggregation of the micro-findings may produce a more unbiased and systematically robust prediction of the global demand of the PGM. [52, 53] Therefore we have analyzed firm-level behavior in detail, and based our studies on vehicle level consumption of the PGM. It also endeavors to combines technological factors and economic factors the authors believe are intrinsically entangled and inseparable from either the macro or micro perspective. Technologically, the demand for the PGM in the auto-industry has been almost exclusively from the engine, yet an analysis may be insufficiently representative if it does not consider both the gasoline engines (three-way catalytic converter) and the diesel engines which is composed of three critical parts (diesel oxidation catalyst, lean-nitrous trap, catalyzed particulate filter). In addition, we have surveyed the past PGM demand under various standards, and have used this survey as a reference point to predict the evolution of regulatory standards of disparate regions of the world that are undergoing different levels of emission regulation. In the last stage of constructing a robust micro-foundation, we have conducted a meta-analysis

to try to comprehend the partial substitutability between platinum and palladium along with its profound implications on the strategic decisions of the firms when the price ratio of these two commodities varies. The macro-stage of the analysis is more of a standardized dynamic materials flow assessment, with a focus on the manufacturing and usage phases of the substance flow diagram.

In a nutshell, the forecast of the global demand for PGM is carried out in three steps. First, we develop a techno-economic model which allows us to estimate the cost optimal (equilibrium) PGM chemistry for a certain type of vehicle under a particular regulation level – which is constructed through an in-depth meta-analysis (i.e., combining results from different studies, in the hope of identifying patterns among study results). Secondly we posit a model of aggregate PGM use over time where which is at least a function of the cost of use per vehicle. The aggregate PGM is obtained by multiplying the PGM demand per vehicle depending on the regulation level and vehicle type and the number of that particular vehicle type subject to the said regulation level. Lastly, we calibrate the model posited in the second step based on historical usage data.

### 3.2. Techno-Economic Micro-Model and Equilibrium Chemistry

The first step of our research has been to obtain a statistically robust description of technologically viable exhaust control systems in terms of PGM use per vehicle through an extensive meta-analysis. This vehicle-level estimation of PGM demand is replicated for a variety of vehicle types, regions, and different levels of regulatory standards. Specifically, the vehicle types include diesel heavy duty vehicles, gasoline



passenger vehicles, diesel hybrid vehicles, gasoline hybrid vehicles, electrical vehicles, and fuel cell vehicles. Region-wise we break down PGM use by: North America, Europe, China, India, and the rest of the world. Regulatory standards are categorized based on the European Standards (Euro III—Euro VI) and the American Standards (US Tier I – US Tier III), the two well-established regulatory standards which are likely to be modeled upon by the other parts of the world.[54] The loading is normalized by total loading divided by engine size.

The author believes one of the central distinctions of the entire modeling approach suggested in this writing from any other DMFA or economic approaches is its consideration of the technical substitution. It is therefore necessary and fitting to briefly sketch out the technological components of this model, namely, which parts of the a certain type of engine consumes how much PGM and for what reason, what is the functionality of the PGM in a particular type of engine, and how their roles are complementary or substitutive, what kind of impact will technological innovations alter the existing equilibrium chemistry, and ultimately, how does the technological component integrate with the economic one.

To substantiate the narrative with an example, we collected a sufficient amount of data on various combinations of platinum and palladium that enable diesel oxide catalyst (DOC) to function in a way that conforms to a specific standard, in this instance, Euro V.[50, 55-62] By plotting the data points on the graph and proper extrapolation, we obtain a functionally optimal expression for the substitution curve of platinum and palladium that minimizes the sum of the mean squared errors of the

afore-mentioned data points. Rhodium is not extensively substitutable with the other two minerals for its functionality is primarily limited in rich or stoichiometric conditions to reduce nitrous oxides, and its presence is also limited in only three way catalytic converter (TWC) of gasoline engine vehicles and lean nitrous trap (LNT) of diesel engine vehicles.[63] Therefore rhodium price change has little noticeable impact on the usage of the other two minerals, and therefore, for simplicity, is temporarily omitted in the current analysis.

A cost-minimization optimization is carried out to forecast for the future PGM demand. The PGM weight per vehicle for gasoline engine vehicles is extrapolated and calculated by using cost minimization the three way catalytic converters (TWC)[64-67]; similarly, the PGM weight per vehicle for diesel engine is computed by collectively minimizing the cost for lean nitrous trap (LNT), diesel oxidation catalyst (DOC), and catalyzed particulate filter (CPF)[61, 68-74]. In a bit more of mathematical jargon, it can be expressed as:

$$dG_t = \text{Min}( P_{Pt,t} M_{Pt,TWC,t} + P_{Pd,t} M_{Pd,TWC,t} ) \quad (1)$$

$$dD_t = \text{Min}( \sum_K ( P_{Pt,t} M_{Pt,K,t} + P_{Pd,t} M_{Pd,K,t} ) ) \quad (2)$$

The variables in these two equations are:

$dG_t$  – the PGM demand per gasoline engine vehicle

$dD_t$  – the PGM demand per diesel vehicle

$P_{Pt,t}$  – the price of the platinum at time t

$M_{Pt, TWC, t}$  – the weight of platinum required to be present in the TWC at time t.

Subscript K in equation (2) encompasses the three primary components that use

PGM in the diesel engine, namely lean nitrous trap (LNT), diesel oxidation catalyst (DOC), and catalyzed particulate filter (CPF). The PGM demand calculated is the optimal combination of platinum and palladium that simultaneously minimizes the cost of the catalysts and at the same time conforms to the regulatory standard of interest.

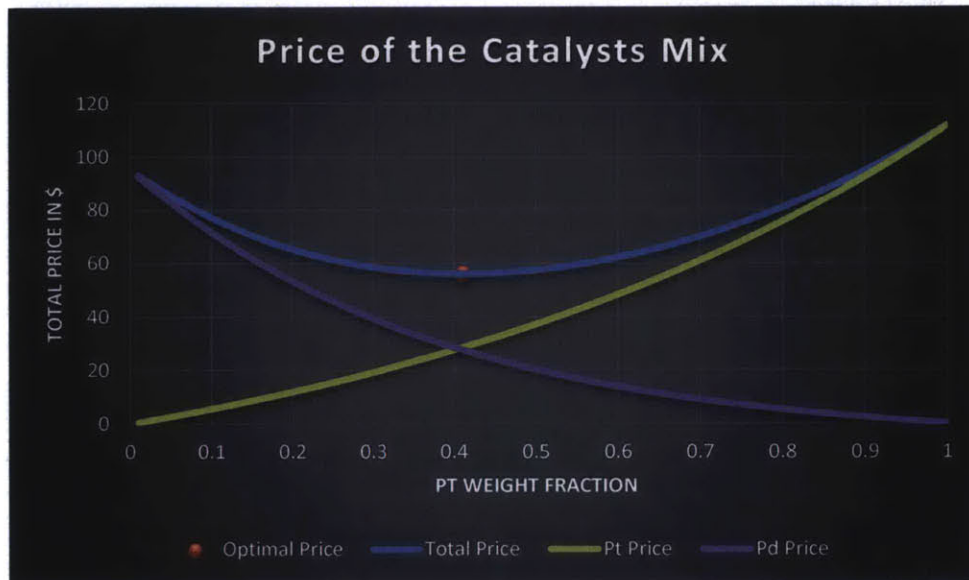


Figure 3: Total PGM Price for TWC under Euro-V standard as a function of Pt weight fraction, only an illustration.

For example, this plot shows the price combination of platinum and palladium to achieve Euro-V standard emission regulation for a three way catalytic converter (TWC). Platinum in general has a stronger catalyzing capability at a broader range of temperature and chemical conditions; hence one portion of platinum can achieve a performance that requires several commensurate portions of palladium to achieve. As has been previously discussed, the various combinatorial mixtures of platinum and palladium to achieve Euro-V standard is extrapolated and calculated based on data obtained through literature research. The total price of the catalyst mix is calculated as

the sum of the product of the price and quantity of each mineral, and is plotted out as a function of platinum weight percentage. The combination of Pt and Pd that minimizes the cost is found iteratively, and this combination is defined as the optimal combination of the TWC converter given the prevailing market price of the relevant minerals. The micro-model is termed “techno-economic” because extrapolation of the amount of PGM required at different compositions of Pt is obtained based on knowledge of substitutability we have acquired from literature; the prevailing prices of Pt and Pd are the principal economic driver, and agents will want to choose a combination that minimizes the raw materials cost while conforms to the regulation standard— hence the name.

