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By

Michele L. Bustamante

A DISSERTATION

Submitted in Partial Fulfillment of the Requirements for the Degree of Doctor of Philosophy in Sustainability

Department of Sustainability
Golisano Institute of Sustainability
Rochester Institute of Technology

May 2016

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SUSTAINABILITY PROGRAM  
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May 2016
ABSTRACT

Golisano Institute for Sustainability
Rochester Institute of Technology

Degree: Doctor of Philosophy
Program: Sustainability

Name of Candidate: Michele L. Bustamante

Title: Criticality of Byproduct Materials: Assessing Supply Risk, Environmental Impact, and Strategic Policy Response for Tellurium

Creating a more sustainable future will require a transition toward more clean energy technologies. As technology shifts, the portfolio of materials needed to support the energy sector will shift as well. To prevent resource scarcity challenges, it is necessary to investigate multifaceted risks for energy materials. In recent years, a tool known as criticality assessment has been used for this purpose, identifying economic vulnerabilities for key energy, defense, and electronic technologies. These studies intend to guide strategic response to reduce risk; however existing methodologies lack a comprehensive systems perspective necessary to inform decisions.

This is particularly true for materials supplied from byproduct mining. Byproduct minerals (e.g. tellurium, indium, gallium) are unintended minor joint products generated while mining and refining major metals (e.g. aluminum, iron, copper). They contribute only marginally to profit, so their extraction is justified strictly by association with the carrier metal ore, linking their supply, both physically and economically, to the system of materials being produced by the joint process. This level of interconnection is not well captured by the single-product focus characteristic of existing criticality assessments, potentially misrepresenting risks for byproducts.

This dissertation aims to inform more appropriate policy response by addressing key gaps in criticality assessment and mitigation for byproduct minerals through the application of various systems modeling tools, including dynamic material flow analysis (dMFA), life cycle assessment (LCA), and scenario-based uncertainty analysis. Resulting contributions address the following specific challenges: (a) supply risk assessment neglects carrier metal production dynamics, (b) environmental risk assessment is sensitive to variability in impact allocation assumptions, and (c) standard, static result metrics are poorly matched for development of dynamic risk mitigation policy. Novel methodologies are demonstrated throughout using a case study of tellurium, a byproduct of copper refining critical to rapidly-growing CdTe thin-film photovoltaics.
ACKNOWLEDGEMENTS

Words cannot express the gratitude I have for my advisor and greatest champion, Dr. Gabrielle Gaustad. Her strength, intellect, compassion, and humor have been and continue to serve as a tremendous inspiration to me both professionally and personally. She has exemplified everything it means to be a leader; pulling the best from me by choosing empowerment as motivation over fear and constantly providing me with opportunities to grow. She also helped me overcome some of the greatest personal challenges of my life, always allowing me the time and space I needed to recover while reminding me that not only was it okay to keep moving forward but that I owed it to myself even when it felt too heavy. Thank you for being exactly the kind of mentor I needed and for never giving up on me.

Throughout this arduous academic marathon known as getting a PhD, I have been incredibly fortunate to also have the support of my committee. Thank you to Dr. Callie Babbitt, who has also served as an attentive teacher and mentor over the years, for being an endless source of inspiration and wisdom. Observing her quickness, discernment, imagination, and eloquence has motivated me to strive for such virtue within myself. To Dr. Elisa Alonso, who graciously agreed to serve states-away as an external committee member, thank you for consistently going above and beyond to support my efforts. Her unique perspective led to feedback that was invaluable and has greatly improved the quality of my work. I sincerely admire her patience and the sacrifices she made to help me grow as a researcher.

To my GIS family of faculty, staff, and students, I thank you for your part in nurturing my passion for sustainability, for challenging me to think deeply and critically about complex global problems, and for arming me with the skills to begin addressing them. I treasure the unique experience I have had in our budding department, and I appreciate all the hard work you have collectively put in to provide a fertile foundation for students to become independent and dynamic professional thinkers. Special thanks to Drs. Thomas Trabold, Eric Williams, Eric Hittinger, Amit Batabyal, Jeffery Wagner, Santosh Kurinec, Seth Hubbard, Nabil Nassar, and Paul Steibetz, who have all directly supported my academic journey in one way or another. To Donna Podeszek and Lisa Dammeyer, thank you for the many long chats, the always helpful advice, and the loving energy you brought to my experience. To my dear friends and classmates, especially Brittany, Liz, and Berlyn for spending the most time dealing with my nonsense, thank
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This work is dedicated in loving memory to my brother, David Bustamante, who passed during my studies. Know that I carry you in my heart every single day, and that I will always find a way to keep you a living part of my life. I love you, big guy.
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CHAPTER 1. Introduction

1.1. Transitioning to a Cleaner Energy Future

The impacts humans have had on the natural environment has fundamentally changed since the dawn of the industrial age. Improvements in health care and sanitation triggered an explosion in global population from 800 million in 1750 (US Census Bureau (USCB) 2013) to 7.3 billion today (United Nations (UN) 2015), representing a major regime shift from near steady-state growth of less than 0.3% per year to growth at a rate of 1-2% growth per year for the past 50 years (UN Department of Economic and Social Affairs 2001). Supporting this population growth alone would have added tremendous pressure to the natural ecosystem; however, simultaneously, societies began shifting away from agrarianism toward more industrial activities, exacerbating this effect. Industrial societies use between 2 to 10 times more energy per capita and 2 to 8 times more materials per capita than agrarian societies (Haberl et al. 2011). As a result, industrialization during the 20th century contributed to a doubling in average per capita material and energy intensity worldwide (Krausmann et al. 2011). Finally, the industrial transition was accompanied by a shift in the kinds of energy and materials being used, from primarily renewable resources to nonrenewable ones. Wood, wind, water, and animal power were replaced by higher energy-density fossil fuels – first coal, then petroleum, then natural gas. Similarly, material usage has shifted from textiles, natural ceramics, and major metals to an ever-diversifying plethora of petroleum-based plastics, complex ferrous and non-ferrous alloys, and high-purity specialty metals. Together these trends set the stage for key sustainability challenges being faced today: namely, anthropogenic climate change and resource scarcity.

The global energy sector contributes heavily to both these issues. Total primary energy supply in 2010 was made up of 29% coal, 34% oil, and 22% gas, for a total of 85% from carbon intensive fossil resources. As a result, energy supply is currently responsible for 35% of annual anthropogenic greenhouse gas emissions, which is greater than any other economic sector (Bruckner et al. 2014). Considering the global, social, and environmental implications of these emissions for climate change, human health damage, and eco-toxicity, transitioning to a more holistically sustainable energy supply chain will be crucial moving into the future. This transition will likely be facilitated by action plans coming out of the international climate agreement reached at COP 21 in December 2015. Over 180 nations committed to the development of intended...
nationallly determined contributions (INDCs), of which energy is a priority to address. While promising as a top down motivation, achieving this transition in practice will be one of the grand challenges of science and engineering in the modern age.

One energy source which many believe should play a significant role in a future clean energy mix is solar. Solar energy has many benefits. First, as a renewable resource, there is no concern about depletion of the fuel source, which in this case is the sun. Further, the sheer abundance of as an energy resource is virtually unmatched. Globally, solar radiation incident on Earth is 520 times the global power demand (27 times if only considering viable land area), which is 4 times more than the power available from wind (Jacobson and Delucchi 2011). Finally, direct emissions from use of solar photovoltaics are non-existent under normal operating conditions, an important advantage over traditional fossil fuel sources of electricity, like natural gas and coal.

There are of course challenges for solar PV as well. This is evidenced by its current negligible contribution to electricity production (0.8% in the US (US Energy Information Administration (EIA) 2016) and 1% globally (Solar Power Europe 2015), respectively, in 2015). Although abundant overall, the solar resource is intermittent at a local scale due to variations in time of day, weather, and season. Additionally, conversion efficiencies are still quite low: commercial module averages remain below 20% (Fraunhofer Institute for Solar Energy Systems (ISE) 2016). Further, in most locations, solar electricity is still significantly more expensive as compared to grid electricity; levelized cost of electricity (LCOE), a normalized measure of electricity price among different technologies, shows solar PV can be up to 6 times more expensive than coal or natural gas (International Renewable Energy Agency (IRENA) 2015).

Fortunately, significant progress has been made in recent years. Crystalline silicon PV module efficiency has increased by 1/3 in the past 10 years, and its price has declined consistently by about 20% for every cumulative doubling of production. In addition to progress within traditional, first generation crystalline silicon technology, many alternative forms of PV technologies have been developing with promising results. For example, second generation technologies made from thin film semiconductors require much less active material (Wadia, Alivisatos, and Kammen 2009) and are often easier and less costly to produce and can be flexible. Progress in thin film technologies has led to record efficiencies above 20% with manufacturing costs as low as $0.40/W. More diverse and complex third generation technologies aim extreme high efficiency (e.g. multi-junction PV) or low costs (e.g. organic PV). Examples of each are
summarized in Table 1. Progress in Gen III technologies has propelled the recent achievement of a 46% efficient multi-junction solar cell and led organic PV to quadruple in efficiency (National Renewable Energy Laboratory (NREL) 2016). As a whole average commercial module prices have declined by 75-80% over the past 5 years (International Renewable Energy Agency (IRENA) 2016). These technical and economic improvement has helped usher in a period of previously unseen solar PV deployment, growing at a compound annual growth rate (CAGR) of 44% between 2000 and 2014, reaching 183 GWp cumulative installed capacity.

Table 1. Overview of solar photovoltaic technologies (National Renewable Energy Laboratory (NREL) 2016).

<table>
<thead>
<tr>
<th>PV Class</th>
<th>Technologies</th>
<th>Elements in Active Layer</th>
<th>Record Cell Efficiency</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Generation I</strong></td>
<td>Crystalline Silicon (c-Si)</td>
<td>Si</td>
<td>21.3% (multi)</td>
</tr>
<tr>
<td></td>
<td>(multi-, mono-)</td>
<td></td>
<td>25.0% (mono)</td>
</tr>
<tr>
<td><strong>Generation II</strong></td>
<td>Amorphous Silicon (a-Si)</td>
<td>Si, H</td>
<td>13.6%</td>
</tr>
<tr>
<td>(thin films)</td>
<td>CdTe</td>
<td>Cd, Te, S</td>
<td>22.1%</td>
</tr>
<tr>
<td></td>
<td>CIS/CIGS</td>
<td>Cu, In, Se, Ga</td>
<td>22.3%</td>
</tr>
<tr>
<td><strong>Generation III</strong></td>
<td>Multi-junction (MJPV)</td>
<td>In, Ga, As, P, Ge</td>
<td>31.6% (2J, non)</td>
</tr>
<tr>
<td></td>
<td>(two-, three-, four+junction)</td>
<td></td>
<td>34.1% (2J, conc)</td>
</tr>
<tr>
<td></td>
<td>(concentrator, non-concentrator)</td>
<td></td>
<td>37.9% (3J, non)</td>
</tr>
<tr>
<td></td>
<td>Dye-Sensitized (DSSC)</td>
<td>In, Sn, Ti, Zn, O</td>
<td>11.9%</td>
</tr>
<tr>
<td></td>
<td>Perovskite</td>
<td>Pb, I, Br, Cl, C, H, N, O</td>
<td>22.1%</td>
</tr>
<tr>
<td></td>
<td>Organic/Polymer</td>
<td>C, H, N, O</td>
<td>11.5%</td>
</tr>
<tr>
<td></td>
<td>Quantum Dot (QD)</td>
<td>Cd, Se, Ti, O</td>
<td>11.3%</td>
</tr>
<tr>
<td></td>
<td>CZTS/Se</td>
<td>Cu, Zn, Sn, S, Se</td>
<td>12.6%</td>
</tr>
</tbody>
</table>

1.2. Implications for Materials

The developments of advanced technologies, for clean energy generation as well as other important applications like electronics and national defense, has enabled the enhancement of performance; however, in many cases, these benefits introduce trade-offs in terms of raw materials scarcity risks. Consider the solar PV example. Traditional Gen I PV uses silicon for its active layer semiconductor. Silicon is the most abundant element in Earth’s crust apart from oxygen. Conversely, many advanced PV technologies rely on less abundant raw materials to form their
active layer semiconductor compounds (Bleiwas 2010) (Table 1). For example, several Gen II technologies employ potentially scarce materials such as cadmium, tellurium, indium, gallium, and selenium to create compounds with higher optical absorption coefficients across more of the solar spectrum, enabling thinner active layers (i.e. thin film PV) (Wadia, Alivisatos, and Kammen 2009; Shih and Mi 2009; Sunshine PV Corp 2012). Amorphous silicon can also be used to make thin film PV, and was an early leader in Gen II solar. However, with the introduction of thin film technologies with higher efficiency and greater efficiency (CdTe and CIGS PV), a-Si lost market share (Fraunhofer Institute for Solar Energy Systems (ISE) 2016). Gen III multi-junction cells often use compounds of indium, gallium, arsenic, and germanium, among others, to achieve higher efficiencies by capturing more of the solar spectrum via layering of compounds with distinct bandgaps (International Energy Agency (IEA) 2010). Across the different advanced PV technologies, the elements highlighted in Table 1 are significantly less abundant than silicon used in traditional PV; in fact, several million times less so in the case of the rarest inputs: tellurium, selenium, and gallium (Haxel, Hedrick, and Orris 2002).

Despite the potential scarcity issue, advanced PV is finding a greater place in the PV market; primarily the thin film technologies, which grew from 4% of the global market in 2003 to 17% in 2009 before settling around 10% for the past 5 years (Fraunhofer Institute for Solar Energy Systems (ISE) 2016). Currently, CdTe is the dominant form of thin film photovoltaic technology on the market with over 10 GW installed worldwide (First Solar 2015a). This technology offers several technical benefits over its competition. CdTe has a near ideal fit to the incoming solar spectrum with an intrinsic bandgap energy of 1.5 eV (Kumar and Rao 2014). The latest modules on the market from First Solar operate at 16.1% - 16.8% efficiency (First Solar 2016). For the first time since 2011, this technology has also regained a cost advantage over inexpensively produced Chinese silicon panels (Martin 2016). CdTe manufacturing costs are reported to be as low as $0.40/W with goals of $0.25/W possible in the near future (Martin 2016). The technology also has a distinct advantage in extreme high temperature and high humidity environments, outperforming its conventional peer, crystalline silicon (Strevel, Trippel, and Gloeckler 2012; First Solar 2015b). Additionally, CdTe has also been touted as the current leader in environmental performance among commercial solar cells with energy payback time of less than 1 year among its strongest claims (V Fthenakis et al. 2009; Held and Ilg 2011; Peng, Lu, and Yang 2013; Goe and Gaustad 2014b; First Solar 2015b).
However, there is significant concern from a materials perspective about CdTe PV. There are diverging opinions about the environmental risks presented by use of potentially toxic materials in CdTe PV. Toxicity related research has primarily focused on risk of cadmium release (Vasilis Fthenakis and Zweibel 2003; Vasilis M Fthenakis 2004; V. M. Fthenakis et al. 2005; Bravi et al. 2010) since it is a potentially fatal, known human carcinogen and kidney antagonist, among other effects, in elemental form (Jarup et al. 1998). Toxicity of elemental tellurium is significant in animal studies, but in human exposure, effects are minimal (Gerhardsson 2014). A few studies have also characterized CdTe toxicity, showing inhalation to have produced acute lung toxicity and mortality at high concentrations in rats and concluded that CdTe is likely to be as toxic as cadmium (V M Fthenakis et al. 1999). However, due to encapsulation, risks of cadmium or CdTe exposure are proclaimed to be low, even in the extreme instance of fire (V. M. Fthenakis et al. 2005; Sinha et al. 2008).

Additionally, as previously mentioned, tellurium is among the rarest elements on Earth. Scarcity makes the ability to meet rapidly growing demand less certain and therefore introduces risk. The long term availability of tellurium for use in PV manufacturing has been questioned and assessed many times throughout the literature with the goal of understanding limits to PV growth. Existing studies have focused on quantifying ultimate availability (i.e. reserves/resources) (Vasilis Fthenakis 2009; Wadia, Alivisatos, and Kammen 2009; Candelise, Speirs, and Gross 2011) or short-term availability (e.g. annual production rates) relative to PV demand (Andersson et al. 1998; Feltrin and Freundlich 2008; Houari et al. 2014). However, most of these studies neglect a key complication in the supply chain of many of these materials: they are produced solely or predominantly as byproducts.

1.3. Byproduct Materials

Theoretically, there are two basic forms of mineral production: one which yields a single valuable product and one which yields more than one valuable product. The former, referred to here as monoproduction, represents as an ideal production pathway where mineral ore is extracted, processed, and refined to obtain a single material. Monoproduction is the simplest form of production because it only has to be optimized for one material product. All costs incurred are attributed to the single final material, and therefore all extraction decisions are driven by profit maximization for that material. Conversely, joint production is a compound production pathway
where a shared mineral ore is extracted and, during processing and refining stages, multiple valuable products are generated. Despite being the simplest economically, monoproduction is a fairly uncommon route in reality. It is far more typical to produce multiple valuable products from a single mining product (N T Nassar, Graedel, and Harper 2015). Particularly for materials that are geochemically rare or dispersed, it is economically advantageous to exploit residues generated throughout the purification processes of major metal production for their trace valuable content. This type of process is often referred to as coproduction; however, to avoid confusion with a distinct subcategory of this form by the same name, the general process will be referred to instead as joint production throughout the present work.

Within joint production there are two further distinctions possible: coproduction and byproduction (Figure 1a). Coproduction is a form of joint production where the outputs are all similarly valuable. In certain situations, there is a clear main product, which dominates in terms of mass and profit generation. There may also be coproducts, which contribute appreciably enough to the economics of the process that they are factored into profit maximization decisions regarding process volumes. The coproduct(s) can sometimes justify the extraction process on its/their own; however, the ability of a coproduct to bear the entire costs of the shared process is not a requirement to be considered a coproduct. Conversely, byproduction is a form of joint production where there is a clear main product and one or more minor byproducts, usually scavenged from a waste stream. Byproducts earn their name because they can never bear the costs of the shared process and are only extracted along with production of the main product and/or coproducts (Petrick et al. 1973; Campbell 1985).

To clarify this distinction, a short term supply curve for a generic mining producer is presented in Figure 1b. Byproduction is described by the segment from 0 to D and D to E. The price at point D is equal to the marginal cost associated with processing the byproduct as opposed to wasting it. For a minor output with price less than D, the costs to produce as a byproduct will outweigh the economic benefit of having processed it; as a result, expected output is fixed at 0 for all prices less than D. At or above price D, the output of byproduct is justified, but it is fixed with respect to the amount of ore being produced. For all prices between price D and price E, there is no economic incentive to process more ore, so output is fixed at quantity A. Between price E and price F, the minor output is considered a coproduct. The costs of processing more ore to generate more minor product are finally met or exceeded by revenue from the joint sale of products, creating
economic incentive to base profit-maximizing process decisions upon multiple outputs. However, in this zone, as price increases, marginal production increases more rapidly until, above price E, it begins to dominate the process and can be considered the main product. Main products have declining marginal production rates with respect to increasing price, consistent with the law of diminishing returns (Campbell 1985).

Figure 1. Joint production and supply inelasticity. (a) Forms of mineral production pathways, including joint production of coproducts and/or byproducts. Color of ore is used to indicate ore grade, i.e. darker gray for higher ore grade of minor joint product (black circles). Size of circles for refined minerals is used to indicate relative value of products. (b) Short term supply curve for different types of products, modified from (Campbell 1985). Between 0 and price at E is the behavior of byproducts, between price E and F is the behavior of coproducts, and above price of F is traditional main or monoprodut behavior. (c) Price inelasticity of byproduct and, to a lesser degree, some coproduct supply induces greater price volatility.
Because they are not mined independently, supply of a joint product is somewhat constrained by economic considerations for the main product. The degree of constraint is different for coproducts and byproducts. Since byproducts do not contribute meaningfully to profit, market forces such as greater demand or higher prices do not affect decisions to process more or less shared ore. This constrains the supply of the byproduct in a manner not directly driven by its own demand, which can result in greater than average price volatility for byproduct materials (Campbell 1985) (Figure 1c). It can also create scenarios where supply is temporarily disrupted due to demand growth in the face of unresponsive supply (M. L. Bustamante and Gaustad 2014a).

Conversely, coproducts are not as constrained because they do factor into process economic decisions (Brooks 1965; Petrick et al. 1973; Campbell 1985). However, they are more constrained than ideal monoproducts would be because the quantity supplied of each coproduct is selected to optimize the overall profit, not necessarily to respond optimally to market forces for any individual product. This results in the same price effects as are observed for byproducts, but to a lesser degree.

Examples of clean energy materials that are jointly produced are plentiful (Table 2). Gallium and indium, used in CIGS thin film PV and various III-V multi-junction concentrator cells, are byproducts of aluminum and zinc production processes, respectively. Cadmium and tellurium, used in CdTe thin film PV, are both byproducts of zinc and copper production respectively. Selenium, used mainly in CIGS PV, is also a byproduct of copper production (Bleiwas 2010). Additionally, coproduct and byproduct rare earth elements, like Nd and Dy, are used in high strength magnets that find application in wind turbines, electric vehicle motors, and battery technologies, and are often produced in conjunction with iron (Table 2). As expected, prices for many of these joint materials are more volatile than for carrier metals. Figure 2 shows price trends from 1990 to 2014 (adjusted for inflation) for two byproducts, tellurium (Figure 2a) and indium (Figure 2b). Tellurium price ranged from as low as $2014 42.41/kg to a peak price of $2014 370/kg in 2011 (215% above its average of $2014 117/kg since 1990), it varied year-to-year by an average of 35% in either direction, and between 2007 and 2008 the price more than doubled (+147%) in a single year. Similarly, indium price ranged from as low as $2014 128/kg to a peak price of $2014 1147/kg in 2005 (130% above its average of $2014 539/kg since 1990), it varied year-to-year by an average of 36% in either direction, between 2004 and 2005 the price nearly quadrupled (+268%) in a single year, and between 2003 and 2006 price ramped up by 800% in 3 years. Compare these results to a non-byproduct material, like tellurium’s carrier, copper (Figure
which peaked in 2011 with tellurium but only to 87% above its 25-year average of $5.03/kg (2011 peak = $9.43/kg), exhibited lower year-to-year variations of on average of 27% when increasing and 12% when decreasing, and, finally, experienced a maximum single year price increase of 76% between 2005 and 2006, which is less than half that shown by tellurium and less than one third that shown by indium.

The greater price volatility exhibited by byproduct materials is concerning because it can slow growth of technologies that utilize these raw materials. Rapid price increases, if sustained for long enough, can even drive manufacturers out of business. This is particularly true for budding technology firms, like clean energy manufacturers. This is an important challenge to recognize for clean energy technologies, which are able to utilize renewable fuels, but still depend upon specialty raw material inputs for manufacturing. Such potentially scarce and important functional materials are often referred to as critical for that application.

Table 2. Jointly produced materials used in clean energy applications and their dominant carrier ores (Bauer et al. 2011; Buchert, Schüler, and Bleher 2009; Talens Peiro, Villalba Mendez, and Ayres 2011; US Geological Survey (USGS) 2016; Bleiwas 2010).

<table>
<thead>
<tr>
<th>Joint Product Elements</th>
<th>Carrier Metals</th>
<th>Clean Technology Applications</th>
</tr>
</thead>
</table>
| Rare Earths (Nd, Dy, Eu, Tb, Y) | Iron Rare Earths (Ce, La) | • Wind Turbines  
• EV motors  
• Batteries |
| Tellurium | Copper Lead | CdTe PV |
| Gallium | Aluminum (Bauxite) Zinc | CIGS PV  
• III – V MJPV |
| Indium | Zinc Lead | Batteries  
Hydrogen catalyst production |
| Cobalt | Nickel Copper | |
Figure 2. Price volatility for byproducts versus a main product. Byproducts: (a) tellurium and (b) indium (M. L. Bustamante and Gaustad 2015). Main product: (c) copper (US Geological Survey (USGS) 2014a).
1.4. Critical Materials & Criticality Assessment

The term critical in a material context has double meaning. First it refers to the crucial, indispensable, vital, or highly important role the material plays in a particular technology, firm, economic sector, or the economy as a whole (e.g. critical component). Further, this means the materials lend functionality that is very difficult or impossible to replace in that context. Finally, critical can also refer to being in or approaching a state of crisis (e.g. critical condition) or relating to a turning point or especially important juncture (e.g. critical point). In other words, a critical material is one that has high economic importance, poor substitutability, and significant risk in its supply chain; a definition which has been used by agencies concerned with criticality such as the US Department of Energy (Bauer et al. 2010; Bauer et al. 2011).

Most commonly, criticality is characterized using a two dimensional framework that considers the material’s scarcity in the context of its economic importance. This is in contrast to a traditional focus on physical measures of scarcity alone. Use of a two dimensional criticality matrix was first put forth by the National Research Council’s 2008 report titled, “Minerals, Critical Minerals, and the U.S. Economy,” where two dimensions of criticality are defined: (I) supply risk (of which scarcity is a factor) and (II) impact of supply restriction (of which demand factors such as substitutability is a factor) (National Research Council (NRC) 2008). Since its introduction, this two-dimensional approach has been applied by government agencies (e.g., Department of Energy (Bauer et al. 2011), United Nations Environmental Programme (Buchert, Schüler, and Bleher 2009), and European Commission (European Commission 2014; Moss et al. 2011) and industry (e.g., General Electric (Konitzer, Duclos, and Rockstroh 2012)) to analyze criticality at various scales (local, corporate, national, and international) for various economic sectors (energy, electronics, etc.) and for various timescales (short-term, mid-term, long-term). However, the most common sector of focus in these and other published studies is, by far, the energy sector because of interests in changing energy mix and potential sustainability trade-offs represented by clean technologies based on scarce, risky materials (Bauer et al. 2010; European Commission 2010; Bauer et al. 2011; Moss et al. 2011; Graedel 2011; European Commission 2014; Goe and Gaustad 2014a).

More recently, criticality research has begun considering the role of environmental factors in supply chain security, as alluded to in the original NRC report (National Research Council (NRC) 2008). The Yale Critical Materials Group has identified some indicators in this category
such as human health and ecosystem damages (Graedel et al. 2012). Since then, other researchers, such as Goe and Gaustad, have stepped in to apply and expand upon this three-dimensional approach to characterizing criticality (Goe and Gaustad 2014a). The Yale Group has produced many publications of this type, focusing on different groups of materials from their own application of the three-dimensional model, which is now composed of more than two dozen indicators (Graedel et al. 2012; Nuss et al. 2014; Harper et al. 2015; Harper et al. 2014; Panousi et al. 2015). The key results of these studies are summarized in three most recent studies that allow for comparison across different related material groups (Graedel and Nuss 2014; Graedel et al. 2015; N T Nassar, Graedel, and Harper 2015).

The evolution of criticality as a multifaceted assessment tool is shown in Figure 3. Several examples of indicators used to quantify each dimension are also shown. In each framework, two theoretical materials, A and B, are placed in space to show the direction of high and low criticality; B is a high criticality material, A is a low criticality material.

