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The V-factor: Towards a New Metric for Gauging the Efficiency and Profitability of Manufacturing Processes for the Bioeconomy

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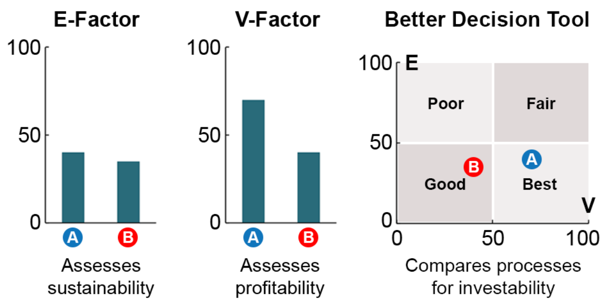
Graphical abstract



Abstract

Several metrics have been formulated to evaluate the environmental impact of chemical manufacturing processes. However, there are no formulas for simplified, back-of-the envelope estimation of their efficiency of resource utilisation and profitability, which are hugely influential when it comes to determining investments and, for academic users, justifying research into new conversion technologies. Herein, we posit a new metric called the valorization (V) -factor to estimate these parameters for manufacturing processes that utilize biomass. Additionally, we also argue that co-assessment of the established environmental (E) -factor, related to waste production in a process, and V-factor will greatly facilitate the development of environmentally and economically sustainable processes for valorization of biomass.

Keywords: valorization, bioeconomy, manufacturing, technoeconomics, profitability, biomass

1 Introduction

Human history has a cycle of innovation and corrections where mass consumption and development has resulted in unforeseen (or limited appreciation for) severe consequences such as species extinction, elevated lead levels in blood, mass deforestation, ozone deterioration, release of carcinogenic compounds, and global warming. In an effort to minimize the environmental footprint of chemical and manufacturing industries, eliminate the generation of hazardous and toxic wastes, and reduce energy consumption, a set of sustainability principles were created to guide the development of greener chemistry practices (Anastas & Warner 1998). These twelve principles, with origins in pollution prevention and regulation, are quite straightforward and include guidelines such as "use renewable feedstocks" or "design benign chemicals". Furthermore, the twelve principles of green chemistry, have had a profound impact on the manner in which chemical processes are now designed

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and operated (Anastas & Lankey 2002, Anastas & Warner 1998), and importantly a variety of metrics have been formulated to assess the compliance of manufacturing processes with these principles (Table S1 in Appendix). The embracement of these straightforward metrics by the chemical industry has greatly improved the atom and energy economies of manufacturing processes (Sheldon 2014). Chemical processes are now designed with an eye to avoid the use of toxic solvents, incorporate renewable feedstocks, and employ catalysts in lieu of stoichiometric quantities of chemical reagents; and products too are now conceived to be more biocompatible and designed for biodegradation. By close examination of by-products formed as possible new reagents, the extensive use of green chemistry metrics has also accelerated the transition of the chemical industry to a circular economy (Sheldon 2016), which will reduce its environmental footprint even further.

Nevertheless, while the reconfiguration of a manufacturing process to minimize its environmental impact delivers two of the three bottom lines (Elkington 1997), people and planet, its impact on the third factor, profits, is not as clearly articulated (Sheldon 2014). Instead, developing processes that utilize resources as productively and profitably as possible – a concept which has its roots in the German term *verwertung* (Sheldon 2016) – could inherently deliver the coveted triple bottom line. To this end, formulas that provide quick, back-of-the-envelope estimates of how productively and profitably a process utilizes resources could be tremendously useful in the design cycle. While metrics such as the EcoScale (Van Aken et al. 2006) or the Green Aspiration Level (Roschangar et al. 2015) provide this information to varying degrees of detail, they are not easy to use; and, paradoxically, despite requiring extensive (and often difficult to procure) data to evaluate, both are semi-quantitative and sensitive to subjectivity in estimates for some of their parameters. Significantly, there are no metrics to assess the efficiency of resource utilization and profitability of processes that valorize biomass, a hugely important domain of the emerging bioeconomy (Bozell & Petersen 2010). Not only are biomass-based alternatives already replacing petroleum-based processes (Karp et al. 2017), but they also open new opportunities to manufacture novel chemicals with superior or designer properties that are otherwise unattainable via petrochemical operations (Carus & Aeschelmann 2017, Carus et al. 2017). In an era in which research on biobased chemical manufacturing is booming, the paucity of metrics to quantify the efficiency with which processes valorize biomass is especially glaring. Our extensive search yielded only two metrics that partially meet this need. The Biotechnological Valorization Potential Indicator (BVPI) measures the degree of suitability of a lignocellulosic feedstock for biorefining (Duarte et al. 2007); whereas the Biomass Utilization Efficiency (BUE) index is an estimate of the percentage of biomass on a molar mass basis that ends up in the desired products (Iffland et al. 2015). Both metrics are grounded in the assumption that treatment of biomass to generate a uniform stream of products typically enhances its value. In contrast, we sought to compare processes based on the degree to which they add value to biomass. To this end, we have conceived a set of simple formulae to quantify the value addition in biomass valorization processes. We label these metrics as V-factors or valorization factors.