After we have obtained a vehicle level estimation of PGM demand, this micro-level demand is projected into the macro-space using equations (1) and (3). We believe a forecast of a macroscopic variable is robust against structural changes when it is constituted by an aggregation of microscopic variables governed by a set of micro-level parameters. In a bit of economics jargon, our belief is equivalent to the Lucas critique to the first order, that a macro-model is meaningful when it has a micro foundation modeled based on a set of structural invariant parameters (deep parameters).[52]

### 3.3. Global PGD Demand Macro-Model

After delineating the micro-scale techno-economic model, we are ready to examine to incorporate the physical aspect of materials flow assessment to aggregate the micro-scale PGM usage to project the global demand of PGM.

The global aggregate PGM usage at time  $t$  can be expressed as a function of the following variables:

$$TD_t = f(VS_{i,t-1}, GR_{i,t-1}, M_{ij,t}) \quad (3)$$

Where the variables are:

$TD_t$  – the total global PGM demand at time  $t$

$VS_{i,t}$  – the vehicle sales of a certain region  $i$  at time  $t$ , including gasoline engine passenger vehicles, diesel engine heavy duty trucks, gasoline hybrid vehicles, diesel hybrid vehicles, electric vehicles, and fuel cell vehicles. These vehicles require PGM usage at different levels depending on their individual catalyst chemistry

$GR_{i,t}$  – the growth rate of the vehicle sales of a certain region  $i$  at time  $t$

$M_{ij,t}$  – the amount of PGM used for a certain type of vehicle  $j$  of a specific region  $i$  under a certain regulation level at time  $t$ . At this level of PGM usage, the economics of the PGM is at equilibrium, namely a state where economic forces such as supply and demand are balanced and in the absence of external influences the equilibrium values of economic variables will not change.

It is important to note and understand that the PGM use of a vehicle can deviate from its optimal cost structure in reality. There are primarily three reasons for the PGM use in a vehicle to deviate from cost optimization. Firstly, manufactures may experience a lag in diagnosing current price trends; in other words, the decision time (the time for the manufacturer to implement a certain decision) may not be zero. Secondly, it takes time to implement a change even if the manufacturer wants to adapt to a varying price. In order to conform to a certain standard while adjusting the recipe

of the catalyst mixture, it takes research and development efforts to achieve such an adjustment. This time lag is termed as the reaction time (the time for the manufacturer to observe the price change and realize it has to react to such a change). Lastly, there is the typical technological and operational inefficiency which may also lead to deviation from the cost optimization composition of the catalyst. Perceived customer values for marginal improvements in emissions performance are well below the marginal cost of achieving those improvements, or in other words, there is no market driven reason for exceeding the regulation.

Deviations from cost optimal value of PGM use are also incorporated into the model.  $M_{i,j,t}$  is expressed as a function of the following variables:

$$M_{i,j,t} = g(P_{t-1}, P_{t-2} \dots P_{t-RDM}, M_{i,j,t-1} \dots M_{i,j,t-n}, RL_{i,t-1}) \quad (4)$$

Where the variables are:

$P_t$  – price level of platinum, palladium, and rhodium at time  $t$ , respectively. The number of lagged price terms that contribute to current PGM usage is dependent on the RDM, namely how long does it take for the decision-makers to catch up with the current optimal PGM combination.

$RL_{i,t}$  – regulation level of region  $i$  at time  $t$

$M_{i,j,t-n}$  – the amount of PGM used in time period  $(t-n)$ .

How exactly  $M_{i,j,t}$  is calculated is the subject of the next section.

To sum up, the global PGM demand can be expressed mathematically as:

$$TD_t = \sum_{i,j,t} VS_{i,t-1} (1+GR_{i,t-1}) M_{i,j,t} \quad (5)$$

The global PGM demand of time  $t$  equals the sum of the products of the expected

vehicle sales of this year times the amount of PGM required for all these different types of vehicles under various regulatory standards. The expected value of vehicle sales is calculated assuming the vehicle sales growth rate of this year equals the growth rate of the past year.

Another further important cautionary note is that the PGM demand per vehicle using equation (1) and (2) is *not* identical with the real PGM weight per vehicle  $M_{ij,t}$  calculated using equation (4). The PGM demand per vehicle is computed assuming perfect information of the price of period  $t$ , which in real life can only be speculated on in period  $t-1$ . It also assumes it takes no time for the firm to diagnose the price trend and modify their current recipe and manufacturing infrastructure to accommodate any recipe change. It further assumes that the firm is operationally efficient, and frictions within and between manufacturing corporates do not exist. The real PGM weight per vehicle  $M_{ij,t}$  comes about with the decision-makers' insight based on past information, and the evolvement of the real weight as time progresses is constrained by both the sensitivity of the decision-makers to the PGM market and the institutional and technological constraints they face to reach that optimal weight. The role of decision time (sensitivity) and reaction time (time takes to overcome constraints and achieve optimal weight compositions) in distinguishing firm-level performance in the market will be further discussed in latter sections. The model also provides flexibility by making decision time, reaction time, and price adjustable variables so as to facilitate future scenario analysis depending on the situation.

### 3.4. Model Evaluation and Calibration

The model strives to provide an accurate picture of future global demand of PGM. Hierarchically, it first breaks down the global fleet into regions of various regulatory standards, and further divides the regional fleet into various types of vehicles with different components that contain different amount of PGM. The fleet projection data are based on the Sustainable Mobility Project (SMP) model developed by the International Energy Agency (IEA) and the World Business Council for Sustainable Development (WBCSD) which we updated recently. The model includes a variety of vehicle types in eleven regions over the world and covers the period 2000-2050.[75] Theoretically, this collective exhaustive and mutually exclusive model (CEME) will produce an unbiased and consistent estimation of future global demand of PGM.

As has been discussed in the previous section, the firms are rational, respond to incentives, and are cost-minimizing agents. They have sufficient motivation to pay close attention to the price evolution of PGM, for more than 60% of the cost of the engine can be attributed to raw materials costs of PGM alone. Firm's response time to changing price can be generally categorized into two groups: decision time and reaction time. As has been briefly described in the previous sections, the decision time is representative of the sensitivity of the firm of interest, or how long it takes the firm to realize the price of PGM has changed. It is mainly determined by how closely the firm has been paying attention to the price change. The reaction time indicates how long it takes for the firm to overcome technological and operational barriers and achieve the cost minimizing weight compositions. It depends on firm's capacity of



adjusting the recipe of the catalyst and investing in research and development activities to catch up with the price trend of PGM given the partial substitutability of platinum and palladium. It also depends on how efficient is communication within the firm, and how fast can the various sectors of the firm reach a consensus to march towards the cost minimizing composition.

The model is calibrated with a matrix of decision year ranging from 0~4 years and reaction year from 1~5 years based on the global PGM demand from 1990 to 2011. For each set of estimations, the mean absolute percentage error (MAPE) is calculated, and repeated-measures analysis of variance test (ANOVA) is conducted. Result shows a decision time of 0 year and a reaction time of 1 year produces the lowest value of MAPE as 0.103%, and is statistically different from any other combinations with 95% confidence ( $F = 7.35$ ,  $F_{crit} = 3.86$ ,  $p = 0.0086$ ). Intuitively, the faster the firm realizes the price change of PGM, and the greater its capacity to adjust its recipe to accommodate the price change, the more likely it is to minimize its deviation of estimation and consequently minimize their costs of production.

MAPE Table	RT = 1 Yr	2 Yr	3 Yr	4 Yr
DT = 0 Yr	<b><u>0.103</u></b>	0.124	0.143	0.159
1 Yr	0.163	0.172	0.183	0.193
2 Yr	0.197	0.209	0.215	0.218
3 Yr	0.223	0.228	0.229	0.230

Table 2: MAPE Table of a matrix of combinatorial variations of reaction time (RT) and decision time (DT) for PGM prices from 1990 to 2011. The optimal reaction-decision time combination is determine to be (RT = 1 Yr, DT = 0 Yr).

However, it is also worthy of pointing out that too fast a reaction time during a periods of volatile PGM prices can lead to inefficiency – for the direction of changing relative prices can swiftly reverse, and a fast reaction in this instance fails to capture that reversion while incurring unnecessary adjustment costs, leading to inefficiency. For instance, the MAPE for monthly PGM spot prices from 2007 to 2011, during which time the financial crisis took place and the PGM spot prices experienced high volatility, has its statistically significant lowest value of 0.185 at a combination of a decision time of 0 year and a reaction year of 3 years.

