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Journal article | **Accepted manuscript (Postprint)**

This version is available at <https://doi.org/10.14279/depositonce-11482>

Buchner, G. A., Zimmermann, A. W., Hohgräve, A. E., & Schomäcker, R. (2018). Techno-economic Assessment Framework for the Chemical Industry—Based on Technology Readiness Levels. *Industrial & Engineering Chemistry Research*, 57(25), 8502–8517. <https://doi.org/10.1021/acs.iecr.8b01248>

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A techno-economic assessment framework for the chemical industry – based on technology readiness levels

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Abstract

For profit-oriented stakeholders techno-economic assessment (TEA) is the most important basis for decisions about research, development and deployment (RD&D). Two key challenges are: Firstly, the rating of RD&D progress which is closely linked to data availability; and secondly, the selection of TEA methods that adequately fit the available data in order to achieve the best possible decision basis. Technology readiness levels (TRLs) are a popular concept for rating the maturity of RD&D according to available data. Since existing TRL scales remain unspecific to technologies, an understanding of TRL in the chemical industry is presented. TRLs are subsequently used in a framework for TEA. Cost estimation is structured (with focus on capital expenditure) and estimation methods are sorted by TRL. Appropriate profitability indicators for the assessment of economic prospects are discussed for each TRL. Static indicators are favored in earlier TRLs, while dynamic calculations are preferred for detailed forecasts later on.

1 Introduction

Well-founded project decisions in all stages of an innovation are crucial to the success of an economic entity engaging in research, development and deployment (RD&D) activities. Decision-makers at profit-oriented stakeholders rely heavily on sound techno-economic assessment (TEA). A choice of inadequate methods often leads to information that triggers unfavorable decisions which often turn out to be very expensive. Money is a scarce resource and has to be used with great care for only the most promising projects. Improving techno-economic assessment methodology will therefore improve RD&D project decisions.

In RD&D, the present (immature) technology delivers parameters that serve as a basis for the forecasting of economic prospects of a planned mature technology. In the chemical industry, these parameters vary considerably along technology maturation due to substantial changes in the nature of the present technology (*e.g.* equipment, mode of operation, feed logistics). For sound TEA, it becomes necessary to distinguish between stages of maturation and consider their consequences for TEA. For example, not all costs can be calculated at all stages: plant costs, which make up the largest share of capital expenditure (CapEx), can be a major part of a technology's cost, however, it is inadequate to include plant costs in early research TEAs when process concepts are not yet available. It therefore becomes crucial to find the point in technology maturation from which then onwards enough data are available for an inclusion of plant costs into the total cost estimate.

Currently the technology readiness levels (TRL) concept is commonly used to distinguish stages of RD&D¹ but presented scales are difficult to interpret for RD&D in the chemical industry. For example, a lot of scales include the word 'prototype'²⁻⁴ whose meaning as "a first full-scale and usually functional form of a new type or design of a construction"⁵ is easily understood in mechanical engineering but lacks a common interpretation in chemical industry

RD&D. As another example, testing a technology in different ‘environments’^{4,6} is not an intuitive idea for chemical plants due to their general immobility. Thus, as a first key challenge, rating RD&D progress in the chemical industry was identified: There is no commonly accepted way of how RD&D progress is monitored. There is a need for a framework that allows for the understanding of how advanced a project is. This framework should incorporate a consistent and comprehensive way of measuring the quality of data available and at the same time evaluate how these data help to understand the technology.

Selecting adequate methods poses a second key challenge for TEA in the chemical industry. In the estimation of cost, conceptual misunderstandings such as mistaking allocated CapEx with depreciation, counting either as operational expenditure (which sometimes leads to double counting of CapEx) or confusing profitability measures with cost ask for a framework relating all TEA components in order to guide practitioners through TEA and help to avoid incorrect calculations. For the case of TEA for CO₂ utilization technologies, a literature review revealed the lack of standardization of economic indicators in early to mid TRL.⁷ In CapEx estimation an example of a commonly encountered problem is assuming technical equipment specifications (‘forced detail’) in order to allow for equipment cost-based cost estimation. Such assumptions often do not depict the actual development and can force into certain, potentially unfavorable, pathways for future development. The choice of methods and indicators is particularly difficult for capital cost estimation and investment appraisal techniques (represented by profitability indicators) because for both fields a variety of methods exists and most methods do not easily reveal when they are suitable to apply. Methods should optimally exploit the existing data in order to lead to the best possible decision basis.