2 Concept

The unabridged V-factor incorporates all variables that influence the profitability of a manufacturing process, namely the costs of its reactants and products ($/kg), its fractional yield, its capital and operating expenditures (CapEx and OpEx, respectively, $/kg for both), tonnage of the product (MT or metric tons), and the tonnage of its product sector (MT). Approximate annual tonnages for some key product sectors are listed in Table 1. The unabridged V-factor is postulated as:

$$\begin{matrix}\text{Unabridged}\\ \text{V-factor}\end{matrix} = \left(\frac{\text{Cost of product}}{\text{Cost of reactant}}\right) \times \left(\begin{matrix}\text{Fractional}\\ \text{yield}\end{matrix}\right) \times \left(\frac{\text{CapEx}}{\text{OpEx}}\right) \times \left(\frac{\text{Tonnage of product}}{\text{Tonnage of product sector}}\right) \quad (1)$$

In this formula, the costs of the product and reactant are on a per-kilogram basis. The CapEx and OpEx are also scaled to a per-kilogram of product basis. CapEx includes costs associated with fixed assets such as land, buildings and manufacturing infrastructure, whereas OpEx includes manufacturing costs, separation costs, R&D investments, plant overheads, labour, insurance, administration costs and taxes. Since CapEx is an asset, it is directly proportional to profitability. On the other hand, since OpEx is a liability, it varies inversely with profitability.

The unabridged V-factor is also directly proportional to the ratio of the dollar values of the products to reactants. This implies that as the cost of the product increases vis-à-vis to the cost of the reactant, the more profitable is the use of the reactant by the process. The fractional yield always ranges between 0 and 1. For processes not involving a chemical reaction, the fractional yield represents the fraction of the starting material that is converted to the desired product. Predictably, the more efficiently the process converts the reactant to the product, the more profitable it will be. Generally, the better the infrastructure used for manufacturing, which translates to higher CapEx, the higher is the fractional yield. Moreover, higher fractional yields, which are indicative of technologically mature processes that do not necessitate large investments on R&D, also incur lower separation costs, and, as a consequence, lower OpEx.

Although the unabridged V-factor adequately describes how efficiently a process valorizes its inputs, it is not easy to calculate. This is especially true for academic users who may not have good estimates for CapEx, or up-to-date information about pricing or product tonnages. It is also evident that the equation has redundancies that could be factored out in most cases. As a result, we have simplified the previous formula by incorporating the fractional dollar output for individual sectors.

We term the simplified metric as the V-factor, and the fractional dollar output is an attribute of the industrial sector in which the product will be sold.

$$\text{V-factor} = \left(\frac{\text{Cost of product}}{\text{Cost of reactant}}\right) \times \text{Fractional yield} \times \left(\begin{matrix}\text{Fractional dollar}\\ \text{output of sector}\end{matrix}\right) \quad (2)$$

This simplification greatly improves the utility of the V-factor and provides academic users with a useful tool to quickly assess profitability during the formulation of green chemistry and engineering research strategies. The fractional dollar output also ranges between 0 and 1. In addition, the sum of the fractional dollar outputs for all sectors of the chemical industry is one. Forecasted global averages of fractional dollar outputs for some common industrial sectors between now and 2050 are listed in Table 2. The impacts of manufacturing volumes, capital and operating expenditures, and investments on R&D on the profits has been assessed previously (Heaton 1991, Valencia 2013), and it has been observed that a sector's profit share of the global chemical market has remained constant over period of 20 years and is expected to remain same over next 25 years. The volume or tonnage at which a product must be manufactured in order to attain economies of scale, the capital and operating expenditures, and investments on R&D that are typically required for a sector greatly influence its profit share. For instance, the profit share is positively correlated with manufacturing volumes. Sectors with higher manufacturing volumes such as petrochemicals typically achieve greater economies of scale compared with speciality chemical producers (Jones 2013). However, higher manufacturing volumes usually incur substantially greater capital expenditures. As a consequence, the profit share for operating in a low-tonnage sector, despite having disadvantages such as higher product and process R&D expenditures, is not significantly lower in comparison. We used sector's profit share data and coined the term fractional dollar output to simplify determination of V factor. The use of the fractional dollar output for estimating the profitability of processes is akin to performing a gate-to-gate life cycle analysis (LCA) in lieu of the more accurate cradle-to-grave LCA.

Table 1. Approximate annual tonnages for various product sectors.

Sector	Tonnage (MT) (Sheldon 1992, Sheldon 2017, Sheldon 1997)
Fuels & petrochemicals	10^7
Commodity chemicals	10^5
Speciality chemicals & polymers	10^3
Pharmaceuticals	10^2

Table 2. Predicted global averages of fractional dollar outputs of selected sectors.

Sector	Fractional dollar output
Basic chemicals, fuels and petrochemicals	0.3
Pharmaceuticals and agrochemicals	0.2
Speciality chemicals	0.2
Polymers and fibres	0.2
Oleochemicals, surfactants & auxiliary chemicals	0.1

3 Examples

V-Factors for some common manufacturing process are plotted in Figure 1. The fractional yields used in these calculations are the highest reported values for that particular process and include examples that have low