Figure 3. The evolution of criticality assessment as a sustainability tool. Theoretical materials, A and B, placed in each framework show B having greater risk or criticality than A.
Criticality can be a somewhat ambiguous characteristic because it is highly dependent upon a stakeholder perspective, i.e. to whom is the material important? The same material can be deemed critical to a particular economic sector, e.g. clean energy (Bauer et al. 2010; Bauer et al. 2011) or defense (US Department of Defense (DOD) 2015; US Department of Defense (DOD) 2013; US Department of Defense (DOD) 2008) but not to a specific company, like GE (Ku et al. 2014; Ku and Hung 2014; Konitzer, Duclos, and Rockstroh 2012), or perhaps what is critical to a nation or international group, like the EU (European Commission 2014; Moss et al. 2011; European Commission 2010) is not necessarily critical to the broader global economy (Harper et al. 2015; Nuss et al. 2014; Graedel et al. 2015; Erdmann and Graedel 2011; Panousi et al. 2015; Harper et al. 2014; N T Nassar, Du, and Graedel 2015; Graedel et al. 2012). For example, indium, tellurium, selenium, gallium, and germanium are examples of solar-critical materials, whereas rare earth elements (REE), such as dysprosium and neodymium, are critical to wind energy (Bauer et al. 2011).

Results of literature review on tellurium criticality are summarized in Table 3. Tellurium has been deemed as highly critical by select studies focusing on the global clean energy sector (Buchert, Schüler, and Bleher 2009; Moss et al. 2011; Moss et al. 2013). However, it has also been deemed as not critical of low criticality by several others focusing on the European nations, specifically (Morley and Eatherley 2008; European Commission 2010; European Commission 2014) and US national defense technologies (US Department of Defense (DOD) 2015). Most studies classified tellurium as somewhere in the middle (Bauer et al. 2010; Bauer et al. 2011; Nedal T Nassar et al. 2012; Graedel et al. 2015; Goe and Gaustad 2014a; Erdmann, Behrendt, and Feil 2011; Morley and Eatherley 2008). Notably, in several of these studies, tellurium was located right near the threshold of the highest criticality group (Erdmann, Behrendt, and Feil 2011; European Commission 2010; European Commission 2014). In these situations, it has been suggested that minor changes in underlying assumptions regarding data or threshold definition could shift tellurium into the higher group (European Commission 2010; Glöser et al. 2015).

The research summarized thus far only represents one family of criticality research: criticality characterization. Another important consideration is criticality mitigation. Research in this space investigates possible strategies for reducing risk in the supply chain, such as finding substitutes for the critical material. An example of this type of research can be found by looking to GE Aviation, who focused on the evaluation of a substitute for high-purity rare-earth oxides in
the synthesis of disilicate, ceramic matrix composites, used for the protection of important engine components (Ku et al. 2014). Other examples look at the role of recycling, reduction of material utilization, and improvement of yield in mitigating supply risk (M. L. Bustamante and Gaustad 2014a; Du and Graedel 2011; Marwede and Reller 2012).

Table 3. Overview of criticality classifications for tellurium across numerous studies in the literature.

<table>
<thead>
<tr>
<th>Criticality Study</th>
<th>Score</th>
<th>Scope</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bauer/DOE 2010/2011</td>
<td>Near-critical</td>
<td>Global/US, Clean energy sector, Short-term (0-5 y), Mid-term (5-15 y)</td>
<td>Supply risk = 50%, importance to clean energy = 75%</td>
</tr>
<tr>
<td>Yale 2012/2015</td>
<td>Medium criticality</td>
<td>Global (long-term), US, Firm (mid-term)</td>
<td>2012: 33% (global), 40% (US), 49-58% (firm) 2015: 45-55% (global), 45% (US)</td>
</tr>
</tbody>
</table>
| European Commission 2010/2014 | Not critical | Global | “a slight change in underlying variables may result in [tellurium] being reclassified as ‘critical’”  
          |             |                | • Threshold: Supply = 10%, Importance = 50%, Environmental = 12%                                                                 |
          |             |                | • 2010: Supply = 5.6%, Importance = 79%, Environmental = 3.5%                                                                       |
          |             |                | • 2014: Supply = 1.9%, Economic = 59.8%, Environmental = N/A                                                                       |
| DOD/DLA 2015           | No net shortfall under base case | US, industry, defense and civilian requirements | • Gross shortfall of 52 tonnes predicted under “Closed Economy” (no imports) scenario  
          |             |                | • Authorized cadmium zinc telluride substrates to national defense stockpile FY 2014                                                 |
| Moss & Tzimas/JRC 2011/2013 | High criticality | EU, Decarbonization of energy sector | Supply = 40%, Importance = 70%  
          |             |                | • Threshold dependent: same vector length as other elements considered “highly critical”                                         |
| Kfw Bank Group 2010    | Medium criticality | Germany | Supply risk – political instability = mid, lack of substitutability = mid, monopoly supply = mid, global warming potential = mid, global consumption = low, total material requirement (TMR) = high |
| Oakdene Hollins        | Low to Medium criticality | Global/UK |                                                                                                                                 |
| Goe & Gaustad          | Medium ranking | Solar materials | 9th of 17                                                                                                                             |
1.5. Research Gaps

Even with the multi-dimensional approach that has developed, understanding the criticality of several clean energy materials can be quite challenging due to the prevalence of byproduct mining in these materials systems. Since byproduct mining involves the production of multiple materials from a singular extraction and/or refining process, its supply is strongly linked to the supply of another material or group of materials. Therefore, in assessing supply risk for the byproduct material, it becomes necessary to consider the material’s production in the context of a dynamic material system rather than in isolation. To date, most criticality assessment methods have failed to do so, neglecting the issue entirely or choosing to address it only superficially. For example, in several multi-dimensional, multi-material criticality assessments, the fraction of production as a byproduct is itself used as an indicator of supply risk, but it is not applied in any meaningful way (Erdmann and Graedel 2011; Graedel et al. 2012; Nuss et al. 2014; Nedal T Nassar et al. 2012; Harper et al. 2014; Harper et al. 2015). Although simpler, this kind of approach which focuses on supply and demand of a byproduct material in isolation does not create a realistic supply chain model, and therefore cannot be expected to consistently produce reliable supply risk results.

Additionally, when evaluating environmental impact dimension of criticality, byproducts introduce a challenge sometimes referred to as “the allocation problem,” where impacts of a single joint production process must be partitioned and assigned to the multiple outputs. There is significant debate in the analytical community regarding the appropriate way to perform this partition, if at all. Further, temporal data variability, such as volatile pricing, may further introduce uncertainty into lifecycle environmental impact assessments of byproduct materials for use in criticality.

Finally, once criticality of a byproduct material has been characterized appropriately, it is important to apply this information in a meaningful way to address the risk that has been identified. This is the ultimate goal of criticality assessment. Current methods are not well suited to inform strategic response aimed at mitigating risk for any material due to highly aggregated presentation of results as well as use of static data and lack of systems perspective.

This dissertation aims to address shortcomings due to lack of systems perspective in each major dimension of criticality assessment (supply risk – as communicated by modeling of scarcity and importance – environmental impact, and informing strategic response) by applying systems modeling tools to expand upon existing methodologies. These approaches will enable researchers
to improve understanding of the sustainability of byproduct materials supply chains and the prospects for their associated technologies. The following chapter (Chapter 2) will address the unique challenges of characterizing byproduct supply by proposing methodology to assess supply risk for byproduct materials by incorporating potentially limiting carrier metal supply dynamics into models of byproduct supply. Chapter 3 addresses challenges posed to quantifying environmental impact due to data variability and modeling decisions regarding allocation; it will also make use of supply modeling from Chapter 2 to improve existing life cycle inventory data. Chapter 4 will address the challenge of translating criticality assessment results to meaningful response by extending the model developed in Chapter 2 to evaluate and compare different supply risk mitigation strategies. Finally, Chapter 5 will tie the findings from each chapter together and conclude with a discussion of remaining work. A visual representation of how each chapter fits together is shown in Figure 4. Given its exemplary status as a critical byproduct material as introduced in this chapter, tellurium will be used as the case study system throughout each chapter.

**Figure 4.** Overview of chapter contributions to goal of improving criticality assessment for byproduct materials within and beyond the three-dimensional framework.
CHAPTER 2. Byproduct Supply Risk: Effects of Carrier Metal Supply Dynamics

2.1. Measuring Supply Risk

Supply risk has historically focused on physical measures of scarcity. One such measure is crustal abundance, or the relative amount of a particular element found in Earth’s crust. Crustal abundance gives the broadest understanding of a material’s rarity, however, it neglects the fact that economic considerations limit supply to exploitation of concentrated ore deposits. In a similar fashion, ore grade measures of the relative amount of a particular substance found in these deposits. Ore grade refines the description of the material’s potential supply and can provide insight into the challenges of resource depletion, where high ore grade deposits are exploited first leading to a gradual decline in average ore grade and leading to larger physical footprint, energy use, and cost of producing the same amount of material. Another related measure of physical scarcity is total mineral resource and reserves, which describe the total quantity of mineral deposits for potential exploitation. Resources include all potential deposits, even those that are not currently economic to exploit, whereas reserves include only deposits that are currently economic to exploit (US Geological Survey (USGS) 2016). Finally, one additional common measure of physical scarcity is depletion time, which calculates how long existing deposits will last at current usage rates. Traditionally calculated as a static index of depletion through a direct ratio of reserves (or resources depending upon the temporal scope) to production, depletion time can also be calculated using slightly more sophisticated approaches that assume, for example, exponential growth of production over time (Alonso et al. 2007) or accounting for secondary supply of material via recycling (Graedel et al. 2012).

The physical scarcity measures described above are effective to communicate long term potential availability; however, in order to understand real world supply risk, it is also important to consider factors that can limit availability of supply in the short term and affect ability to meet demand in carefully balanced markets from year to year. These types of limitations are not mineralogical but rather geosociopolitical, economic, and environmental. Examples of indicators used in this space include the Herfindahl-Hirschman Index or HHI, which is a measure of market concentration in global supply of the material. If a single country dominates global supply, as is

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1 This chapter has been adapted from a manuscript published in Applied Energy in 2014. To avoid a distracting degree of repetitive self-citation throughout the chapter, a blanket reference to the original publication is provided here: (M. L. Bustamante and Gaustad 2014a).
the case for China in many mineral markets, notably including rare earth elements, then any events that occur within that country (extreme weather events, epidemics, war), its mining market (mine closures, strikes), and international trade policies (tariffs, export quotas) has the potential to strongly impact the global supply. For this reason, HHI is often combined with location-specific measures of stability, such as the World Governance Indicators for political stability and absence of violence (WGI-PSAV), the Fraser Institute Policy Potential Index (PPI), or the PRS Group International Country Risk Guide (ICRG), to highlight potential for geopolitical and sociopolitical risk for supply. Environmental regulation can also factor into these supply restrictions, but are often presented separately in criticality frameworks. Another potential source of limitation, which is less well studied, is the impact of forms of production on potential supply; namely risk of supply restriction from byproduction as discussed in Section 1.3.

For example, in recent years promising growth of thin film cadmium telluride solar PV has generated concern about the ability for tellurium supplies to meet the demand of the rapidly growing PV market. Several studies have focused on its potential scarcity of the material (Buchert, Schüler, and Bleher 2009; European Commission 2010; Moss et al. 2011; Nedal T Nassar et al. 2012; Talens Peiro, Villalba Mendez, and Ayres 2011; Ullal and Von Roedern 2007), while others have questioned whether this scarcity makes the technology unsuitable for large-scale development as indicated by reserve data (Candelise, Speirs, and Gross 2011; Wadia, Alivisatos, and Kammen 2009; Vasilis Fthenakis 2009). A number of studies have gone further to use this scarcity to try to determine physical limits to CdTe PV growth (Vasilis Fthenakis 2009; Andersson et al. 1998; Feltrin and Freundlich 2008; Houari et al. 2014). Some look only at the ultimate global resource potential (Andersson et al. 1998; Feltrin and Freundlich 2008). The more advanced studies of this type (Vasilis Fthenakis 2009; Houari et al. 2014; Andersson 2000) recognize that there are constraints to supply over time, creating dynamic resource limitations. However, most studies, even the dynamic ones, have largely failed to capture the true complexity of the tellurium supply chain because of inadequate focus on the way it is produced, which is strictly as a byproduct.

2.2. Supply Risk for Byproduct Materials

Currently, supply risk relating to byproduction are not well captured in criticality studies. For frameworks that consider this factor at all, inclusion may be limited to coarse static metrics,
like binary indications of byproduct supply (yes or no) (American Physical Society (APS) and Materials Research Society (MRS) 2011; Buchert, Schüler, and Bleher 2009) or measures of supply share from byproduct sources (National Research Council (NRC) 2008), which is referred to as companion metal fraction (CM) in the Yale model (Graedel et al. 2012).

The nature of byproduction is necessary and important to understand in the context of supply risk because it implies inelasticity of supply. Extending the previous example, the quantity of tellurium supplied to the market is very insensitive to changes in its own price. Therefore, despite having a higher market value, tellurium is in such low availability relative to the carrier metal, copper, that, even in the case of increased tellurium demand, additional copper ore extraction is not likely to be justified economically as a means of increasing byproduct tellurium supply (Buchert, Schüler, and Bleher 2009; Bleiwas 2010). As a result, the amount of tellurium available for use in CdTe PV and other applications at any given time is not directly linked to the demand for the mineral itself but rather is constrained by supply as dictated by demand for the carrier metal. This introduces risk of supply–demand gaps, which come in addition to risks caused by the mineral’s inherent scarcity. Certainly, prior to large scale deployment of this technology, these risks and more must be thoroughly investigated from multiple angles to avoid trading in one energy security issue (i.e. reliance of foreign oil) for another (i.e. scarcity-induced supply disruption).

Unlike most previous studies, this chapter does not aim to determine the physical limit to technological growth but rather develop a model to describe the magnitude of short-term supply risk posed by historically-observed supply and demand trends in a way that can be used meaningfully in criticality assessment frameworks. To begin, Sections 2.3 and 2.4 provide a discussion of some of the major challenges of byproduct material systems supply chain analysis, focusing specifically on the copper/tellurium system and its application in solar photovoltaic technology. In Section 2.5, methodology is proposed for assessing risk and mitigation potential in the copper–tellurium byproduct system. In Section 2.6, the base case supply and demand scenarios for tellurium are developed and then manipulated to evaluate dynamic sensitivity to each key parameter identified in Sections 2.3 and 2.4. Finally, the work is concluded with a broad discussion of the risks identified, as well as potential for their mitigation through traditional means. The goal is to create a model of supply risk and understand its sensitivities for potential insight into criticality of tellurium and materials like it.
At this point, it is important to re-emphasize that this issue of byproduct criticality is not unique to the copper/tellurium system. It can also be observed in many other clean energy critical material systems, such as aluminum/gallium and zinc/indium (Moss et al. 2011; Buchert, Schüler, and Bleher 2009). With a few modifications, specific to the material system of interest, the methodological framework used in this work could be applied to other byproduct material systems. For instance, despite quantification specific to Cu/Te extraction and processing, the sensitivity analysis presented in Section 2.6 highlights challenges present in many of these material systems. Extension of this methodology would make it possible to more broadly assess the implications of byproduct mining on the future of clean energy production and energy security.

2.3. Challenges for Modeling Byproduct (Tellurium) Supply

Modeling byproduct supply is inherently more challenging than main product supply for a number of reasons. First, materials produced exclusively as byproducts are typically minor metals with low global supply; as such sometimes only one company will produce that material in a given country, leading to proprietary withholding of production data. This is the case for tellurium, where production is withheld from several known producing nations, including the US, Australia, Belgium, Chile, China, Colombia, Germany, India, Kazakhstan, Mexico, the Philippines and Poland (US Geological Survey (USGS) 2016). However, in the years leading up to its cessation of reporting, the US contributed between 40-60% of global reported production, so it should not be neglected (International Copper Study Group (ICSG) 2012). Due to these many data gaps, after 2003, USGS could no longer reliably report global tellurium production from direct national-level reporting data (US Geological Survey (USGS) 2011b). This precludes use of historical global production data as a method to project future supply for tellurium, a technique used for main product materials, like copper, and requires estimation as a function of carrier metal (copper) production trends. However, not all methods of producing copper are the same in terms of implications for tellurium supply, so it is important to understand technology-specific trends in copper supply as well.

2.3.1. Carrier metal (copper) supply chain is diversifying

Although overall demand for copper has grown at a relatively constant rate of 3% per year for the past century, the specific production techniques employed to meet this demand have only
changed dramatically over the past fifty years. Today most copper ore comes from Chile, where extraction accounts for about 1/3 of all the copper ore mined in 2010. Other important producers include China, Peru and the United States (Edelstein 2011). The exact composition of copper ore varies geographically, but all ore can generally be classified as one of two types: copper sulfide (which include chalcopyrite, chalcocite and bornite ore) and copper oxides (cuprite, azurite and malachite ore) (Davenport and Biswas 2002). Each type of ore contains a different average fraction of copper and tellurium, as well as a varying amount of other elements, including silver, nickel and selenium. Generally speaking, copper sulfide ores contain more copper and more tellurium, and are considered to be of higher quality (Bleiwas 2010; International Copper Study Group (ICSG) 2012). The type and composition of the ore dictates the technology that will be used to extract it.

Copper sulfide ores are typically mined by physical processes, followed by crushing and grinding into finer particles, and finally mixed with water to form slurry. The resulting slurry is aerated with chemical additives to promote separation during a process called froth flotation, whereby the copper is floated to the top and is recovered as concentrates. The concentrates are then treated pyrometallurgically to further increase the copper content. This is accomplished by drying, smelting at high temperatures and oxidizing in a conversion furnace to drive off iron and/or sulfur. The resulting 99% pure blister copper is then shaped into cathodes and connected into electrolytic cells. During the next process, called electrolytic refining (or electrorefining), the copper from the relatively impure anode is dissolved into the electrolyte solution and deposited on the purer cathode. During this process, a slime containing copper and many impurities is produced (Davenport and Biswas 2002).

Conversely, with oxide ores, copper is more commonly extracted hydrometallurgically by leaching with a sulfuric acid solution. The leachate undergoes solvent extraction, whereby the copper is transferred into an organic phase, leaving behind nearly all impurities and then re-leached with sulfuric acid to a more highly concentrated form. The dissolved copper is then extracted from this leachate by electrowinning (or electroplating) onto the cathode in a highly pure form (Davenport and Biswas 2002). The name for this overall process is solvent extraction-electrowinning (SX-EW).

The remainder of refined copper is produced from recycled scrap metal, which offsets the need for primary ore extraction. First, the scrap is pretreated, as necessary. This can include
cleaning, manually or mechanically sorting into more concentrated streams with other scrap, shredding and burning off contaminants (US Environmental Protection Agency (EPA) 1995). Once pretreated, the scrap is then smelted and fire refined. However, in certain circumstances, if the scrape grade is high enough it will also be electrolytically refined (US Environmental Protection Agency (EPA) 1995; Schlesinger et al. 2011).

The decisions made by copper producers to extract ore and to process it in certain ways are typically motivated by profit maximizing behaviors with respect to the primary product alone. However, since byproduct elements (such as tellurium) also enter the anthroposphere as a result of this same extraction, it is important to view their supply from a system’s perspective. In order to make sense of the often complex interactions that occur in such a dynamic economic/environmental system, it can be useful to develop a system diagram. System diagrams, often used in industrial ecology research, classify relationships between subsystem components and can act like “food webs” for industrial systems. Ultimately, these diagrams can be examined and used in conjunction with data and mathematical relationships (when available) to create a useful quantitative model. Such a diagram is provided in Figure 5 for the copper-tellurium byproduct system.

**Figure 5. Simple system diagram of the copper-tellurium byproduct system, depicting the relationships between copper mining activities and tellurium supply as well as downstream use.**

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2 There are many other factors, including market forces and regulatory tools, that may exist in real systems.
The diagram shows that although all three copper production methods have positive effects on copper supplies, only one has a positive effect on tellurium supplies: the electrolytic refining of copper sulfide ores. This is because during the electrolytic refining process a residual byproduct slime forms from copper anode impurities, like tellurium, which are insoluble in the electrolyte solution. By contrast, the other copper production techniques – SX-EW and copper recycling – either do not or cannot produce byproduct tellurium. Research at Oak Ridge National Lab has concluded that SX-EW production offers no meaningful potential for byproduct recovery of any trace elements, including tellurium (Ally et al. 2001). This is because the copper oxide ore that is typically processed this way contains little to no tellurium to begin with. Any trace elements that do get leached out are lost during the solvent extraction process because they are not absorbed well into the organic phase. Similarly, secondary refining does not contribute meaningful amounts of tellurium because the copper has already been refined from the impure ore form, and thus it has already been stripped of the trace elements of interest.

Therefore, if the global copper market can be thought of in a simplified manner as an overall demand that must be met by the sum of three, substitutional supply options, then an increase in the use of non-traditional (SX-EW and/or recycling) production as a fraction of total production would have negative implications for tellurium supplies and ultimately CdTe PV producers who rely on the material to manufacture their solar cells; thus the negative relationship indicated in the diagram.

Looking to historical data, it is revealed that copper supply from each of the three production methods has been increasing over time but each at a different rate (Figure 6). Prior to the 1960s, virtually all copper was mined as concentrates from sulfide ores, making electrolytic refining the dominant technique for primary production. Solvent extraction technology was in its infancy at that point so EW production was negligible, and only a few hundred metric tonnes of secondary copper was produced. Since then, secondary supplies have grown at a rate consistent with overall growth, allowing the technique to maintain a fairly constant share of refinery production (fluctuating between 13-18%). Conversely, solvent extraction continued to play a modest role in mining only until the mid-1990s when rapid growth began, taking the technique from 10% of mining production to 22% in less than 20 years. As a result, electrowinning has become a much more significant player in the production of refined copper and electrolytic refining.
of primary ore concentrates dropped by 10%; a fraction of total production. Over the past fifty years, the introduction of alternative supply technologies has shifted the balance of mining and refining to the point where only 60% of total refined copper comes from primary concentrates refined electrolytically, down from 80% in 1960 (International Copper Study Group (ICSG) 2012). Since SX–EW is used for the mining of lower quality ore, and much of the high quality copper ore in the US and Chile have already been exploited (International Copper Study Group (ICSG) 2012), it is likely that this technique may become more dominant as a primary extraction and refining process in the future. Additionally, although secondary production has historically maintained, if not slightly decreased, its share of total copper production, this technique could see growth of importance in the future if regulatory or market forces incentivize greater use of copper recycling.

Given the importance of the choice in copper production method on the availability of byproduct anode slime, and ultimately on the supply of tellurium, a strong focus is applied to copper production scenarios in this study. This focus is critical to understanding the tellurium supply chain and its broader implications on the potential for tellurium-based solar technology growth.

Figure 6. Historical copper supply trends disaggregated by production technology. (Left) Copper supply since 1960, plotted as a function of production technique using data presented in ICSG’s World Copper Factbook (International Copper Study Group (ICSG) 2012). (Right) Share of total copper supply produced by each technique since 1965.
2.3.2. Byproduct (tellurium) recovery technology can be improved

Aside from the source of copper, another significant technological factor is the specific method used for recovering tellurium from the anode slime generated during primary electrolytic refining of copper. Technologically, the most important parameter is the yield, or recovery efficiency, which dictates how much of the available tellurium is extracted from the ultimate resource. The natural occurrence of the mineral in ore is geochemically determined, which thereby sets an upper limit on supply. However, yield is one of the only parameters tellurium producers can attempt to improve (through increased recovery rate of tellurium from the anode slime byproduct) in order to meet rapidly growing demand in the face of supply constraints (Vasilis Fthenakis 2009; Ojebuoboh 2008). This can be accomplished in any number of ways; for example, by expanding operations to process more of the available anode slime (Bleiwas 2010) or by exploring alternative processing techniques to improve efficiency, like the addition of copper choppings to decopperizing leach solution has in the past (Shibasaki, Abe, and Takeuchi 1992). Any approach will require some investment however, so the decision to invest in yield improvements is weighed against the potential for increased profits from augmented tellurium supply.

Historically, yield of tellurium from ore content has been low: between 35% and 55% (M Woodhouse et al. 2012; Candelise, Winskel, and Gross 2012; Guilinger 2000). Theoretically, yields close to 100% could be achieved at the process level (Wang 2011; Candelise, Winskel, and Gross 2012); practically, an upper limit of roughly 80% at a systems level has been estimated, given sufficient demand and/or commodity price increases (Vasilis Fthenakis 2009; M Woodhouse et al. 2012). Therefore, if demand for cadmium telluride PV continues to increase rapidly into the future, driving prices up, producers will be more likely to see incentive to invest in one or more ways to improve yield of this mineral. A change in this parameter would have a substantial impact on future tellurium supply and is, therefore, worth investigating more closely.

2.4. Challenges Modeling Byproduct (Tellurium) Demand

Tellurium has found use in a changing variety of applications over time. Traditionally, its highest volume application was in ferrous alloying, however, other applications have since emerged, including its use in thermoelectric devices and photoreceptors (US Geological Survey (USGS) 2005). Most recently, tellurium use has shifted more toward CdTe PV since it is the most
difficult application to substitute. Despite claims in the most recent US Geologic Survey (USGS) publication that demand from the solar sector represented “the major end use” of tellurium (US Geological Survey (USGS) 2016), the exact fraction is not thought to constitute more than half of total demand. Literature values range from about 25% (Moss et al. 2011; European Commission 2010) to 40% (M. W. George 2012; Selenium-Tellurium Development Association (STDA) 2010).

![Tellurium demand chart](image)

**Figure 7. Tellurium demand.** *Top* Estimation for 2010 - 2016 (Selenium-Tellurium Development Association (STDA) 2010; Moss et al. 2011; European Commission 2014; Merchant Research & Consulting ltd 2016). *Bottom* Variation over time from different sectors as reported in Kavlak & Graedel (Kavlak and Graedel 2013).
Consideration of tellurium demand fraction from solar would have a significant impact on supply estimations. For example, using the literature values cited about would result in a direct decrease of supply estimations by a factor of 2.5 – 4. However, this parameter is highly uncertain. Since there are several end-use applications for tellurium, the fraction of demand coming from each sector in a given period is dependent upon the dynamics of several different markets. Different external factors influence the demand for each of these products which traditionally utilize tellurium. A further complication of estimating this parameter’s evolution over time is the substitutability of tellurium in many of its applications, particularly metal alloying. Substitution implies that if the demand for a particular end-use product increases in a given year, the demand for tellurium from that sector may not increase commensurately. These factors make estimation of this parameter highly uncertain.

Although it is unlikely, the present work assumes that 100% of tellurium produced each year will be available in the future for solar production. This is a significant limitation that needs to be addressed in future iterations. However, it is plausible that fractional demand for tellurium from solar would grow in the future. As the only application without a direct substitute for tellurium (US Geological Survey (USGS) 2016), CdTe PV manufacturing may be much less sensitive to changes in price. This supply inelasticity encourages increased dominance of the PV end-use application in the face of scarcity-induced price increases, supporting an optimistic future PV sector tellurium demand prediction.

Additionally, this assumption reflects the work’s focus on supply chain parameters that can be directly controlled. The implications of changes to those parameters are of the greatest importance to policy makers, who can use the newfound information to improve supply chain security. Regardless, the resulting supply estimations made in the present work do not fully account for the complex and dynamic nature of sectoral demand. They must therefore be considered carefully in light of this shortcoming and evaluated in the context of other simplifying assumptions.

2.4.1. Demand for solar PV is changing rapidly

Despite the fact that solar energy currently accounts for less than 1% of total global demand, it is one of the fastest growing renewable sources around the world. Since 2000, installed global PV capacity has grown exponentially; from 1400MW in 2000 to 7000MW in 2006 to
40,000MW in 2010 and finally to over 100,000MW in 2012 (Masson et al. 2013). Roughly 90% of all PV installations worldwide have occurred in the past 5 years. Since demand for solar technology is largely a function of economics and regulatory incentives, the development of its overall demand will depend on the evolution of prices and policies implemented in the future.