Therefore, a framework for TEA in RD&D projects is presented in this paper. In the first chapter, TEA in the chemical industry is described: After providing a structure, contents and general remarks on TEA, characteristics of TEA in the progress of RD&D are described. An understanding of maturity rating and technology readiness levels (TRL) in the chemical industry is presented and serves as a framework for data availability based sorting of methods. Cost estimation is a major part of every TEA and is therefore described in detail in a second chapter: After general considerations, cost estimation is broken down into major blocks that are separated by methodology. Recommendations for operational expenditure depending on TRL are given in the following; for the commonly used factored estimation of indirect operational expenditure items factors are compiled. This framework then focusses on in-depth analysis of capital expenditure estimation by explaining a detailed structure of capital expenditure and sorting estimation methods into the TRL framework according to how their inputs correspond with TRL descriptions, resulting in a table for sound method selection along the RD&D progress. Following cost estimation, recommendations for an approach on market analysis are given in a subsequent chapter. Finally, adequate profitability indicators are provided for each TRL.

2 Techno-economic assessment methodology in the chemical industry

2.1 What is techno-economic assessment? Structure and contents

The question whether or not a technology should be invested in is answered depending on its assessment. An assessment is defined as “making a judgement about something”⁸, a judgement is defined as “process of forming an opinion or evaluation”⁹, an evaluation is defined as “determination of the value [...] or quality of something [...]”¹⁰. As for the scope of this framework, it is concluded that assessment means assigning a positive or negative value to a certain criterion. A criterion reflects the meaning of one or multiple indicators. Indicators are measurable states that help answering whether or not criteria are met.¹¹ In conclusion, fields of

assessment contain criteria that can be referred to as positive or negative. Important assessment fields are economic viability, ecologic sustainability or social acceptance^{12,13}; examples of important indicators in the chemical industry are profitability indicators (economic viability), global warming impact (ecologic sustainability) or combinations like CO₂ abatement cost¹⁴.

For profit-oriented stakeholders technical criteria can not be assigned positive or negative meanings: A technical criterion to be met can for example be whether a ‘reaction is fast’ (reaction speed, quantitative or qualitative). The reaction rate is a suitable indicator for this criterion: A reaction rate that is perceived as high or meets a given target value answers positively to the criterion. The criterion that is therefore met indicates high space-time-yield but at the same time can come along with downsides such as demanding construction material or complex installations for heat removal. As a consequence, a certain reaction speed taken for its own does not have any value. It can though be used as parameter in the calculation of indicators that are associated with criteria that are suitable for assessment.

While feasibility is a knock-out criterion if understood as purely technical criterion, it cannot positively decide whether a technology should be implemented or not and is therefore no genuine assessment field. Some technical indicators, such as energy efficiency, can though give valuable hints for the cost decreasing potential that may be exploited in future development, but still can not definitely attest economic viability. Hence, the ‘T’ in ‘TEA’ solely refers to the fact that the economic assessment is done for a technology and is based on data collected from it. Differences between technologies only appear in technical indicators that do not directly affect profitability calculation. For the purpose of this framework, TEA methodology is therefore unspecific to single technologies or technology fields, such as biotechnology or electrochemistry, and should therefore not differentiate between those.

In general, TEA follows the same logic that is applied for life-cycle assessment (LCA) as described in ISO standards 14040/14044:^{15,16} goal and scope definition (I), life-cycle inventory analysis (II), life-cycle impact assessment (III), interpretation phase (IV). While this is a good description for every assessment with regard to methodology, the specific contents need to be detailed for different assessment types. For TEA, at first the technology is rated in TRLs (1) in order to understand the maturity of the current RD&D and the depth of knowledge gained. Then goal, scope and scenario definition (2) of the TEA is required. The goal defines the aim and purpose of the TEA; it reflects on the reason for the TEA and states the decision that is prepared with it. Scope and scenario definition includes the subquestions a TEA has to answer, resources available for the subsequent work as well as the setting in which an investment is carried out and system boundaries of the assessment. Since scope and scenario restrictions affect the calculation both directly, for example by adding time effects, and indirectly by influencing the analysis of process and market parameters, they have to be defined at the beginning of a TEA. Steps 1 and 2 form the general goal and scope of the TEA (I). Parameters defined in step 2 must be aligned with other assessments (A) in order to ensure that all assessments can be combined in a single decision (B) later.

The RCOV framework by Demil and Lecocq draws the main components of business models.¹⁷ It distinguishes between the “volume and structure of revenues” on the one hand and the “volume and structure of costs” on the other hand as content that is to be combined in order to result in a “margin”.¹⁷ As the framework presented here is about assessing economic activities, the basic thoughts of a business model as a formalized realization of economic activities can be translated: For this framework, the activities that are carried out in order to obtain volume and

structure of revenues or costs are parts of the TEA. The volume and structure of revenues is called ‘market analysis’ whereas the volume and structure of costs is called ‘cost estimation’.