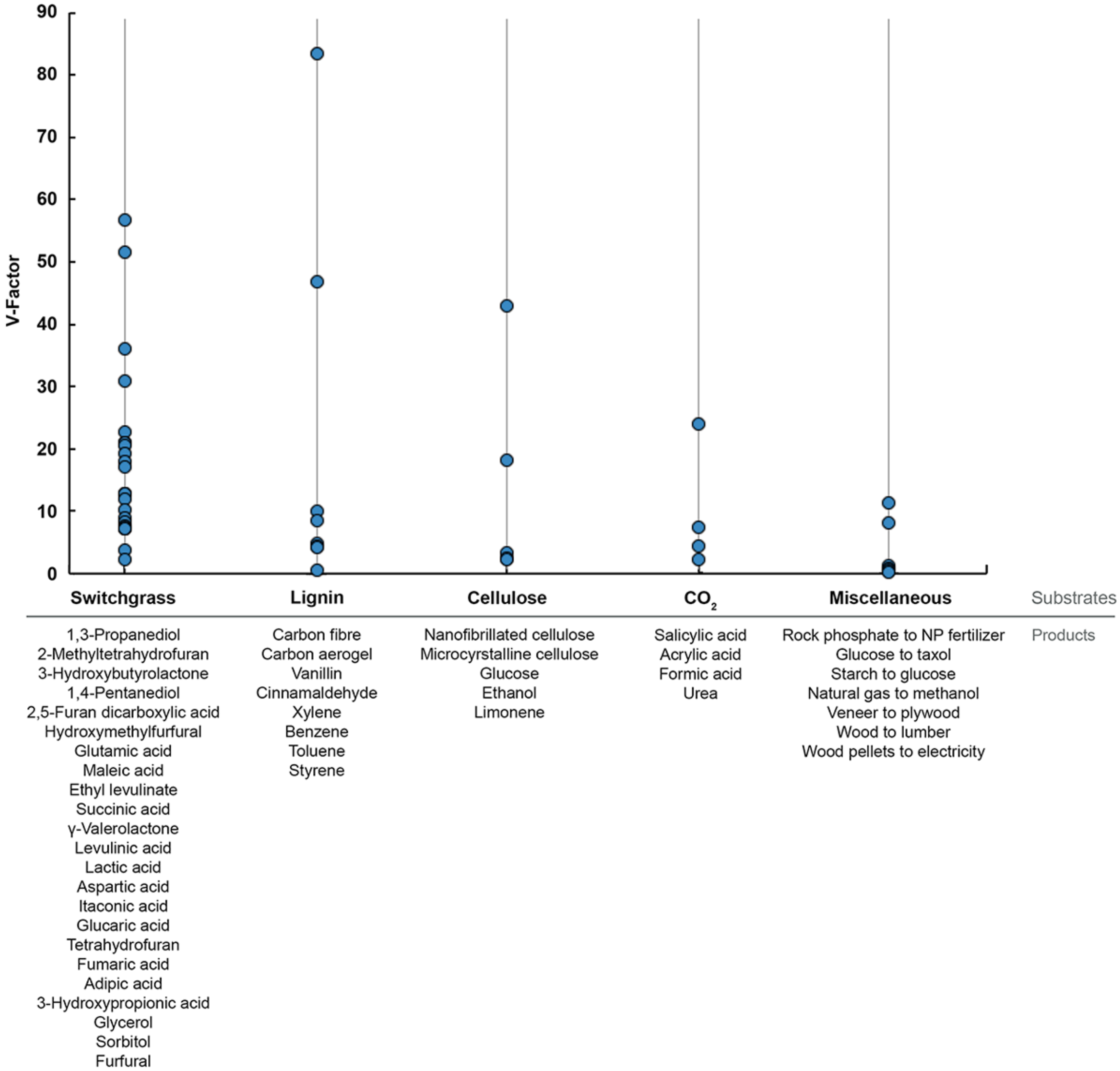

Figure 1. V-Factors for the manufacture of selected products obtained at the highest reported fractional yields. Detailed information about the conversion processes and the raw data employed to calculate the V-factors have been compiled in Table S2 in the appendix. The product labels are listed in descending order of their V-factors and correspond to the order of the ordinate points plotted for each substrate.

technology readiness levels (Héder 2017). Information about the conversion processes and the raw data employed to calculate the V-factors have been compiled in Table S2 in the appendix. From a chemical engineering standpoint, analysis of the V-factors plotted in Figure 1 also confirms the wisdom of selectively exchanging – or converting – less reactive C-C and C-H σ-bonds in the substrate for more reactive C-C π-bonds to generate a small set of products, but at higher yields, as opposed to arbitrarily exchanging of σ-bonds for π-bonds to generate a plethora of products (Kolb et al. 2001). Comparable insights are discernible for the other substrates listed in Figure 1.

4 Variations to the Formula

Although the V-factor is a useful comparative metric, it has some limitations, chief among which are that it relies on empirical data. Additionally, it can only be used to compare either processes that manufacture different products from the same reactant or processes that make the same product from different starting materials. A comparison between processes that manufacture identical products from the same reactants necessitates inclusion of CapEx and OpEx. Since CapEx is quite difficult to estimate for academic users, we empirically determined that eliminating CapEx from the equation still provides a reasonably accurate approximation for comparative valorization by the processes. This modification to the calculation yields a formula for a "process-function" V-factor, whose labeling is rationalized similarly to process or path-dependent thermodynamic functions (Sychev 1991). In fact, one could simply replace the ratio of CapEx to OpEx with the reciprocal of manufacturing costs incurred on a per-kilogram of product basis, which can be estimated quite readily by academic users.

$$\text{Process-function V-factor} = \left(\frac{\text{Cost of product}}{\text{Cost of reactant}}\right) \times \left(\text{Fractional yield}\right) \times \left(\frac{1}{\text{Manufacturing costs}}\right) \times \left(\frac{\text{Tonnage of product}}{\text{Tonnage of product sector}}\right) \tag{3}$$