The same is true for the demand of each individual PV technology. PV research has led to the development of many diverse technologies: from polycrystalline silicon to single crystal silicon to organic and dye-sensitized cells and high-efficiency multiple junction devices. The demand for each technology will depend upon its efficiency, cost, reliability, and intended application. For example, multi-junction PV reaches record-high efficiency by absorbing more of the solar spectrum and by combination with strong solar concentrators and high precision solar trackers, but such high efficiency also comes with a high price (International Energy Agency (IEA) 2010). These two facts make multi-junction PV particularly well suited for large scale centralized generation. By contrast, amorphous silicon technology is inexpensive and lightweight so it is better suited to decentralized and/or mobile applications (International Energy Agency (IEA) 2010). The changing demand for each of these end-use applications, in conjunction with the unpredictable commercial development of emerging technologies into the future, create significant uncertainty in demand for solar PV and also, indirectly, for the materials used within the technologies.

2.4.2. Material intensity of PV is developing rapidly

One of the most commonly overlooked parameters in a dynamic predictive analysis is technological progress. As any technology, including solar photovoltaics, progresses over time, it can evolve in any number ways: physical form, unit price, performance, efficiency, etc. A change in any of these parameters is likely to have a very significant effect on the outcome of the forecasting model; particularly one with a long time horizon, over which dramatic change in several parameters is virtually guaranteed. One parameter in particular that will greatly affect supply and demand flows is material intensity, which refers to the amount of a particular material contained in a unit of product. Dematerialization, or the reduction in material intensity, has been observed to occur rapidly in many common products like appliances, electronics, and automobiles over the past century (Bernardini and Galli 1993).

For PV, in the past 40 years, record efficiencies for CdTe have climbed from 8% to 22%. Next-generation technologies such as organic and multi-junction PV have emerged with the latter
reaching 46% efficiency (Scanlon 2012) (National Renewable Energy Laboratory (NREL) 2016). These increases in module efficiency have direct implications on material intensity. Higher efficiency cells require lower film area per unit power resulting in less material usage. Another way material intensity can be reduced is via reduction of film thickness. However, there are tradeoffs as reliability of electrical performance generally declines with film thickness (M Woodhouse et al. 2012; Morales-Acevedo 2006; Amin, Sopian, and Konagai 2007). Using less of the high embodied energy materials in these active layers can in turn lower manufacturing cost (M Woodhouse et al. 2012; Candelise, Winskel, and Gross 2012) and, ultimately, environmental impact. Material intensity, specifically, will directly affect forecasted demand as well as the resulting supply chain dynamics.

2.5. Methods

Methodology developed to investigate future tellurium supply-chain security is detailed in this section. It provides broad perspective on byproduct systems by capturing and relating both copper and tellurium flows, and it is distinct in its isolation of individual supply and demand parameter impacts.

2.5.1. Dynamic Material Flow Analysis

The proposed model is a dynamic material flow analysis (dMFA), which is augmented by sensitivity and scenario analyses. Dynamic material flow analysis (dMFA) is a useful tool for modeling the way elements, substances, or materials move through a system over time. In dMFA modeling, time series relationships are developed to relate critical model parameters to the passage of time and to one another, which ultimately allow for a simple description of a complex and dynamic system. In supply chain analysis, the dMFA approach is particularly helpful for modeling systems with dynamic, secondary inflows from end-of-life recycling. This activity significantly affects the mass balance that is used to determine stocks and flows.

Examples of such studies include Gaustad and colleagues’ treatment of contaminating trace element accumulation in recycled aluminum (Gaustad, Olivetti, and Kirchain 2011) and Ayres et al.’s treatment of global copper stocks and future primary and secondary flows (Ayres, Ayres, and Råde 2002). The latter made reference to tellurium as a byproduct of copper production but remained focused on the copper lifecycle and did not quantify tellurium stocks and flows; partially
because in 2002 tellurium use in solar was minor. After the growth potential for CdTe PV was realized in the 10 years following Ayers et al.’s report, Marwede & Reller developed a dMFA model to quantify end-of-life tellurium flows from this emerging solar application (Marwede and Reller 2012). The present work adds value by expanding the scope of their model to look further upstream in the supply chain at tellurium flows as they relate to copper production flows. By considering trends in the entire byproduct system a clearer picture can be painted about the supply chain for this promising end use of tellurium. The effect of key challenge parameters – outlined in Section 2.2 – on supply chain metrics, such as material availability and the ratio of consumption to production, is characterized. A goal of this modeling framework is to identify common, troubling conditions that are prevalent in all byproduct production systems, so an attempt is made to present the methods in a generalizable format. However, in light of recent interest in cadmium telluride solar technology and increasing diversity in the copper supply chain, the details of the methods are tailored to and discussed in the context of the copper-tellurium byproduct system. Throughout this work, the terms “supply” and “demand” are generally used to refer to supply of tellurium not copper and demand for tellurium not copper or solar panels, unless otherwise specified.

2.5.2. Modeling byproduct (tellurium) supply and supply sensitivity

Because of their relevance to multiple byproduct systems, only the following two supply streams are considered in this model: (1) the traditional method of primary extraction (i.e. isolation of tellurium from copper anode slimes) and (2) recycling from highly concentrated end-of-life products (i.e. CdTe PV modules). Although the latter has been historically unimportant, it is beneficial to quantify the future contributions that could be made to overall supply from recycled sources because this pathway also has environmental implications. First, recycling helps to prevent the potential release of a known toxin, cadmium (Cd), into the environment via incineration or crushing and leaching in a landfill. Elemental cadmium is a known carcinogen as well as a kidney antagonist (Jarup et al. 1998); very little is actually known about the toxicity of non-elemental cadmium. Fortunately, empirical work has indicated that the amount of harmful cadmium emissions released during PV disposal is not nearly as great as was originally thought (Vasilis Fthenakis and Zweibel 2003), however, recycling is still the preferable end-of-life choice. Second, recycling can be utilized to offset the need for development of alternative, primary tellurium
mining efforts. These supply streams will undoubtedly have large physical and ecological footprints than the more traditional pathways. Additionally, there are non-environmental benefits to recycling; i.e. improved resiliency of CdTe supply chain from more diversity in tellurium supply.

2.5.2.1. Estimating primary byproduct (tellurium) supply from parent metal (copper) proxy data

The total primary supply of tellurium, $S$, produced in a single year, $t$, can be summarized as in Equation 1.

$$S(t) = \sum_i \alpha_i(t)\gamma_i(t)x_i(t)C_i(t); \text{ where } \alpha \text{ and } \gamma \in (0,1) \quad \text{Equation 1}$$

It is calculated by multiplying the total global copper production, $C$, in that time period by the average tellurium content of the copper ore, $x$, the recovery yield of tellurium from copper ore, $\gamma$, and the fraction of total copper production from electrolytic refining of primary sulfide ore, $\alpha$. This byproduct supply model was developed because it emphasizes the close physical relationship between the supply of the parent metal (copper) and the supply of the daughter mineral (tellurium). It also provides the means to circumvent use of direct production data for the daughter product, which is necessary in the case of tellurium since sufficient data is not publically available. The product of $C$, $x$, and $\alpha$ represents the upper limit of tellurium supply availability (Guilinger 2000). The addition of the fractional yield parameter captures the various technological and economic limitations that prevent actual production from being the total amount available. In Equation 1, the subscript, $i$, represents the producing mine, as each of these parameters varies from mine to mine. However, in this study, due to lack of sufficient plant-level data, aggregate global figures are used instead.

Since a major focus of this study is on implications of non-traditional copper production processes, $\alpha$ has been defined indirectly by the secondary and SX-EW production shares, $\delta$ and $\lambda$, respectively (Equation 2). In turn, the dynamic expressions for $\delta(t)$ and $\lambda(t)$ are defined by linear growth equations, where each has a unique growth rate, $g$, describing their observed or predicted progress (Equations 3 & 4). Linear growth was chosen for these parameters based on historical observation (see 2.6.1.1. Base case byproduct (tellurium) supply further discussion).
% Primary Electrolytic Cu Production: \( \alpha(t) = 1 - (\delta(t) + \lambda(t)) \) \hspace{1cm} \text{Equation 2}

% Secondary Cu Production: \( \delta(t) = \varepsilon_1 + g_{sec}t \) \hspace{1cm} \text{Equation 3}

% Primary SX-EW Production: \( \lambda(t) = \varepsilon_2 + g_{sx-ew}t \) \hspace{1cm} \text{Equation 4}

Change in yield is handled a little differently. For most scenarios, yield will be considered constant as a simplification. However, for this particularly powerful control parameter, three additional, differently “shaped” growth scenarios were also imagined, ranging from conservative to aggressive, to capture the uncertainty in technological improvement and subsequent implementation.

1. No improvement: \( \gamma(t) = \gamma_0 \)
2. Steady improvement: \( \gamma(t) = \gamma_0 + g_{lin}t \)
3. Rapid early improvement: \( \gamma(t) = \gamma_0(1 + g_{con}t)' \)
4. Rapid late improvement: \( \gamma(t) = \gamma_0(1 + g_{con}t)' \).

Growth form 1 represents constant yield; this is the base case assumption. Growth form 2 represents gradual improvement in yield over time, approximated by a linear function. Growth forms 3 and 4 represent rapid growth in the near and distant future, respectively, approximated by hyperbolic growth functions. Sensitivity of tellurium supply to changes in growth form is also discussed with in Section 2.6.2.1.1. Primary byproduct (tellurium) supply sensitivity to growth of non-traditional copper production (secondary and SX–EW copper), \( g_{sec} \) & \( g_{sx-ew} \).

Tellurium supply is sensitive to changes in each of the defined parameters. Supply sensitivity is modeled as a function of time and of abstract parameter, \( p \) (Equation 5). Again, the subscript \( 0 \) represents the base case value of a parameter. Within the definition of supply (Equation 1), two dynamic parameters contain these growth rates: (a) primary electrolytic share of copper production, \( \alpha \), and (b) recovery yield of tellurium from copper ore, \( \gamma \).

\[
\%\Delta S(p,t) = \frac{S(p,t) - S(p_0,t)}{S(p_0,t)}
\] \hspace{1cm} \text{Equation 5}

Since this study is most concerned with its sensitivity to changes in the following key parameters because they represent factors over which there is some human control: (a) SX–EW
share of copper production, \( \lambda \), (b) secondary share of copper production, \( \delta \), and (c) recovery yield of tellurium from copper, \( \gamma \). Each of these parameters can be assumed to follow a specific path over time, with a characteristic growth rate, \( g \). It is from the changes of these paths over time that most can be learned. Therefore, in this analysis, the growth rate parameter, \( g \), rather than the production share parameter is taken as a key parameter, \( p \), for probing supply sensitivity; except in the case of yield, which will serve as the key parameter directly.

2.5.2.2. Estimating secondary byproduct (tellurium) supply from end use (PV) residence time data

CdTe solar panels, like all products, will eventually reach the end of their useful life. If the material is not recovered and recycled, the tellurium and other valuable components will be landfilled, reducing the overall available stock. To determine the amount of tellurium leaving the system in a given year, material flow analysis techniques can be employed which rely on estimates of panel lifetime, similar to Marwede and Reller (Marwede and Reller 2012).

Panel lifetime has previously been characterized in the literature by a normal distribution (Marwede and Reller 2012); however, more recently available data from First Solar indicates that about 1/3 of panel failures via breakage occur before even being installed (during transport or installation process), suggesting a skew in lifetime distribution toward earlier stages (Sinha and Wade 2015). This information was not available analysis was originally performed, a normal distribution, so a normal distribution is assumed here. A shift in this assumption will likely affect results but is left for future work.

Assuming normal lifetime distribution, the amount of secondary tellurium available in a given year, \( EOL(t) \), is equal to the amount contained in panels produced \( T \) years ago multiplied by the probability of a panel reaching end-of-life after \( T \) years. This can be expressed using a simple Gaussian function weighted by the tellurium content of the panels, as in Equation 6. There, \( \mu \) represents mean lifetime in years and \( \sigma \) represents standard deviation.

\[
EOL(t) = \sum_{T=t}^{n} \left[ \frac{M(t-T)}{\sigma \sqrt{2\pi}} \exp\left(-\frac{1}{2} \left(\frac{T-\mu}{\sigma}\right)^2\right) \right]
\]

Equation 6
2.5.3. Modeling byproduct (tellurium) demand & demand sensitivity

This analysis assumes annual demand for CdTe solar technology will grow in the future. Realistically, the number of installations and rate of growth are unknown. As such, the growth can be modeled in any number of ways. However, one reasonable approach is to use a simple logistic function because it generates the characteristic “S-shaped” curve frequently associated with emerging technology growth (Packey 1993). Equation 7 presents this approach in the form of a three parameter, general form logistic function.

\[
D(t) = \frac{K}{1 + e^{-(\beta_0 + \beta_1 t)}}
\]

Here, \(K\) represents a saturation level or plateau in annual solar demand, hereafter referred to as the steady state demand. \(K\) has units of gigawatts per year, and \(t\) represents time in units of years. \(\beta_0\) and \(\beta_1\), represent fitting parameters that determine when and at what rate, respectively, CdTe PV demand growth will occur. The resulting time series curve, \(D\), represents CdTe PV demand in any given year, in units of gigawatts per year (Figure 8).

Next, the projected yearly tellurium demand, \(M(t)\), is calculated as shown in Equation 8 by multiplying solar power demand, \(D(t)\), by the material intensity of the PV on a power-specific basis, \(\bar{m}\), calculated as shown in Equation 9. In Equation 9, \(A\) is film area (m²), \(\tau\) is film thickness (µm), \(\rho\) is film density, \(n\) is mass fraction of tellurium in the active layer film, and \(P\) is the nominal power rating of the panel in kilowatts. Note that \(\bar{m}\) has equivalent units of metric tonnes per gigawatt.

\[M(t) = \bar{m} \cdot D(t) \]
To deal with the considerable uncertainty associated with many of these parameters ($\rho$, $\tau$, $\Pi$), a range of values was collected from the literature and used to generate various scenarios for material intensity. In this model, one parameter is selected to serve as a proxy for all other possible changes in material intensity: film thickness, $\tau$. In reality, many other factors also contribute to intensity, including the module’s electrical efficiency and the efficiency of material deposition during manufacturing (Candelise, Winskel, and Gross 2012). This assumption may limit the analysis by reducing the complexity of the $m$ improvement scenarios, but, in doing so, it makes the current modeling effort much more tractable.

A key metric in this study is the sensitivity of tellurium demand, $%\Delta M$, to changes in a single modeling parameter, $p$. Percent change is used to quantify sensitivity, and changes are measured relative to the base case values. Equation 10 shows the general form for calculating demand sensitivity to the change in generic parameter, $p$, from $p = p_0$ (base case value) to some arbitrary value, $p$.

$$%\Delta M (p, t) = \frac{M (p, t) - M (p_0, t)}{M (p_0, t)}$$

Parameters of interest in this study are (a) Steady State Annual Solar Demand, $K$, (b, c) Demand Growth Fitting Parameters, $\beta_0$ and $\beta_1$ and (d) Active Layer Film Thickness, $\tau$, because they were identified in Section 2.4 as being uncertain and critical to modeling future tellurium demand dynamics. When calculating demand sensitivity, $%\Delta M$, to a given parameter, $p$, all other parameters remain at their baseline levels.

### 2.6. Data, analysis, and discussion

To learn from the above methodology, it should be applied to real data; in this case, materials and process data specific to the copper-tellurium byproduct supply chain. This allows for the establishment of a reference case, referred to as a base case or baseline scenario in this
work, against which other scenarios can be compared. Section 2.6.1 details the process and presents the base case results.

Valuable lessons can be gleaned from comparison of scenarios based on isolated key parameter changes. This analysis is detailed in Section 2.6.2. Each section is further separated into supply and demand subsections. Sensitivity to changes in supply and demand parameters lends insight into factors that most influence risk in the byproduct supply chain. Generally speaking, supply and demand will refer to byproduct tellurium supply and demand, unless otherwise specified. The scope of this analysis is limited to a 50-year period, beginning in 2010.

2.6.1. Establishing the base case scenario

For this analysis, two baseline scenarios were established: one for tellurium demand and one for tellurium supply, based only on observed historical data and trends. These estimates may or may not represent the true path of supply or demand into the future; however, they provide a benchmark for comparison and assessment of potential growth and technological progress. Additionally, sensitivity analysis can help to identify parameters that have the potential to significantly modify risk in the supply chain. The dynamic sensitivity analysis presented here also gives an idea as to the power of a given parameter to affect change at different points in time.

2.6.1.1. Base case byproduct (tellurium) supply

Global tellurium supply data is available from the USGS for most of the 20th century; however, the reported data still has high uncertainty. Several nations, despite known production, are not included in the global supply total estimates because they do not report the data. These include major producers, such as Russia, other former-Soviet countries, and the US, which considers the data proprietary and ceased reporting after 1975 (US Geological Survey (USGS) 2011b). As of 2003, no data for global tellurium production is reported at all due to this lack of sufficient information (US Geological Survey (USGS) 2015b). Unfortunately, this predates most of the demand generated by solar production (Shibasaki, Abe, and Takeuchi 1992). In recent years, tellurium supply has been estimated less directly. The most popular approach is to use copper tank house data because, as a byproduct of primary electrolytic copper refining, tellurium production is strongly linked to copper production. Current estimates from these sources range from 450 to 550 metric tonnes per year (Bleiwas 2010; M. W. George 2012).
The base case tellurium supply used in this work was generated using a similar technique, which has been described mathematically in Section 2.5.2. Total copper production levels, \( C(t) \), dating back to 1900 were collected from both the USGS (US Geological Survey (USGS) 2011a) and the International Copper Study Group (ICSG) (International Copper Study Group (ICSG) 2012). The growth rate of overall copper production was regressed and assumed to continue into the future under the base case supply scenario. Additionally, the ICSG provided detailed graphical production data from 1960 to 2011, disaggregated by each copper production technology (primary electrolytic, secondary, and primary SX–EW) allowing for more in-depth analysis (International Copper Study Group (ICSG) 2012). Recall from Section 2.3.1. Carrier metal (copper) supply chain is diversifying that the growing importance of SX–EW as a copper production source, as well as steady levels of secondary copper production, have caused the share of total copper production from primary electrolytic refining to decline. Although it seems likely that primary electrolytic production will remain a dominant source in the short-term, its role in long-term future production is more uncertain. If historical copper production trends continue, electrowon copper production will rival primary electrolytic production (Table 4).

### Table 4. Results of historical copper supply regression and projection.

Linear regression of technology-specific copper production share data shows decline of primary electrolytic dominance, steady or slightly declining secondary production, and growth of SX–EW production.

<table>
<thead>
<tr>
<th>Production Technology</th>
<th>Historical Growth Rate</th>
<th>Observed 2009</th>
<th>Projected 2050</th>
</tr>
</thead>
<tbody>
<tr>
<td>% Primary Electrolytic, ( \alpha )</td>
<td>-0.37%/y (lin)</td>
<td>66%</td>
<td>53%</td>
</tr>
<tr>
<td>% Secondary Electrolytic, ( \delta )</td>
<td>-0.04%/y (lin)</td>
<td>16%</td>
<td>13%</td>
</tr>
<tr>
<td>% Primary Electrowon, ( \lambda )</td>
<td>+0.41%/y (lin)</td>
<td>18%</td>
<td>34%</td>
</tr>
<tr>
<td>Total Production, ( C(t) )</td>
<td>+2.66%/y (exp)</td>
<td>18.3 Mt</td>
<td>37.8 Mt</td>
</tr>
</tbody>
</table>

Taking these factors into consideration will make the forecasts presented in this work quite different than an approach which estimates constant share of production or neglects the heterogeneous primary copper supply chain in calculation of future tellurium supply. Once it was confirmed that the total copper production data from this more detailed ICSG graphical source was consistent with the total production data from the USGS (Edelstein 2011), the technique-specific time-series data was manipulated to show the share of the total copper production from each technique over time. Each historical series of production share was then regressed linearly to obtain a baseline growth rate for each production technology, presented in Table 4.
As with the total, historic growth rates of each technology’s production share over time was assumed for the base case. Additionally, the ore’s tellurium content, $x$, is assumed as a constant 182 ppm tellurium (Guilinger 2000), and yield, $\gamma$, is also assumed to be constant in the base case scenario, halted at a conservative value of 35%. Although some sources have cited current recovery of tellurium at rates up to 55% (Vasilis Fthenakis 2009; Ojebuoboh 2008; Michael Woodhouse et al. 2013), 35% is used because tellurium recovery does not occur at all mining sites (Greenpeace and European Photovoltaic Industry Association (EPIA) 2011). Demand sensitivity to changes in this parameter are explored in Section 2.6.3.1. Finally, the baseline tellurium supply projection was obtained by multiplying the projected primary electrolytic production share, $\alpha$, with the other supply parameters as in Equation 1. This scenario is presented alongside the baseline demand scenario in Figure 9.

![Graph showing baseline demand and supply projections](image)

**Figure 9. Base case tellurium projections: supply and demand.** A base case scenario for both tellurium supply and demand were created from observed historical data and trends. They are compared above, revealing a potential for supply gap conditions beginning as early as 2018.
2.6.1.2. Base case byproduct (tellurium) demand

Historical data for cadmium telluride PV production was obtained from First Solar, Inc. (First Solar 2012). In order to fit the data to a logistic growth curve, appropriate values for steady state demand, \( K \), and fitting parameters, \( \beta_0 \), and \( \beta_1 \), had to be estimated. Since its value has real world meaning, \( K \) was estimated first from published forecasts. A moderate estimate of \( K \) was obtained by combination of a relatively conservative forecast of total solar growth with an optimistic forecast of thin film market share. The conservative solar estimate was generated by the IEA, which estimated that demand would level off at about 150 GW/y by 2050 (International Energy Agency (IEA) 2010; Candelise, Winskel, and Gross 2012). The aggressive thin film forecast of 30% was cited by Candelise as the opinion of an industry expert given in 2010 (Candelise, Winskel, and Gross 2012; Greenpeace and European Photovoltaic Industry Association (EPIA) 2011). The accompanying values of \( \beta_0 \) and \( \beta_1 \) were found by minimizing the sum of the squared error of the observed data points. The resulting three parameters, summarized in Table 5, were fed into Equation 7, generating the base case solar demand curve through 2060.

Table 5. Base case PV demand growth parameters fitted from observed data.

<table>
<thead>
<tr>
<th>Modeling Parameter</th>
<th>Practical Significance</th>
<th>Baseline Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( K )</td>
<td>Steady State Demand</td>
<td>50 GW/y</td>
</tr>
<tr>
<td>( \beta_0 )</td>
<td>Delay of Demand Growth</td>
<td>-7.5</td>
</tr>
<tr>
<td>( \beta_1 )</td>
<td>Rate of Demand Growth</td>
<td>0.4</td>
</tr>
</tbody>
</table>

Since the focus of this work is on demand for tellurium, this baseline CdTe solar demand curve was converted to demand for tellurium using power-specific material intensity as in Equation 9. For the base case, a constant material intensity was assumed, using a constant film thickness as proxy. A wide range of thicknesses was found in the literature (Moss et al. 2011; Bleiwas 2010; Morales-Acevedo 2006; Amin, Sopian, and Konagai 2007; Marwede and Reller 2012; Razykov et al. 2011; Noufi et al. 2007), but the most common were between 2 and 5 \( \mu \)m. As a result, an average film thickness of 3 \( \mu \)m was assumed for the base case. Section 2.6.3.1.4. explores demand sensitivity to the value of this parameter. Assuming average values for the remaining material intensity parameters (Table 6), resulted in a base case material intensity of 90.7 tonnes of tellurium per gigawatt of nominal power. This ultimately led to the calculation of a baseline scenario of tellurium demand, as shown in Figure 9.
Table 6. Data ranges used to calculate material intensity. Film thickness sources: (Moss et al. 2011; Bleiwas 2010; Morales-Acevedo 2006; Amin, Sopian, and Konagai 2007; Marwede and Reller 2012; Razykov et al. 2011; Noufi et al. 2007). Film density sources: (Speirs et al. 2011; Sigma-Aldrich 2015). Film area and power rating source: (First Solar 2014).

<table>
<thead>
<tr>
<th>Film Thickness, $\tau$</th>
<th>1-10 µm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Film Density, $\rho$</td>
<td>5.6 – 6.25 g/cm³</td>
</tr>
<tr>
<td>Film Area, $A$</td>
<td>0.72 m²</td>
</tr>
<tr>
<td>Nominal Power Rating, $\Pi$</td>
<td>62 – 93 W</td>
</tr>
</tbody>
</table>

2.6.2. Sensitivity analysis of byproduct (tellurium) supply chain

The first step in analyzing the supply chain sensitivity is gaining an understanding of the supply chain behavior under its base case conditions. Figure 9 displays both baseline supply and baseline demand for tellurium, overlaid for easy comparison. This scenario, which represents the continuation of historical trends, predicts that tellurium supply will nearly triple over the 50-year time frame. It does so by sustaining an approximately linearly increase at a rate of just under 30 additional metric tonnes of tellurium produced per year. Note that this linear increase is observed despite exponential trends assumed for parent metal copper production, $C(t)$, a key parameter used to estimate tellurium supply (Equation 1). This indicates a strongly conflicting trend in one or more of the remaining supply parameters, namely primary electrolytic copper production share, which is predicted to decline under baseline conditions. This decline results from continued growth of SX–EW copper production at historical rates in addition to stable contributions from secondary copper production.

Over the same time period, the baseline scenario predicts CdTe installations will continue to increase at historic growth levels, logistically. The rapid early growth that is projected is enough to create supply gap conditions as early as 2018. Further, by 2030 tellurium demand from solar is projected to be more than triple the expected supply for that year. This is a central result because it demonstrates clearly that the current growth path of this solar technology is not sustainable without dramatic changes in the tellurium supply structure.

A few important questions emerge: Exactly what kinds of supply-side changes are needed? What is possible? And, what are the implications if demand growth turns out to be different than what has been historically observed? These types of questions lend themselves perfectly to sensitivity analysis. The parameters chosen for sensitivity analysis are those discussed in Sections
2.3 and 2.4. 4, and reiterated below, which can and may be manipulated by supply- or demand-side entities in the future in unknown ways.

Supply Parameters
- SX–EW Cu growth rate, \( g_{sx-ew} \)
- Secondary Cu growth rate, \( g_{sec} \)
- Te yield / recovery efficiency, \( \gamma \)
- Te yield growth regime

Demand Parameters
- Steady state demand, \( K \)
- Delay of growth, \( \beta_0 \)
- Rate of growth, \( \beta_i \)
- Material intensity, \( \bar{m} / \) film thickness, \( \tau \)

Sensitivity to these parameters is explored via specific scenarios in which the value of one input is varied at a time. In this way, results may not capture the co-mingled impacts of the dynamic system, but individual trends can be better understood. This is a major distinction between this work and that of Houari et al., who use a highly complex system dynamics (SD) model to investigate the supply-constrained limits to CdTe PV growth (Houari et al. 2014).

The following section outlines the supply chain sensitivity, first, to several supply-side parameter changes and, then, to several demand-side parameter changes. Together, the results provide a range of supply chain impacts that can be expected under any reasonable scenario.

2.6.2.1. Sensitivity to byproduct (tellurium) supply growth parameters

The base case supply modeled in Section 2.6.1.1 represents the direct projection of historical copper production trends assuming pessimistic tellurium yield. The following analysis puts that scenario in context by demonstrating supply sensitivity to changes in growth rate of production technologies and recovery yield. Potential impact of future PV recycling is also assessed.