Cost estimation (3) and market analysis (4) are carried out based on the given scope and scenario. They return intermediate results that are inputs to the economic impact calculation called ‘profitability analysis’. Thus, cost estimation and market analysis can be seen as inventory (II) of the TEA. Cost estimation and market analysis may each be divided into the same steps (I-IV) as the total TEA. The phases of cost estimation are described as follows: Cost estimation methods are selected in the goal and scope step of the cost estimation (3.I) which depends heavily on the general goal and scope of the TEA and on the availability of data, which was analyzed with the TRL concept. The input data needed for the cost estimation method(s) selected are collected in the cost inventory (3.II) and processed to effective cost (3.III, cost impact). Cost estimation can only directly be followed by an interpretation (3.IV) if used as an instrument for the comparison of process options that do not have different market implications. As market analysis is not the focus of this work, it is only touched upon briefly in a later chapter. Aligning market analysis methodology with LCA phases is left to future research. Market analysis and cost estimation are carried out in parallel since they are equal inputs to the next step and related in both directions: Material costs are derived from market analysis and cost ranges often help understanding the target market as price is a dimension of market segmentation¹⁸.

Economic impacts result from the combination of parameters arising from the evaluation of processes in which a product is produced (especially production cost) and markets where the product is sold (especially selling price, sales volume).^{19,20} In the profitability analysis (5) the actual calculation of economic impact is carried out by relating revenue to cost (*cf.*¹⁷) in profitability indicators. Additionally, there are economic factors that are difficult to translate into

monetary terms (*e.g.* availability of qualified personnel²¹) and therefore left to qualitative evaluation which is not in the scope of this contribution.

The value of a profitability indicator is then discussed in the interpretation phase (6). Interpretation includes the evaluation of impact results and discusses the TEA approach; however, it does not include active RD&D choices, but together with results from other assessments (A) serves as basis for decisions about RD&D continuation. The evaluation of risk is part of the interpretation phase as it discusses the chances of impacts not being realized. The project decision step (B) must also include recommendations and directions for further RD&D (C) to be subsequently carried out. The RD&D results give feedback whether or not a concept is technically feasible (D) and potentially lead to redefinition of recommendations or stopping RD&D. At this point, technical feasibility does not include any economic considerations, but only checks whether an RD&D pathway is scientifically possible. The progress of RD&D is monitored in TRLs (1).

The described assessment procedure is not performed at fixed dates or stages in RD&D but should rather be seen as an ongoing and iterative process.²² The proposed structure of TEA in the chemical industry is shown in Scheme 1 (numbers 1-6, related activities A-D).

In order to ensure that TEA and LCA can be weighted in a decision, they should feature the same assessment goal and scope. Substantial overlaps of both assessments can primarily be found in their inventories: Commonly, at least mass and energy balances are required for both assessments. Following the analysis of data availability by TRL rating, a joint collecting of inventory data can be carried out. In the following phase (III), these data are ‘tagged’ with potentials such as cost (TEA) or global warming potential (LCA) in order to yield the respective impacts. This approach helps providing the same depth of analysis, exploiting synergies and thus

leading to a common ground for following decisions. A shared scope and calculation basis is especially important when calculating composite assessment indicators such as CO₂ abatement cost. Recommendations for additional synergies, combined indicators or approaches on challenges arising such as differences in system boundaries or cut-off criteria are left to future research.

Scheme 1. Structure of techno-economic assessment (1-6, dotted line box), and associated activities (A-D), phases analog to LCA:^{15,16} I – goal and scope, II – inventory, III – impact, IV – interpretation

In LCA, interpretation is a specific step in the assessment that is conducted after the life-cycle impact assessment step, but at the same time also a description of interim quality control that practitioners apply in every phase of their work and which allows for the correction of approaches in all phases.²³ For TEA, it is suggested to complete all phases of assessment and decide upon major methodological changes reflecting the results of the TEA in order to avoid the danger of the result of an altered TEA not being suitable to answer the initial question(s). Changes are included in the goal and scope definition of the next TEA iteration.

2.2 TEA in research, development and deployment (RD&D)

This framework addresses projects within phases of research, development and deployment. In this framework, ‘research’ excludes basic research which is not target-oriented as it focusses on understanding natural phenomena²⁴; as for the scope of this framework, ‘research’ is limited to applied research which focusses on altering understood natural phenomena in order to achieve a certain outcome (*cf.* ²⁵). The term ‘development’ describes the conversion of research into ‘the creation of new and/or improved products and processes’²⁵. Applied research and development are subsumed under the abbreviation ‘R&D’. Bringing a developed technology into effective action in an environment with tangible result is called ‘deployment’ in this work (*cf.* ²⁶) and here is together with applied R&D abbreviated as ‘RD&D’.