In reality, firms are constrained by their resources and capacity, therefore not always likely to achieve the optimal decision-reaction time combination. In this model, however, we assume perfect rationality and unlimited capacity of adjustment of the firms, and use the long-term optimal decision-reaction time combination (i.e., decision time = 0 year, reaction time = 1 year) to forecast for the global PGM demand.

## 4. Results

### 4.1. Techno-Economic Micro-Model

The first-step vehicle-level PGM demand analysis is done for four critical components as has been mentioned earlier: three way catalytic converters (TWC) for gasoline engine; lean nitrous trap (LNT), diesel oxidation catalyst (DOC), and catalyzed particulate filter (CPF) for diesel engines. In order to understand the micro-level PGM demand per vehicle under different regulations, it is crucial to obtain a sensible and accurate estimation of the amount of PGM that is required. The PGM demand per vehicle varies from engine size, region, technology, regulations, and recipe; therefore, to grapple with so many variables it is necessary to examine an extensive volume of existing research on this subject. These researches provide us with a deep appreciation of the mechanisms of PGM in these four major PGM-consuming components and give us a profound understanding of the evolution of emission control catalyst technology and how it is likely to unfold in the future.

There are three central characteristics that any catalyst for emission control has to satisfy, and current these requirements can be jointly fulfilled by a deliberately designed mixture of Pt, Pd, and Rh.

1. High activity for the removal of the pollutants in very short residence times  
(large volumetric flows of the exhaust in relation to the size of catalyst which could be accommodated in the available space);
2. Resistance to poisoning by residual amounts of sulfur oxides in the exhaust;

3. Less prone (but not entirely immune) to deactivation by high-temperature interaction with the insulator oxides of Al, Ce, Zr, etc., of the washcoat.

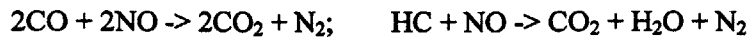
It is also critical to understand the individual strengths and weaknesses of Pt, Pd, and Rh, and such knowledge is summarized in the following table:

	Platinum (Pt)	Palladium (Pd)	Rhodium (Rh)
HC, CO Conversion Lean ( $\lambda=1.7$ )	+	0	-
NO <sub>2</sub> Formation Lean ( $\lambda = 1.7$ )	+	-	0
HC, CO, NO <sub>x</sub> Conv Stoi ( $\lambda = 1$ )	0	+	+
HC Conversion Rich ( $\lambda = 0.9$ )	0	+	0
NO <sub>x</sub> Conversion Rich ( $\lambda = 0.9$ )	-	0	+

Table 3: An exhibition of the relative strengths and weaknesses of Pt, Pd, and Rh under different conditions. Lean burn refers to the burning of fuel with an excess of air in an internal combustion engine, and rich burn refers to the opposite. Stoichiometric burn refers to an air to fuel ratio of 14.64:1. The excess of air in a lean burn engine combusts more of the fuel and emits fewer hydrocarbons. High air-fuel ratios can also be used to reduce losses caused by other engine power management systems such as throttling losses.

Exhaust treatment in gasoline vehicles is predominantly accomplished using a ceramic monolith coated with Pt and Pd to oxidize HCs and CO, and Rh to reduce NO<sub>x</sub>. The system removes three pollutants (HCs, CO, and NO<sub>x</sub>) simultaneously, and is hence referred to as a three way catalytic converter (TWC). Different manufacturers use different Pt:Pd:Rh ratios, and the exact compositions are proprietary. The chemical functionality of the TWC can be succinctly described by the following chemical equations.

Reduction reaction:



Oxidation reaction:



Three-way catalytic converter functions the best at the stoichiometric condition. Its oxidizing capability declines at rich condition, and its reducing ability wanes at lean condition.

Exhaust treatment in diesel vehicles is achieved using a system comprising of several different components. The diesel oxidation catalyst (DOC) removes HCs and CO, and therefore is solely composed of platinum and palladium. It functions at lean burn condition, and therefore is rich in air and oxygen. Its oxidizing environment coupled with a higher operating temperature compared to TWC makes Pd a less competitive candidate compared to Pt despite its lower raw materials cost. In addition to oxidizing HCs and CO to CO<sub>2</sub> and H<sub>2</sub>O, the DOC oxidizes NO to NO<sub>2</sub>. As will be soon discussed, in the passive regeneration approach in diesel particulate filter, it is critical to have high NO to NO<sub>2</sub> conversion in the DOC, and this is also best achieved by using Pt catalyst. Therefore, systems relying on passive regeneration typically have high Pt loadings in the DOC as well.

One further complication of the diesel engine is it emits a lot more particulate matters compared with gasoline engine. Diesel engines can produce diesel particulate matter (or black soot) from their exhaust. The black smoke consists of carbon compounds that were not combusted because of local low temperatures where the fuel is not sufficiently atomized. These local low temperatures occur at the cylinder walls and at the outside of large droplets of fuel. At these areas where it is relatively colder, the mixture is rich (contrary to the overall mixture which is lean). The rich mixture

has less air to burn and some of the fuel turns into a carbon deposit. Removal of soot is achieved using a diesel particulate filter (DPF). The soot is oxidized either passively in a continuous fashion using  $\text{NO}_2$ , which is NO previously oxidized by DOC, as the oxidant at ~350 to 400 Celsius, or actively by periodically heating up the DPF to ~650 Celsius and using  $\text{O}_2$  as the oxidant. In the active approach, regeneration of the DPF is needed, so additional fuel is injected late in the engine cycle, passes through the engine largely unburnt, and oxidized by the DOC which heats the exhaust system. In order to minimize of HCs and CO slipping through the system, mostly Pt and some Pd are added as catalysts in DPFs on vehicles using active regeneration. In short, DPF using the negative approach does not need PGM as catalysts, whereas DPF using the positive approach needs PGM (mostly Pt and some Pd). DPF using the positive approach is of our interest, and in the auto-industry is typically referred to as catalyzed particulate filter (CPF).

Finally, the mixture of NO and  $\text{NO}_2$  ( $\text{NO}_x$ ) has to be taken care of. This is achieved either using either a selective catalytic reduction component (SCR) which relies on ammonia as the reducing agent with a non-PGM zeolite catalyst, or using a lean nitrous trap (LNT). LNTs contain Pt and Pd to oxidize NO to  $\text{NO}_2$ , which is trapped in the LNT as a nitrite, and Rh does the final shot to catalyze reduction of nitrous oxide into nitrates. The nitrates are liberated periodically when the trap is regenerated by heating that decomposes the nitrates. Our analysis focuses on LNTs, for SCRs do not require any PGM.

An extensive literature research has been done for these four components under

various regulatory standards (Euro III—Euro VI & US Tier I—III). We take the average value of each component and the corresponding standard to obtain the average PGM usage in that said component. With every increment of regulatory standard level, we have discovered that empirically an average of an additional of 0.3g of platinum, 0.8g of palladium, and 0.2g of rhodium have to be added to the original formula to conform to the tightening regulatory standard. To give a flavor of the magnitude of average PGM demand per vehicle, the average of the PGM weight in vehicles across regulations is presented in the following figure. Note the weights are calculated for Euro V. Also the loading has been calculated to be gram/liter. In other words, the PGM loading represented in the following chart is an average loading of an engine. Mathematically this statement can be expressed as:

$$\text{PGM Loading} = \text{Total PGM Loading of an Engine} / \text{Size of the Engine}$$

The size of engines varies depending on the purpose of the vehicle, the style and design, the manufacturer, and the targeted customer. The engine size parameter in the model is captured by the calibration factor as will be discussed later.

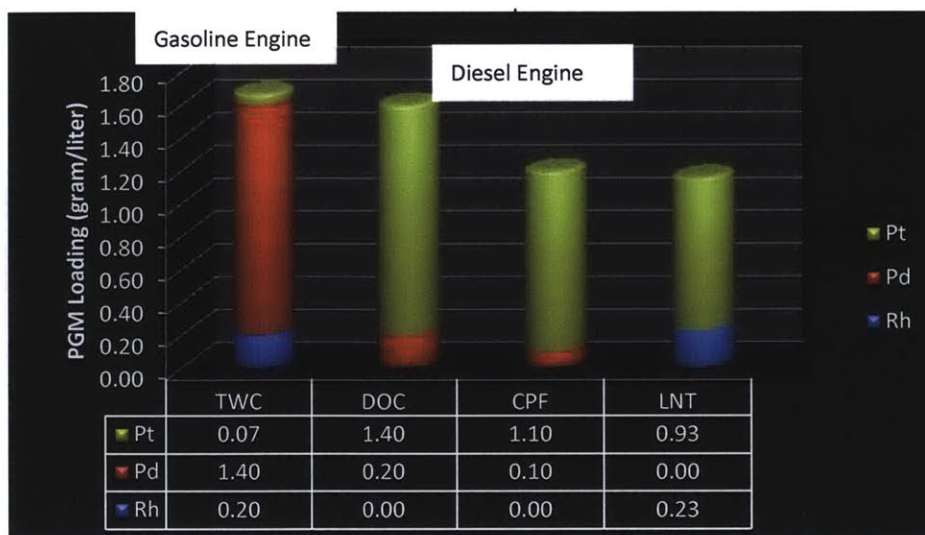


Figure 4: PGM loadings in the four most widely used automotive components. TWC = three catalytic converter, DOC = diesel oxidation catalyst, CPF = catalyzed particulate filter, and LNT = lean nitrous trap. Note most positive numbers have a standard deviation of approximately 20 to 30% of its value.