If no information on product tonnages is available, which is quite common for new products, the fractional dollar output could be used instead.

$$\text{Process-function V-factor (with fractional dollar outputs)} = \left(\frac{\text{Cost of product}}{\text{Cost of reactant}}\right) \times \left(\text{Fractional yield}\right) \times \left(\frac{1}{\text{Manufacturing costs}}\right) \times \left(\text{Fractional dollar output of sector}\right) \tag{4}$$

Either form of the process-function V-factor can be used to assess competing processes that have the same inputs and products but incur vastly different separation costs. More generally, the process-function V-factor can also be used as a first step to compare processes with similar products and processes with similar inputs. In order to illustrate the utility of the V-factors, let us compare the conversion of glucose to 5-hydroxymethylfurfural (HMF) using a heterogeneous catalyst and the production of limonene from glucose via fermentation (Table 3). HMF is an important platform chemical that is produced from a variety of renewable feedstocks at relatively modest scales and has been suggested to be used in the replacement of plastic bottle containers for soda pop (Xue et al 2016, Yadav et al. 2004). Limonene, on the other hand, is produced industrially via extraction from the peels of citrus fruits (Pourbafrani et al. 2010). Although the annual tonnages of HMF and limonene vary merely by about an order of magnitude, the former is a bulk chemical whereas the latter is a speciality chemical whose price and quality fluctuates seasonally. These fluctuations have forced manufacturers of limonene to pursue other alternatives, one of which is microbial fermentation. Although the microbial synthesis of limonene is not cost-competitive at the moment, it is expected to rival and eventually supplant the current mode of manufacture by riding the wave of synthetic biology (Jongedijk et al. 2016). It should be noted that the tonnage and cost for limonene reported in Table 3 refer to its production using the current, extraction-based route, whereas the fractional yield is the highest reported value for microbial fermentation.

Accordingly, equation 2 is used to calculate the V-factors for the conversion of glucose to HMF (V_1) and production of limonene from glucose (V_2) as follows:

$$V_1 = \frac{3.5}{0.5} \times 0.7 \times 0.3 = 1.47 \tag{5}$$

$$V_2 = \frac{6.5}{0.5} \times 0.06 \times 0.2 = 0.16 \tag{6}$$

The corresponding process-function V-factors for the conversion of glucose to HMF and production of limonene from glucose are estimated using equation 3 to be:

$$\text{Process-function } V_1 = \frac{3.5}{0.5} \times 0.7 \times \frac{1}{1.5} \times \frac{9\times10^5}{10^5} = 29 \tag{7}$$

$$\text{Process-function } V_2 = \frac{6.5}{0.5} \times 0.06 \times \frac{1}{2.15} \times \frac{5\times10^4}{10^3} = 18 \tag{8}$$

Table 3: Conversion of glucose to HMF and limonene.

Process	Product	Cost of reactant ($/kg)	Cost of product ($/kg)	Fractional yield	Product tonnage (MT)	Fractional dollar output	Sector tonnage (MT)	Manufacturing costs ($/kg)
1	HMF	0.5	3.5	0.7 (Xue et al. 2016)	9×10^5 (Factor & Equilibrium Research Report 2017)	0.3	10^5	1.5 (van Putten et al. 2013)
2	Limonene	0.5	6.5	0.06 (Alonso-Gutierrez et al. 2013)	5×10^4 (Global Market Insights 2016)	0.2	10^3	2.15 (Jongedijk et al. 2016)

Likewise, if we use fractional dollar outputs (equation 4) instead, the process-function V-factors for the two processes are estimated to be:

$$\text{Process-function } V_{1,\,\text{FDO}} = \frac{3.5}{0.5} \times 0.7 \times \frac{1}{1.5} \times 0.3 = 0.98 \quad (9)$$

$$\text{Process-function } V_{2,\,\text{FDO}} = \frac{6.5}{0.5} \times 0.06 \times \frac{1}{2.15} \times 0.2 = 0.07 \quad (10)$$

All forms of the V-factor provide the same inference for the previous example, namely that it is more profitable to convert glucose to HMF rather than limonene using currently available technologies. The conversions of glucose to HMF and limonene could not be more dissimilar from a logistical perspective; yet, all forms of the V-factor correctly predict their comparative profitability. The predictive capability of the V-factors is even better for more realistic comparisons that process developers usually make. However, we would like to stress that since the V-factor is a comparative metric, it is imperative to make similar assumptions and use the same form of the V-factor for the processes being compared.

5 Use of the V-factors in Decision-making

It is apparent that for the multiple products and/or substrates case, the V-factor mirrors the crack spread (Canadian Fuels Association 2013, Murat & Tokat 2009) in oil refining, which is defined as the difference between the price of crude oil and the price of all products that are produced from it. The profitability of oil companies is intricately linked to their crack spread – the wider the spread, the more profitable they are, and, oil companies dynamically alter their product spectra in response to market conditions in order to widen their crack spreads. However, unlike the crack spread, which aids to focus operational strategy, the V-factor can also be utilized to focus research strategies, as is illustrated by the examples of HMF and limonene. If the selling prices for a particular product in two competing market domains were comparable, the domain with the higher fractional dollar output would be the logical choice. Although it appears that the net difference between the fractional dollar outputs of individual sectors is small, their impact on the V-factors is sizable. For instance, the fractional dollar output for the petrochemical sector is 1.5 times higher than that of the pharmaceutical sector. Like the crack spread, the V-factor also clearly identifies levers for maximizing profits.