Assessment in RD&D deals with the evaluation of economic activity that will be conducted in the future and is therefore – in contrast to evaluating past activities – naturally afflicted with uncertainty.²⁷ In the course of an RD&D process the availability of data increases, allowing for the choice of methods that consider more data and inversely reduce uncertainty. In order to minimize risk, maintain competitiveness and reduce RD&D cycle times, it is crucial to select methods that best utilize available data.²⁸ This especially holds true for RD&D projects in the chemical industry where sound and early decisions about project stop or reorientation are

necessary in order to save large amounts of money. The RD&D cost as well as cost for later correction of infeasible or disadvantageous (compared to potential alternatives) RD&D increase by one order of magnitude for each RD&D phase with larger equipment.²⁹

Capital cost estimation frameworks are known from plant engineering and rely on engineering progress (defined as percentage of deliverables completed) or estimation purpose in gated projects.^{30–35} Using adequate methods in the assessment is difficult: The estimation purpose often does not fit the available data; one classic example is the expectation of detailed estimates in early R&D. Practitioners lacking knowledge about suitable methods is a common problem. This bears risks in two directions: Overly complex and time-consuming methods often lead to forcing assumptions that narrow the path for future development, whereas too simple methods that do not consider all known relevant data lead to lack of information. Cost estimation is an example of major importance for strong dependence of economic assessment on innovation progress.^{36–38} The overall availability of data for the process side is best described by technology readiness levels (TRLs), making TRL rating a crucial part of TEA.

2.3 Technology readiness levels (TRLs)

Technology readiness levels are a popular concept for the analysis of technological maturity of research and development projects in academia, industry and government.⁴ Technology readiness is commonly rated in nine levels, covering all innovation stages from the initial idea to a fully working technology. TRLs were first defined by NASA for the analysis and comparison of various fields of technology and science that are integrated for space exploration, including mechanical, electrical and chemical engineering as well as aviation or medicine.² Enabling the comparison of various disciplines at the same time is only possible with criteria that remain unspecific to technologies. TRL ratings based on such criteria are prone to vagueness, misinterpretation and even purposely misleading. For a variety of sectors specific TRL criteria

were therefore defined, for example for energy and defense systems,^{6,39} biomanufacturing⁴⁰ or the steel industry⁴¹. TRL scales that are also popular in the evaluation of projects in the chemical industry are presented by NASA,^{2,3} the US Department of Energy⁶ or the European Commission in the Horizon 2020 programme⁴. A report of the European association of research and technology organizations (EARTO) identified the need for the specification of TRLs for the chemical industry.¹

The scale should intrinsically depict the level of information available about the technology. However, beginning and end of technical progress and maturation cannot be determined objectively. Thus, beginning and end of the scale have to be defined according to other criteria. Criteria that define beginning and end of a scale according to a specific purpose that the RD&D has to fulfill are suitable. In case of the original NASA scale, a mature technology is at hand if it proves to be working in a space mission. For profit-oriented stakeholders technological maturity rating commences as soon as target-oriented research ideas arise of how basic research can be exploited on the market. In accordance, a technology is seen as mature as soon as it is running in an economically relevant environment and performing economically sustainable market-related activities. Titles, descriptions, tangible work results and typical workplaces for nine TRLs in the chemical industry are suggested in Table 1 (*cf.* ^{7,42}). More detailed qualitative and quantitative criteria still need intensive research and are therefore left to future publications. The presented TRLs are distinguished by the level of information that is characteristic for steps that are passed in typical RD&D projects in the chemical industry. Basic research is conducted before the TRL scale begins. Applied research is then conducted from TRL 1 up to TRL 4. There is no clear line that separates research and development in terms of TRL as information of both categories is needed in order to advance technological maturity in preliminary process development. While

only rough process concepts are at hand at TRL 3, systematic development starts with TRL 4. TRLs 8 and 9 are seen as deployment stages because the technology is actively brought into effect in the economic environment. However, during plant commissioning at TRL 8 there are often still substantial advances in knowledge. For this reason, TRL 8 also holds characteristics of a development phase. Sorting cost estimation methods in the TRL scale provides guidance for the selection of adequate methods and ensures maximal exploitation of available data in all RD&D stages.

Table 1. TRL titles, descriptions, tangible work results and workplaces for the chemical industry

TRL	1	2	3	4	5	6	7	8	9
Title	Idea	Concept formulated	Proof of Concept	Preliminary Process Development	Detail Process Development	Pilot Trials	Final Engineering	Commissioning	Production
Description	Opportunities identified, basic research translated into possible applications (<i>e.g.</i> by brainstorming, literature study)	Technology concept and/or application formulated, patent research conducted	Applied laboratory research started, functional principle / reaction (mechanism) proven, predicted reaction observed (qualitatively)	Concept validated in laboratory environment, scale-up preparation started, conceptual process design (<i>e.g.</i> based on simulation with simple models)	Shortcut process models found, simple property data analyzed, detailed simulation of process and pilot plant using bench scale information	Pilot plant constructed and operated with low rate production, products tested in application	Parameter and performance of pilot plant optimized, (optional) demo plant constructed and operating, equipment specification including components that are type conferrable to full-scale production	Products and processes integrated in organizational structure (hardware and software), full-scale plant constructed, startup initiated	Full-scale plant audited (site acceptance test), turn-key plant, production operated over the full range of expected conditions in industrial scale and environment, performance guarantee enforceable
Tangible work result	Idea/rough concept/vision/strategy paper	Technology concept formulated, list of solutions, future R&D activities planned	Proof of concept (in laboratory)	Documentation of reproduced and predictable (quantitative) experiment results, first process ideas	Simple parameter and property data, process concept alternatives evaluated	Working pilot plant	Optimized pilot plant, (optional) working demo plant, sample production, finalized and qualified system and building plan	Finalized and qualified system and building plan	Full-scale plant tested and working
Workplace	Sheets of paper (physical or digital), whiteboard or similar	Sheets of paper (physical or digital), whiteboard or similar	Laboratory	Laboratory/miniplant	Laboratory/miniplant	Pilot plant, technical center	Pilot plant, technical centre, (optional) demo plant (potentially incorporated in production site)	Production site	Production site