Palladium usage has drastically increased in the 1990s as the engineers discovered it to be a cost-effective oxidation catalyst. The spike in Pd price in 2000-2001 caused a substantial drop in its use in 2002 which has since recovered. Therefore, as the chart indicates, Pd has become the predominant oxidizing agent in TWC, or gasoline engines. Due to reasons described above, Pt remains the dominant oxidation catalyst in the three diesel engine components. Rh plays the role of a reducing agent in both gasoline and diesel engines.

So far the analysis has informed us nothing more than the prevailing PGM loading under different regulations. To say anything about how the PGM loading is likely to evolve in the future requires a more sophisticated micro-scale understanding of interplay of various social-economic and physical parameters subject to the respective catalyzing capabilities of the PGM. It is important to recapture a central



assumption of the model that agents in this model behave like homo-economicus who are profit-seeking and cost minimizing. Based on interviews with experts in this field, the principal drivers of the price of the engine are the PGM, weighing a staggering 60%. Therefore the agents will respond to price signals, and adjust their recipe while conforming to the prevailing standard in order to minimize their costs of manufacturing. The model takes into account of operation and technological inefficiency as well as communication and negotiation costs in decision time and reaction time, but the model also assumes that any costs incurred by the aforementioned activities do not outweigh the economic benefits brought by a redesign of the PGM recipe. In addition, as has been discussed in detail, Rh serves as a reduction agent, and is a complimentary good to Pt and Pd. The demand of Rh, therefore, is price-signal independent, and can be modeled using only physical feedback based on available and projected fleet models with a focus primarily hinged on automobile demand characteristics and regulatory pressures of different regions of interest. The real trade-off, as has been borne out by time and facts, is between Pt and Pd, which have a large degree, though not perfect, substitutability. It is natural, therefore, to investigate the historical prices of Pt and Pd, and use this as a best estimator to explore how will likely price ratio adjustments of Pt and Pd influence the behavior of the agents and hence the global demand of these two minerals.

The figure below shows the historical price ratio (price ratio = Pt price/ Pd price).

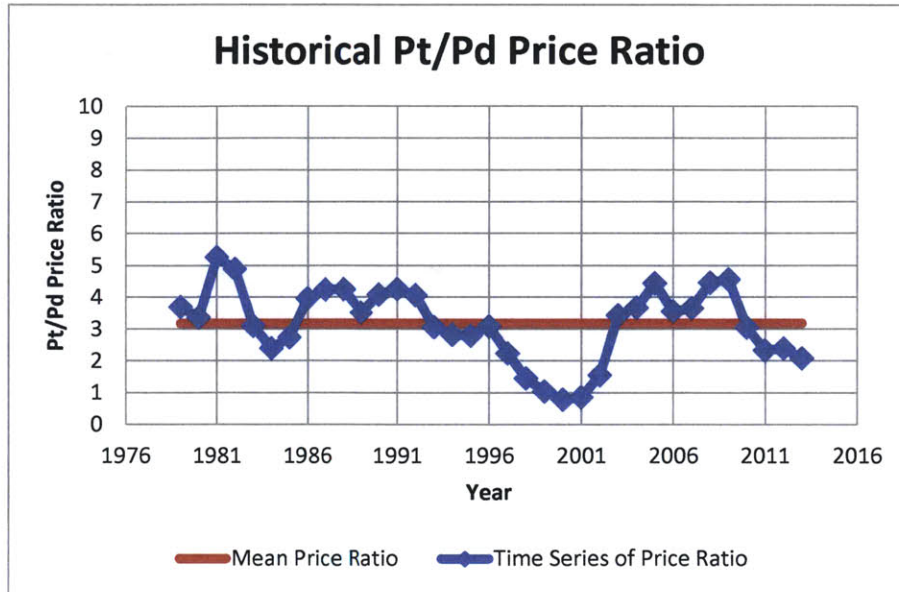


Figure 5: Historical Pt/Pd price ratio.

Historically, the price ratio between platinum and palladium varies from a minimum of 0.799 to a maximum of 5.273 with a mean of 3.190 and a standard deviation of 1.15.[58, 76, 77] In the past few years, it seems the price ratio has walked around 2.00. In order to understand the likely evolution of the price ratio in the future, a time series assessment has been carried out in order to select the best model to simulate the price ratio movement. A vector error correction model (VECM) has been applied, and it indicates that the price time series of Pt and Pd are not co-integrated, namely, the movement of one time series will not necessarily cause a corresponding movement in the other time series. Therefore an autoregressive integrated moving average (ARIMA) model can be applied to the time series price data of both Pt and Pd for a dynamic forecast. Based on Akaike information criterion (AIC) and Bayesian information criterion (BIC), the price time series of Pd is best modeled as an ARIMA(2,1,0) model, whereas the price time series of Pt is best model as an ARIMA (1,1,0) model. Here the (p,d,q) respectively represent the number of

autoregressive terms, the order of integration, and the number of moving average terms. The palladium price follows optimally an autoregressive integrated moving average model (ARIMA (2, 1, 0)) with two autoregressive terms, differenced once, and zero moving average term with the following coefficients and uncertainties:

$$(P_{Pd, t+1} - P_{Pd, t}) = 0.22 (P_{Pt, t} - P_{Pt, t-1}) - 0.32435 (P_{Pt, t-1} - P_{Pt, t-2}) + 17.44 (\pm 90.98) \quad (1)$$

The platinum price follows optimally an ARIMA (1, 1, 0) model with the following coefficients and uncertainties:

$$(P_{Pt, t+1} - P_{Pt, t}) = -0.12 (P_{Pt, t} - P_{Pt, t-1}) + 29.91 (\pm 125.54) \quad (2)$$

The estimation of the price ratio between  $P_{Pt, t+1}$  and  $P_{Pd, t+1}$  through 2015 to 2030 is simulated with Monte Carlo method over 10,000 trials for each year, assuming the uncertainties in the white noise terms are normally distributed. We hope to examine the impact of price ratio ( $P_{Pt, t+1} / P_{Pd, t+1}$ ) change on global demand, therefore we take a closer look at five difference dynamic scenarios. For 2015, the Monte Carlo simulation yields a  $\mu = 2.29$  and a standard deviation of  $\sigma = 0.35$ . It means there is 95% confidence that the price ratio will land in the range [1.60, 3.00]. We have incorporated an even range of the price ratio when we run the simulation, and at this stage, we only examine what is the optimal composition of Pt and Pd in the catalyst and temporarily disregard firm-level inefficiencies. We first examine gasoline engines, and will then turn to a detailed investigation of the diesel engines.

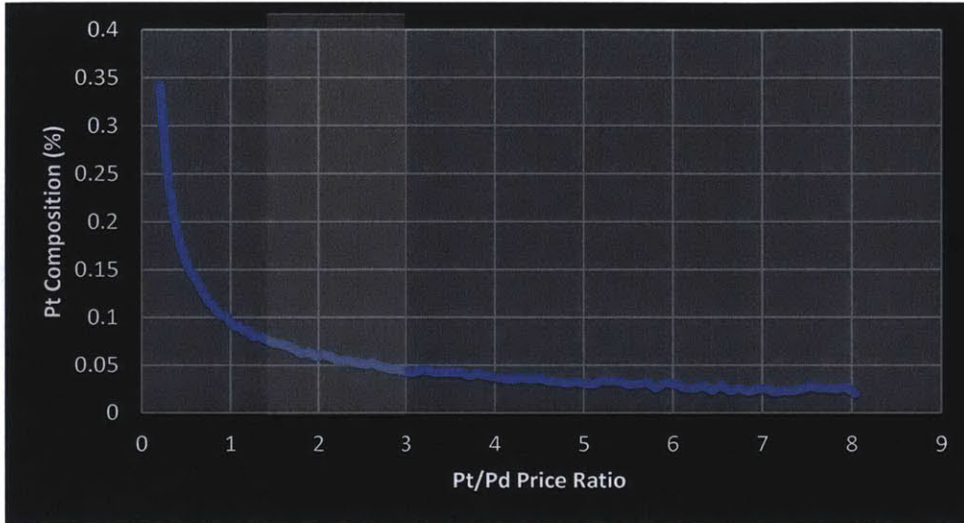


Figure 6: Pt weight fraction as a function of Pt/Pd price ratio for gasoline engines.