The impending implementation of a carbon pricing and taxation scheme across much of the industrialized world (World Bank et al. 2017) has prompted aggressive investments in carbon capture, sequestration and conversion technologies, an example of which is industrialized photosynthesis using genetically engineered microorganisms (Sarkar & Shimizu 2015). Several new ventures are commercializing the manufacture of alcohols in this manner. While the first generation of these companies targeted production of alcohols as biofuels, current operators are producing and marketing alcohols as high-grade, mid-commodity chemicals rather than biofuels. For instance, the wholesale price of pharmaceutical-grade ethanol is roughly three times that of fuel-grade ethanol (S&P Global Platt's 2015a, 2015b); and the ratio of the V-factors for manufacturing pharmaceutical- (V_3) and fuel-grade ethanol (V_4) from carbon dioxide is:

$$\frac{V_3}{V_4} = \left(\frac{\text{wholesale price of pharmaceutical-grade ethanol}}{\text{wholesale price of fuel-grade ethanol}}\right) \times \left(\frac{0.2}{0.3}\right) = 2 \quad (11)$$

Since distillation and downstream processing account for a very small fraction of the costs pharmaceutical- and fuel-grade ethanol (McAloon et al. 2000), manufacturers should choose to compete in the former domain. Additionally, since product pricing is heavily influenced by regional factors that control demand and supply, as well as availability of resources, the V-factor for a process will change from region to region (Figure 2). For each case that has been analyzed, the fractional yield is assumed to be constant. However, the V-factors vary since the values of the reactants and products vary from region to region owing to the unique market conditions that exist therein. For instance, it is more profitable to generate electricity via the combustion of wood pellets in Europe than in India even though pellets cost more in Europe.

Likewise, methanol production in the United States is amongst the most profitable in the world. Methanol is efficiently produced from natural gas via steam reforming or by direct partial oxidation of methane. The United States boasts of some of the largest deposits of shale gas

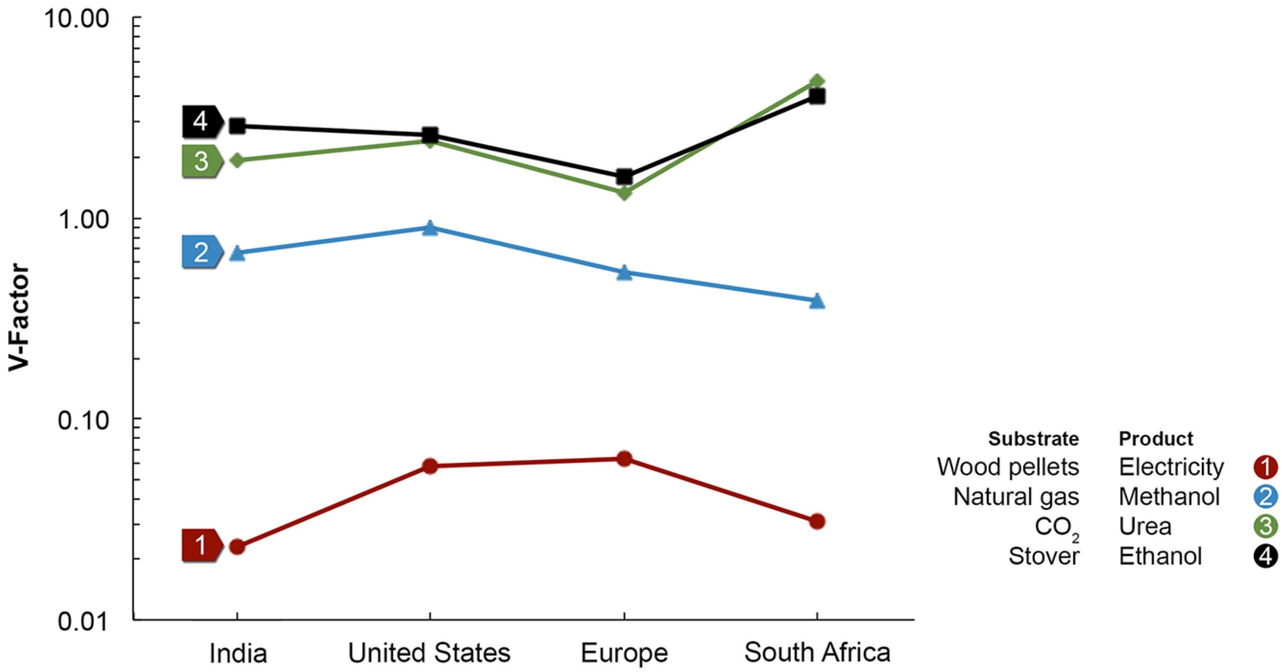

Figure 2. The V-factor for a manufacturing process varies with geography. For each process, the fractional yield is usually constant with respect to location. However, the values of the reactants and/or products vary from region to region since pricing is heavily influenced by regional factors that control demand and supply. The raw data employed for the calculation of the V-factors is presented in Table S3 in the appendix.

in the world, and the cost of natural gas is quite low on account of the country's surplus production and supply of shale gas. Similarly, the V-factor for urea production is the highest in South Africa due to cheaper availability of carbon dioxide from coal; and converting stover to ethanol is more profitable in developing economies due to cheaper collection costs for biomass.