Sensitivity of tellurium supply is analyzed by varying each modeling parameter through a reasonable range. Note that supply of tellurium can be calculated from copper proxy and byproduct material relationships as described in Equations 1-4. The new supply cases are compared with the base case supply and presented as a percent change (Equation 5). The results show the impact of using different assumptions in long-term modeling of complex byproduct market systems.
2.6.2.1.1. Primary byproduct (tellurium) supply sensitivity to growth of non-traditional copper production (secondary and SX–EW copper), $g_{sec}$ & $g_{sx-ew}$.

To determine the sensitivity of tellurium supply to changes in growth rate of each non-traditional copper production technology, copper supply scenarios covering a small (magnitude), but significant (percentage) range of growth rates were generated and compared to the baseline historical projection scenario. The results are presented in Figure 10.

**Figure 10. Tellurium supply sensitivity to growth rate of non-traditional copper production technologies.** (a) Sensitivity to growth rate of secondary copper as share of production (constant SX–EW) and (b) Sensitivity to growth rate of SX–EW copper as a share of total production (constant secondary).

In varying the growth rate of each copper production technique, secondary and SX–EW, the growth rate of the other was assumed to remain at the base case level, allowing for direct displacement of primary electrolytic copper production. As expected, reduction in growth rate from base case levels results in an increase in tellurium supply because neither method yields recoverable tellurium.

However, note that the same magnitude growth rate results in very different supply sensitivities for secondary and SX–EW growth. Negative growth rates result in greater positive response from SX–EW than from secondary while positive growth rates result in greater negative response from secondary than from SX–EW. For example, a sustained decline in use of SX–EW (negative $g_{sx-ew}$) could have significant long term effects on tellurium supply, up to an 80% increase (Figure 10b), whereas the same growth rate for secondary copper would result in only a 20–30% increase in tellurium supply (Figure 10a).
In both cases, the sensitivity reaches a lower limit of 100%. This is simply stating that supply is reduced to zero because of primary electrolytic refining is no longer used. This would occur by 2060 with a sustained +1%/year increase in share of production for secondary growth or a +1.5%/year increase for SX–EW production share. This seems counterintuitive at first because SX–EW already accounts for a greater share of production than secondary copper. However, it is important to remember that the baseline growth rate of SX–EW was significantly higher than that of secondary copper production, which was slightly negative. Therefore, a shift of SX–EW growth rate to 1.5% represents a comparable shift to 1%, relative to the baseline. To put these growth rates in context, secondary copper production share has fluctuated by up to 3.3% from year to year but has never sustained growth for more than a few years at a time. Therefore, a shift to growth rate of 1% production share per year (an immediate and sustained increase) would represent a dramatic deviation from the status quo. This would occur only under the influence of heavy regulations calling for increased copper recycling. Similarly, although demand for SX–EW copper has growth significantly over its history, the fastest sustained growth rate ever observed occurred during the 1990s and was equal to 1.0%/y. A sustained growth rate of 1.4%/y would only occur if a paradigm shift in mining occurred and copper sulfide ore availability grew scarce enough to make primary extraction and electrolytic refining of this ore uneconomical.

2.6.2.1.2. Primary byproduct (tellurium) supply sensitivity to byproduct (tellurium) yield, $\gamma$.

If demand for CdTe PV increases enough to drive tellurium prices upward, increased investment in recovery technology may become profitable. This would have a positive effect on primary tellurium supply. As discussed in Section 2.3.2, yield estimates range from 35% to 80% in the literature and can theoretically reach almost 100%. The sensitivity of tellurium supply was evaluated according to Equation 5 to determine the effects of changes in this parameter. Since yield is related to supply in the same way $K$ and $\bar{m}$ are related to demand, the percent change in supply is static and proportional to the percent change in the parameter. An increase to 50% recovery from all production locations results in a 43% increase in tellurium supply relative to the base case. An increase to 80% recovery would more than double base case supply, and perfect recovery of available tellurium would increase supply by 171%.

The implications for market balance are displayed in Figure 11 (top left). Despite dramatic reduction in the magnitude of the supply–demand imbalance, supply gap conditions are shown to
emerge for all of the yield values modeled, even 100%. The latter demonstrates that, even with perfect yield, if the observed historical trends in utilization of nontraditional copper supply technology continue, supply from copper anode slimes will be unable to meet baseline demand as soon as 2023. All the available traditionally extracted tellurium in copper slimes will be less than the amount demanded for solar production in only 10 years. Even if you consider that this source only represents 90% of total primary tellurium supply (US Geological Survey (USGS) 2016), the additional 10% only pushes back the gap by 1 year (Figure 12).

Figure 11. Sensitivity to changes in recovery yield, γ. (Top left) tellurium market balance sensitivity to recovery yield, γ. (Top right) tellurium supply sensitivity to recovery yield improvement regime. (Bottom) tellurium market balance sensitivity to recovery yield improvement regime.
After this point, alternatives to traditional byproduct supply must be considered. There are several options: (a) increase recovery from other byproduct sources (lead, bismuth, etc.), (b) develop primary telluride ore to mine tellurium, and (c) recycle end-of-life PV panels. From an environmental perspective, improvement of recovery yield and recycling are preferable to increased primary mining of tellurium. These options reduce material waste as well as the ecological footprint associated with production of this resource. However, there are trade-offs. Yield and recycling are ultimately limited by availability, technology, and cost. The risk mitigation potential of secondary supply is assessed in the following section.

Figure 12. Yield limitations. The solid line plots the necessary yield to meet demand from copper byproduction alone. The dashed line considers the 10% of tellurium production from other primary (mainly byproduct) sources. In both cases, the available primary byproduct supply is not sufficient.

The previous supply sensitivity to recovery yield assumed that the yield remained at that value over the entire time period. In reality, the parameter is likely to change over time, and has the potential to mitigate risk in the short term. Recall the four growth regimes that will be considered for this parameters pathway over time: no progress (the previous analysis), steady progress, rapid early progress, and rapid late progress. The no improvement scenario serves as a lower bound representing status quo and base case. Steady improvement represents a case of conservative progress. This might be observed if the burden for traditional source (copper
byproduct) yield is offset by lower than expected tellurium demand due to modest solar demand
growth or gradual entry of other tellurium supply sources (secondary or alternate primary). Finally,
the two rapid improvement cases represent scenarios of disruptive technology introduction and differ in when they occur.

Since the different growth forms have such different treatments of the growth rate parameter, sensitivity to change in this parameter can only be made assuming a particular type of growth form. A more useful comparison is to compare the different types of growth regimes, which all approach the same point by the same year (100% by 2110 was selected for illustrative purposes), and then to observe the magnitude of the impact that these different types of supply augmentation could have on overall tellurium supply in the next 50 years. The resulting sensitivities are presented in Figure 11(top right). The trends show that improving yield toward the goal by any growth regime would result in at least a 30% increase in tellurium supply by 2060. This is a significant increase, but it is not enough to overcome the projected 150% imbalance between demand and supply in that same year (Figure 11(bottom)). Further, the most rapid demand growth is likely to occur in the short-term future, so the earlier the onset of recovery improvements the better it is for reducing risk of supply disruption. It was observed that rapid early growth of recovery efficiency could push back the onset of supply gap conditions by 2 years and reduce the peak market imbalance by 50%.

2.6.2.1.3. Secondary byproduct (tellurium) supply potential.

Secondary tellurium from recycled PV panels represents a viable supplementary supply option in the future because of its high material intensity relative to other applications, many of which are dissipative. Under the baseline demand scenario, the end-of-life flows from PV shown in Figure 13 (left) are expected for panels with lifetimes of 25 ±5 years. End-of-life flows begins to grow to meaningful levels around 2030. As expected, the growth of these flows over time mirrors the growth of demand over time, but with a delay. Note that this curve merely represents the global potential for secondary tellurium supply; actual secondary supply will be at least 5% lower to account for inefficiencies in the recycling process. More likely, secondary supply will be
drastically lower to reflect incomplete collection of end-of-life panels; especially at the global scale.

Regardless, end-of-life flows can be used to approximate the upper limit of secondary tellurium supply. By 2045, secondary flows from PV recycling could double baseline projected tellurium supply. In 2060, 98% of baseline projected demand for tellurium could be met from secondary sources (Figure 13 (right)). This is made possible by the logistic assumption about annual demand growth. If demand growth eventually stagnates, material in end-of-life panels can directly replace material needed for new panels. This later-term potential for supply augmentation is a perfect complement to the early potential of yield improvement. Through the middle of the next decade, supply can be met from traditional byproduct means alone if yield is helped along to follow a path like the one shown in Figure 12, which is optimal for meeting demand.

Figure 14 explores the implications for tellurium market balance of pursuing just recycling to augment base case supply as well as yield improvement and recycling simultaneously. Because secondary supply growth occurs late and but supply gap conditions emerge early, the addition of secondary supply does nothing to prevent gap conditions in the short term. It does however, help
to shorten the length of time spent in gap conditions: by several decades as compared to the baseline primary tellurium supply. It can even add a 5 to 10 year improvement over the best case recovery scenario. However, for short-term prevention of gap conditions, improvements in recovery yield are the most powerful tool in the arsenal from the supply perspective.

Since, as a byproduct, demand for tellurium does not directly dictate how much copper ore is extracted, the environmental benefits of using recycled supply are not from displacement of ore extraction but rather from displacement of waste. However, reuse of tellurium does allow for greater deployment of clean solar PV per unit of extraction. Primarily, the availability of a secondary tellurium supply reduces the risk of supply interruption by making the supply chain more robust.

2.6.3.1. Sensitivity to byproduct (tellurium) demand growth parameters

Since the solar energy market is still largely maturing, future demand for photovoltaics is highly uncertain. Specifically, the way in which overall demand will evolve over time, and to what extent, is unknown and also challenging to predict. Even more challenging is predicting the demand for a particular technology, like cadmium telluride, because of the increasing diversity of
the solar market. Nevertheless, a great deal of information can be gleaned from an understanding the systems sensitivities to different types of changes.

Sensitivity of demand for tellurium was analyzed by varying each modeling parameter through a reasonable range. Note that demand for tellurium can be calculated from PV demand as described in Equations 7-9. The new demand cases are compared with the base case demand and presented as a percent change (Equation 10). The results show the impact of using different assumptions in long-term modeling of complex byproduct market systems.

2.6.3.1.1. Steady state CdTe power demand, \( K \).

Because of the considerable uncertainty, the range of values for the steady state annual power demand or saturation level, \( K \), is quite large: from 5 to 100 GW/y. Since the base case material intensity was assumed to be 90.7 tonnes tellurium per gigawatt, this corresponds to a steady state tellurium demand range of 270 to 9000 metric tonnes of tellurium demanded per year. The low estimate accounts for recent skepticism about thin film market share in the future (Masson et al. 2013). If a conservative total demand scenario is combined with a pessimistic CdTe market share of less than 5%, steady state demand of 5 GW/y is feasible. The upper estimate represents an aggressive growth scenario, similar to that proposed by EPIA Greenpeace (which results in 250 GW/y demand in 2050). This level of demand would require CdTe technology to take hold at least 40% of the PV market share (International Energy Agency (IEA) 2010; Candelise, Winskel, and Gross 2012): a difficult task when up against mature competitor crystalline silicon as well as other emerging PV technologies (CIGS, organic, dye-sensitized, multi-junction, etc.). This 100 GW/y is treated as an upper bound of expected growth in this time frame. The base case value of 50 GW/y was compared with these two extreme values and two moderate values. All five scenarios begin to see plateauing of tellurium demand between 2025 and 2030. To meet these scenarios in real life, both rapid development and large scale development would be required.

As defined in Equation 8, any changes to the steady state PV demand will result directly in proportional changes to tellurium demand. Additionally, these demand sensitivities are independent of time. Across the range of scenarios, tellurium demand could reach a maximum of
as much as double what is estimated in the base case or as low as 10% of the base case. The practical importance of these variations is the implications for market balance – or the ratio of tellurium demand to supply for a given year. Under each demand scenario the risk of supply gap conditions emerging is different. For some scenarios these conditions may not ever be expected to emerge within the timeframe.

To visualize this, the market balance for each $K$ scenario is presented in Figure 15 (top left). Supply gap conditions are observed anywhere the market balance metric exceeds 100%. The figure indicates that, if historical tellurium supply and PV demand growths continue, CdTe PV annual installation must stabilize between 10 and 25 GW/y to avoid supply-gap conditions. The critical point for this parameter is 14 GW/y, at which point PV deployment is maximized and tellurium supply is expected to meet or exceed demand throughout the entire timeframe. Surprisingly, this is found to be on the lower end of the range found in the literature for steady state demand, indicating a gross overestimation of what is possible given material constraints of this dynamic byproduct system. However, this analysis exposes only the
limitations of the traditional tellurium supply chain from copper anode slime with poor, non-improving tellurium recovery yield.

Another way to think about this uncertain range of steady state PV demand is from a sustainability perspective. In most scenarios there are trade-offs among different environmental and social benefits. For example, high $K$ value can be environmentally beneficial because it means higher a deployment of environmentally-benign PV panels and possible substitution of electricity from fossil fuel sources. Additionally, there may be social benefits if the PV is deployed in developing countries to improve electrification. However, as indicated by the emergence of supply gap conditions, rapid deployment of high levels of CdTe PV can put too much pressure on the delicate byproduct system resulting in price volatility or supply shortages. Further, not recycling panels at the end of their useful life will result in faster depletion of the scarce tellurium.

2.6.3.1.2. Delay of critical byproduct application (CdTe PV) demand growth, $\beta_0$.

Another important parameter is the demand growth fitting parameter, $\beta_0$, which represents delay of CdTe PV demand growth. Changes in $\beta_0$ will shift the time of deployment initiation without any effect on the ultimate level of steady state demand or rate of growth. The sensitivity of demand to $\beta_0$ was assessed by varying the parameter value, holding all else equal, from -5 to -11.5 or an equivalent of +33% to 53% (Figure 16 (left)). The demand sensitivity to these changes is shown in Figure 16 (right). This range is broad but this parameter is particularly uncertain, and even using these significant changes only provides a range of growth initiation from 2000 to 2020. It is certainly possible with various political and economic scenarios that growth of this technology, or solar as a whole, would not grow rapidly until much later; however, for the discussion at hand this range serves its purpose.

Realistically, changes to $\beta_0$ can be thought of in a few ways. One way is the gain or relinquishing of economic dominance for a specific solar technology. For instance, during most of the last decade cadmium telluride PV had a cost advantage over the incumbent crystalline silicon. However, in recent years, silicon prices have dropped, allowing the technology to regain its economic advantage over CdTe. If over the next few years, research and development allows First Solar to increase efficiency and/or reduce film thickness, further driving down manufacturing costs, CdTe may shift back into the economic lead and resume growth as before. This scenario is shown on Figure 16 (left) as the highlighted path. The implications of such a shift would be a 70%
reduction in short-term anticipated demand, which would significantly reduce risk of tellurium supply interruption. Similar delays could be caused by economic recession or removal of subsidies and/or tax incentives for solar PV.

![Figure 16. Tellurium demand sensitivity to PV growth delay, $\beta_0$. (Left) the four demand scenarios were generated from changing parameter $\beta_0$. The path highlighted in yellow represents a real life example of shift in the parameter, expounded upon in the text. (Right) percent change in tellurium demand as a function of time is presented for three different values of $\beta_0$, the so-called “delay of growth” parameter. The percentage values overlaid on the figure represent the magnitude of variation in parameter $\beta_0$ relative to the base case scenario, to emphasize the non-linearity of its relationship with the magnitude of change in demand response.](image)

In general, sensitivity to $\beta_0$ varies over time because of its direct effect on the start of rapid growth. The higher the absolute value of $\beta_0$, the later demand growth begins. Therefore, demand estimations in the short term are most strongly affected by changes to this parameter. Additionally, the sooner the growth occurs (parameter reduction) the greater the demand response is to smaller changes in $\beta_0$. In this way, demand is more sensitive to reductions of $\beta_0$ than to increases of equal or greater magnitude. This is because a reduction of $\beta_0$ corresponds to an earlier start of logistic demand growth and, since the rate of growth is rapid, the effects on demand are quickly revealed. Conversely, demand sensitivity is negligible after 2040 for all of the modeled scenarios. This is because they all share the same growth rate, $\beta_1$, and steady state demand, $K$, allowing them all to reach the same constant level of demand by that time. However, the later the beginning of growth (larger absolute value of $\beta_0$), the later the convergence to this insensitive steady state demand level.

Market balance sensitivity to this parameter is displayed in Figure 15 (top right). The results show that the sooner rapid implementation of CdTe PV begins (lower absolute value of $\beta_0$), the sooner rapid demand growth begins and, since the rate of growth is rapid, the effects on demand are quickly revealed. Conversely, demand sensitivity is negligible after 2040 for all of the modeled scenarios. This is because they all share the same growth rate, $\beta_1$, and steady state demand, $K$, allowing them all to reach the same constant level of demand by that time. However, the later the beginning of growth (larger absolute value of $\beta_0$), the later the convergence to this insensitive steady state demand level.
delay parameter, $\beta_0$) the greater the risk of supply interruption and the sooner that supply gap conditions could emerge. Again, this is due to the relatively slow and decoupled expansion of byproduct tellurium supply. Holding all else equal, it would take a $\beta_0$ value of -23.5 (a 213% absolute value increase) to prevent supply gap conditions through 2060, which corresponds to a growth scenario beginning in 2050. Therefore, with the anticipated supply restrictions, it may not be practical for CdTe PV to begin rapid deployment for many decades.

The environmental implications of demand as discussed in the previous subsection on steady state demand still apply. However, for this parameter, because there is a change in sensitivity over time, the main issue is risk of supply chain interruption and thereby energy security. This is highest under an immediate growth scenario, where demand nearly doubles supply (Figure 15 (top right)). Generally, wherever demand for tellurium exceeds primary supply, there is risk of supply interruption and/or volatile commodity pricing.

### 2.6.3.1.3. Rate of critical byproduct application (CdTe PV) demand growth, $\beta_1$.

Companion fitting parameter $\beta_1$ controls the rate of demand growth. The base case value was taken as an upper limit case since forecasts for PV seem quite optimistic. Although only a small range of values was tested ($0.4 > \beta_1 > 0.1$), sensitivity over this range was observed to be very significant; for example, demand modeled with the lowest growth rate (a 75% decrease in $\beta_1$) was 85–99% less than the base case demand throughout the timeframe (Figure 17).

![Figure 17. Tellurium demand sensitivity to PV growth rate, $\beta_1$. (Left) tellurium demand scenarios for PV growth rate, $\beta_1$, and (Right) sensitivity of tellurium demand to changes in $\beta_1$.](image)
The different demand scenarios generated by varying $\beta_1$ can be thought of as the installation path necessary to meet a renewable goal by 2030, 2040, 2060, and 2100, respectively. In contrast to the previous discussion on parameter $\beta_0$, this type of scenario aims to meet these goals by starting now. By this analogy, setting the goal just 10 years later ($\beta_1 = 0.3$) results in a reduction of up to 75% in short-term demand. Similarly, setting the goal 30 and 70 years later results in up 95% and 99% reduction in demand, respectively. The peak demand reduction occurs later and lasts longer for each successive target timeframe.

The impacts of these goals on byproduct tellurium market balance is quite significant; particularly, in delaying supply gap conditions and reducing the market imbalance, or supply-demand mismatch. Figure 15 (bottom left) displays the ratio of tellurium demand to baseline tellurium supply over time for each demand scenario. All but the slowest growth scenario will result in supply gap conditions emerging before 2040. The earliest onset of gap conditions occurs in the base case scenario at 2018. The highest growth rate possible without entering gap conditions is $\beta_1 = 0.13$, a 68% decrease from the baseline PV growth rate. This indicates that if deployment of this technology is to continue without disruption in the presence of base case tellurium supply, then it must occur more than half as slowly as it has been observed to be going in the past decade.

### 2.6.3.1.4. Material intensity of critical byproduct application (CdTe PV modules)

Demand for tellurium from PV is directly related to material intensity as in Equations 8 and 9. In CdTe PV, the thickness of the cadmium telluride active layer is one of the most crucial parameters for determining material intensity. Film thickness values found in the literature ranged from 1 to 10 µm (Moss et al. 2011; Bleiwas 2010; Morales-Acevedo 2006; Amin, Sopian, and Konagai 2007; Marwede and Reller 2012; Razykov et al. 2011; Noufi et al. 2007); other data ranges collected for parameters critical to material intensity are included in Table 3. The lower limit of 1 µm is typically cited because below this thickness the effectiveness of the material’s electronic performance begins to break down (M Woodhouse et al. 2012; Morales-Acevedo 2006; Amin, Sopian, and Konagai 2007). Using a range of densities reported in the literature results in 5% variability in the material intensity as a function of film thickness.

As with the steady state demand parameter, $K$, because of the direct relationships between film thickness, material intensity, and demand for tellurium (Equations 8 & 9), the magnitude of demand change caused by a change in thickness is equal to the percent change in thickness from
the base case value, and it is independent of time (summarized in Table 7). The results range from a two thirds reduction in maximum demand in the case of 1 µm film thickness to more than tripled demand in the case of 10 µm. Each scenario assumes constant film thickness over the 50-year time period. Although film thickness reduction is expected to be the case in reality, the actual film thickness may currently be higher than it is assumed to be in the base case, in which case a pathway can be drawn in a similar manner as depicted in Figure 16 (left) to model progress over time.

Again, as with parameter \( K \), the more informative analysis of tellurium demand sensitivity is that of market balance. The results of this analysis are displayed in Figure 15 (bottom right) along with the other parameters and their scenarios. Previous analyses have revealed supply gaps emerging in the base case demand scenario, which assumes a film thickness of 3 µm. Therefore, not surprisingly, all scenarios assuming film thickness greater than 3 also result in supply gaps, but with larger imbalances. Since reduction of material intensity is often thought to be a useful tool in reducing risk in the tellurium supply chain, the market balance of scenarios \( \tau < 3 \) are the most relevant to observe. This analysis shows that even dematerialization to the commonly accepted lower limit of 1 µm film results in supply gap conditions emerging. However, the reduction to 1 µm is successful at pushing back the onset of these conditions from 2018 in the base case to 2024 and the magnitude of the imbalance is reduced by two-thirds to more manageable levels, as compared to the base case.

Table 7. Tellurium demand sensitivity to material intensity.

<table>
<thead>
<tr>
<th>Thickness (µm)</th>
<th>1 µm</th>
<th>2 µm</th>
<th>3 µm</th>
<th>6 µm</th>
<th>10 µm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Material Intensity (g/cm³)</td>
<td>0.03</td>
<td>0.06</td>
<td>0.09</td>
<td>0.12</td>
<td>0.3</td>
</tr>
<tr>
<td>Demand Change</td>
<td>-67%</td>
<td>-33%</td>
<td>0%</td>
<td>100%</td>
<td>233%</td>
</tr>
</tbody>
</table>

From an economic standpoint, material intensity is one of the most important demand parameters. The more material in a product the greater the pressure on the supply chain and the greater the material input costs for the solar producer. As compared to traditional photovoltaics, thin film technologies already have an advantage in material intensity, by their very nature.

2.6.3.1.5. Conclusions about byproduct (tellurium) demand sensitivity.

One of the central results of each of these analyses is the year of gap condition onset for a given scenario. This result can be thought of as a metric of risk because most supply-side
parameters are constrained by mining infrastructure and technology and cannot react to change as quickly. Furthermore, there is little incentive to react at all because of the low profitability of byproduct tellurium relative to parent metal copper. The more time available to develop supplementary tellurium supply (primary mined tellurium, more non-copper byproduct tellurium, secondary tellurium), the more likely the system is to avoid these predicted supply gap conditions. Therefore, the lower this parameter (i.e. the sooner the year) the greater the risk to the supply chain.

The date of onset of gap conditions risk metric for each scenario is presented in Figure 18. For reference, all the scenarios are summarized in Table 8, labeled as scenario 1–4 for each parameter. If less than four scenarios were generated the 4th is left blank. Also, if a scenario does not induce supply gap conditions it is left out of Figure 18. Generally speaking, most of the scenarios modeled in this work lead to increased supply chain security as compared with the baseline scenario. Gap onset dates range from 2011 for the most aggressive $\beta_0$ scenario to 2036 for the least aggressive $\beta_1$ scenario.

**Figure 18. Year of supply gap condition onset for demand parameter scenarios.**
Table 8. Demand scenarios.

<table>
<thead>
<tr>
<th>Demand Scenarios</th>
<th>Baseline</th>
<th>K1</th>
<th>K2</th>
<th>K3</th>
<th>K4</th>
<th>B0-1</th>
<th>B0-2</th>
<th>B0-3</th>
<th>B0-4</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K$ (GW/y)</td>
<td>50</td>
<td>100</td>
<td>25</td>
<td>10</td>
<td>5</td>
<td>50</td>
<td>50</td>
<td>50</td>
<td>N/A</td>
</tr>
<tr>
<td>$\beta_0$</td>
<td>-7.5</td>
<td>-7.5</td>
<td>-7.5</td>
<td>-7.5</td>
<td>-7.5</td>
<td>-5</td>
<td>-9</td>
<td>-11.5</td>
<td>N/A</td>
</tr>
<tr>
<td>$\beta_1$</td>
<td>0.4</td>
<td>0.4</td>
<td>0.4</td>
<td>0.4</td>
<td>0.4</td>
<td>0.4</td>
<td>0.4</td>
<td>0.4</td>
<td>N/A</td>
</tr>
<tr>
<td>$\tau$ (\mu m)</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>N/A</td>
</tr>
</tbody>
</table>

Sensitivity of gap onset was also probed by comparing the change in gap year and the percent change of the demand parameter. Since the values were different for each of the scenarios the average was taken for each parameter and error bars were included to indicate the range (Figure 18). By this metric, the demand parameter that has the greatest effect per relative unit change on when or if gap conditions emerge is the rate of PV demand growth, $\beta_1$. This fact can be qualitatively gleaned from a look at all of Figure 15, but this quantitative metric is a novel and useful way to measure risk and compare the effectiveness of a particular parameter at affecting risk.

![Figure 19. Sensitivity of supply gap onset to demand parameters.](image)

*Gap sensitivity is the ratio of change in gap (years) to percent change in the demand parameter.*
Figure 19 indicates that PV growth rate, $\beta_t$, has the greatest impact of the demand parameters to affect risk, for better or worse depending on the direction of the parameter change. Despite its potential for delaying onset of supply gap conditions, the rate of PV demand growth is not easily controlled. In fact, of the leverage points modeled in the present work, material intensity as approximated by film thickness is the only demand parameter that really can be directly controlled by an agent in this supply chain, and according to Figure 19, it has a much smaller impact.

This motivates the importance of looking to supply-side solutions early on in addition to preventing policies that encourage rapid growth of this technology until the supply can keep up. This reduction in growth rate may happen naturally in response to price signals. As tellurium approaches gap condition point, its price, given inelastic supply, will increase dramatically. Tellurium contributes between 4-27% of CdTe manufacturing costs (M. L. Bustamante and Gaustad 2015) However, it has been shown that even increasing the price of tellurium by over 300% only results in about 50% increase in manufacturing price (Candelise, Winskel, and Gross 2012). This increase may still be enough to tip the scales away from CdTe PV toward a less expensive technology (for more about how raw material input price can affect competitiveness of solar technologies (see the following published analysis comparing CdTe and CIGS PV from firm, consumer, and broader policy perspective (M. L. Bustamante and Gaustad 2015)).