Modifications to existing technologies result in new technologies. Modifications can thus be treated like overall new technologies and have to pass the same RD&D steps, from a first modification idea to a running modified system. However, as major aspects of the technology may already contain characteristics of later TRLs, technology modifications may more quickly pass earlier TRLs.

3 Cost estimation methodology in the chemical industry

3.1 General considerations about cost estimation

Two concepts of cost estimation methodology have been proposed in the evaluation of early project stages: shortcut and full-scope. Both approaches usually lead to valuable and corresponding decisions about R&D continuation; however, they deal with insecurity in different ways. In the following, ‘method error’ describes the inaccuracy that results from excluding cost items from the calculation while ‘indicator error’ depicts the inaccuracy of a value which results from its calculation with insecure parameters. Shortcut methods use simple calculations and neglect yet unknown cost items, leading to small indicator errors but large overall method error with respect to absolute estimates. Full-scope methods on the other hand try to estimate all cost items with the lowest possible error. The average error of indicators as well as the method itself decreases with increasing data availability (as shown in detail for capital expenditure estimation).

Assessment is carried out in comparison to a different solution (existing or also in RD&D) to the same problem. This object of comparison is called ‘benchmark’, defined as “something that serves as a standard by which others may be measured or judged”⁴³. In shortcut methods, the benchmark must be analyzed with the same cost items as the examined product(s) whereas full-scope relates to absolute benchmark data that are relevant to the respective market and are typically obtained from market analysis. In full-scope assessment, decisions depend strongly on the decider’s risk aversion (*i.e.* error allowance) whereas shortcut methods lead to sharp distinction by giving small error bars. In this work the focus lies on full-scope assessment from TRL 3 on in order to show the decreasing indicator error over TRL. The alternative approach of shortcut assessment and decreasing method error will be discussed in another contribution. TRLs 1 and 2 are excluded from full-scope because process concepts are yet to be drafted. In principle, in full-scope estimation all cost items have to be included; however, cost items that are

estimated not to have a major economic impact can be omitted in earlier TRLs (similar to a cut-off criterion in LCA). No exact guidance can be given here because characteristics differ a lot between technologies.

3.2 Cost structure

In order to analyze if a technology is economically viable, the total cost of producing and selling a product (cost of goods sold, COGS) have to be estimated. COGS are separated into manufacturing cost (cost of goods manufactured, COGM) and general expenses that cannot be allocated to a specific manufacturing operation.^{37,44,45} General expenses mainly include administration, marketing and sales (M&S) as well as general research^{37,44}; they are usually estimated as a share of COGM, COGS or sales price (*cf.* table for factors in the supporting information). COGM can be further divided by their spending date and frequency into initial investment cost, called ‘capital expenditure’ (CapEx) and cost spent for ongoing operation, called ‘operational expenditure’ (OpEx).^{37,45,46} It is important to include the CapEx when calculating COGM because the plant is necessary for the production of the product and can therefore be allocated to the product. For the representation of investments allocated to product cost some authors choose the word ‘depreciation’, which is not used here because it does not mean cost but depicts loss in value and is especially used as an allowance when calculating taxable earnings. Components of CapEx and methods for its estimation are discussed later in this chapter. Operational expenditure is commonly divided by the way it is allocated to the product into direct OpEx which is directly depending on the amount of product produced (also called “variable”^{46,47}) and indirect OpEx which is spent independent thereof (also called “general”⁴⁵). It is suggested to further split direct OpEx into material cost and cost for energy and utilities (E&U) in order to generate cost items that are separated by the methodology used for their estimation and the data they are based on.

Research and development (R&D) is divided into product and process R&D that is conducted before the production phase (general R&D) and R&D that is done in order to ensure ongoing operability (operating R&D). The first is considered general expense; the latter is allocated to the product and is part of indirect OpEx. It is here subsumed under operating intellectual property cost together with royalties and/or patents. These costs depict a special case and are shown separately (Scheme 2, dotted line) because they are usually recursively factorized to cost that they are part of.^{37,48–50} Depending on individual contracts, royalties can in some cases depend directly on the amount of product produced or sold. A complete structure of COGS is shown in Scheme 2.