Based on graph, it is clear that gasoline engine of current technology has stabilized Pt composition around 4.8% to 7.5%. The price ratio has been around 2.00 recently, corresponding to a 5.0% platinum in the catalyst. This is corroborated by our literature research, which indicates a platinum composition of approximately 5.2%. The simulation based on the micro-model also tells us that even if the price of Pt rises to an extremely high level, the substitution curve asymptotically approaches the price ratio axis at a slow pace. It is unlikely, given the incomplete substitutability, that the Pt can be entirely substituted out of the TWC absent of significant scientific or technological innovations.[78] On the other hand, we want to know how a decrease in price ratio will shift the Pt composition. Suppose the price of the platinum, which is currently much higher than that of the palladium, drops significantly, or if the price of palladium, due to some external perturbations, rises to a level that is equal or even higher than that of the platinum. Our simulation indicates that a commensurate price, or a price ratio of 1, will tip the balance toward using more Pt from 5% to 10%; even

if the price of Pt becomes half of that of Pd, which has not transpired even during the Russia Pd crisis, the composition of Pt in the catalyst will not exceed 15%. Therefore we can almost be certain to conclude that given the recent price ratio, the prevailing regulatory standard, and the current technological level, Pt will likely remain a supplemental minority when it is used as a TWC catalyst with a percentage range from 3% to 15% (95% confidence interval corresponding to a percentage range from 4.8% to 7.5%).[79-81] We have also noticed that the platinum composition of the gasoline engine whose functional catalyzing component is TWC alone can be described with a correlation coefficient of 0.9914 by the following equation

$$\log(\text{Pt\_Composition}) = -1.005 - 0.699 \log(\text{Price\_Ratio}) \tag{3}$$

The Pt composition characteristic of the diesel engine, however, emanates quite a different flavor, and is virtually impossible to be expressed in a single functional form.



Figure 7: Pt weight fraction as a function of Pt/Pd price ratio for diesel engines.

The most conspicuous trait the graph entails is that we are almost certain, given the status-quo, that the diesel engine relies most heavily on Pt at a staggering percentage of approximately 97%, and this composition is unlikely to radically

change as long as the price ratio does not diverge to too high a value (i.e., >4.5). [62, 82-84] Note the composition is calculated by taking into account of all three components (DOC+CDF+LNT).

$$\text{Pt Composition} = \frac{\text{Pt}_{\text{DOC}} + \text{Pt}_{\text{CDF}} + \text{Pt}_{\text{LNT}}}{\text{Pt}_{\text{DOC}} + \text{Pt}_{\text{CDF}} + \text{Pt}_{\text{LNT}} + \text{Pd}_{\text{DOC}} + \text{Pd}_{\text{CDF}} + \text{Pd}_{\text{LNT}}} \times 100\% \quad (4)$$

The entire curve can be roughly divided into four regions. When the price of platinum is lower than that of palladium, it is desirable to use exclusively platinum without mixing in any palladium, for there is no economic incentive to substitute an inferior type of catalyst at a higher cost. When the price ratio ranges from 1.00 to 3.00, the DOC component starts to permit palladium addition with economic viability, for Pd also has oxidizing ability and can function properly, though not optimally, under the burning condition of a diesel engine. When the price ratio jumps up to more than 3.00 but smaller than 4.35, it becomes desirable to mix palladium into platinum in not only DOC but also CPF to conform to the regulatory standard while minimizing costs. When the price of platinum becomes more than 4.35 times that of palladium, one enters the “collapse regime”, and in this regime, with the increase of the Pt/Pd ratio, it becomes exponentially desirable to mix in palladium in all three components of the diesel engine. The exact price ratio that these regime-shifts transpires is only empirical to a first-order, and is out of the scope of this thesis to provide a scientific treatment.

#### 4.2. Global PGM Demand Macro-Model

To project the future global demand of Pt, Pd, and Rh, one needs to consider the influence of four factors: (i) changes in the relative prices of Pt and Pd; (ii) changes in

future emission regulations, and (iii) changes in the split of vehicle technology.

In this section, a projection assuming the current prices, regulation standard, and share of vehicle technology will persist is first provided as the Base Case. Recall the fleet projection data are based on the Sustainable Mobility Project (SMP) model developed by the International Energy Agency (IEA) and the World Business Council for Sustainable Development (WBCSD) which we updated recently. The model includes a variety of vehicle types in eleven regions over the world and covers the period 2000-2050. In this model, the number of light-duty vehicles (LDV) on the road grows from 647 million in 2000 to 1.2 billion in 2020 and 2.3 billion in 2050. The OECD (Organization for Economic Co-operation and Development) regions show little growth, but the fleet expands significantly in developing regions[75].

To address the first factor, a set of five scenario analyses with five different values of price ratios are carried out, and the PGM global demand for each scenario is calculated.

Afterwards, to address the second factor, a scenario where the regulatory standard rises to such an extent that the PGM demand per vehicle increases by 50% is constructed, and the total demand is projected.

Lastly, to address the third factor, we consider and compare three different cases: (i) there is no change in the current gasoline-diesel split in the different markets in our Base Case; (ii) factor of two increase in diesel vehicles from base scenario at the expense of gasoline vehicles globally by 2030 (High Diesel); (iii) the scenarios for success of alternative technologies, in this case we consider battery electric vehicle

technology (High Alternative I) and fuel cell vehicle technology (High Alternative II).

#### 4.2.1. The Base Case

The Base Case is constructed using the current relative prices among all three minerals, and also assumes, in plain words, that whatever the current trends are will be the trends of the future.

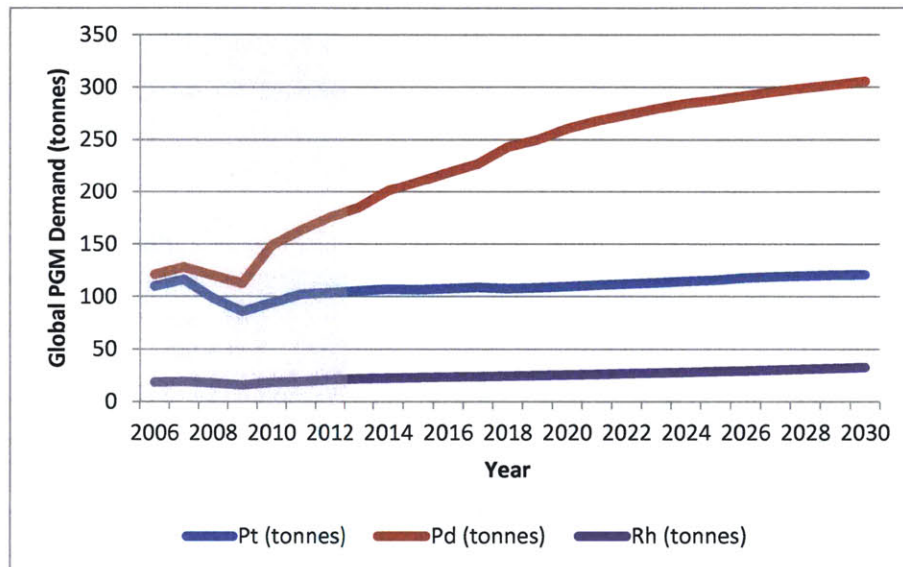


Figure 8: The Base Case Global PGM Demand. The growth trends in demand for Pt and Rh seem to be somewhat mild, whereas the global demand for Pd is likely to increase almost three-fold. Shaded area indicates historical data.

The base case global PGM demand shows the growth rate in demand for Pt is the lowest at approximately 1.63%/year. The global demand growth rate for Pd is the strongest at approximately 4.89%/year. The growth rate for Rh sits somewhere in between, and is at roughly 3.42%/year. This prediction is supported by our previous reasoning as well – most developing countries will be the main drivers for PGM demand growth, countries such as China and India rely mostly on gasoline engine which uses almost exclusively Pd. Given the current price ratio of Pt over Pd, it is



likely firms will invest in improving the catalyzing capability of Pd under various situations and seek to substitute Pt by Pd in diesel engines to achieve cost-minimization. This further pushes up the demand for Pd and pushes the demand for Pt downward. Rhodium demand is largely driven by only vehicle production increase in the developing countries. Its functionality is unlikely to be substitutable by the other PGM, and its demand growth rate is therefore between that of Pt and Pd.