2.7. Discussion & Future Work

The central results of this chapter indicate that growth of CdTe PV, a promising thin film solar technology, will likely be stifled by the periodic availability of tellurium rather than by its overall availability as many have focused on in the traditional context of criticality. The mineral is geologically scarce but it is the dynamics of its byproduct supply chain that create the biggest risks to expansion. The current supply infrastructure for tellurium is insufficient to meet even conservative demand growth for the emerging CdTe PV technology. However, the foremost CdTe PV company is American, so it is possible that entities within the United States may have some interest in promoting this technology’s success. In order to do so, action must be taken immediately to provide supplementary supply to traditional byproduct sources.

From an environmental perspective, the top priorities should be improving CdTe PV recycling infrastructure and increasing recovery yield of available tellurium from byproduct
sources. Next action should be the development of more primary tellurium mines because, although it is less resourceful and more physically impactful, this source would represent a larger and more robust source of supply. Even with use of higher recovery efficiency and recycling, this option may be unavoidable unless stockpiled mineral is readily available and sufficient to cover production/consumption imbalance for a given year. Stockpiling is another useful technique for supplementing supply, with no investment in new technology or infrastructure necessary. Conversely, little can or should be done on the demand side. If this technology cannot deliver the demand for PV, it will be replaced by competitors, such as traditional silicon. However, dematerialization, via film thickness reduction or otherwise, offer significant potential to reduce risk of supply interruption if pursued in the short term as shown in Figure 16 (bottom right).

Broadly speaking, these results illustrate how byproduct minerals like tellurium face a higher risk of supply disruption due to the decoupling of their primary supply and demand. As such, their end-use applications are inherently exposed to potential supply interruption or dramatic price volatility and such conditions were observed in this analysis. Such supply issues or price spikes pose great risks to firms, particularly start-ups like the budding clean tech companies that utilize byproduct input materials.

For CdTe technology specifically, such disruptions would only effect overall PV growth as customers would likely purchase an alternative PV system if demand for CdTe systems was unable to be met. Supply interruptions would not disrupt production of energy from already installed PV systems in the same way a fuel supply interruption would disrupt non-renewable power plants. In this way, PV has an advantage in terms of overall energy security. With most energy-critical byproduct supply-chains, both recycling from their respective clean-tech applications and improvements in yield offer significant potential to reduce supply risks and price volatility by supplementing current levels of primary supply. However, as in this case for tellurium due to rapidly expanding use in CdTe PV, these mitigation strategies may not fully eliminate the emergence of supply gap conditions because parent metal supply trends can diminish long term prospects of availability. Recycling has particular potential for ensuring supply chain sustainability in the long-term and should be considered for any technology based on a critical byproduct material. Conversely, investments in increased byproduct yield and end use dematerialization can help bridge the gap in the short term.
The methodology presented here represented a novel approach to modeling the sensitivity of a byproduct supply chain to changes in supply and demand parameters into the mid-term future. While valuable in its analysis, the approach could be improved upon in several ways. For instance, several alternative primary tellurium supply chains exist but were not directly modeled in this analysis. USGS mentions the minor recovery of tellurium from lead refineries and various metal smelters (US Geological Survey (USGS) 2016). Additionally, Fthenakis and Anctil summarize the tellurium resource available in gold–telluride ore (V Fthenakis and Anctil 2013). Some inclusion of these resources is likely part of the future supply chain and the current analysis underestimates that fact. Also, in reality, growth of supply from primary sources is constrained by several factors potentially not captured by historical trends. For instance, the development of new mining sites is dependent on geological availability, economic feasibility, as well as political restrictions. It also takes a great deal of time. Inclusion of constraints to growth, capturing some of these factors, would improve upon the model’s predictive powers; however, the objective of the analysis was to demonstrate sensitivity to changes over time and reality is likely captured within the range presented.

In general, the model successfully represents a framework by which the supply risk of complex byproduct systems can be analyzed. The methodology should be thought of as a tool that can be applied to many systems, where it is at the author’s discretion to define the goal and scope of the analysis. For example, the time frame and geographic scope of the assessment can be contracted or expanded from that chosen here to better suit available data or interests of the investigator. The results of this and similar analyses can help to inform policy decisions by demonstrating the dynamic role of recycling as a secondary supply source and indicating under what conditions supply interruption is most likely to occur. The latter can allow policy makers and producers to be aware of dangerous developing conditions and allow for better decisions to be made in anticipation. In this way, knowledge of the supply-chain sensitivities itself helps to make the supply chain more secure and sustainable into the future.

Additionally, work like this, which demonstrates scenarios and conditions indicative of danger may encourage investment in abatement strategies (like improving byproduct yield of recycling technology and infrastructure). The sooner a projected gap onset and the larger the potential imbalance, the greater is the risk. Changes to parameters that delay gap onset and reduce imbalance magnitude are useful to reducing risk. Whether or not changing them in real life is easy
or even possible is another discussion individualized to each parameter. Policy makers can help to steer the relevant plays in the right direction by developing mechanisms that incentivize these risk-mitigating practices and developments.
CHAPTER 3. Characterizing Environmental Risk: Effects of Allocation & Temporally-Specific Data Variation

3.1 Environmental risk in criticality assessment

Supply risk has traditionally been, and still remains the primary focus of criticality assessment; however, environmental factors are increasingly being considered. The use of environmental risk as a component of criticality assessment was first introduced by the European Commission’s first report on critical materials for the European Union in 2010. In this report a measure of “environmental country risk” was evaluated in addition to traditional supply risk from geophysical, economic, and sociopolitical factors to capture potential for restricted access to deposits on the basis of increased environmental regulation. The environmental country risk was calculated using a metric from known as the “environmental performance index” or EPI (European Commission 2010). EPI is a country-specific indicator that is intended to measure disparity between current environmental performance and established policy goals using over 20 indicators pertaining to human health and ecosystem vitality. EPI is then applied to individual materials using a weighted market concentration approach for global supply. For example, of 180 countries ranked in 2016, Finland was ranked highest with a score of 90.68%, the US ranked 26th with a score of 84.72%, China ranked 109th with a score of 65.1%, and lowest reported score of 27.66% was for Somalia (Hsu and et al. 2016). Since approximately 85% of rare earth oxides (REO) mined during 2015 came from China, another 8% came from Australia, 3.3% from the US, 2% from Russia, and 1.6% from Thailand (US Geological Survey (USGS) 2016), REO would receive an environmental country risk score equal to the sum of the product of each country’s EPI score (e.g. for China, 65.1) and the square of that country’s REO market share (e.g. for China, 0.85^2). However, in the most recent version of this report published in 2014, the group eliminated use of the environmental country risk indicator due to concern that its indicators were not truly relevant for the mining industry (European Commission 2014).

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3 This chapter is adapted from a forthcoming publication in Solar Energy Materials and Solar Cells. As in the previous chapter, to avoid distracting repetitious self-citation, a blanket reference to the original manuscript is provided here: (M. L. Bustamante et al., n.d.). Note: in this chapter there are a few exceptions where reference to a secondary case study of terbium, a rare earth element, are called out using internal citation in the body of the chapter as necessary.
In the original 2010 report, the European Commission also considered using life cycle assessment (LCA) to generate environmental risk indicators that capture relative environmental impact of different materials. LCA is a powerful modeling framework for comprehensive evaluation of environmental impact for products. The tool considers everything from raw material extraction to generation of energy used during manufacturing and transportation all the through waste management at the end of the product’s useful life. The group investigated use of twelve midpoint level indicators, similar to those captured by the ReCiPe 2008 method, but ultimately rejected the idea due to lack of data for some materials of interest (e.g. beryllium, germanium, and rhenium) and fundamental disagreement with use of a material-specific cradle-to-gate perspective instead of a product-specific cradle-to-grave perspective. The former perspective compares elements on a one-to-one by weight basis when in reality different materials are used in different amounts in same and differing products. Further, only environmental impacts of extraction and mineral production processes are captured, neglecting impacts during manufacturing, use, and disposal (European Commission 2010).

Although these concerns are valid, environmental factors can have real impacts on material availability. Consider, the case of indium; since 2003, global primary indium supply has been dominated by China, peaking at 90% in 2005 and currently holding around 50%. During 2009, hundreds of indium producers were shut down by a series of newly-introduced environmental regulations on the non-ferrous metals industry leaving just 21 open by 2010. This supply restriction is thought to have led to a temporary price spike observed during 2009, which triggered Japan to begin stockpiling indium (Tolcin 2011). Meanwhile, China increased export quotas in 2010 to protect domestic supply (Duan et al. 2016) and indium prices reached a peak of $720/kg in 2011 (US Geological Survey (USGS) 2014b). Fortunately, due to availability of prompt scrap for recycling, impacts were diminished. However, most other critical materials do not have comparable secondary streams to stabilize their markets in the face of similar restrictions. Therefore, even if there are still challenges with straightforward cradle-to-gate LCA methods to quantify environmental risk for critical materials, it may still serve as a useful indicator of potential risk for future restriction due to environmental impact of production.

In recent years, a few other studies have emerged using LCA-inspired metrics to quantify environmental risk. The majority come from a group at Yale, where they utilize the same methodology but focus on different case studies groups of related materials. These studies use a
separate environmental implications axis, creating a 3-dimensional criticality space, but also capture elements of environmental risk factors in the other two axes (supply risk and vulnerability). The supply risk axis captures environmental risk as a component of the policy potential index (PPI), which is a mine- and region-specific indicator developed by the Frasier Institute to capture appeal of different regions for mining activity based on policies including, but not limited to, environmental regulations. Separately, the Yale framework evaluates environmental implications associated with production using ReCiPe endpoint indicators of human health and ecosystems damages per kilogram of material. These same results are also considered in the context of environmental tradeoffs of substitution within the vulnerability axis, as an indicator called environmental ratio (ER) (Graedel et al. 2012). Aside from the Yale studies, a group from RIT has identified and quantified potentially useful environmental risk indicators for criticality assessment in a recent study: CERCLA toxicity points, primary embodied energy, and energy savings from recycling. The CERCLA toxicity score captures a complementary use phase and end of life perspective of impact in the case of release of the material rather than impact generated during extraction and production of the material. The primary embodied energy metric captures a measure of environmental impact highly relevant to the target audience of solar photovoltaics specialists, who use energy input to determine energy payback time (EPBT), a measure of environmental performance of their technology. Energy savings from recycling are calculated using primary energy data and empirically developed relationships to estimate benefit or recycling, another policy relevant metric. Of these three environmental risk metrics, primary embodied energy and energy savings are both derived from LCA data (Goe and Gaustad 2014a).

In these existing criticality studies that consider environmental impact as informed by LCA, results are pulled directly from LCA modeling software using existing unit processes without consideration for modeling decisions underlying these processes. One key challenge regards modeling environmental impact for minor and specialty metals. Since these materials are often geologically less abundant, they may not form ore deposits that would allow direct mining. Instead, the most economical pathway to recovery of these materials is as coproducts or byproducts of major metal extraction and refining processes (Bleiwas 2010; M. L. Bustamante and Gaustad 2014a; N T Nassar, Graedel, and Harper 2015). These forms of joint production are challenging to assess using LCA because the tool is inherently product-focused. Therefore, when evaluating a shared process, the environmental impacts must be distributed among the multiple outputs of each
process in some way. This situation is sometimes referred to as “the allocation problem,” (e.g. Guinee, 2006 (Guinée 2006)). There is no universally acceptable method to conduct this impact partitioning, so it inevitably introduces a degree of variability through practitioner judgment about methodology and associated data selection (Curran 2007).

The goal of this chapter is to propose potential solutions to key methodological and data-driven variabilities in LCA of jointly produced metals. The discussion begins with a more thorough review of the unique challenges byproduction poses for LCA; namely, need for allocation, choice of allocation method, and parametric variability in time sensitive allocation data. Then, the impact of these modeling decisions on LCA results is demonstrated for tellurium (Te). Finally, best practices are recommended to address the identified challenges in LCA of similar material systems. These insights are intended to inform behavior that will improved reliability of environmental impact results for criticality assessment based on LCA results.

3.2. Byproducts & Challenges for LCA

Byproduction is inherently challenging for LCA because the modeling framework dictates that the environmental impacts of processes must be attributed to individual products. The International Standards Organization (ISO) has developed a procedure to guide practitioners facing this challenge and to encourage uniformity across studies (Finkbeiner et al. 2006); however, their guidelines are not prescriptive and, as a result, leave a great deal of choice to the practitioner. This is problematic because it is well established that allocation choices can dramatically affect results (Luo et al. 2009; Morais, Martins, and Mata 2010; Wardenaar et al. 2012; Stamp, Althaus, and Wäger 2013; Zaimes and Khanna 2014).

The ISO guidelines for dealing with multi-output processes first recommends avoiding allocation of impacts, if possible (Finkbeiner et al. 2006). Common methods for avoiding allocation include system expansion and system subdivision (Bo Weidema 2000; B. P. Weidema and Schmidt 2010). System expansion identifies a substitute process for producing the coproduct and compares it to the joint process, either claiming a credit for avoided production or adding it to the system to provide the second function via an alternate pathway. However, many joint products of multifunctional processes are minor byproducts that are never produced independently; therefore, any alternate production processes also face the allocation problem, shifting rather than solving it. Allocation can also be avoided in some scenarios though more detailed process
modeling, known as process subdivision. Subdivision involves further separation, where possible, to isolate sub-processes that lead directly to the production of the individual joint products. Again, this is often not possible because the joint products are separated during a single process step, i.e. anode slime created during electrolytic refining of copper or generation of flue gases during smelting.

When allocation avoidance is not possible, ISO dictates allocation based upon “physical causal” relationships, where possible (Ekvall and Finnveden 2001; Finkbeiner et al. 2006). In other words, impact should be partitioned based upon the degree to which each product drives the process. Distinction should be made to identify joint production processes where the secondary product is produced at a rate dependent or independent of the major product, where the former is considered causal. If a physical relationship cannot be established, any other relationship can then be used. As a result, there is still considerable debate within the LCA community as to which allocation method is most appropriate to use, if any, and under what circumstances (Bo Weidema 2000; Ayer et al. 2007; Curran 2007; B. P. Weidema and Schmidt 2010). The two most commonly used allocation methods are governed by tradition: mass-based allocation and economic (or market value-based) allocation. Mass allocation distributes impact to each product according to its share of total output on a mass basis whereas economic allocation distributes impact based upon share of total revenue generating potential. Mathematically these are represented as shown below:

Mass Allocation: \[ AF_{m,i} = \frac{X_i}{\sum_i X_i} \]
where \(AF_{m,i}\) = mass allocation factor for product \(i\) with mass output \(X_i\)

Economic Allocation: \[ AF_{e,i} = \frac{P_i X_i}{\sum_i P_i X_i} \]
where \(AF_{e,i}\) = economic allocation factor for product \(i\) with mass output \(X_i\) and market price per unit mass \(P_i\).

In LCAs of metals and mining, economic allocation has unofficially been established as the allocation method of choice (Classen et al. 2009; Bigum, Brogaard, and Christensen 2012; Nuss and Eckelman 2014). This trend has been justified by the idea that profit seeking behavior drives joint mining processes and therefore economic factors are fair basis upon which to partition impact. Further, it has been asserted that economic allocation is justifiable when the volume of the joint
process actually varies in proportion to changes in the revenue contributions from the different products, which is typically the case when no alternative production route or substitutes for the material exist (B Weidema and Norris 2002). However, revenue-based allocation may not be appropriate for all joint production scenarios because it neglects cost considerations that factor into profit-driven decision making, such as increasing production volume, which are distinct for byproducts and coproducts.

Coproducts have the ability to bear costs of processing, but byproducts do not (Brooks 1965; Campbell 1985). In the absence of cost data, it may be impossible to definitively classify a joint product being modeled in LCA as a coproduct or a byproduct. Therefore, other forms of allocation need to be considered as well. For instance, allocation on the basis of physical relationships may be more appropriate for byproducts. When the minor product is scavenged from a waste stream, as is the case for tellurium recovered from copper refinery anode slime, there is no way to vary the output of the byproduct-containing stream (e.g. copper anode slime) except to process more main product (e.g. refine more copper concentrates), which would create a large oversupply of the main product (e.g. copper cathode) and cause the refiner to incur costs unjustifiable by the marginally profitable sale of byproduct (e.g. anode slime) to further processing facilities, meaning realistically it would not happen regardless of price.

Another obstacle that prevents variation in joint process volume in byproduction systems is the fact that there are typically multiple stakeholders along the supply chain. Perhaps if one stakeholder managed the entire process from joint ore extraction to byproduct metal refining, it could be considered justifiable to extract more ore just to produce more byproduct; however, it is highly unlikely and contrary to the economic definition of a byproduct (Petrick et al. 1973; Campbell 1985). The economic justification is highly dependent upon the relative masses of the joint products, which can vary by several orders of magnitude (i.e. ~2.5 grams of anode slime containing ~20 - 80 milligrams of tellurium are yielded per kilogram of copper cathode refined (Classen et al. 2009)). In these cases, where the byproduct is so minor in mass that even very large changes in price of the byproduct are not enough to justify additional processing, using economic allocation would unfairly penalize byproducts (albeit by a small amount) when their production is more of a function of mass ratios. In reality, each process step is managed by a different stakeholder to their best benefit; extending the tellurium example, the copper miner is different than the copper refiner who is different than the anode slime processor and tellurium refiner. Each
upstream actor acting in his own best interest economically sets a physical limit to the amount of tellurium being made available downstream. The copper miner’s profit maximization is irrespective of the ore’s tellurium content. Therefore, even if the optimal extraction of copper ore does not provide enough tellurium to meet demand, driving prices up wildly, it would not factor into the copper miner’s decision on process volumes. It also would not likely factor into the copper refiner’s decision to process more or less copper concentrates since its primary purpose is to produce copper and anode slime is just an unavoidable but marginally valuable output of that process. The only time the byproduct metal’s value likely factors in would be in the further processing steps where tellurium-containing compound, copper telluride, has characteristics more like a coproduct. For other joint materials supplied in a similar fashion, choice of allocation method cannot be blindly assumed to be compatible with the industry-standard economic approach; however, as emphasized earlier, in absence of definitive classification, it should still be considered because it may apply under certain conditions.

When using the traditional economic allocation approach, impact determination can be further complicated by the prevalence of commodity price volatility. Significant changes in price of joint products can create variability in results by attributing the burden differently to each coproducts depending upon the time period selected. Many studies use average prices to address this issue (Classen et al. 2009; Stamp, Althaus, and Wäger 2013; Nuss and Eckelman 2014); however, the choice of averaging period is also subjective. A few studies have touched on this topic (Stamp, Althaus, and Wäger 2013; Nuss and Eckelman 2014), but they did not consider how choice of distinct averaging periods could change results, not surprisingly understating the potential impact of this factor. Further, dramatic shifts in price over time can cause a joint product to be considered a coproduct instead of a byproduct and vice versa, making choice of appropriate allocation method a time-specific decision as well.

3.3. Life Cycle Assessment Methodology

LCA involves four general steps: goal and scope definition, life cycle inventory, life cycle impact assessment, and interpretation. Goal and scope definition establishes several important aspects of an LCA. First, it requires clear declaration of the purpose for the assessment; i.e. what will be done with the results. Next, it explicitly defines the system to be studied, including boundaries (both physical and temporal), processes, and flows that will and will not be modeled
and justification for these decisions. Ideally, by the end of goal and scope definition it should be clear to the modeler what data needs to be collected to accomplish those goals. This data collection is accomplished during the next step, life cycle inventory. In the life cycle inventory it should be clear what assumptions are being made about the data and its modeling. Once all the life cycle data has been inventoried, the environmental impacts are assessed for all the reference flows defined in the previous two steps. Life cycle impact assessment requires selection of an impact assessment method to translate reference flows of material and energy into environmental impacts determined to be relevant as defined in the goal and scope. The final step, which is really utilized all along the way, is interpretation. This means interpretation of results to glean implications for addressing the goals of the model as well as interpretation of modeling at each step in the process. This methodology may sound linear, but, in reality, interpretation is continually important to determine whether previous steps need to be revised in the face of modeling limitations (Matthews, Hendrickson, and Matthews 2014).

3.3.1. Goal and scope definition

The goal of the LCA case study is to improve current life cycle inventories, illustrate common challenges in modeling impacts of byproduct materials, and demonstrate ways to potentially deal with these challenges. These goals are accomplished by performing globally representative cradle-to-gate LCA, using a functional unit of 1 kg tellurium, where environmental impact is assessed for different allocation method and temporal data assumptions. Temporal scope is limited to 2006 – 2014 to encompass two averaging periods: 2006 - 2010, which has been used in a recent study (Nuss and Eckelman 2014), and 2010 - 2014, which represents the most recently available 5-year averaging period. The scenarios demonstrate the importance of these decisions on LCA results and implications for further decision making.

As in the previous chapter, the scope of this analysis was limited to this primary production pathway, which is via extraction from a copper refining byproduct known as anode slime. System boundaries were drawn to bound the investigation around the following four sequential processes: (1) copper mining from sulfide ore, (2) copper refining via electrolytic method, (3) anode slime processing to separate valuable components, and (4) tellurium refining to produce semiconductor-grade material. Along this production pathway, many instances of allocation are required because the first three unit processes generate coproducts without substitutable production pathways,
preventing system expansion, and often without clear causal delineation, preventing subdivision. Figure 20 shows the system diagram encompassing the modeled processes.

![System Diagram](image)

**Figure 20. Tellurium LCA system diagram** showing modeled processes and valuable outputs for byproduction of tellurium from copper ore.

### 3.3.2. Allocation methods

To probe variation in LCA results introduced by allocation assumptions, a host of allocation scenarios are created and applied to the two case study systems. These scenarios, summarized in Table 9, use different allocation method and temporal scope assumptions for data. To facilitate comparison, a baseline scenario is selected against which all other scenarios will be measured. Economic allocation was used for this baseline scenario to be consistent with most mining or metal production LCAs. To represent a state-of-the-science model, the most recent inflation-adjusted 5-year averaging period of 2010-2014 is used to determine allocation factors. Additionally, to represent a situation where more recent time period data are not available, a distinct averaging period scenario is created which utilizes inflation-adjusted 2006-2010 data. Next, to represent a situation where a practitioner might not have access to historical data to create averages, new allocation scenarios are also created using data from individual years between 2006 and 2014, covering the whole time-frame of the study. Finally, to test the effects of alternate allocation method decisions, the second most common approach, mass allocation, is also generated for comparison for each time period assumed.

As shown in Table 9, all tellurium allocation scenarios are associated with a specific time period. Even the mass allocation scenarios for the tellurium case study utilize time-specific data because the anode slime processing unit process block was designed in accordance with ecoinvent (Classen et al. 2009) to reflect realistic output levels of coproducts that reconcile with actual
observed supply. This approach utilizes global production ratios to adjust anode slime joint products in proportion to changing anode slime content and yield, preserving mass balance while capturing realistic trends in supply. For the baseline mass and economic scenarios, a time period of 2010 - 2014 is utilized for all time sensitive data. For the alternate mass and economic scenarios, a time period of 2006 - 2014 is utilized for all time sensitive data. Individual year economic and mass scenarios utilize data from the associated year only, with no averaging.

**Table 9. Summary of LCA scenarios considered.** Each scenario is constructed using different allocation & time-related data assumptions.

<table>
<thead>
<tr>
<th>Scenario Code</th>
<th>Scenario Description</th>
<th>Allocation Method</th>
<th>Temporal Scope</th>
</tr>
</thead>
<tbody>
<tr>
<td>ECON_base</td>
<td>Baseline scenario: Economic allocation using averaging over most recent 5 year time period for time sensitive data, mainly prices</td>
<td>Economic</td>
<td>2010 - 2014</td>
</tr>
<tr>
<td>ECON_alt</td>
<td>Alternate economic allocation using averaging over different 5 year time period for time sensitive data, mainly prices</td>
<td>Economic</td>
<td>2006 - 2010</td>
</tr>
<tr>
<td>ECON_year</td>
<td>Economic allocation using individual year specific values for time sensitive data, mainly prices</td>
<td>Economic</td>
<td>2006 - 2014 (individual years)</td>
</tr>
<tr>
<td>MASS_base</td>
<td>Mass allocation using averaging over most recent 5 year time period for time sensitive data, where applicable, mainly production ratios</td>
<td>Mass</td>
<td>Te: 2010 - 2014</td>
</tr>
<tr>
<td>MASS_alt</td>
<td>Mass allocation using averaging over different 5 year time period for time sensitive data, mainly production ratios</td>
<td>Mass</td>
<td>Te: 2006 - 2010</td>
</tr>
<tr>
<td>MASS_year</td>
<td>Mass allocation using individual year specific values for time sensitive data, where applicable, mainly production ratios</td>
<td>Mass</td>
<td>Te: 2006 - 2014 (individual years)</td>
</tr>
</tbody>
</table>

**3.3.3. Life cycle inventory**

Simapro 8.0 LCA modeling software is used to conduct the LCA case studies in line with ISO guidelines (Finkbeiner et al. 2006). Raw unallocated unit processes from ecoinvent (v. 3.01 available online) are used as a starting point to create custom process blocks in the software, updating data where available to reflect best knowledge of the case study material production systems (ecoinvent 2015). Crucial case study specific modeling improvements are detailed in Sections 3.2.3 and 3.3.3. Allocation factors for each process step were assigned according to methods described in the previous Section 3.1.2 and case study specific Sections 3.2.2 and 3.3.2.

Several changes were made to model tellurium production to the best of present research abilities. First, the upstream copper extraction processes (orange blocks in Figure 20) were connected to the downstream byproduct extraction processes (blue blocks in Figure 20). The existing modeling in ecoinvent employed a cut-off approach, separating the copper refining block
from the anode slime generation block when in reality they result from the same process. Next, copper refining was modified so that only copper refining processes resulting in tellurium production were included. This was accomplished by substituting all irrelevant copper inputs, such as copper mined by solvent-extraction (SX-EW), with copper mined as concentrates (1:1 w/w). Further, prices and production figures used in inventory calculations prescribed by ecoinvent (Classen et al. 2009) were updated as necessary.

Production data was obtained from USGS for all coproducts except copper and tellurium. This alternative sourcing was selected because USGS production figures did not describe the appropriate process for copper (mining reported versus refining) and were incomplete for tellurium (plagued by proprietary withholding). For copper production, USGS figures represent total mine output not refinery output and the latter is what is being modelled when production figures are used in calculation. For tellurium production, many nations known to produce tellurium do not report their production figures, including the United States, and therefore an accurate global production estimate cannot be made from the reported data (US Geological Survey (USGS) 2015a). In lieu of reported tellurium data, the ICSG electrolytically refined copper production data was used as proxy for tellurium production according to methodology previously described in Chapter 2 (M. L. Bustamante and Gaustad 2014a).

Finally, an additional coproduct, selenium, was added to the anode slime processing step to more accurately reflect global coupled production. Each year, more selenium is available and ultimately produced from the same anode slime (M. W. George 2012), making it inappropriate to exclude selenium from allocation considerations in an LCA of tellurium. The resulting reference flows and prices for each allocation scenario are shown in Figure 21.