Scheme 2. Structure of estimated cost of goods sold, double lined boxes: major cost of goods manufactured items, dashed line: operating intellectual property, often factored to superordinate items

3.3 Operational expenditure estimation and TRLs

Material cost are determined according to the mass balance. At TRL 1 the technology idea does not have to be translated into reaction schemes and resulting mass balance. At TRL 2 the mass balance is given by the stoichiometry of the reaction (comparable to the atom economy concept⁵¹). In laboratory to pilot stages (TRLs 3-6), the actual mass flows resulting from experiments are used, factors for process-specific waste or start-up losses of comparable technologies can be applied. In more advanced stages (TRLs 6-9), simulations can estimate more accurate values.

E&U cost are determined according to energy balance. At TRL 2, the reaction enthalpy can already be considered and priced with an average for the energy source mainly associated to the

reaction.⁵² At TRLs 3 and 4, this idea can be extended to additional unit operations with simple thermodynamic calculations (*e.g.* energy demand for evaporation *via* mass flow, heat capacity, vaporization enthalpy and temperature difference), optionally including correction factors for equipment efficiency. If energy costs are not expected to be a major part of the COGM, they can in earlier stages be roughly estimated with factors applied to material cost since energy from fossil resources and the major material feedstocks in the chemical industry are related. In later stages (TRLs 5-9) E&U cost are derived from the design of single equipment and process simulation. The demand for utilities can be neglected in early stages, factorized based on energy in mid stages (TRLs 3-5), since E&U are closely linked,^{36,53} and taken from simulation in later stages (TRLs 6-9).

All other, indirect OpEx (*e.g.* laboratory, overhead, maintenance) can be estimated *via* factors applied to CapEx or major (indirect) OpEx items⁵⁴ at TRLs 3-7. Typical cost items and a variety of individual factors are available from literature.^{22,36–38,44,45,47–50,55–58} Factors from literature serve as an orientation and have to be adapted to the present scenario. A detailed compilation of factors is available in the supporting information. As scenario definition advances, single cost items can be calculated.⁴⁶ For TRL 8, all major cost items have to be calculated in detail. Assuming E&U cost and/or indirect OpEx from similar plants can be reasonable at TRLs 3-6, depending on the degree of similarity and given data quality.

3.4 Capital expenditure structure

In literature, different nomenclature and structures are proposed for the components of CapEx; when combining different systems it is important not to forget or double estimate cost items. Capital expenditure (also called ‘total invested capital’, TIC) can be divided into fixed capital investment (FCI), working capital and startup expenses as well as contingency.^{37,47} While FCI is calculated in detail, working capital and startup expenses as well as contingency are commonly

estimated *via* factors applied to FCI. FCI is separated in inside battery limits (ISBL) and outside battery limits (OSBL, also called off-site) cost.^{46,47} ISBL includes all cost items that are necessary to build the plant's core production facilities and everything that is directly needed for production; it includes physical components (direct cost, DC) and services needed for building the plant (indirect cost, IC). DC consist of equipment cost (EC, *e.g.* for vessels, pumps or heat exchangers) and components surrounding purchased equipment (other direct cost) such as instrumentation, piping and electrical installations. IC items include engineering, supervision and construction (including insurance) expenses as well as legal and contractor fees and miscellaneous overhead. OSBL items include the infrastructure that is needed to connect the plant to the outside world, such as roads, railroads, docks or general service facilities like power plants or fire protection.^{37,46,47,59} Both ISBL and OSBL contain DC and IC. It is advised to distinguish between ISBL and OSBL on a higher level than DC and IC because the nature of what is built inside battery limits and off-site differs. Thus, factors for IC applied to DC or EC are often different for ISBL and OSBL. OSBL cost depend strongly on the regional scenario since cost items for infrastructure differ between locations. For ISBL equipment and equipment related cost depend indirectly on the location of the plant by altering prices for equipment shipping and construction, while items like buildings (housing the plant), land purchase and yard improvement depend directly on the scenario. For rough location comparisons ISBL cost can be considered independent of location. OSBL cost are often estimated in total as a factor applied to ISBL cost.^{21,46,47,60} A complete structure of CapEx is shown in Scheme 3.