Since the V-factor depends on demand-supply dynamics, it is also a function of time. This means that, like money, the V-factor too can be extrapolated with respect to time, which allows the user to make temporal projections about the profitability of the process. This attribute of the V-factor aids the user to make informed decisions that are more robust to market trends. Finally, the E- and V-factors for the manufacture of a selective list of compounds, including those on the highly publicized Department of Energy's list of top 12 chemicals (Werpy & Petersen 2004) that can be procured from biomass are plotted in Figure 3.

The high oxygen content of biomass and its distinct chemical bonding patterns make it recalcitrant to most of the thermochemical transformations that are commonly employed in biorefining. As a consequence, desirable biomass valorization necessitates use of specially tailored catalysts and novel chemistries (Rinaldi 2014, Rinaldi et al. 2016), neither of which have been developed to a satisfactory standard, as well as significant quantities of reagents, which greatly lowers the atom economy of biorefining. Expectedly, processes for the production of the top 12 chemicals exhibit mid-level E-factors and have low V-factors. Such a co-evaluation of E- and V-factors provides a clearer understanding of the triple bottom line and prioritizes R&D to transition the process to exhibit low E-factors and high V-factors.

6 Conclusions

In conclusion, the V-factors enable users, especially academic users, to critically assess the productive use of resources and thereafter formulate informed and focussed research strategies. These metrics are particularly useful for evaluating manufacturing processes that valorize biomass, a hugely important domain of the emerging bioeconomy. Estimating the profitability of

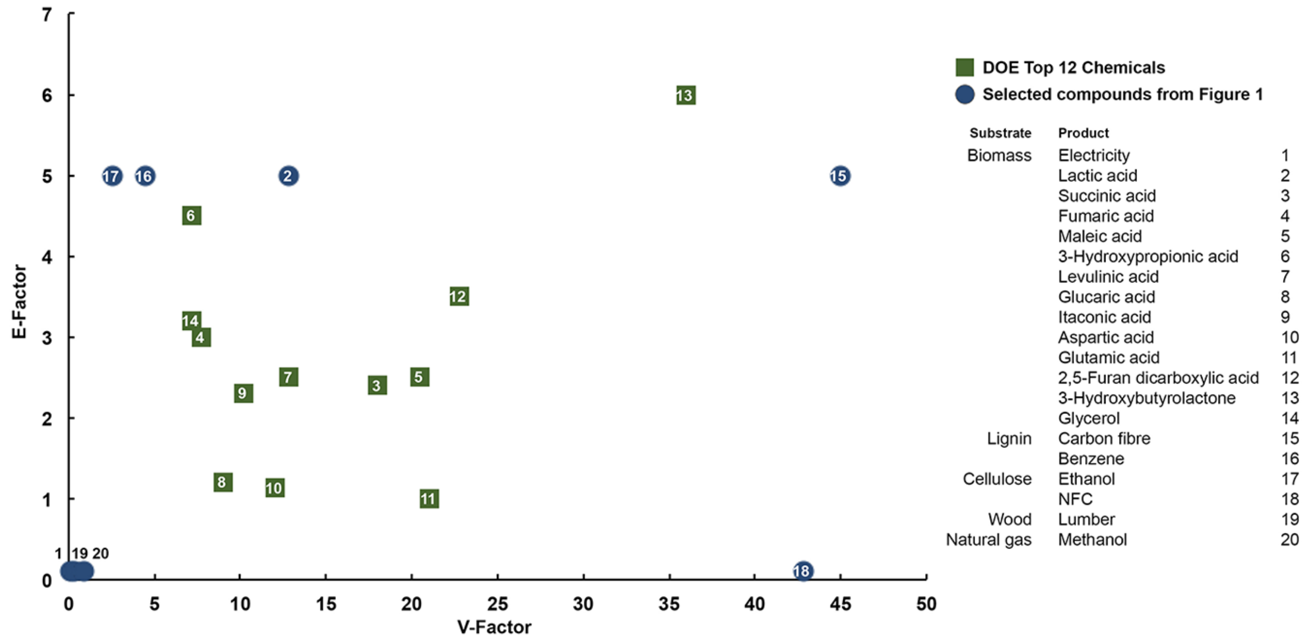

Figure 3. E- and V-factors of selected products. Processes for the production of the Department of Energy's top 12 value-added chemicals from biomass exhibit moderate E-factors and low V-factors. This insight establishes a roadmap for technology development to improve fractional yields in order to further lower E-factors and increase V-factors. Switchgrass is the starting material for all products with the exception of electricity, which is generated from wood pellets. The raw data employed for the calculation of the E- and V-factors is presented in Table S4 in the appendix.

manufacturing processes using conventional methodologies requires elaborate market analyses, which may not be feasible for academic researchers to conduct. The V-factors fill a clear gap for such users and allows them to judiciously direct their research efforts. Moreover, a co-assessment of the E- and any one of the four V-factors presented herein provides a roadmap for technology development that could simultaneously reduce the environmental footprint and improve profitability of chemical manufacturing.