### 3.3.4. Life cycle impact assessment

Cumulative energy demand (CED) is selected to serve as the impact assessment method for the present analysis. CED is a very common, single issue impact assessment method, which accounts for the net energy generation and consumption throughout the product’s modeled life cycle (Jungbluth and Frischknecht 2010). This method is selected for a few different reasons. First, CED, also known as embodied energy or primary energy, is a useful input for several decision metrics of potential interest to solar professionals. These include energy return on investment.
(EROI), a measure of life cycle net energy generation; energy payback time (EPBT), a form of breakeven analysis to determine time to net energy balance; and energy savings of secondary materials as compared to primary materials, a means for motivating recycling. Further, CED offers a certain level of methodological simplicity. As a single issue impact assessment method, the focus remains on allocation sensitivities, which is aligned with the goal of the present LCAs. Finally, although it lacks the comprehensivity of a broad impact assessment method like ReCiPe or TRACI, CED has been shown to represent an effective proxy for other key environmental impact metrics, such as global warming potential (GWP), a measure of greenhouse gas (GHG) impacts (Huijbregts et al. 2010).

3.4. Results & discussion

CED results for the averaged time period scenarios are summarized in Figure 22. The
change in CED, relative to the base case, suggests the variation associated with two different aspects of allocation: (1) choice of method (e.g. mass versus reference case), and (2) price variation (i.e. recent versus prior 5 year timeframe). Both economic scenarios resulted in very similar CED, with only a 2% decrease observed when using the older timeframe. This was surprising since tellurium price varied by more than 50% in either direction over the course of the two time periods being considered.

The greatest CED is obtained from allocation by mass. Choosing to allocate based on mass of each product instead of value of each product results in a near 6-fold increase in CED estimation over the base case economic scenario. This is somewhat counterintuitive; since tellurium is a very minor coproduct in terms of mass but has a fairly high value compared to copper, it was expected that economic allocation would assign a greater impact to tellurium. However, since tellurium is extracted from the anode slime as a compound, copper telluride (CuTe), and it is coproduced along with silver and selenium during this process, the results depend upon the relative trends in price and production among the coproducts. Silver has a much higher price than CuTe (estimated based upon recoverable tellurium content) and also a higher output relative to tellurium in the reference case, skewing the economically-allocated impact away from tellurium. These finding highlights the importance of system perspective in modeling of complex production systems as well as the potentially powerful impact associated with allocation method selection.

Figure 22. Tellurium CED results for each data-averaged allocation scenario.
Further analysis based on individual annual price and production values yields smaller variation than choice of allocation method. Under economic allocation assumption, results range from 11% above the reference case (2011 data) to 10% below (2007 data). This variation is not as large as might be expected from looking at tellurium price variation alone over the same time period. Pure tellurium price averaged $1998 122/kg from 2006 - 2014, peaking at $1998 253/kg (+107%) in 2011 to more than double the period average, and sinking to nearly half the average in 2007 at $1998 67.50/kg (-47%) (US Geological Survey (USGS) 2015b). Conversely, under mass allocation, in which only the production ratios change, the year to year CED deviation from average is much smaller. The maximum deviations in each direction are observed in 2007 (-5.6%) and 2013 (+1.4%). Using an averaging period of 2006 - 2010 instead of the baseline 2010 - 2014 for mass allocation resulted in a 3% reduction in expected CED, which is double that of economic, but still small. The larger difference between averaging periods suggests more recent trends in production data may skew results more than price trends or that price trends counteract some of the production trends. After all, economic allocation is simply a price weighted mass allocation.

Existing models employ cut-off methods to avoid allocating impacts for joint production at the mine or refinery. This is concerning because, depending on the scope of the LCA and allocation method, upstream processes can contribute a significant amount to the overall impacts for byproducts (see. Fthenakis & Anctil (V Fthenakis and Anctil 2013). The present study also integrates updated allocation factors for the mass and economic scenarios, including temporal effects within its mass allocation via changing production ratios to reflect variation in anode slime content and yields over time. As a result, tellurium displayed temporal variation in CED by mass allocation for the individual years. Although small (3% decrease for MASS_alt), choice of averaging period affected mass-based CED for tellurium more than it did for economic based CED (1% decrease for ECON_alt). Tellurium did not see much variation: at most an 11.2% change from the baseline. Additionally, economic to mass CED ratio is 1 to 5.8 for tellurium. Surprisingly, the highest CED was realized for a mass allocation scenario.

To understand, trace the tellurium-bearing joint products through each multi-output process; copper concentrate from copper mining, anode slime from copper refining, and copper telluride from anode slime processing. The tellurium-bearing output is typically the lowest priced among its coproducts; in the copper mining step, molybdenite is 6 - 18 times more valuable per unit ($/kg) than copper concentrate, and, in the anode slime processing step, silver and selenium
are 45 - 138 times more valuable than copper telluride is estimated to be (Figure 24). The exception is anode slime which has similar price per unit to copper cathode (only 1.2 to 2.7 times greater) but opposing rank in relative mass outflows (2.6 - 2.9 grams anode slime produced per kilogram copper cathode), creating a value difference between the products of 130 - 340 times greater for copper cathode as compared to the tellurium-bearing anode slime. Note that, in the case of copper telluride and anode slime, valuation was determined in line with Classen et al (Classen et al. 2009)
methods, which assumed a value of the intermediate product (anode slime and copper telluride) that is 10% of the pure value of the contained metals (silver, selenium, and tellurium). Sensitivity of results to this kind of methodological assumption are not probed in the present study, but since they directly determine price, selection of a different valuation method may also strongly affect economic allocation results.

Additionally, the tellurium-bearing joint products is always the lower contributors to total process mass output, except in the first process where copper concentrate is the major output. Tellurium, as a component of the lower valued outputs and, in most cases, the lower magnitude flows, would display a weakened allocation factor using economic versus mass allocation. This result highlights how decision of allocation method might change the results differently for different systems, especially in the case of a comparative LCA. Choosing to allocate based on industry norms may still yield mixed results.

Figure 24. Unit price behavior for joint products of each unit process in tellurium production, demonstrating the importance of accounting for price volatility and system perspective in LCA of joint product materials.
Breaking the results down by process contributions can also provide interesting insight into the impacts of allocation decisions. Figure 25 shows CED for all economic allocation scenarios (top) and mass allocation scenarios (bottom) considered. Under the economic allocation scenarios, CED is dominated by the tellurium refining stage, which contributes between 73-90% of total cradle to gate impact. In these scenarios, anode slime processing contributes the least with only 0.3-0.8% of the total impact. This skew toward the refining step can be explained, as previously, by the lower relative prices of the tellurium component as compared to the other joint products of the processes. Under the mass allocation scenarios, CED is instead dominated by the copper mining stage, which contributes between 54-59% of total cradle to gate impact for tellurium. In these scenarios, anode slime processing still contributes the least to the total, but makes up a larger percentage of 4.4-4.5%. Further, total impact by mass is much larger, so this higher percentage contribution from anode slime processing is much more significant in terms of CED: 0.4-1.2 MJ/kg from anode slime processing under economic allocation versus 34-37 MJ/kg under mass allocation. Comparing between the two methods, process-specific impact contributions are more sensitive under economic allocation than mass. This is the opposite of the result for overall CED (mass was more sensitive); however, the switch can be explained by the difference in magnitude between mass and economic. Economic CED is much smaller, therefore, smaller changes in energy contribution from each process, represent larger percentage contributions to the total small CED.

3.5. Best practice recommendations

The findings from this case study identifies three common challenges for LCAs of byproduct materials: (1) existing LCI process data, if it exists, may not fully incorporate joint production; (2) choice of allocation method dramatically affects results; (3) temporal variation in allocation data can also strongly impact results, but only in data series with non-normal distributions. To address these challenges, several broad practices are recommended (Table 10) and described in greater detail in the following subsections. It is anticipated that these practices will contribute to the growing effort to standardize and improve solar LCA (e.g. International Energy Agency PV Power Systems (IEA PVPS) Methodology Guidelines on Life Cycle Assessment of Photovoltaic Electricity (Frischknecht et al. 2016)).
Figure 25. CED by process for tellurium under different allocation scenarios. (Top) Economic. (Bottom) Mass.
Table 10. Summary of best practice recommendations for critical byproduct material LCA.

<table>
<thead>
<tr>
<th>Challenges</th>
<th>Best Practices</th>
</tr>
</thead>
</table>
| Joint production poorly modeled in existing LCI modules | ● Examine temporal and methodological assumptions of existing modules before using  
● Connect upstream and downstream joint production process inputs  
● Use multi-output processes to model joint production systems  
● Substitute real process data wherever possible |
| Allocation method can dramatically change results | ● Selecting allocation methods to reflect causality when possible  
● If not possible, report at least two methods with justification; no method is technically correct  
● Use results from each method to provide bounds for expected results  
● Use ranges during decision making to improve reliability |
| Time sensitive data assumptions can dramatically change results | ● Consider historic price volatility for coproducts  
● If averaging, use inflation-adjusted values  
● Where possible, provide bounded results from min and max values of time sensitive data |

3.5.1. Modifying existing LCI processes to account for joint production

When evaluating environmental impact for a product or material, a common first step before conducting an entirely new and full LCA is to review the available literature and browse existing LCI databases for results. Theoretically, one could pull these published results directly or utilize the existing process blocks; however, this can be dangerous, particularly for joint product materials, without thorough consideration about the system modeling, allocation method, and allocation data assumptions. For example, Table 11 summarizes CED results from several published LCAs. Only economic allocation values were found to have been reported for tellurium. However, the time period assumptions for the price data or any other time sensitive modeling parameters are not always transparent. Those who do report have utilized different time period averages, e.g. 2004 - 2006 (Classen et al. 2009), 2006 - 2010 (Nuss and Eckelman 2014), 2008 - 2010 (V Fthenakis and Anctil 2013), and report results varying from 124 - 435 MJ/kg of tellurium.

After determining a need for more modeling detail than can be provided from literature values, the next step is likely to use an LCA modeling software resource, like Simapro or GaBi. Simapro, for example, comes preloaded with several LCI databases, such as Agri-footprint, which focuses on agricultural products and processes, ELCD, which focuses on European data, USLCI, which focuses on US data, and ecoinvent, which represents a broad variety of sectors and regional data. While the unit processes available in these databases can serve as helpful starting points, it is not advisable to utilize these processes blindly without consideration for the allocation methods or assumptions (temporal, geographic, or otherwise) embedded within them. As demonstrated in
Table 11. CED results compared to results from other studies in the literature.

<table>
<thead>
<tr>
<th>Source</th>
<th>Allocation Method</th>
<th>Temporal Scope</th>
<th>Results CED (MJ/kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ecoinvent 2.0 (Classen et al. 2009)</td>
<td>Economic</td>
<td>2004 - 2006</td>
<td>124</td>
</tr>
<tr>
<td>ecoinvent 3.1 (Simapro 8.0.5)</td>
<td>Economic</td>
<td>2012 - 2014</td>
<td>*105 – 185</td>
</tr>
<tr>
<td>Goe &amp; Gaustad, 2014 (Goe and Gaustad 2014a)</td>
<td>Economic</td>
<td>2010 - 2013</td>
<td>157</td>
</tr>
<tr>
<td>This study: ECON_base</td>
<td>Economic</td>
<td>2010 - 2014</td>
<td>140</td>
</tr>
<tr>
<td>This study: ECON_alt</td>
<td>Economic</td>
<td>2006 - 2010</td>
<td>138</td>
</tr>
<tr>
<td>This study: MASS_base</td>
<td>Mass</td>
<td>2010 - 2014</td>
<td>815</td>
</tr>
<tr>
<td>This study: MASS_alt</td>
<td>Mass</td>
<td>2006 - 2010</td>
<td>790</td>
</tr>
<tr>
<td>This study: x_year, extreme low</td>
<td>x = Economic</td>
<td>2007</td>
<td>127</td>
</tr>
<tr>
<td>This study: x_year, extreme high</td>
<td>x = Mass</td>
<td>2013</td>
<td>825</td>
</tr>
</tbody>
</table>

* Depending upon geographic assumption: Canadian or rest of the world regional perspective.

the presented case studies, these assumptions can lead to highly variable results. The concern is the variation could potentially lead to inappropriate decision making.

This is particularly true for many minor and joint product metals used in advanced solar technology, where if they even exist, stock unit processes typically handle joint production inappropriately. Tellurium represented a scenario where joint production modeling required improvement. Specifically, the ecoinvent database often utilizes a cutoff method, which separates the upstream carrier ore extraction and processing from the joint product extraction and processing. Cutoff would be an appropriate method if the joint products were instead wastes of no market value, but, since they are not, they must be treated as multifunctional processes. In best case scenario, there will be fragment processes representing each end of the cutoff, which can be manually connected. This was the case for tellurium, where copper refining is modeled to produce a waste anode slime, and then a separate anode slime processing block is available, but its input anode slime does not ever connect back to copper joint production.

Once it is determined that independent modeling is required for a given system, whether basing the unit processes off existing database modules or starting from scratch, two practices are recommended. The first is when joint production scenarios are encountered, choose to model the
process as a multi-output module rather than embedding allocated inputs and outputs into two separate modules, if this is possible in the modeling software. In single output allocated modules, the allocation factors are buried within the stagnant input and output values. However, with multi-output processes, the allocation factor is held separate from the pre-allocated flows and made readily available to the practitioner. This allows for greater transparency in modeling, and it also provides valuable accessibility to create multiple allocation scenarios and test the limits of data assumptions, ultimately assessing the variability of the end results.

Finally, if a more accurate representation is known for certain modeling processes from expert study or first-hand experience, incorporate the most realistic process data into the system model. In many cases this can include improved yields. In other cases, like the tellurium case study presented in this study, this included use of alternate methods of reference flow estimation based on more complete system modeling knowledge. For solar LCA, this approach will most likely add value when modeling processes regarding solar material growth or processing. However, it is valuable to add these contributions at every level where there is knowledge with greater specificity. In the case of this paper, the data contribution comes from expertise in supply chain modeling of raw material inputs.

3.5.2. Managing allocation variation: method selection

As suspected, the case study confirmed that choice of allocation method can dramatically change LCA results. This was shown to be especially true for the more minor joint products. For example, choosing mass allocation over a typical economic allocation (baseline scenario) resulted in a 5-fold increase for tellurium CED estimates. However, technically speaking there is no “correct” method of allocation. There are justifications, which may be better or worse for a particular application. According to Weidema & Norris “what has been missing, is a unifying theory that can explain what allocation key is justifiable in each specific situation,” (B Weidema and Norris 2002). Research in the area of allocation remains fragmented, trying to identify methods with “better” justifications or describe scenarios in which already established methods are better justified; however, at its core, allocation is just a work around for an impossible problem. The issue is when the cause is not obvious, and a method is chosen arbitrarily or by convention, it is often not clear whether one method overestimates impacts or the other underestimates them even for the same process. This is troubling because when different people can calculate the same result
in different ways and get very different answers, there is risk of unethical reporting and use of these results to mislead decision making to suit the practitioner’s purposes. For example, if considering environmental advantage of a substitute material, choice of allocation method and temporally-specific input data can be used to skew results and may result in a decision that creates greater environmental impact. This best practice emphasizes the importance of these specific issues (allocation and related temporal data assumptions) as part of the more general transparent reporting guidelines for solar PV LCA (Frischknecht et al. 2016).

Earlier in this study, it was thought that the nature of the joint production process, i.e. coproduction versus byproduction, might offer helpful insight into the appropriate choice of allocation method. As suggested in Section 3.2, the economics of byproduction versus coproduction are such that economic allocation makes sense for coproducts and mass allocation makes sense for byproducts. However, it can be very challenging to classify the joint outputs from individual processes. First, without cost information at the individual process level, the economic distinction between coproducts and byproducts is somewhat unclear. Further, not all processes can be wholly characterized one or the other; there can be processes with both coproducts and byproducts. Additionally, when breaking down production of a material such as tellurium, that is referred to as a byproduct at a systems level, to the individual process level, the joint product may not yield directly from the same process as its carrier metal. For example, to produce tellurium copper ore is mined, refined, then anode slime is processed and tellurium is refined. The process for mining of copper ore yields copper concentrates and molybdenum concentrates. Refining of copper concentrates yields pure copper cathode and anode slime. Anode slime processing yields silver, selenium, and a copper telluride precipitate. Copper telluride refining yields only refined tellurium; there are no byproducts or coproducts. In brief, despite being broadly referred to as a byproduct of copper, at no point in the individually modeled processes described above is pure tellurium ever yielded from the same process that yields pure copper. Therefore, even though tellurium behaves as a system level byproduct, i.e. no more or less copper ore would be mined to recover more tellurium, at the process level relevant for modeling LCA tellurium and copper are not actually direct coproducts and its joint production form cannot be used as a basis for allocation decisions directly in LCA. However, at its core and in reality beyond LCA modeling, this distinction speaks to economic drivers of the production processes and has potential in this space barring further analysis and investigation.
In lieu of a proposing a better way to determine appropriate allocation strategies, always report results from use of at least two allocation methods, e.g. mass and economic, or a more causally justifiable method, and to use these scenarios as boundary values for the result in decision making. Although it may be frustrating to work with a range rather than a single value, it will encourage decision makers to design a solution or identify conditions where the entire result range can be encompassed in a safe decision zone. Even if this complete agreement scenario cannot be reached, using a range can give an idea of the chances of being correct. This can be used to identify conditions and tipping points for success that may lead to more nuanced decision making.

3.5.3. Managing allocation variation: temporal data selection

A key result of this paper is the analysis of price variability on LCA results for price volatile joint product material. In the case of tellurium, despite large price variations for the pure material, counter-influencing price trends among coproducts created small sensitivity of overall result, assuming consistent year data was used. However, this may not be the case for other materials. In a rare earth example, terbium CED results could be changed by up to 45% in either direction depending on the year selected between the period of 2006 and 2014 (M. L. Bustamante et al., n.d.). Clearly, for certain joint product materials, particularly those with dramatic price trends even under allocation adjustment (Fig 9), the time period assumed can affect results dramatically as well. This effect was understated in previous analyses (Stamp, Althaus, and Wäger 2013; Nuss and Eckelman 2014). However, the case study results demonstrate that it is crucial when modeling joint production processes to consider historic price volatility and account for time value of money.

Traditionally, it has been thought that averaging could effectively erase this variability and lead to more time-stable results. However, solely relying on averages can be problematic for a few reasons. One is the demonstrated challenge that selecting an averaging period can appreciably change results. For example, even assuming a somewhat recent price averaging period of 2006-2010 rather than 2010-2014 for the REE LCA resulted in a 25% decrease in terbium CED estimation (M. L. Bustamante et al., n.d.). Another reason is that the average by definition does not represent reality but an approximation and truly only reflects scenarios with normal distribution. Capturing a reasonable range of extremes can be helpful to ensure the full range of results is captured as well.
A simple way to do this is to collect historic price data from resources, such as USGS, identify period highs and lows, and select those years to extend the bounds of the allocation scenario results. For tellurium, the extreme lower bound of 127 MJ/kg is found via single year data point from 2007 under economic allocation, and the extreme upper bound of 825 MJ/kg is found via single year data point from 2013 under mass allocation (Table 11).

3.6. Conclusions, Broader Impacts & Future Work

LCA is one of the best tools decision makers have to objectively assess environmental impacts and make decisions based on this information to manage them. Whether at the firm level or for broader policy development, it is critical the data used to make these decisions is as realistically representative as possible for it to be reliable. This chapter has reiterated how allocation decisions have the ability to dramatically affect results, particularly for materials that represent valuable but price volatile minor outputs of joint production processes, like tellurium. As such, decisions informed by LCA results are at risk of being affected and need to be robust to methodological and inherent data variability. The results of these case studies should bring greater awareness to the unique sources of variation in modeling LCA for these materials, i.e. price volatility, other time sensitive data, and allocation decisions. The best practices prescribed in Section 3.5 offer several practical methods, including use of bounding techniques for allocation assumptions, to avoid misuse of LCA results and provide more nuanced and reliable basis for decision making. The case study of tellurium reveals factors that can help predict behavior of systems like it which also depend upon price trends of coproducts. Notably, an additional case study of rare earth element, terbium, analyzed using the same methodology reveals that certain joint products can be affected differently by the same modeling choices. Specifically, tellurium CED was found to be greater by mass allocation than economic, but the opposite was true for terbium due to differences in the materials’ upstream history and price relative to other coproducts (for more detail on the terbium case study see Bustamante et al. (in press) (M. L. Bustamante et al., n.d.)).

Despite demonstrating a significant influence of allocation and temporal modeling decisions on the environmental impact assessment of jointly produced solar raw materials, like tellurium, these materials only constitute a small portion of the ultimate PV modules and larger installed systems. Studies of CdTe PV environmental impact (Peng, Lu, and Yang 2013; V
that the tellurium-containing semiconductor material is not a major contributor to panel or system
environmental impacts. Using the results of the present analysis, however, tellurium alone can be
shown to contribute between 30% and 74% of the embodied energy attributable to the thin film
CdTe layer material depending upon choice of allocation factor and temporal scope of data.
Further it is difficult to extrapolate the full implications at the product level without extending the
methodology to other relevant system inputs, like cadmium, which is a joint product of zinc and
lead refining and may be subject to similar variability. However, it seems likely that even
incorporating these large raw material variabilities, due to the dominating effects of impacts from
other system components, CdTe PV will likely maintain its environmental advantages as compared
to other technologies, like silicon and CIGS PV. Regardless, even if variability in environmental
impact determination of raw materials are not significant enough to affect PV product-level LCA
results, it can still affect signals of importance to global market actors, i.e. criticality, that may
have serious implications for solar manufacturers’ supply chains.

Criticality is increasingly considered by firms and national organizations, like the US DOE
and DLA, who take strategic actions in response to perceived risk. LCA is commonly used to
quantify these environmental impacts included in criticality assessments, creating interrelated
challenges. For example, toxicity scores can affect substitutability of a critical material, making
products more or less dependent upon the original material and affecting its vulnerability to supply
disruption.

Generally speaking, while tools like LCA exist that enable us to evaluate potentially
beneficial strategies for byproduct critical materials, such as recycling, decisions and assumptions
within LCA can affect whether or not we consider a strategy effective. For example, energy
savings from production of secondary material as compared to primary production is one potential
benefit of recycling. Such a potential benefit would need to be verified from a life cycle
perspective using a method like CED. Future work is needed to understand how and to what
degree variabilities, like those demonstrated in this chapter, which affect LCA of joint product
materials can trickle back in and affect criticality results. Just as LCA can be used to inform
decision making regarding environmental impact, criticality assessments can be used to inform
decision making regarding supply chain security. Therefore, the same principles apply regarding
their need for reliability and robustness to inherent variability.
In addition to allocation as a source of variability, future studies should direct attention to other sources of variation, including geographic factors such as ore grade, yield, energy mix, transportation assumptions, to understand how LCA uncertainties propagate differently through to decision metrics aimed at, for example, reducing environmental and/or broader criticality risk. Further, other indicators could be useful for informing criticality risk mitigation. For instance, breaking down results to look at CED from each unit process would help to target energy hotspots in these material production systems. If for instance, mining is found to contribute the greatest degree to impact, there is incentive to invest into extraction technologies. Similarly, if refining is the issue, then perhaps reduction of refined material use per product, or dematerialization, by manufacturers is the answer. Other potential indicators include GHG emissions, which can help education based campaigns, such as carbon footprint labeling for products, and resource depletion, which perhaps could inspire a similar campaign for critical material usage in products.
CHAPTER 4. Informing Strategic Response to Criticality: Quantifying Complex Supply Risk Reduction Potential

4.1. Challenges for Addressing Criticality Risk

While the previous chapters have focused on addressing challenges to characterization of criticality risk for byproduct materials, the present chapter will shift focus to the complementary pursuit of addressing challenges to mitigation of criticality risk. This is a primary motivation of performing criticality assessments. Criticality assessment enables stakeholders to identify materials with the greatest risk with the intention of using this information to guide future action. This future action can come from the bottom up through the technical community (i.e. scientists and engineers) or it can come from the top down through the policy community (i.e. federal government, state/local government). The two pathways are also interconnected since policy can drive technical response and technical findings can inform policy. Further, if criticality is being assessed and addressed at the firm level, as in GE (Ku and Hung 2014), the policy response could be company policy coming down from leadership. In this chapter, all of these perspectives will be discussed together as different forms of strategic response to criticality.

Despite being a key motivator for such analyses, criticality assessment frameworks are not currently structured well to inform strategic response with any degree of nuance. Results are often presented in a highly aggregated fashion (e.g. single score or position in 2-D/3-D space), providing little to no direct insight about how to resolve the risk being identified (National Research Council (NRC) 2008; Graedel et al. 2012; Bauer et al. 2010; European Commission 2010; Bauer et al. 2011; European Commission 2014). This is problematic since there are virtually endless potential approaches that different agents, including policy makers and firm-level technical actors, can take to resolve identified risk. Right now, at most, they can look to the scores from each indicator (if available) leading to a high score and try to compare them to one another to determine which lever to pull; for example, if supply risk is scored very high because recycling rate is 0, companion metal fraction is 100, and supply concentration is high, what should be done? Develop recycling technology? infrastructure? policy? Diversify supply by taxing imports from a particular nation to allow domestic suppliers to compete? Stop using the material altogether? The best response is not immediately clear because it is not possible to directly compare these three disparate
challenges. Each approach will have its own costs and benefits, and further analysis is needed to quantify these.

Additionally, byproduct nature of critical materials is not often considered when developing mitigation response. For example, one common approach to mitigating risk is substitution. Currently, criticality assessments, if they address substitutability will identify a single substitute for each material considered and qualitatively describe how effective it is in that application. Often times, for the same reason that they form together naturally in ore deposits, coproducts of the same joint mining pathway will be used as substitutes for one another. Examples of this include selenium and tellurium as well as various rare earth elements substituting for one another. For these materials, if a supply stream is being restricted for one, it is likely being restricted for the other. This is not to say that substitution cannot be an effective solution for byproduct materials; however, when considering substitutions and any other mitigation solution, byproduct character becomes an important factor to consider. Further, not all strategies will work for these materials. For instance, mining volumes cannot directly be increased because of the economic production constraints previously discussed.

A technique is needed which addresses both of these challenges. Continuing the case study of tellurium, this chapter will demonstrate how extension of supply chain modeling especially formulated for byproducts, as in Chapter 2, can be used to help evaluate different mitigation strategies for byproduct materials. Strategic responses representing both technical and policy type actions will be used to test the framework with the goal of identifying which response is most effective overall at reducing supply risk. Additional modification of the present evaluation approach can be used to evaluate reduction in environmental risk as well, creating a full picture of criticality risk reduction, but this will be left for future work.

4.2. Leverage Points for Strategic Response in Byproduct Supply Chains

In order to inform strategic response, it is helpful to first identify key leverage points for action. When considering supply risk reduction, these leverage points can be technical factors of the supply chain, such as the key parameters identified previously in Chapter 2 (i.e. byproduct yield or material intensity of the demand application) or they can be thought of more broadly as

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4 This section draws upon discussion already published in TMS 2016 REWAS proceedings. Citation: (M. L. Bustamante and Gaustad 2016).
lifecycle stages (i.e. raw material extraction to end of life). Figure 26 displays a few examples of potential strategies for response to supply risk within this lifecycle framework. Examples of technical mitigation strategies include substitution and improving material efficiency in production. Examples of traditional policy response include regulations governing end-of-life management of products, such as landfill bans and municipal collection programs. Examples of firm-level policies can include best practices for employees transporting and installing solar panels to prevent premature end-of-life via breakage (e.g. vehicle tracking and punishment for excessive speeding in company vans) as well as extended producer responsibility programs, where, for example, the product manufacturer or distributor is required to take back products from consumers at end-of-life for recycling or remanufacturing.

Figure 26. Criticality mitigation strategies employable throughout material lifecycle.