Scheme 3. Structure of capital expenditure, typical estimation items

3.5 Capital expenditure estimation and TRLs

Methods used for CapEx estimation can be distinguished between transformation and estimation methods. Transformation methods are used for the adaption of complete plant estimates or single cost items to a different scenario, most importantly time, location and capacity. The input to transformation method is of the same nature as its output. No congruent definition of cost estimation methods or types/classes of methods can be found in literature. In this framework, cost estimation methods are defined – in contrast to transformation methods – as ways of concluding cost from characteristic parameters or ‘extrapolating’ to cost from the cost for a part of a plant. Most capital cost estimation methods focus on the estimation of ISBL cost (often excluding engineering costs), while other CapEx components are commonly estimated *via*

factors.^{45,47} The object of cost estimation is usually (part of) an operatable full-scale plant (TRL 9). Four types of cost estimation methods are separated: short methods, global factor methods, functional unit counting methods and component factored methods (*cf.* ⁴²).

There are methods that use one (or few) characteristic parameter(s) as input and return cost; these are called ‘short methods’ in the following. Most of these short methods consist of power functions (usually pre-factor (a), capacity (K) and exponent (b) as exemplarily depicted in eq. 1) that depict the economies of scale effect which in the chemical industries is roughly estimated by the volume to surface ratio of spherical equipment.⁶¹ Methods including the number of functional units or equipment cost are excluded here and listed separately as they form distinctive groups.

*short method, example
structure*

$$FCI = a * K^b \quad \text{eq. 1}$$

Global factor methods use total EC (sum of all EC) as input and apply factors (f) for the estimation of other direct and indirect cost items of ISBL or FCI (as shown in eq. 2). Total EC have to be estimated beforehand.

*global factor method,
example structure*

$$FCI = \sum_j f_j * \sum_k EC_k \quad \text{eq. 2}$$

Functional unit counting methods are based on the number of functional units (also referred to as “process steps”, *e.g.* ⁶², N) and other characteristic process parameters (PP) such as maximum process temperature and pressure or throughput as inputs; an example structure is given in eq. 3. There is no commonly accepted definition of a ‘functional unit’; authors of the respective methods give slightly different definitions or no definition at all. The following wordings comprehend most of the methods listed. The ACostE (2000) gives the following definition of functional units:⁶³ “A functional unit is a significant step in a process and includes all equipment

and ancillaries necessary for operation of that unit. Thus, the sum of the costs of all functional units in a process gives the total capital cost.” Another concise description is given by Sinnott & Towler:⁴⁷ “A functional unit includes all the equipment and ancillaries needed for a significant process step or function, such as a reaction, separation or other major unit operation.”

$$\begin{array}{l} \text{functional unit counting} \\ \text{method, example structure} \end{array} \quad FCI = a * N * function(pp_1, pp_2, \dots) * K^b \quad \text{eq. 3}$$

Component factored methods use single equipment cost or process module costs as inputs and apply different factors for the estimation of equipment-related, detailed direct and indirect cost items of ISBL or FCI (see eq. 4).

$$\begin{array}{l} \text{component factored} \\ \text{method, example structure} \end{array} \quad FCI = \sum_j \sum_k f_{j,k} EC_k \quad \text{eq. 4}$$

Table 2 gives CapEx estimation methods sorted in TRLs. The sorting is based on the fit of information known, represented by the TRL, to inputs needed for the respective cost estimation method.

Table 2. Capital cost estimation methods^{21,31,62,64–102} in the TRL framework,⁴² extended

TRL	1	2	3	4	5	6	7	8	9
Short methods			Kiddoo ⁸⁸ , Tolson & Sommerfeld ⁹⁷ , Bridgwater I ⁶⁹ , Herbert & Bisio ⁸³		Gaensslen ⁷⁶ , Lange ⁹¹				
Global factor methods				Burgert ⁷² , Cran ⁷⁴ , Helfrich & Schubert ⁸² , Hirsch & Glazier ⁸⁵ , Lang ⁹⁰ , Viehweger ⁹⁸ , Mach ¹⁰³ , Prinzing, Rödel & Aichert ³¹ , Marouli & Maroulis ⁹²	Chilton ⁷³ , Johnstone ⁸⁶ , Montfoort & Meijer ⁹⁴ , Garrett ²¹ , Kamman & Erb ⁸⁷	Groen & Tan ⁷⁸ , Miller ⁹³			
Functional unit counting methods				Allen & Page ⁶⁴ , DeCicco ⁷⁵ , Klumppar, Brown & Fromme a,b) ⁸⁹ , Petley ¹⁰⁴ , Stallworthy ⁹⁵ , Viola ⁹⁹ , Wilson ¹⁰⁰ , Zevnik & Buchanan ¹⁰² , Timms ⁹⁶ , Gore ⁷⁷ , Bridgwater III ⁶⁷	Bridgwater II ⁶⁸				
Component factored methods			Hill ⁸⁴ , Bridgwater IV ⁷⁰ , Taylor b,c) ⁶²						
Estimation error [%]			-50/+100	-30/+50	-20/+30	-15/+20	-10/+15		

(Process concepts not yet available)

TRL 6 methods with high quality data, detailed single factors for single equipment (offer/tender based equipment cost), software-based including rigorous process design and capital estimation tools (simulation)

(Plant built)

multiple methods from one publication are marked alphabetically in the order of their appearance in the publication

TRLs 3-7 depict the range in which capital cost estimations are applied. The given TRL for each method is the earliest recommended TRL for the application because it is possible to be applied at this TRL without making technical assumptions that narrow the path of future development. The application of a method in a later TRL than listed here can be beneficial and leading to significantly better estimates, especially if the methods allows for the inclusion of

additional data. A method cannot be selected following the level of information that is theoretically possible to have but is rather chosen with best fit to the practically accessible data level. While this should ideally be the same within a single organization, it is often not possible for external estimators due to restricted data accessibility.