Nomenclature

CapEx:	Capital expenditures ($/kg)
OpEx:	Operating expenditures ($/kg)
MT:	Metric ton
HMF:	Hydroxymethylfurfural
V_1:	V factor for conversion of glucose to HMF
V_2:	V factor for conversion of glucose to limonene
Process-function V_1:	Process-function V-factor for conversion of glucose to HMF
Process-function V_2:	Process-function V-factor for conversion of glucose to limonene
Process-function $V_{1,\ FDO}$:	Process function V-factor for conversion of glucose to HMF using fractional dollar output
Process-function $V_{2,\ FDO}$:	Process function V-factor for conversion of glucose to limonene using fractional dollar output
V_3:	V-factor for manufacturing pharmaceutical grade ethanol from carbon dioxide
V_4:	V-factor for manufacturing fuel grade ethanol from carbon dioxide

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Appendix

Table S1: Green chemistry metrics.

Metric	Formula	Ref.
Atom economy (A + B → C)	$= \frac{\text{MW of C}}{\text{MW of A + MW of B}} \times 100$	1
E-factor	$= \frac{\text{kg waste}}{\text{kg product}}$	2, 3
Effective mass yield (%)	$= \frac{\text{mass of product}}{\text{mass of non-benign reagents}} \times 100$	4
Atom utilization (%)	$= \frac{\text{mass of desired product}}{\text{total mass of all products}}$	5
Carbon efficiency (%)	$= \frac{\text{amount of carbon in product}}{\text{total carbon present in reactions}} \times 100$	6
Mass intensity	$= \frac{\text{total mass involved in a process or step (kg)}}{\text{mass of product (kg)}}$	6
Reaction mass efficiency (A + B → C)	$= \frac{\text{mass of product C}}{\text{mass of A + mass of B}} \times 100$	7
EcoScale	$= 100 - \sum \text{individual penalties}$ (unifies several green chemistry metrics and works on a penalty system)	8
Green Aspiration Level (GAL)	= tGAL × complexity where, $\text{tGAL} = \frac{\text{E-factor}}{\text{average complexity}}$ complexity = (% ideality) × (total # of reactions) $\text{\% ideality} = \frac{\text{(\# of construction reactions) + (\# of redox reactions)}}{\text{total \# of reactions}}$	9

Table S2. **V-Factors for the manufacture of selected products using the conversion platform with highest reported fractional yield.**

Process	Value of reactant (USD/kg)	Value of product (USD/kg)	Transformation efficiency	Fractional dollar output	V-factor	Ref.
Switchgrass to 1,3-propanediol	0.035	22	0.3	0.3	56.57	10
Switchgrass to 2-methyltetrahydrofuran	0.035	20	0.3	0.3	51.43	11
Switchgrass to 3-hydroxybutyrolactone	0.035	6	0.7	0.3	36	12
Switchgrass to 1,4-pentanediol	0.035	12	0.3	0.3	30.86	13
Switchgrass to 2,5-furan dicarboxylic acid	0.035	3.8	0.7	0.3	22.8	14
Switchgrass to hydroxymethylfurfural	0.035	3.5	0.7	0.3	21	15
Switchgrass to glutamic acid	0.035	3.5	0.7	0.3	21	16
Switchgrass to maleic acid	0.035	4	0.6	0.3	20.57	17
Switchgrass to ethyl levulinate	0.035	3	0.75	0.3	19.29	18
Switchgrass to succinic acid	0.035	3.5	0.6	0.3	18	19
Switchgrass to γ-valerolactone	0.035	2.5	0.8	0.3	17.14	11
Switchgrass to levulinic acid	0.035	2.5	0.8	0.3	12.86	20,21
Switchgrass to lactic acid	0.035	3.2	0.7	0.2	12.8	17
Switchgrass to aspartic acid	0.035	2	0.7	0.3	12	17
Switchgrass to itaconic acid	0.035	1.7	0.7	0.3	10.2	22
Switchgrass to glucaric acid	0.035	1.5	0.7	0.3	9	23
Switchgrass to tetrahydrofuran	0.035	1.4	0.7	0.3	8.4	24
Switch grass to fumaric acid	0.035	1.5	0.6	0.3	7.71	25
Switchgrass to adipic acid	0.035	1.1	0.8	0.3	7.54	26
Switchgrass to 3-hydroxypropionic acid	0.035	1.4	0.6	0.3	7.2	27
Switchgrass to glycerol	0.035	1.2	0.7	0.3	7.2	17
Switchgrass to sorbitol	0.035	0.65	0.7	0.3	3.9	28
Switchgrass to furfural	0.035	0.4	0.7	0.3	2.4	24
Lignin to carbon fibre	0.03	25	0.5	0.2	83.33	29
Lignin to carbon aerogel	0.03	35	0.2	0.2	46.67	30
Lignin to vanillin	0.03	15	0.1	0.2	10	31
Lignin to cinnamaldehyde	0.03	8.5	0.15	0.2	8.5	32
Lignin to xylene	0.03	0.8	0.6	0.3	4.8	33
Lignin to benzene	0.03	0.75	0.6	0.3	4.5	33
Lignin to toluene	0.03	0.7	0.6	0.3	4.2	33
Lignin to styrene	0.03	0.2	0.8	0.1	0.53	34
Cellulose to nanofibrillated cellulose	0.035	25	0.6	0.1	42.86	35
Cellulose to microcrystalline cellulose	0.035	4	0.8	0.2	18.29	36
Cellulose to glucose	0.035	0.5	0.8	0.3	3.43	37
Cellulose to ethanol	0.035	1	0.3	0.3	2.57	38
Cellulose to limonene	0.035	6.5	0.06	0.2	2.23	39
CO_2 to salicylic acid	0.02	4	0.4	0.3	24	40
CO_2 to acrylic acid	0.02	1.5	0.5	0.2	7.5	40
CO_2 to formic acid	0.02	0.5	0.6	0.3	4.5	40, 41
CO_2 to urea	0.02	0.2	0.8	0.3	2.4	40, 41
Rock phosphate to nitrophosphate fertilizer	0.08	3.75	0.8	0.3	11.25	42
Glucose to taxol	0.5	1000	0.02	0.2	8	43
Starch to glucose	0.1	0.5	0.8	0.3	1.2	44
Natural gas to methanol	0.15	0.5	0.9	0.3	0.9	45
Veneer to plywood	60	400	1	0.1	0.67	46
Wood to lumber*	100	300	1	0.1	0.3	46
Wood pellets to electricity	0.12	0.0923	0.25	0.3	0.058	47