Some strategies shown will apply for all kinds of critical materials, like recycling, dematerialization, and substitution; however, others, such as direct mining development and byproduct yield improvement, are specifically aimed at byproduct critical materials. Within each lifecycle stage, examples specific to byproducts can be identified. The following paragraphs will review some of these examples within the technical community; specifically, material science and
engineering as an example. In terms of policy response, the easiest points of intervention for supply risk reduction are typically at end-of-life and point of use, for example, incentives for home solar installation can drive up demand. However, at all points, policy can also induce negative effects. For example, environmental regulation policies may impact supply of carrier materials, and further restricting byproduct availability and incentives to install solar may drive up demand, making it even harder for constrained byproduct supply to keep pace.

During the initial phase of a product’s lifecycle, extraction, raw materials are obtained from the natural environment. In the case of metals and minerals, this extraction is typically accomplished via a physical mining process. For byproduct materials, options are somewhat more limited. Two extraction phase intervention strategies are development of direct mining resources and exploitation of alternate byproduct mining. Developing direct mining resources can be a particularly effective strategy in the face of rapidly growing demand because primary production reduces supply risk by creating more flexibility in the supply chain. Whereas byproduct flows are constrained by the needs of another material, direct mining supply is unattached and optimized to respond to market forces. Developing direct mining as a mitigation strategy requires specialized materials expertise. First, geological and mineralogical research may be required to discover new resources using advanced imaging and exploration techniques. Next, once a suitable primary resource has been identified, knowledge of extractive metallurgy will be required to plan the optimal mining approach, e.g. surface or underground, mining as concentrates or in situ leaching. Alternatively, supply can be expanded through the use of other byproduct mining pathways. This would not change the total amount of ore extracted but rather the decision to recover a material as a byproduct or not. Just as increased prices can drive development of resources previously deemed unfit for primary mining, increased prices can motivate recovery of byproduct resource from outputs previous deemed as wastes due to lower concentration, i.e. slags, residues, exhaust gases. Alternate byproduct mining can reduce supply risk by diminishing the influence of any single byproduction system or process. Developing these pathways also requires extractive metallurgy to characterize potential waste resources, plan the extraction approach (method, reagents, conditions, etc.), and ensure optimal extraction efficiency.

The next lifecycle stage, processing, elevates raw materials to a usable form. For byproduct materials, this involves separation of the main product from the byproduct(s). Two potential processing phase intervention strategies are improvement of byproduct yield and recovery of
losses from scrap or wastes. Yield is the overall ratio of byproduct ultimately in usable form as compared to the initial pre-extraction availability, which incorporates individual process efficiencies and losses. Byproduct extraction efficiency is just one component of a larger indicator known as byproduct yield. Recovery of losses from scrap or waste streams is similar to byproduct mining and requires similar skills.

The manufacturing phase, which is when all the processed raw materials get incorporated into product form, is another powerful area for implementation of technical mitigation because so many of the fundamental processes involve science & engineering processes, e.g. forming, joining, casting, heat treatment, coating, deposition, and crystal growth. Two common mitigation strategies tied to the manufacturing phase are dematerialization, or reduction of material intensity, and substitution. Dematerialization and substitution both offer supply risk reduction by reducing demand for the critical material per unit of the product, allowing supply growth to catch up to that of demand. However, whereas dematerialization necessarily uses less material overall, substitution may require use of a greater amount of the substitute material to achieve the same performance. Alternately, development of new and better substitutes for non-energy-critical applications can have a beneficial effect on supply risk reduction overall by reducing competition for the material with the rapidly growing critical applications. Both strategies may require advances in synthesis and processing techniques, such as chemical vapor deposition or wafer design. Additionally, thin films expertise is very valuable in consideration of dematerialization processes. Finally, at least for solar materials, it will ultimately be important to research fundamental optoelectronic properties to ensure they will not unacceptably diminish or breakdown with dematerialization and to design perhaps new materials for substitution.

The use phase is the period in which the product itself is being utilized by a consumer. This makes it the hardest phase to intervene during as a materials scientist. However, certain approaches taken during manufacturing may actually see most change in impact during the use phase by modifying the product’s lifetime. Lifetime modification is an interesting example, however, because the direction of modification can have counterintuitive effects. On the one hand, extending the lifetime of a good should theoretically reduce demand by preventing the consumer from needing to replace it, e.g. disposable versus durable plastic grocery bags. However, while a material is sequestered in a product for a longer time, it cannot be made available for reuse or recycling until after a long delay. From a materials perspective, various processing techniques can
be applied to extend the product lifetime, e.g. coating for corrosion and/or degradation resistance. Additionally, research into degradation and failure mechanisms would be helpful to design more robust solar cells and modules. Further, use of low quality material or poor manufacturing can reduce useful life for these kinds of technologies. Finally, substitutions and dematerialization carried out during manufacturing may indirectly affect product lifetime. For example, frameless glass thin film PV, although lighter in weight, is considered to be more fragile (Collins 2009).

End-of-life refers to the final stage in a linear model of a product’s lifecycle when it ceases to be useful to the current owner in the current form. In reality, end-of-life can often mean new beginnings for many materials and products via recycling and remanufacturing. Recycling and remanufacturing both work to mitigate supply risk by displacing demand for virgin raw materials with recovery of individual substances or product components from end-of-life products. Additionally, providing a secondary supply of material or parts helps to diversify the supply chain making it potentially more resilient and less vulnerable to disruption. Recycling is a very popular research topic, however, in terms of reducing supply risk, recycling can be challenging to predict because it is so highly dependent upon the product lifetime.

4.3. Methods

To achieve the goal of this study, which is to create an evaluation framework for supply risk mitigation strategies, first a baseline scenario of supply and demand must be created. Next, alternate scenarios representing the effect of implementation must be created for comparison. Then metrics must be defined which can describe the change in risk between the pre- and post-implementation scenarios. Finally, these metrics are used to compare effectiveness and benefits of different strategies.

4.3.1. Establishing baseline risk

Models of baseline supply and demand are constructed using methods from Chapter 2, with a few key modification in an effort to address some potential limitations of the model published in that chapter. Modifications are summarized in Table 12. Baseline supply and demand projections are superimposed to reveal emergence of supply gap conditions, indicating that mitigation is necessary.
Table 12. Modeling improvements from Chapter 2 tellurium supply risk study (M. L. Bustamante and Gaustad 2014a).

<table>
<thead>
<tr>
<th>Previous Study</th>
<th>This Study</th>
<th>Calculation</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tellurium supply from copper only: S</td>
<td>Total tellurium supply approximated: S’</td>
<td>S’ = S/f</td>
<td>f value from USGS; This study: Baseline f = 90%; Range f = none; Previous study (equivalent): f = 100%.</td>
</tr>
<tr>
<td></td>
<td>Fraction of tellurium supply from copper: f</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tellurium demand from solar only: M</td>
<td>Total tellurium demand approximated: M’</td>
<td>M’ = M/n</td>
<td>n value from (Candelise, Winskel, and Gross 2012) and (Merchant Research &amp; Consulting ltd 2016); This study: Baseline n = 40% Range n = 40% and 90% Previous study (equivalent): n = 100% in previous study</td>
</tr>
<tr>
<td></td>
<td>Fraction of tellurium demand from solar: n</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tellurium supply from recycled PV (assumes perfect collection &amp; recovery): R</td>
<td>Tellurium supply from recycled PV: R’</td>
<td>R’ = R*r</td>
<td>This study: Baseline r = 0.1% Range r = 0.1% and 100% Previous study (equivalent): Baseline r = 0% Range r = 0% and 100%</td>
</tr>
<tr>
<td></td>
<td>Tellurium recovery rate from PV recycling: r</td>
<td>S’ = S/f + R’</td>
<td></td>
</tr>
</tbody>
</table>

The onset of supply gap conditions is one of three risk metrics used to characterize baseline supply risk. The number of years from model start until the onset of supply gap conditions communicates the time frame available for development of alternate supply resources or for product innovations to reduce demand while still allowing demand to grow at present rate; the sooner the onset the faster action is needed if the current course is considered desirable. Another way is to quantify the degree to which demand exceeds supply, or the peak market imbalance. In Chapter 2 this was reported as the ratio of demand to supply. Here it will be measured as the difference between demand and supply. This can communicate the additional supply capacity in tonnes needed to stay on track or the amount of material that needs to be stockpiled for future use. Last, the duration of the hypothetical supply gap conditions can also be predicted by the model. This suggests the degree of permanence needed from a solution. For example, is a temporary ramp up in marginal production sufficient or do is investment in developing totally new direct mining resources required?
4.3.2. Selecting Strategic Response Mechanisms

Three mitigation strategies were selected to serve as illustrative examples in this analysis: byproduct yield improvement, dematerialization via film thickness reduction, and recycling rate policy. In each instance, the associated parameter values – yield, film thickness, and recycling rate, respectively – were varied through a range dictated by the previous literature to create multiple scenarios. A unique supply or demand scenario was generated for each improvement as necessary. It should be noted that a major simplification was made with regard to modeling implementation; rather than modeling a gradual transition to the improved state within these scenarios, implementation is modeled as a discrete jump beginning in year one (2016 in this chapter). This assumes that any time delay necessary for development of technologies, infrastructure, procurement and policy frameworks has already occurred. It may not be realistic; however, it represents an upper bound and simply enables demonstration of the methodology for comparing different strategies, which is the primary objective of this chapter.

4.3.3. Measuring Risk Reduction Effectiveness

Next, effectiveness of individual mitigation strategies is probed by, first, identifying the model parameters which are affected by each approach, then perturbing the model in a way that represents the effect these policies would have on the associated parameters. The results are supply and/or demand scenario for the byproduct that differ from the baseline, creating shifts in the previously identified risk metrics – (1) onset of supply gap conditions, (2) degree of market imbalance, and (3) duration of supply gap – as well. Efficacy of the policy scenarios are then assessed using three companion metrics: (1) delay of supply gap onset, (2) reduction in peak market imbalance, and (3) reduction in supply gap duration; all calculated as percentage change from a baseline scenario. However, there are also at least 3 different ways to describe effectiveness of each risk reduction strategy (Table 13).

First, there is the maximum benefit, which is the largest reduction observable using the strategy. This represents an upper bound on risk mitigation potential and can be communicated as a raw result (e.g. x years delay of supply gap onset) or relative to the baseline risk level (e.g. y more years delay of supply gap onset than in baseline scenario). Another potential measure is the average benefit, which is calculated as the change in the raw risk metric, such as years of delay in supply gap onset, over the percentage change in the relevant model input parameter, such as yield,
from its baseline. This allows for comparison across the different risk reduction strategies, each of which is based upon different parameters with different units and ranges. Finally, the normalized average benefit, which represents marginal benefit from implementing a strategy, can be calculated as the percentage change in the risk reduction measure over the percentage change in the input parameter. Normalized average benefit results in a unitless measure, which allows for comparison between the risk metrics for a given risk reduction strategy, which have different units, as well as across the different strategies. Ultimately this enables the calculation of a single measure of risk reduction effectiveness for each strategy that encompasses impact in each of the three risk metrics.

Table 13. Metrics used to measure risk mitigation potential of different strategies. \( B \) is benefit in terms of years of delay in onset of gap conditions, tonnes reduced from peak market imbalance, or years reduction in gap duration. \( p \) represents a given value of an input parameter value (film thickness, yield, recycling rate) and \( p_0 \) represents the baseline value of that parameter.

<table>
<thead>
<tr>
<th>Risk Mitigation Metric</th>
<th>Equation</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum Benefit</td>
<td>[ \max_p B(p) ]</td>
<td>years or tonnes</td>
</tr>
<tr>
<td>Average Benefit</td>
<td>[ \frac{\Delta B}{\Delta p/p_0} ]</td>
<td>years/% or tonnes/%</td>
</tr>
<tr>
<td>Normalized Average Benefit</td>
<td>[ \frac{\Delta B/B_0}{\Delta p/p_0} ]</td>
<td>%/%</td>
</tr>
</tbody>
</table>

4.4. Results & Discussion

4.4.1. Updated Baseline

The resulting baseline scenario to which we will compare changes in risk measurement is shown in Figure 27. As compared to the baseline shown in Chapter 2, supply gap onset begins earlier. This is primarily driven by the assumptions regarding demand. Demand for tellurium from solar is modeled according to the fitted logistic growth model assumed in Equations 7-9 of Chapter 2. However, this overall demand is then set equal to 40% of total demand; therefore under this assumption, as demand for tellurium from PV increases, demand for tellurium overall increases at the same rate. This is not necessarily a realistic assumption, but neither is assuming that 100% of tellurium supply is available for use in solar, as was used in Chapter 2. In future iterations of this model, more detailed description of the share of demand parameter would enable evaluation of substitution within this framework. Since tellurium has substitutes in every other
major application, it is likely that the demand growth in solar will create an even greater shift toward solar (US Geological Survey (USGS) 2016). The effect of demand assumptions was partially mitigated by assumptions about supply as well. In Chapter 2, the baseline scenario assumed tellurium supply from copper represented 100% of global supply. In reality it is thought to be between about 90% (US Geological Survey (USGS) 2016).

4.4.2. Dematerialization

Dematerialization was approximated as reduction of CdTe PV thin film layer of CdTe. In reality efficiency improvement may also play a large role. As in Chapter 2, the baseline scenario assumes 3 microns, but here a range from 5 microns to 0.67 microns is considered for potential scenarios. Although it is traditionally considered that 1 micron is the limitation of film thickness without deterioration of PV cell electrical performance, reduction to 0.67 was proposed as a goal for supply risk reduction (Zweibel 2010). Figure 28 shows market balance scenarios representing the full range of film thicknesses found in the literature are shown as compared to the baseline in black.
Recalling the risk measures, it is possible to qualitatively observe how film thickness affects risk; positive values equal supply gap conditions, where the scenarios cross from negative to positive is the onset of gap conditions, the inflection point represents peak market imbalance, and the distance between the onset and where the scenarios cross back from positive into the negatives is the duration of supply gap conditions. However, to quantify risk reduction potential, so risk reduction potential as a function of strategy relevant input parameter – in this case film thickness – must be calculated. Figure 29 shows results for delay of supply gap onset relative to the baseline scenario of 3 micron film thickness. To the right, where there is higher film thickness, supply gap is projected to emerge during the first year same as in the baseline scenario only because it cannot happen sooner as modeled. However, when film thickness is reduced below 3 microns, it goes through a linear period of improvement before approaching infinity at the smallest film thickness. This means that, if film thickness below 1 micron can be achieved without tradeoffs due to efficiency loss, even aggressive PV growth like what has been modeled in the baseline scenario can proceed without inducing supply gap conditions at all.
Figure 29. Effectiveness of dematerialization as a means to delay supply gap onset.

Next the reduction in peak market imbalance is shown in Figure 30. A maximum decrease in peak market imbalance of about 3700 tonnes can be achieved, which is actually larger than the baseline value. This is because in the two thirds scenario the entire baseline peak is eliminated and a supply surplus is projected. Finally, reduction in gap duration is shown in Figure 31. Results show a slightly less linear trend than for market balance due to this metric’s greater dependence upon the non-linear shape of the market curve, experiencing reductions in the gap from both directions through later onset and sooner ending. A maximum reduction in gap duration of 86 years is achievable, which corresponds to 100% of the baseline gap, again because of the complete avoidance of gap conditions.
Figure 30. Effectiveness of dematerialization to reduce peak market imbalance.

Figure 31. Effectiveness of dematerialization to reduce duration of supply gap conditions.
4.4.3. Yield Improvement

This same analysis is performed for byproduct yield improvement by creating scenarios that represent the full range of 35 – 80%, as discussed in Chapter 2 (Figure 32). Whereas, before, a near parallel downward shifts with reduction of material intensity was observed, with yield improvement, benefits grow over time. This is due to the dominating influence of demand early on. As a result, less benefit is realized in terms of supply gap onset delay: topping out at 3 years. Peak imbalance reduction is less than half that seen with dematerialization, maxing out at 1666 tonnes. However, this still represents a 48% improvement over its own baseline. Finally, a significant reduction in gap duration of 52 years, which is larger than the 3 years of delay in supply gap onset achieved, only represents a 60% improvement over its baseline value making less effective than the 300% relative change seen for onset delay.

Figure 32. Effectiveness of byproduct yield improvement for reducing supply risk, showing all scenarios considered.
4.4.4. Recycling Rate Policies

Finally, the introduction of mandates or at least goals for recycling rate of PV are modeled (Figure 33); perhaps like what has been developing in the EU as part of broader e-waste legislation. For the baseline, a near zero recycling rate of 0.1% is assumed to reflect the current reality that most panels are still in their useful life. The range for scenarios was developed all the way through 100% to reflect a full recycling mandate; in reality, some losses in collection and material recovery are inevitable. The most striking difference between the recycling scenario evolution and the previous strategies discussed is the lack of any benefit to delay of gap onset. This is due to the long product lifetime before secondary material becomes available. Similarly, recycling does little to reduce the degree of market imbalance expected; reducing the measure by a maximum of 13 tonnes as compared to several thousand by the other approaches reviewed. Where recycling does play a useful role is in reduction of gap duration. Up to 31 fewer gap years are possible through full recycling mandate. Despite only representing a 36% change from its baseline, of the measures, this represents the greatest form of risk reduction achievable through recycling. However, this is less than the maximum gap duration reduction observed from both dematerialization and yield.

Figure 33. Effectiveness of CdTe recycling rate for reducing supply risk for tellurium, showing all scenarios considered.
These are important results because, for as much discussion as surrounds recycling of PV, the approach will have little value in the short to mid-term future in terms of stabilizing tellurium supply risk.

### 4.4.5. Comparing Strategies

One valuable result of this assessment is to determine, if, how, and why the choice of evaluation metric matters to decision making. For example, does use of average benefit lead to the same conclusions about strategy effectiveness as normalized average benefit does? In this case the answer is yes. For each risk reduction metric individually, dematerialization consistently provides the greatest benefit followed by yield reduction and then recycling rate improvement. However, it is important to emphasize that despite the greater magnitude of average benefit produced from gap duration reduction versus gap onset delay in each case, it actually represents a smaller relative improvement over the baseline condition and therefore normalized average benefit to gap duration reduction is lower than gap onset delay. Truly, despite having the same units, results across risk metric categories in terms of average benefit cannot be compared due to their differing baseline and/or units, so the normalized indicator should be used if comparison is the goal.

![Figure 34. Average benefit for each indicator (clusters) and mitigation strategy (columns).](image)

Dematerialization Yield Improvement Recycling Rate

Delta Onset (years) Delta Imbalance (tonnes) Delta Duration (years)
An additional interesting result is the ability to generate a single measure of risk reduction effectiveness for each mitigation strategy by summing the normalized indicators. The results confirm the greater effectiveness of dematerialization under current conditions, followed by yield improvement, and then recycling. Further, they communicate in a single measure just how much better it is in terms of supply risk reduction. These results provide a foundation for strategic stakeholders to determine where they will get the greatest marginal benefit in terms of supply risk reduction. An interesting next step would be to factor in other attributes of each mitigation strategy, such as marginal cost and environmental impact, to evaluate complex tradeoffs.

![Graph showing normalized average benefit for mitigation strategies.](image)

**Figure 35.** Total normalized average benefit for the mitigation strategies: dematerialization, yield improvement, and recycling rate.

### 4.5. Conclusions

Results show that rapid demand growth, driven by solar PV, rendered supply-side mitigation strategies (byproduct yield improvement and recycling) much less effective than demand-side solutions, like dematerialization and substitution. Overall, the results serve as a
reminder that there is no universal mitigation strategy for all materials and applications; instead, optimal results should be obtained by targeted and temporally-relevant strategic development.

The results quantitatively show that in scenarios where rapid demand growth is expected in the face of limited supply, the most powerful and effective interventions will logically involve reductions of demand. However, in order to see the kind of benefits presented here, these reductions would need to occur as soon as possible. The model doesn’t currently assume a slow dynamic transition but rather a discrete jump to the alternate scenarios beginning in year 1. This isn’t necessarily realistic but it provides bounds for our expectations and creates goals.
CHAPTER 5. Final Remarks

5.1. Summary of Contributions

This dissertation represents three major methodological contributions to criticality assessment of byproduct materials. Chapter 2 introduced a more detailed approach to estimating byproduct (tellurium) supply in the face of evolving carrier metal (copper) supply and incomplete reporting. This was able to be used in conjunction with demand scenario projection from the critical application (CdTe solar PV) to characterize shorter term supply risk by identifying a range of potential scenarios and their associated year of supply gap condition onset, where demand for that year exceeds supply. Chapter 3 introduced a more complete LCA of a byproduct (tellurium) by including LCI flows based upon more accurate Chapter 2 supply estimates, by connecting upstream carrier metal extraction processes with downstream byproduct extraction processes, and by considering uncertainty in results due to variability from byproduct price volatility, choice of data timeframe, and allocation methods used. Best practice recommendations made in this chapter for LCA of jointly produced metals enables assessments of environmental impact that specifically addresses uncertainty for byproduct materials improving their usefulness in three-dimensional criticality assessment frameworks. Finally, Chapter 4 presents approach to quantitatively evaluate potential effectiveness of supply risk mitigation strategies informed by dMFA scenario modeling in Chapter 2. The approach takes a multifaceted perspective, using three metrics to measure risk, three metrics to measure risk reduction, and three metrics to measure effectiveness of each strategy, assuming there is a scenario analysis that depicts possible supply-demand imbalance. This method is one step toward a better design of specific policies and mitigation strategies in response to criticality as determined by criticality assessment by focusing on parameters that are levers for policy makers and engineers. Together these chapters fill gaps important for understanding and dealing with criticality of byproduct materials. If the applications they find use in are considered valuable to societal missions, like achieving sustainability, then it is important to identify how far off the current path is from reaching these deployment goals, to identify the challenges to meeting those goals, and to understand the potential leverage points for overcoming these challenges. This work aims, as a whole, to do that from a multidimensional, sustainability perspective.

Additionally, since the methods were developed and tailored to the byproduct system of tellurium from copper refining, there are also interesting contributions in terms of case specific
results. In Chapter 2, despite long term depletion time estimates on the order of 129 years for tellurium (Nedal T Nassar et al. 2012), modeling supply as a function of copper production technologies revealed a risk of short term supply gap conditions emerging between 2011-2036 depending upon reasonable developments in key supply (i.e. growth of copper recycling, growth of SX-EW copper, and tellurium yield from copper ore) and demand parameters (i.e. material intensity, CdTe PV growth onset, rate, and steady state plateau). The model is most sensitive to demand parameters, however, disruptions are still expected to emerge even if PV demand growth slows to half its historical rate or the SX-EW copper technique is eliminated from future use. In Chapter 3, an updated tellurium LCA was produced using more recent data (2010-2014 for base case) and more accurate tellurium supply data from Chapter 2 methodology. Additionally, non-tellurium yielding SX-EW copper inputs were replaced by copper concentrates, anode slime was treated as a byproduct rather than a waste by eliminating the cutoff between copper refining and anode slime processing. Finally, selenium was added as a joint product of the anode slime processing to reflect real world supply. The results were generating for 22 different allocation scenarios, varying method (mass and economic) and time period assumptions (2006-2010 average data, 2010-2014 average data, or individual year data between 2006-2014) to reveal uncertainty in results from underlying byproduct-related variability factors in LCA. Tellurium CED varied from 127-825 MJ/kg across all scenarios, with change in temporal scope creating at most +/-10% variation in results. The tellurium case study LCA highlights the driving role of price ratios between joint products in determining the effect of allocation method selection. Finally, Chapter 4 generated an updated baseline supply-demand scenario for tellurium where supply gap conditions were expected to begin in 2016. Pursuing this baseline demand would result in an annual imbalance peaking to 3500 tonnes around 2030, and disappearing by 2100. Three strategies – dematerialization via film thickness reduction, byproduct yield improvement, and recycling mandates – were tested to evaluate how effective they were at reducing supply risk, as measured by the onset of supply gap, peak market imbalance, and duration of supply gap conditions previously mentioned, and it was revealed that dematerialization was 3 times more effective at reducing risk overall for this system (3x more effective than yield improvement) and recycling mandates were not effective at all due to the currently low rate of recycling and lack of impact on gap delay or peak imbalance reduction.
While valuable, the tellurium-specific contributions are not nearly as impactful as the lessons that can be learned and applied to other case studies. The frameworks developed in this work can theoretically be adapted to apply to any other byproduct materials with only minor modifications. Given the current state of the PV market, if tellurium supply were to reach a crisis point, or increase in price so much that it drove out profitability of manufacturing CdTe PV, solar growth as a whole would not have to stop; rather, incumbent crystalline silicon would regain larger market share or another advanced technology would replace CdTe if it reached competitive pricing. Even in this scenario, the work presented here would still have value for other communities. Tellurium is representative of the broad class of materials produced as byproducts. As shown in Table 14, there are many byproduct materials critical to clean energy applications; however, the same materials are also critical to varying degrees for defense technologies. Tellurium, specifically, is critical to a compound known as CdZnTe (CZT), which is used as a substrate in thermal imaging devices. Tellurium also finds defense applications in thermoelectric coolers for infrared detectors, integrated circuits, laser diodes, and medical instrumentation. Additionally, CZT has been included in a list of materials for potential acquisition for the National Defense Stockpile in 2016 to meet the demands of the US military, industry, and essential civilian needs during a national emergency (US Department of Defense (DOD) 2015).

Table 14. Jointly produced materials critical to defense applications (Defense Logistics Agency 2012).

<table>
<thead>
<tr>
<th>Joint Product Elements</th>
<th>Carrier Metals</th>
<th>Defense Technology</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rare Earths (Nd, Dy, Eu, Tb, Y)</td>
<td>Iron</td>
<td>• SmCo, NdFeB Magnets</td>
</tr>
<tr>
<td></td>
<td>Rare Earths (Ce, La)</td>
<td>• YGG for comm. &amp; radar</td>
</tr>
<tr>
<td>Tellurium</td>
<td>Copper Lead</td>
<td>• CdZnTe infrared device substrates</td>
</tr>
<tr>
<td>Cadmium</td>
<td>Zinc Lead</td>
<td></td>
</tr>
<tr>
<td>Gallium</td>
<td>Aluminum (Bauxite)</td>
<td>• Air &amp; missile defense radar, infrared imaging</td>
</tr>
<tr>
<td></td>
<td>Zinc Lead</td>
<td></td>
</tr>
<tr>
<td>Indium</td>
<td>Zinc Lead</td>
<td></td>
</tr>
<tr>
<td>Cobalt</td>
<td>Nickel Copper</td>
<td>• Infrared imaging, communications</td>
</tr>
</tbody>
</table>
5.2. Future Work

In addition to the work completed here, there are several questions that remain to be answered and would require considerable additional analysis warranting their own separate study beyond what is presented here. This work will be briefly discussed in the following sections in the context of their relationship to existing work.

5.2.1. Novel Criticality Metrics

As demonstrated in Chapter 2, complex dynamic modeling offers benefits for assessing short term supply risks in the context of growing importance from an emerging demand application; however, benefits gained from complexity always come with tradeoffs in terms of additional time necessary to collect and analyse more data. Since criticality assessment is relative, many materials are typically evaluated in a single study increasing the need for data inputs many times over. In order to facilitate incorporation of some of the novel byproduction system insights discussed here into traditional criticality frameworks, it would be beneficial to determine if a more streamlined approach could be taken. Are there certain key parameters or combinations of parameters used in the supply-chain model presented here that are not yet included in existing studies but drive results of overall criticality behavior and can be used as novel criticality metrics?