#### **4.2.2. Changes in the Relative Prices of Pt and Pd**

Recall the average price ratio obtained using the Monte-Carlo Simulation as discussed in the previous section is  $\mu = 2.3$  with a standard deviation of  $\sigma = 0.3$ . A set of five scenario tests are carried out with the following price ratio values:  $(\mu - 2\sigma, \mu - \sigma, \mu, \mu + \sigma, \mu + 2\sigma)$ , or equivalently, (1.7, 2.0, 2.3, 2.6, 2.9). Note the third scenario is also the Base Case we have discussed in 4.2.1.

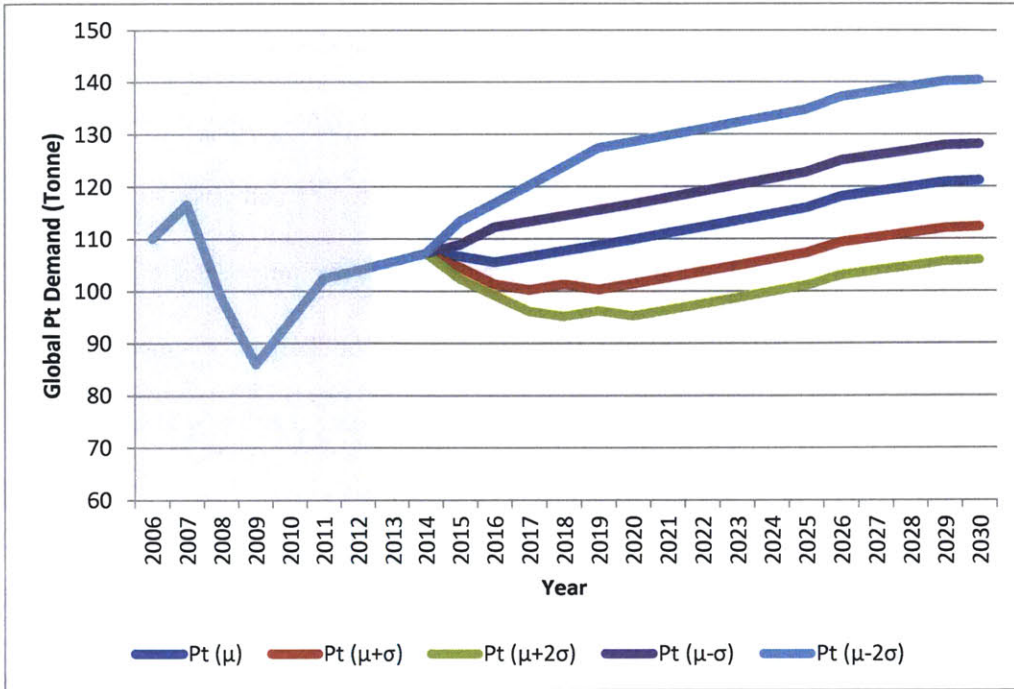


Figure 9: Global demand of Pt under five different price ratios.

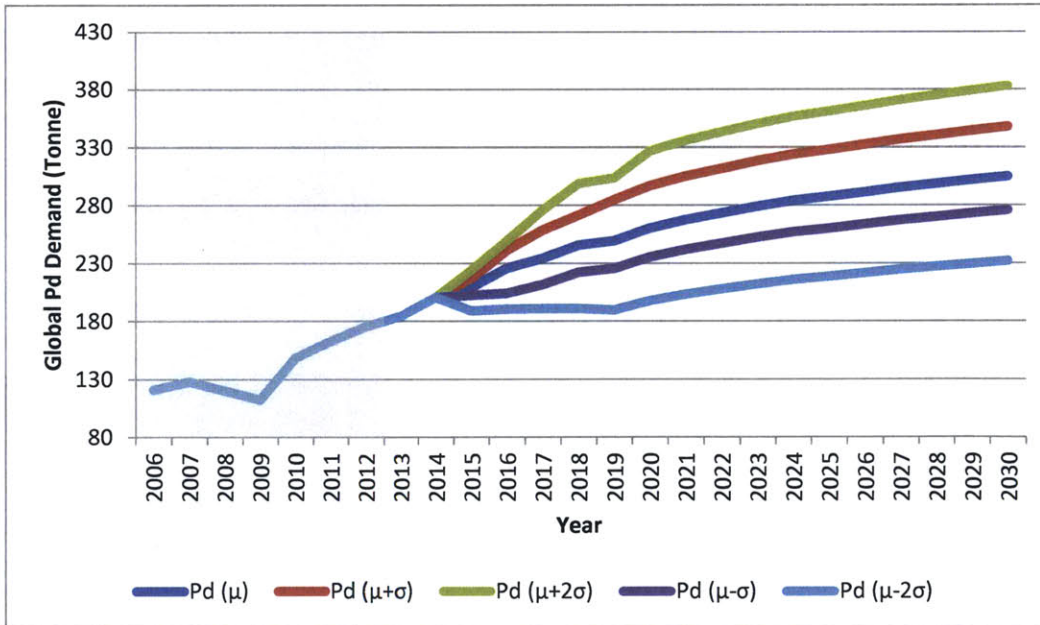


Figure 10: Global demand of Pd under five different price ratios.

As one would expect, given that the agents in this model seek to minimize their costs, varying price ratio is a key driver for their decision-making process and

influence the global demand for each mineral greatly. It is also worth pointing out that given a price ratio shift, the influence of such a shift on the demand of Pd is considerably greater than that of Pt. For example, when the price ratio drops to 1.7, namely the relative price of Pt becomes considerably lower (there is only 2.5% of probability that the price ratio can go anywhere below that value), it is favorable to use more Pt and less Pd. The increase of demand for Pt at 2030 compared with the Base Case is about 19 tonnes, whereas the decrease of demand for Pd at 2030 is about 73 tonnes. The decrease of demand for Pd is about four times of the increase of demand for Pt. On the other hand, if the price ratio rises to 2.9 (there is only 2.5% of probability that the price ratio can go anywhere beyond that value), namely the relative price of Pt becomes considerably higher, and then it is favorable to substitute Pt by Pd. The decrease of demand for Pt at 2030 compared with the Base Case is about 15 tonnes, whereas the increase of demand for Pd at 2030 compared with the Base Case is about 78 tonnes. The increase of demand for Pd is about five times of the decrease of demand for Pt. It is also clear that as the price ratio increases, the demand growth rate of Pd increases at a faster pace than the decrease of the demand growth rate of Pt. The reason for such a non-linearity and non-unit substitution relationship is mainly attributed to the incomplete substitutability of these two minerals, and the stratifying catalyzing capability between Pt and Pd.

#### **4.2.3. Changing Emission Regulation**

The PGM requirement for each regulation standard is the product of two balancing forces: the technological innovations in this field that enable using less

PGM to achieve the same emission standard; the more and more stringent emission standard enacted by EPA as time progresses. Therefore it is instructive to consider a case where the increasing efficiency becomes no longer sustainable, and a tightening emission regulation can be satisfied *only* by increasing the PGM use per vehicle. We consider such a case where the PGM use per vehicle increases linearly from 2015 to 2030 by 50%, and run a simulation.

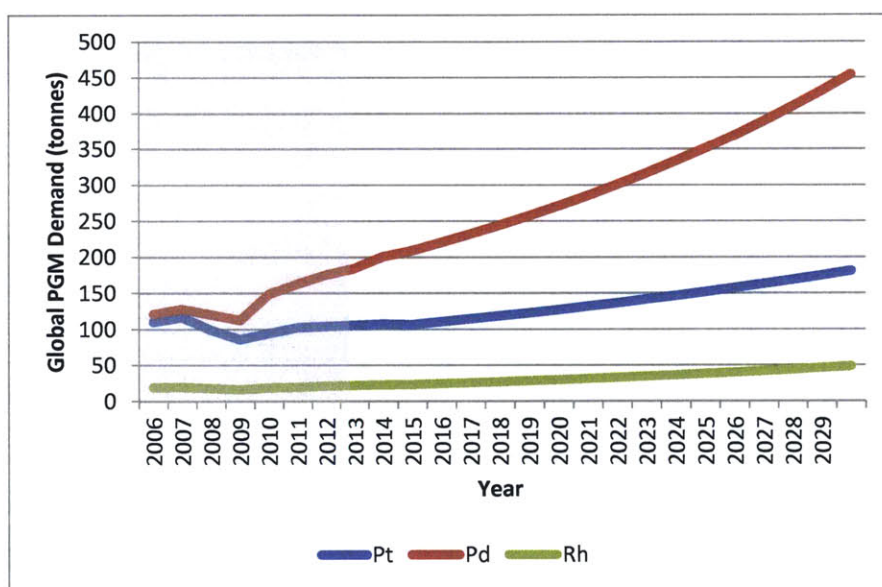


Figure 11: Global demand for PGM when the PGM usage per vehicle increases linearly by 50% from 2015 to 2030.