**Value of reactants and products in USD/thousand board feet.*

Table S3. Variation of V-factor with geographical location (Ref.: 47, 48-53).

Wood pellets to electricity

Region	Value of reactant (USD/kg)	Value of product (USD/kg equivalent)	Transformation efficiency	Fractional dollar output	V-factor
India	0.2	0.0615	0.25	0.3	0.023
US	0.12	0.0923	0.25	0.3	0.058
Europe	0.22	0.185	0.25	0.3	0.063
South Africa	0.15	0.0615	0.25	0.3	0.03

Assumptions for estimation of the V-factor for conversion of wood pellets to electricity:
Electricity costs for India, US, Europe & South Africa are 0.08, 0.12, 0.24 and 0.08 USD/kWh, respectively
1.3 kg of biomass is required to generate 1 kWh electricity

Natural gas to methanol

Region	Value of reactant (USD/kg)	Value of product (USD/kg equivalent)	Transformation efficiency	Fractional dollar output	V-factor
India	0.2	0.5	0.9	0.3	0.675
US	0.15	0.5	0.9	0.3	0.9
Europe	0.25	0.5	0.9	0.3	0.54
South Africa	0.35	0.5	0.9	0.3	0.39

Assumptions for estimation of the V-factor for conversion of natural gas to methanol:
Cost of natural gas in India, US, Europe & South Africa is 3.9, 2.9, 4.95 and 6.9 USD/MMBtu, respectively
1 MMBtu is equivalent to 28.33 m^3 of natural gas
Density of natural gas at STP is 0.7 kg/m^3

CO_2 to urea

Region	Value of reactant (USD/kg)	Value of product (USD/kg equivalent)	Transformation efficiency	Fractional dollar output	V-factor
India	0.025	0.2	0.8	0.3	1.92
US	0.02	0.2	0.8	0.3	2.4
Europe	0.036	0.2	0.8	0.3	1.33
South Africa	0.01	0.2	0.8	0.3	4.8

Stover to ethanol

Region	Value of reactant (USD/kg)	Value of product (USD/kg equivalent)	Transformation efficiency	Fractional dollar output	V-factor
India	0.025	0.8	0.3	0.3	2.88
US	0.035	1	0.3	0.3	2.57
Europe	0.045	0.8	0.3	0.3	1.6
South Africa	0.02	0.9	0.3	0.3	4.05

Assumptions for estimation of the V-factor for conversion of stover to ethanol:
Theoretical transformation efficiency is assumed

Table S4: **E- and V-factors values of selected products depicted in Figure 3 (Ref.: 48-53).**

#	Process	Value of reactant (USD/kg)	Value of product (USD/kg)	Transformation efficiency	Fractional dollar output	V-factor	E-factor
1	Wood pellets to electricity	0.12	0.0923	0.25	0.3	0.058	0.1
2	Switchgrass to lactic acid	0.035	3.2	0.7	0.2	12.8	5
3	Switchgrass to succinic acid	0.035	3.5	0.6	0.3	18	2.4
4	Switchgrass to fumaric acid	0.035	1.5	0.6	0.3	7.71	3
5	Switchgrass to maleic acid	0.035	4	0.6	0.3	20.57	2.5
6	Switchgrass to 3-hydroxypropionic acid	0.035	1.4	0.6	0.3	7.2	4.5
7	Switchgrass to levulinic acid	0.035	2.5	0.6	0.3	12.86	2.5
8	Switchgrass to glucaric acid	0.035	1.5	0.7	0.3	9	1.2
9	Switchgrass to itaconic acid	0.035	1.7	0.7	0.3	10.2	2.3
10	Switchgrass to aspartic acid	0.035	2	0.7	0.3	12	1.13
11	Switchgrass to glutamic acid	0.035	3.5	0.7	0.3	21	1
12	Switchgrass to 2,5-furan dicarboxylic acid	0.035	3.8	0.7	0.3	22.8	3.5
13	Switchgrass to 3-hydroxybutyrolactone	0.035	6	0.7	0.3	36	6
14	Switchgrass to glycerol	0.035	1.2	0.7	0.3	7.2	3.2
15	Lignin to carbon fibre	0.03	25	0.5	0.2	83.33	5
16	Lignin to benzene	0.03	0.75	0.6	0.3	4.5	5
17	Cellulose to ethanol	0.035	1	0.3	0.3	2.57	5
18	Cellulose to nanofibrillated cellulose	0.035	25	0.6	0.1	42.86	0.1
19	Wood to lumber*	100	300	1	0.1	0.3	0.1
20	Natural gas to methanol	0.15	0.5	0.9	0.3	0.9	0.1

*Value of reactants and products in USD/thousand board feet

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