5.2.2. Expanded Market Model

The supply and demand models presented in Chapter 2 and even the modifications made in Chapter 4 represent certain improvements over existing modeling approaches, however they are not perfectly comprehensive. For example, in the current model, total demand for copper is assumed to continue growing at its historical rate of 3% per year; however, this monolithic treatment of copper demand modeling neglects potential for growth from infrastructure demands for emerging economies, as was seen in China, as well as declines due to declining ore grade and recently low prices. Similarly, the current model only captures demand growth for the critical solar PV application in any detail. Data availability limitations are challenging to overcome for tellurium demand (US Geological Survey (USGS) 2005), so Chapter 4 utilized a linear factor, \( n \), to capture fraction of total demand from PV applications. However, this implied total demand for tellurium grew at a rate proportional to PV demand, which is not likely to be true since emerging technologies grow faster and substitution is likely occurring in other applications. Capturing these
elements is important to improving the accuracy of the tellurium model since all production systems are connected (Figure 36).

Figure 36. Visualizing how mitigation strategies affect joint production systems. As byproducts, tellurium and selenium, extraction phase is the same as copper processing phase in lifecycle perspective. Additionally, tellurium and selenium are substitutes for one another as indicated by the dotted line connecting them.

5.2.3. Substitution

One key mitigation strategy for short- and long-term strategic material availability issues not addressed in this dissertation is substitution. If a firm can easily use another material in their product, this can offset production bottle-necks due to physical scarcity or other supply-chain inefficiencies. Addition of market modeling to capture substitution would improve
characterization of the $n$ parameter representing share of tellurium demand from solar in Chapter 2 supply risk model. This would also enable evaluation of substitution as a mitigation strategy using Chapter 4 methodology.

However, understanding what materials may serve as substitutes, and the ease of that substitution is a complex process. There are many factors dictating substitutability. First, there is technical substitutability which is currently characterized using qualitative scales for by most studies. While this provides an important starting point, quantitative treatment of substitution on the basis of functionality would be more useful to identify criticality risks since most materials cannot substitute one-to-one for one another. Additionally, interdependence of substitutes could be assessed to show how substitutions in multiple systems may be affecting criticality of one another over time. Next, since environmental regulation can also play a large role in determining suitable substitutes (UKCSF, 2010), future work will propose alternative environmental impact metrics that more appropriately capture life cycle impacts of using critical elements, focusing on factors of importance to product designers (e.g. recyclability, toxicity of the product itself not just the emissions from its production). Finally, most studies focus on what is known as elemental substitution – i.e. one element or material for another in a given product – however, there is potential for substitution at the product level, process level, and system level all of which may ultimately impact material demand, availability and criticality in complex ways not currently captured (Nassar, 2015).

For preliminary work in this space see work published in the photovoltaics specialists conference (PVSC 42) proceedings comparing the economic sensitivity of potential substitute thin film technologies, CdTe and CIGS PV, to price volatility of critical input materials, tellurium and indium. Understanding of their sensitivity of firm, consumer, and policy level decision metrics to byproduct raw material price volatility can be an indicator of ability to absorb cost increase, and competitiveness of each technology (M. L. Bustamante and Gaustad 2015).

5.2.4. Evaluate policy tradeoffs

The results of the Chapter 4 analysis communicate benefit in terms of supply risk reduction normalized to a specific mitigation parameter (film thickness, yield, recycling rate) and risk metric (onset of gap conditions, peak market imbalance, duration of gap conditions), and used this as a measure of a strategy’s merit. In reality, there are various other factors to consider when
developing policy that will lead to more sustainable outcomes. For example, although recycling may not have the best efficacy at mitigating supply risk in the short term, it will likely provide benefits in terms of environmental impact by displacing primary supply, and this should not be overlooked. However, it may be more expensive than other strategies. Extending the normalized average benefit metric to include similar measures of marginal environmental and/or economic performance would enable a more balanced evaluation of sustainability tradeoffs between different mitigation strategies and would improve its ability to inform policy design. Marginal environmental impacts can be collected from consequential or economic input-output LCI databases. Marginal costs can be collected from cost models or financial records. Tradeoff space would be explored using multicriteria optimization.

5.2.5. Other case studies

Although the methodology developed throughout this dissertation was designed with tellurium in mind, it was also intended to be broadly applicable to other byproduct systems. While byproduct systems share one source of common supply risk, they may differ in many other aspects of their supply chains that impact its supply risk; for example, whereas recycling of tellurium is virtually non-existent, indium, which is a byproduct of zinc, has nearly half of its global supply come from prompt scrap recycling due to poor deposition efficiency in making flat screen devices (Duan et al. 2016). Methodology will be extended to additional case studies with similar joint production nature but distinct system features; example, indium which has significant secondary supply (prompt scrap), and rare earths, which have more coproduct character for some elements and byproduct character for others.

5.2.6. Recycling versus Clean Energy Critical Supply

Additionally, there are several interesting questions left to be answered with respect to environmental tradeoffs. For instance, copper recycling and solar energy generation are both generally considered to be positive environmental behaviors. The former offsets the need for primary mining and the latter offsets the need for fossil fuel energy generation. However, because of the interconnected nature of this byproduct system, increasing secondary copper production negatively affects supply of tellurium and thus ability to produce CdTe PV reliably and at an affordable price. Do the environmental gains from increasing recycling of copper outweigh the
environmental benefits of clean solar energy generation? How do conflicting policy goals factor in? What is the optimal balance? Thorough life cycle assessment and multi-criteria decision modeling work is needed to answer these questions.
APPENDIX A. More on yield improvement potential for tellurium\(^5\)

To assess opportunities for future improvement, a closer look at the extractive processes used to recover tellurium from copper anode slime is needed. Such quantification could inform proactive strategies to reduce the risk of supply interruption or steep price increases.

The amount of tellurium available for extraction in copper ore is a function of natural geochemistry. It represents an inherent upper limit to local supply and cannot be manipulated technologically. One factor that can be manipulated, however, is the efficiency of tellurium separation and recovery from copper anode slimes. This parameter, hereafter referred to as yield, can be represented by the generalized function in Equation 11.

\[
Yield = f (Technology, \text{ Process Parameters})
\]

Equation 11

In the long term, yield is one of the best tools that producers can leverage to control tellurium supply in the face of uncertain byproduct slime supply. Like tellurium content, the specific technology or process selected establishes an upper limit for recovery. From there, process parameters can be manipulated to produce more or less of the given value element. Once determined, the yield parameter can be used to infer supply according to the following relationship in Equation 12. In the short term, supply can be controlled by processing more or less slime.

\[
Supply = \text{Slime Amount} \times \text{Slime Content} \times \text{Yield}
\]

Equation 12

What are the different kinds of “technologies” that limit recovery of tellurium from copper anode slime? As with copper extraction and refining, there are several and the exact choice of a process will depend upon on the specific composition of the feedstock – in this case the anode slime. Wang reviews three major types of leaching processes, summarized in Table 15. According to Wang, acid pressure leaching has become the most popular method for decopperization. It utilizes a small amount of sulfuric acid under pressure in an autoclave in the presence of excess oxygen to dissolve copper and tellurium. By contrast, acid aeration leaching utilizes more sulfuric

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\(^5\) This section draws upon discussions published in TMS 2014 proceedings but with update figures and is included for reference. (M. L. Bustamante and Gaustad 2014b)
Table 15. Leaching processes, listed in order of maximum theoretical yield.

<table>
<thead>
<tr>
<th>Leaching Process</th>
<th>Maximum Yield</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acid Aeration</td>
<td>100%</td>
<td>(Wang 2011)</td>
</tr>
<tr>
<td>Alkaline Pressure</td>
<td>99.9%</td>
<td>(Davenport and Biswas 2002; Wang 2011)</td>
</tr>
<tr>
<td>Acid Pressure</td>
<td>&gt;90%</td>
<td>(Wang 2011)</td>
</tr>
</tbody>
</table>

Acid requires a long “digestion” time, but does not require use of pure oxygen, opting for air instead and is carried out at atmospheric pressure. Finally, alkaline pressure leaching utilizes an alkaline solvent, such as sodium hydroxide, rather than sulfuric acid to form a hydrated sodium tellurium compound (Wang 2011). It should be noted that anode slime contains many valuable metals including silver, gold, and selenium, and as such, the process selection and design decisions are driven by the economic optimization.

Once the leaching is complete, there are additional steps that must be taken to produce refined tellurium. For each step in the process of producing refined tellurium from copper anode slimes there is potential to lose more and more content. Thus the overall supply is more accurately described with a series of yield terms. Rather than add redundant terms the overall yield can be calculated as shown in Equation 13, where $i$ represents the set of all process steps.

$$Yield = \prod_{i} ProcessYield_i$$  \hspace{1cm} \text{Equation 13}

This fact may be one reason that, despite the reported high theoretical efficiencies, yield is typically reported by most studies of industry to be much lower. Figure 37 summarizes the yield reportings in the past 40 years. The works included by no means represent an exhaustive list, but rather a representative one. The blue area plots the government reports and journal articles that present or apply a yield value. The red area plots the results of bench scale experimental or theoretical studies. Generally speaking, the former group represented much more conservative, and probably realistic, values between 33-60%. Unfortunately, the values provided in these studies cannot be reliably linked to any one extraction technology. Conversely, the experimental studies naturally provide a great deal of process detail, but will only describe yield of one step in the tellurium recovery process: typically, leaching efficiency. The bench-scale studies all reported values above 70%, going as high as 95% in work conducted by Rhee et al. (Rhee et al. 1999). Several of the studies
are plotted as a very large range because they include the variation of several process parameters, such as temperature, leaching time, and additive weight. For instance, Hait et al. reports on acid aeration leaching with and without the addition of (a) MnO$_2$ and (b) HCl, varying the process parameters previously mentioned. The group found that without any additives tellurium recovery was quite poor (10%) regardless of temperature. With the sole addition of MnO$_2$, the maximum recovery achieved was 75% at the highest temperature, acid concentration, and additive weight studied. With the addition of both MnO$_2$ and NaCl, the maximum tellurium recovery observed had increased to 79% (Hait et al. 2002).

![Figure 37. Graph of tellurium yield as published in a broad sample of the literature. Yield values presented in governmental reports and applied analyses, shown in black, range from 33-60% (Bleiwas (Bleiwas 2010), Coakley (Coakley 1976), Fthenakis (Vasilis Fthenakis 2009), Ojebuoboh (Ojebuoboh 2008), USGS (M. George 2013), Guilinger (Guilinger 2000), Jensen (Jensen 1985), and Woodhouse (Michael Woodhouse et al. 2013)). Conversely, yield values from small-scale experimental studies, patents, and theoretical studies, shown in grey (or double line), all claim to produce yields over 70% (Biswas (Biswas et al. 1998), Fan (Fan et al. 2013), Hait (Hait et al. 2002), Hoffmann (Hoffmann 1989), Rhee (Rhee et al. 1999), Robles-Vega et al. (Robles-Vega, Sanchez-Corrales, and Castillon-Barraza 2009), and Stafiej et al. (Stafiej, Claessens, and White 1999)).]
Several applied studies have mentioned 80% yield as a reasonable upper limit for tellurium extraction from copper anode slimes in the near future (Vasilis Fthenakis 2009; Ojebuoboh 2008; Michael Woodhouse et al. 2013). As such studies were demonstrated on a small scale with leaching experiments, there is still some room for doubt. First, the sources amassed in the top plot of Figure 37 seem to indicate that, currently, overall yields including all steps of tellurium recovery and processing, may be quite low. Reaching a global average of 80% in the near future would therefore require aggressive and optimistic improvements by a majority of producers. Additionally, it cannot be guaranteed that efficient bench-scale processes will provide the same performance once they are scaled up. Certainly the same level of recovery cannot be assumed for the whole tellurium production process because of the multiple steps required. However, despite these doubts there is also reason for hope. If rapid increase in demand from solar or other applications is in fact observed and furthermore, if it is coupled with slower growing supply, then simple economic analysis indicates that tellurium prices could become high enough to incentivize investment in scaling up newer and higher yielding technologies. Even if they do not provide the near ideal performance alluded to in Wang’s review, any improvements will help take pressure off supply by making better use of what is available.
### APPENDIX B. LCA Supplement

#### B.1 Unit Processes

**Table 16. Summary of modified ecoinvent unit processes used to generate the case study LCAs.**

<table>
<thead>
<tr>
<th>ecoinvent unit process</th>
<th>online source (<a href="https://v30.ecoquery.ecoinvent.org/Details/UPR/%E2%80%A6">https://v30.ecoquery.ecoinvent.org/Details/UPR/…</a>)</th>
<th>new unit process</th>
<th>Modifications used to create new unit process from ecoinvent unit process</th>
</tr>
</thead>
</table>
| copper mine operation, GLO | 645d0a72-6b4c-4333-b9d3-71d5f999b851/8b738ea0-f89e-4627-8679-433616064e82 | copper mining | • created modified global production block based on production-weighted average of inputs and outputs from regional blocks (also available online)  
• Used ICSG World Copper Factbook 2013 to estimate production weightings for each region (ecoinvent region = ICSG region: AU = Oceania, RAS = Asia, RER = Europe, RLA = Latin America, RNA = North America, RoW = Africa).  
• Electricity (high and low voltage separately) approximated using ‘rest of world’ region market blocks  
• Electricity values based on global averaging based on regional production (regional electricity demand = sum of subregional demands)  
• Copper concentrate intermediate calculated using Nuss & Eckelman (2014) methodology with inflation-adjusted prices for the appropriate years |
| copper production, primary, GLO | 505ad36f-5c60-4617-8355-4c30715d2725/8b738ea0-f89e-4627-8679-433616064e82 | copper refining | • linked to output from new copper mining block  
• other modifications: same as copper mining |
| processing of anode slime, primary copper production, GLO | d47fb544-b50d-400b-b33a-283538e6832f/8b738ea0-f89e-4627-8679-433616064e82 | anode slime processing | • linked to output from new copper refining block  
• included coproduct: selenium  
• modified allocation factors based on Te production estimated from Bustamante & Gaustad (2014) |
| tellurium production, semiconductor-grade, GLO | 8b191b2c-7d4d-4238-95ee-eeoe0e60e570/8b738ea0-f89e-4627-8679-433616064e82 | tellurium refining | linked to output from new anode slime processing block |
B.2. Inventory Data

Table 17. Reference flows and unit price ($1998/kg) for all unit process outputs.

<table>
<thead>
<tr>
<th>MASS (kg)</th>
<th>Copper Mining</th>
<th>Copper Refining</th>
<th>Anode Slime Processing</th>
<th>Te Refining</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Copper Concentrate</td>
<td>Molybdenum Concentrate</td>
<td>Copper Cathode</td>
<td>Anode Slime</td>
</tr>
<tr>
<td>2006</td>
<td>1.00E+00</td>
<td>4.11E-03</td>
<td>1.00E+00</td>
<td>2.56E-03</td>
</tr>
<tr>
<td>2007</td>
<td>1.00E+00</td>
<td>4.11E-03</td>
<td>1.00E+00</td>
<td>2.57E-03</td>
</tr>
<tr>
<td>2008</td>
<td>1.00E+00</td>
<td>4.11E-03</td>
<td>1.00E+00</td>
<td>2.60E-03</td>
</tr>
<tr>
<td>2009</td>
<td>1.00E+00</td>
<td>4.11E-03</td>
<td>1.00E+00</td>
<td>2.75E-03</td>
</tr>
<tr>
<td>2010</td>
<td>1.00E+00</td>
<td>4.11E-03</td>
<td>1.00E+00</td>
<td>2.89E-03</td>
</tr>
<tr>
<td>2011</td>
<td>1.00E+00</td>
<td>4.11E-03</td>
<td>1.00E+00</td>
<td>2.76E-03</td>
</tr>
<tr>
<td>2012</td>
<td>1.00E+00</td>
<td>4.11E-03</td>
<td>1.00E+00</td>
<td>2.84E-03</td>
</tr>
<tr>
<td>2013</td>
<td>1.00E+00</td>
<td>4.11E-03</td>
<td>1.00E+00</td>
<td>2.84E-03</td>
</tr>
<tr>
<td>2014</td>
<td>1.00E+00</td>
<td>4.11E-03</td>
<td>1.00E+00</td>
<td>2.78E-03</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>PRICE ($/kg)</th>
<th>Copper Concentrate</th>
<th>Molybdenum Concentrate</th>
<th>Copper Cathode</th>
<th>Anode Slime</th>
<th>Silver</th>
<th>Selenium</th>
<th>Copper Telluride</th>
<th>Tellurium</th>
</tr>
</thead>
<tbody>
<tr>
<td>2006</td>
<td>1.62</td>
<td>24.66</td>
<td>5.61</td>
<td>0.02</td>
<td>302.00</td>
<td>43.80</td>
<td>3.60</td>
<td>72.00</td>
</tr>
<tr>
<td>2007</td>
<td>1.64</td>
<td>29.30</td>
<td>5.69</td>
<td>0.02</td>
<td>339.00</td>
<td>57.30</td>
<td>3.23</td>
<td>64.50</td>
</tr>
<tr>
<td>2008</td>
<td>1.53</td>
<td>26.62</td>
<td>5.33</td>
<td>0.02</td>
<td>365.00</td>
<td>53.90</td>
<td>7.95</td>
<td>159.00</td>
</tr>
<tr>
<td>2009</td>
<td>1.14</td>
<td>10.94</td>
<td>4.04</td>
<td>0.02</td>
<td>359.00</td>
<td>38.70</td>
<td>6.00</td>
<td>120.00</td>
</tr>
<tr>
<td>2010</td>
<td>1.65</td>
<td>14.56</td>
<td>5.74</td>
<td>0.03</td>
<td>485.00</td>
<td>62.30</td>
<td>8.25</td>
<td>165.00</td>
</tr>
<tr>
<td>2011</td>
<td>1.88</td>
<td>13.89</td>
<td>6.49</td>
<td>0.05</td>
<td>819.00</td>
<td>106.00</td>
<td>12.65</td>
<td>253.00</td>
</tr>
<tr>
<td>2012</td>
<td>1.66</td>
<td>11.16</td>
<td>5.75</td>
<td>0.04</td>
<td>713.00</td>
<td>85.20</td>
<td>5.30</td>
<td>106.00</td>
</tr>
<tr>
<td>2013</td>
<td>1.50</td>
<td>9.02</td>
<td>5.24</td>
<td>0.03</td>
<td>537.00</td>
<td>55.80</td>
<td>3.90</td>
<td>78.00</td>
</tr>
<tr>
<td>2014</td>
<td>1.43</td>
<td>10.43</td>
<td>5.00</td>
<td>0.02</td>
<td>424.00</td>
<td>40.84</td>
<td>4.05</td>
<td>81.00</td>
</tr>
</tbody>
</table>
### B.3. Allocation Factors

**Table 18. Allocation factors for each unit process output in the time averaged scenarios.**

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Copper Mining</td>
<td>Copper Concentrates</td>
<td>99.6%</td>
<td>97.1%</td>
<td>99.6%</td>
<td>94.6%</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Molybdenum Concentrates</td>
<td>0.4%</td>
<td>2.9%</td>
<td>0.4%</td>
<td>5.4%</td>
</tr>
<tr>
<td></td>
<td>Copper Refining</td>
<td>Copper Cathode</td>
<td>99.7%</td>
<td>99.4%</td>
<td>99.7%</td>
<td>99.6%</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Anode Slime</td>
<td>0.3%</td>
<td>0.6%</td>
<td>0.3%</td>
<td>0.4%</td>
</tr>
<tr>
<td></td>
<td>Anode Slime Processing</td>
<td>Silver</td>
<td>63.1%</td>
<td>96.0%</td>
<td>60.9%</td>
<td>94.7%</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Selenium</td>
<td>21.1%</td>
<td>3.8%</td>
<td>23.0%</td>
<td>4.9%</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Copper Telluride</td>
<td>15.8%</td>
<td>0.3%</td>
<td>16.1%</td>
<td>0.4%</td>
</tr>
<tr>
<td></td>
<td>Tellurium Refining</td>
<td>Tellurium</td>
<td>100.0%</td>
<td>100.0%</td>
<td>100.0%</td>
<td>100.0%</td>
</tr>
</tbody>
</table>

**Table 19. Allocation factor for each unit process output in the individual year scenarios.**

<table>
<thead>
<tr>
<th>MASS</th>
<th>Copper Mining</th>
<th>Copper Refining</th>
<th>Anode Slime Processing</th>
<th>Te Refining</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Copper Concentrate</td>
<td>Molybdenum Concentrate</td>
<td>Copper Cathode</td>
<td>Anode Slime</td>
</tr>
<tr>
<td>2006</td>
<td>99.6%</td>
<td>0.4%</td>
<td>99.7%</td>
<td>0.3%</td>
</tr>
<tr>
<td>2007</td>
<td>99.6%</td>
<td>0.4%</td>
<td>99.7%</td>
<td>0.3%</td>
</tr>
<tr>
<td>2008</td>
<td>99.6%</td>
<td>0.4%</td>
<td>99.7%</td>
<td>0.3%</td>
</tr>
<tr>
<td>2009</td>
<td>99.6%</td>
<td>0.4%</td>
<td>99.7%</td>
<td>0.3%</td>
</tr>
<tr>
<td>2010</td>
<td>99.6%</td>
<td>0.4%</td>
<td>99.7%</td>
<td>0.3%</td>
</tr>
<tr>
<td>2011</td>
<td>99.6%</td>
<td>0.4%</td>
<td>99.7%</td>
<td>0.3%</td>
</tr>
<tr>
<td>2012</td>
<td>99.6%</td>
<td>0.4%</td>
<td>99.7%</td>
<td>0.3%</td>
</tr>
<tr>
<td>2013</td>
<td>99.6%</td>
<td>0.4%</td>
<td>99.7%</td>
<td>0.3%</td>
</tr>
<tr>
<td>2014</td>
<td>99.6%</td>
<td>0.4%</td>
<td>99.7%</td>
<td>0.3%</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>ECON</th>
<th>Copper Concentrate</th>
<th>Molybdenum Concentrate</th>
<th>Copper Cathode</th>
<th>Anode Slime</th>
<th>Silver</th>
<th>Selenium</th>
<th>Copper Telluride</th>
<th>Tellurium</th>
</tr>
</thead>
<tbody>
<tr>
<td>2006</td>
<td>94.1%</td>
<td>5.9%</td>
<td>100.0%</td>
<td>0.0%</td>
<td>94.4%</td>
<td>5.3%</td>
<td>0.3%</td>
<td>100.0%</td>
</tr>
<tr>
<td>2007</td>
<td>93.2%</td>
<td>6.8%</td>
<td>100.0%</td>
<td>0.0%</td>
<td>93.4%</td>
<td>6.4%</td>
<td>0.2%</td>
<td>100.0%</td>
</tr>
<tr>
<td>2008</td>
<td>93.3%</td>
<td>6.7%</td>
<td>100.0%</td>
<td>0.0%</td>
<td>93.9%</td>
<td>5.5%</td>
<td>0.6%</td>
<td>100.0%</td>
</tr>
<tr>
<td>2009</td>
<td>96.2%</td>
<td>3.8%</td>
<td>100.0%</td>
<td>0.0%</td>
<td>95.9%</td>
<td>3.7%</td>
<td>0.4%</td>
<td>100.0%</td>
</tr>
<tr>
<td>2010</td>
<td>96.5%</td>
<td>3.5%</td>
<td>100.0%</td>
<td>0.0%</td>
<td>95.4%</td>
<td>4.2%</td>
<td>0.4%</td>
<td>100.0%</td>
</tr>
<tr>
<td>2011</td>
<td>97.1%</td>
<td>2.9%</td>
<td>100.0%</td>
<td>0.0%</td>
<td>95.1%</td>
<td>4.5%</td>
<td>0.4%</td>
<td>100.0%</td>
</tr>
<tr>
<td>2012</td>
<td>97.3%</td>
<td>2.7%</td>
<td>100.0%</td>
<td>0.0%</td>
<td>96.0%</td>
<td>3.8%</td>
<td>0.2%</td>
<td>100.0%</td>
</tr>
<tr>
<td>2013</td>
<td>97.6%</td>
<td>2.4%</td>
<td>100.0%</td>
<td>0.0%</td>
<td>96.7%</td>
<td>3.1%</td>
<td>0.2%</td>
<td>100.0%</td>
</tr>
<tr>
<td>2014</td>
<td>97.1%</td>
<td>2.9%</td>
<td>100.0%</td>
<td>0.0%</td>
<td>96.8%</td>
<td>3.0%</td>
<td>0.2%</td>
<td>100.0%</td>
</tr>
</tbody>
</table>
Figure 38. Allocation factors visualized over time showing relative trend between joint products of each unit process. Top: ECON_year. Bottom: MASS_year.
APPENDIX C. Strategic Response Supplement

C1. RESULTS

Table 20. Summarizing results from assessment in Chapter 4 of mitigation strategies.

<table>
<thead>
<tr>
<th>MAXIMUM BENEFIT</th>
<th>Units</th>
<th>Δ Onset</th>
<th>Δ Imbalance</th>
<th>Δ Duration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Technical</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Dematerialization</td>
<td>-</td>
<td>Infinity (no gap)</td>
<td>3685 tonnes*</td>
<td>86 years*</td>
</tr>
<tr>
<td>Yield Improvmt</td>
<td>-</td>
<td>3 years</td>
<td>1666 tonnes</td>
<td>52 years</td>
</tr>
<tr>
<td>Policy</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Recycle Rate</td>
<td>-</td>
<td>0 years</td>
<td>13 tonnes</td>
<td>31 years</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>AVERAGE BENEFIT</th>
<th>Units</th>
<th>Δ Onset</th>
<th>Δ Imbalance</th>
<th>Δ Duration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Technical</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Dematerialization</td>
<td>%/%</td>
<td>7.8%*</td>
<td>.014%</td>
<td>.010%</td>
</tr>
<tr>
<td>Yield Improvmt</td>
<td>%/%</td>
<td>2.8%</td>
<td>.004%</td>
<td>.046%</td>
</tr>
<tr>
<td>Policy</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Recycle Rate</td>
<td>%/%</td>
<td>0%</td>
<td>4E-8%</td>
<td>4E-6%</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>NORMALIZED AVERAGE BENEFIT</th>
<th>Units</th>
<th>Δ Onset</th>
<th>Δ Imbalance</th>
<th>Δ Duration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Technical</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Dematerialization</td>
<td>%/%</td>
<td>7.8%*</td>
<td>.014%</td>
<td>.010%</td>
</tr>
<tr>
<td>Yield Improvmt</td>
<td>%/%</td>
<td>2.8%</td>
<td>.004%</td>
<td>.046%</td>
</tr>
<tr>
<td>Policy</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Recycle Rate</td>
<td>%/%</td>
<td>0%</td>
<td>4E-8%</td>
<td>4E-6%</td>
</tr>
</tbody>
</table>

* Only applies to limited scope
C2. Alternate baseline scenario for Chapter 4

Figure 39 shows alternate baseline risk scenario using assumptions from Chapter 2. Onset of supply gap conditions occurs 2 years later than in Chapter 4 baseline, peak market imbalance is half of what it is in Chapter 4, and duration of supply gap conditions is about 30% what it is in Chapter 4. The difference comes from the fact that Chapter 4 assumes logistic growth of all tellurium demand proportional to PV at 40%. It is valuable to include this consideration since it has such a large impact on results, however, this current treatment is insufficient to describe growth of non-emerging tellurium applications demand growth.

Figure 39. Supply risk under baseline scenario, using assumptions from Chapter 2.
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