As one would expect, such a linear increase in PGM loading per vehicle results in an also almost linear increase in the global demand of PGM as well, for the global demand of PGM is simply a multiplication of vehicle sales and PGM loading/vehicle, summed over all regions. Therefore, a 50% increase in PGM loading per vehicle will correspond to a 50% increase in total PGM demand world-wide, assuming the fleet model is still reasonably simulated by the SMP model. It is important to note that this simulation is entirely physically based, and has no economic factor behind it; in other

words, the emission regulation is taken as entirely exogenous, and there are no endogenous repercussions. We have assumed an entirely linear increase of PGM loading per vehicle, and the growth rate is set. In reality, the corresponding identical linear increase of global PGM demand will have different influence on the price of different minerals depending on its own market structure and the interaction of its market structure with the others. This will result in changing relative prices among the minerals, and this will further influence the behavior of the agents in the model which will further influence demand and price. However, as a first order approximation just to get a flavor of the increase of PGM demand if efficiency cannot keep pace with tightening regulation, we believe such a treatment is sufficient.

#### **4.2.4. Changes in the Split of Vehicle Technology**

In this section we will first consider the High Diesel Case and then the High Electric Vehicle Case, and compare these two cases to our Base Cases.

Due to higher efficiency, many automotive manufacturers believe there will be an increase in the amount of diesel demand in the future. In North America the diesel share is less than 5%, and it is approximately 50% in Europe[85, 86]. Although many developing countries still rely heavily on gasoline engines, diesel engines do provide many comparative advantages that may make them the star of tomorrow. Some benefits brought by diesel engines are:

- Diesels get great mileage. They typically deliver 25 to 30 percent better fuel economy than similarly performing gasoline engines
- Diesel fuel is one of the most efficient and energy dense fuels available today. Because it contains more usable energy than gasoline, it delivers better fuel economy.

- Diesels have no spark plugs or distributors. Therefore, they never need ignition tune-ups.
- Diesel engines are built more ruggedly to withstand the rigors of higher compression. Also, because of the way it burns fuel, a diesel engine provides far more torque to the driveshaft than does a gasoline engine.

Therefore, it is reasonable that we devote a section to a scenario where the share of diesel vehicles increases by a factor of two from 2015 to 2030 at the expense of gasoline vehicles.

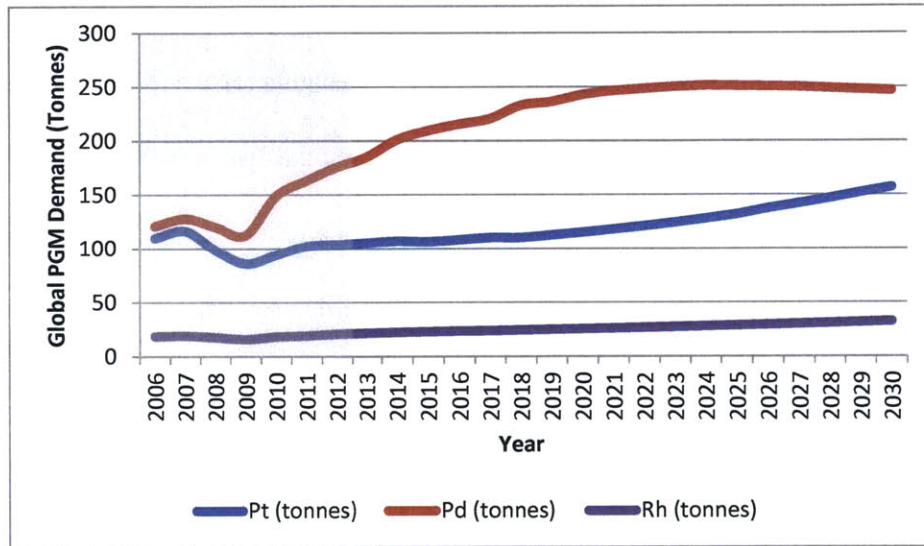


Figure 12: Global PGM demand when the annual sales of diesel vehicles increase by a factor of two from 2015 to 2030 at the expense of gasoline vehicles.

From the simulation results, one can easily observe a distinct feature of this scenario: the growth rate of the global demand of Pd gradually decreases, and by about 2026 the global demand of Pd starts to tank; on the other hand, the global demand of Pt gradually increases at a faster pace. The global demand of Pd at 2030 decreases by about 60 tonnes (or ~20%), and the global demand of Pt in the same year increases by about 36 tonnes (or ~30%) compared to the Base Case. Diesel engines use mostly Pt and little Pd, whereas gasoline engines use mostly Pd and little Pt, therefore an increase of diesel vehicles on the road *at the expense of* gasoline vehicles

sales will naturally leads to a decreasing demand for Pd and an increasing demand for Pt, absent of technological innovations that make it preferable to use mostly Pd in diesel engines.

#### 4.2.5. Alternative Technology Case

In this case we consider two alternative technology cases. First we consider how the global PGM demand will respond to the rise of an alternative vehicle such as battery electric vehicles which barely use any PGM, holding other vehicle technologies constant; secondly we consider how the global PGM demand will evolve if the market share of fuel cell vehicles considerably increase, holding other vehicle technologies constant.

Consider a case where the share of battery electric vehicles increases by a factor of ten (High Alternative I) at the expense of gasoline and diesel vehicles proportional to their current market share, we obtain a global PGM demand forecast for the High Alternative I Case:

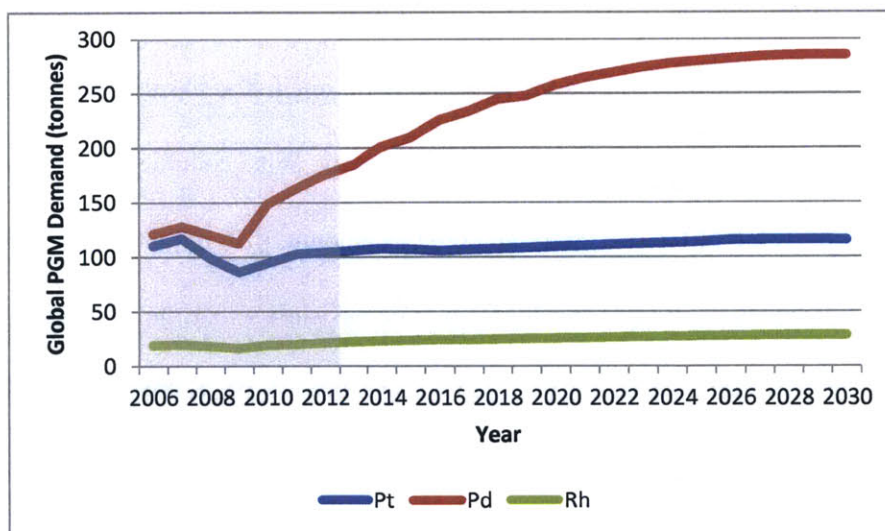


Figure 13: Global PGM demand if the market share of electric vehicles increase by ten folds in the next fifteen years.

This scenario indicates that given the minor share of electric vehicles, even if their market share increases by ten folds at the expense of gasoline and diesel vehicles, the impact on the global PGM demand is not likely to be dramatic. Indeed, the simulation of this model suggests that the global Pt, Pd, and Rh demand will decrease by about 5.2%, 6.6%, and 7.3% compared to the base case, respectively. Therefore, it is perhaps safe to conclude that even a relatively rapid share expansion (in this case, a market share growth rate of 11%/year) of the electric vehicle market will not necessarily contribute a significant drop in terms of the PGM global demand.

In the second scenario, we assume the market share of fuel cell vehicles increases by a factor of ten, and examine its impact on global PGM demand. Fuel cell vehicles does not use catalytic converters, for the only exhaust it produces is water. Most current research has been done for proton exchange membrane (PEM) fuel cell vehicles; therefore we confine our discussion in PEM-FCV. However, fuel cell uses Pt as a catalyst at the anode to knock off the hydrogen atoms' electrons, leaving positively charged hydrogen ions and free electrons.[87] A membrane placed between the anode and cathode only allows the ions to pass through. The electrons must travel along an external circuit – generating an electric current. What complicates the picture is the rapid decrease of the originally humongous amount of Pt required as a catalyst in fuel cell vehicles. A study done by C. E. Thomas shows that the Pt loading has decreased greatly over the past ten years from 65g (2005) to 39g (2008) to 24g (2010) and a projected 16g in 2015[88]. We assume the Pt loading will stay at 16g, bearing in mind a caveat that our forecast will be an upper-bound for the Pt global demand given



the said ten-fold market share increase.

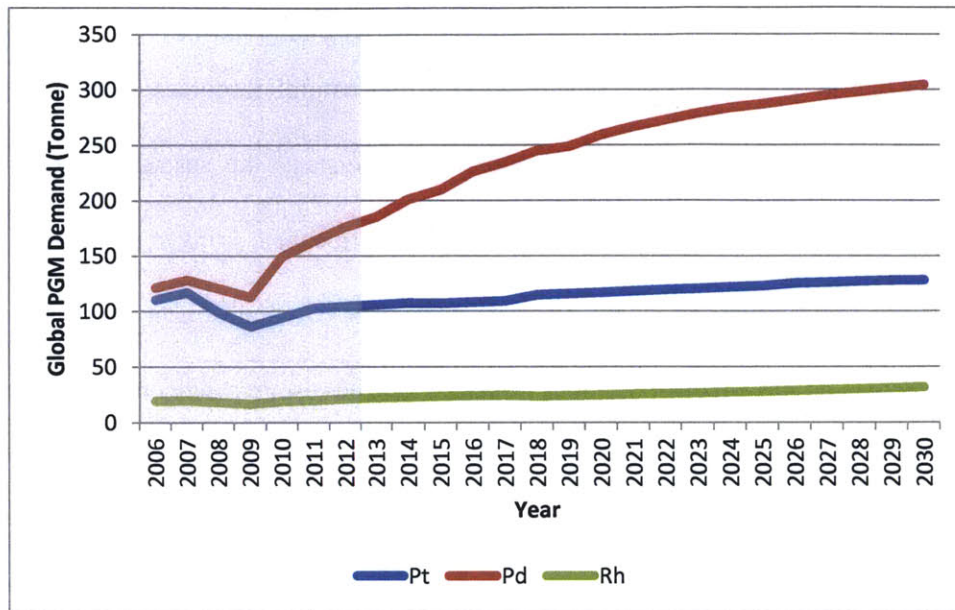


Figure 14: Global PGM demand for a case where the market share of fuel cell vehicles increases by ten folds.

The simulation reveals that a ten folds increase in the market share of fuel cell vehicles will have minor impact on the global PGM demand for Pd and Rh, and a slightly greater impact on the global PGM demand for Pt. Based on this simulation, the demand for Pd and Rh will decrease by 0.42% and 0.88%, respectively, whereas the demand for Pt will increase by about 5.6%, all being compared to the Base Case. The demand increase in Pt, however, is an upper-bound given the rapidly evolving technology that consistently decreases the Pt usage per fuel cell vehicle over the past ten years.

## 5. Conclusions and Future Work

### 5.1. Conclusions

In a world where consumption of exhaustible natural resources increase in an almost exponential fashion, it is essential to understand the sustainability of our consumption pattern in the long run, and to be able to enable firms to make informed purchasing and design decisions in the short run. The two mainstream approaches we have reviewed have their individual weaknesses. The resource economists' approach suffers from its abstracted treatment of the technological influence on resource economics. It frequently fails to recognize the imperfect substitutability among minerals, the derived demand characteristics of different resources, and is at many occasions too forward looking and dismissive of short-term volatilities. The existing dynamic materials flow assessment literatures indicate a vast majority of them adopt a top-down approach which is not robust against the Lucas critique. In addition, they either treat economic and physical feedbacks somewhat separately, or simply ignore one and focus on only the other.

In this thesis, we propose a bottom-up prospective dynamic materials flow assessment modeling approach to investigate and project the global PGM demand to assist manufacturers and firms relying on these raw materials to make informed decisions. The model aims to integrate technology and economics on a micro-level, and aggregate the micro-scale PGM use to obtain a robust and accurate projection of the macro-level PGM demand. It overcomes the deficiencies of the resource economists' approach by conducting an in-depth meta-analysis that considers the

partial substitutability between Pt and Pd, and the complementarity of Pt with respect to Rh, and Pd with respect to Rh and integrates such materials characteristics into the microeconomic model. It reflects the derived demand characteristic of these minerals by investigating the automotive sector – the dominant PGM-consuming industrial sector. On the other hand, it addresses the deficiencies of the current DMFA approaches by aggregating micro-level behaviors to obtain the global PGM demand to make the model robust to structural changes, and considers both physical and economic feedback. It also incorporates short term volatility by conducting scenario analyses of relative price changes and examines the impact of such changes on the global PGM demand.

Some of the key conclusions obtained from this model are:

- (i) The global demand of Rh is unlikely to be very responsive to price changes caused by substitutability – it is mainly a complimentary catalyst to Pt and Pd;
- (ii) Given the price ratio of the past, and absent major technological innovation, the gasoline engine is likely to rely heavily on Pd and little Pt, whereas the catalyst in the diesel engine is likely to be composed mostly of Pt and little Pd;
- (iii) When the relative price between Pt and Pd increases, the global demand of Pt will decrease, and the global demand of Pd will increase, the ratio of the absolute value of changing demand reflects the catalyzing effects of Pt and Pd;

- (iv) When the emission regulation tightens, and if such a tightening regulation cannot be offset by increasing efficiency provided by a fixed amount of PGM usage, the PGM use per vehicle will increase, and such a vehicle level PGM use increase will be reflected in the global PGM demand;
- (v) If diesel vehicle sales see a considerable increase at the expense of gasoline vehicle sales, absent technological innovations that make Pd effective in diesel engines, the growth rate of global demand of Pt will increase, and the growth rate of global demand of Pd will decreased, with the Base Case as a reference.
- (vi) The rise of alternative vehicle technology is unlikely to dramatically reshape the PGM demand in the foreseeable future. However, given the prevailing technology, a rise of sales of fuel cell vehicle compared to the Base Case will decrease the global demand of Pd and Rh, but will increase the global demand of Pt; a rise of sales of electric vehicle will decrease the global demand of all three PGM.

## 5.2. Future Work

It is critical to keep in mind that a model is simply an abstract and simplified representation of a complicated reality. Therefore it is almost certain that there are strengths and weaknesses in each modeling methodology, and the modeling approach proposed in this thesis is not exempted from this iron-clad rule.

The fleet level data is obtained from the SMP fleet model, and if there is an

inaccuracy in the SMP data, then the model that builds on it is certainly likely to suffer from the inaccuracy caused by the SMP data.[86] Likewise, the meta-analysis, though encompasses a vast number of literatures, is not immune to imprecision and data with sub-optimal quality. Future work can be done to improve any imprecision caused by the existing analysis.

The emission regulation scenario (section 4.2.3) is at best a first-order approximation, for the model has largely treated the regulatory standard as a exogenous variable, namely, it is not determined within the system. This treatment, the author believes, is reasonable, but the exogeneity of it makes a realistic and accurate treatment of it difficult, if not impossible. After all, the tightening regulation is partially a political outcome achieved by various institutional schemes. In addition, the upgrade of emission regulation in each region of interest is, after a detailed and serious historical assessment, ultimately arbitrary. Future work can consider how to better incorporate the emission regulation variable into the system.

This model stands out among the others for it is techno-economic on a micro-level. However, though the model has done its best to capture the state-of-the-art technological condition in this industry, it is incapable of capturing or envisioning any future technological innovations, and therefore has to treat any future technological innovations as true “innovations” in a time-series analysis sense. Future work can be directed towards a more sophisticated treatment of technological factors to make the model an even better integration of the technological and economic world.

Lastly, a global demand forecast is scary because of a simple reason – the world is too big, and the interactions within the world too complicated. The current model has divided the world into five distinct regions – the two most developed lumps, United States and Europe, and the two fastest developing countries, China and India, and the rest is lumped altogether into ROW. If a more accurate global demand is required, then a further breakdown is necessary. It is important to keep in mind that there is always a trade-off between sophistication and robustness. Future work can be directed towards discovering if a better division of the world, in the sense that it provides a more representative and holistic description of the world, is possible, and how will such a division change the outcomes we have thus far obtained.

After all being said, the flexibility offered by the model, combined with the ease of use of spreadsheet, should provide a convenient jumping board that future adventurers can take advantage of to embark on a journey that leads to greater splendor.

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