Assigning a TRL to cost estimation methods takes into account the recommendations that authors give in their method description regarding if and how the method can be adapted or if given factors are to be applied without considering adapting them to the present case. The table lists the most common estimation methods but does not claim to be complete. Textbooks that summarize cost estimation methods are not listed here if they include (mostly minor) changes to factors without proposing a new structure for cost estimation.

Capital expenditure estimation is possible as soon as process development is started. TRLs 1 and 2 are described as completion of ideation or opportunity identification and concept formulation respectively; they do not include process concepts and are therefore left empty in Table 2. As at TRL 8 the plant is built and is operated at TRL 9, CapEx is then already spent and not estimated but calculated as sum of the past cash flows used to build the plant. Excluding TRLs 1,2,8,9 leaves five distinct levels for cost estimation which corresponds well with the well-established AACE International classification that distinguishes five estimation classes³⁴. Despite the corresponding implications for cost estimation, TRLs 3-7 are not synonymous with given estimation classes due to the different underlying scales, technological maturity *versus* completion of project deliverables respectively.

Not all authors give estimation errors of their methods and often stated errors are unrealistic^{104,105}. The estimation error is asymmetric because under-estimation is more dangerous than over-estimation (more than 100% over-estimation is not possible). The relative difference

between absolute positive and absolute negative error decreases with increasing overall certainty. Error intervals given in Table 2 correspond with the AACE International recommendation that describes types of cost estimation methods depending on their complexity³⁴.

Estimated plant cost can be transformed regarding time, location and capacity to the desired scenario. The methodology of transforming plant costs in time (construction date) and location is independent of TRLs. These adaptations of (parts of) CapEx estimates to a given scenario concerning date and location are usually done by multiplying the cost estimate with a ratio of indexes for equipment cost packages (*e.g.* Chemical Engineering Plant Cost Index (CEPCI), Marshall and Swift Cost Index, Nelson-Farrar Index) or country/location characteristics (*e.g.* Process Engineering US Gulf Coast Basis or Northwest Europe Basis or Aspen Richardson's International Construction Cost Factor Location Manual).

The very popular and easy-to-use power rule ("six-tenths rule"^{106,107}) returns cost, but is methodologically a transformation method since the same cost item is transferred to a different scenario; input and output are of the same nature. It can be used for complete plants or single equipment. For complete plants an exponent of 0.6 is often chosen.^{106,107} Exponents for different types of plants are given in literature³⁵. It is important to bear in mind that this rule is best applied if the cost of the main components of a plant scale in that way. For this reason, excluding OSBL or increasing the exponent when applied to FCI or CapEx is recommended. An exponent exceeding 0.6 is for example depicted in various short methods for cost estimation (*e.g.* ^{83,97}). For large scaling factors the plants component types change; this approach can then be seen as a cost estimation method. However, it is not advised to use this method for dissimilar plants. Depending on the similarity of the plants (process) and scenarios (construction date, location) as well as quality of data (data source) this method can lead to reasonable estimates at TRLs 3-6.

4 Market analysis and scenario definition

For profitability analysis in the context of the techno-economic assessment of a chemical process, benchmark identification, sales price and sales volume are the key market parameters. Inadequate pricing is a major challenge^{18,108} for techno-economic assessment and should therefore be conducted with care. While other qualitative indicators such as freedom to operate analysis might be added to the market analysis, benchmark, price and volume are sufficient for analyzing and comparing production processes and products from a market perspective in the phases of chemical R&D (TRLs 1-7), in the following referred to as ‘market analysis’. If the assessment scope involves the company and competitors, which is important for late development and deployment phases (TRLs 7-9), addressing questions such as, strategies for market entry, collaborations or competitor response, analysis frameworks from strategic management literature, such as value chain analysis, five forces, SWOT, or business model canvas should be included in the assessment; however, these assessments lie outside the scope of this paper.

Following the classification of Cussler and Moggridge, the four general types of chemical products are base chemicals (*e.g.* ethylene), chemical microstructures (*e.g.* polyurethane, sunscreen), active pharmaceutical ingredients (*e.g.* penicillin, acetylsalicylic acid), and chemical devices (*e.g.* lithium-ion batteries); in the following examples will be provided for each type.¹⁰⁹

As a first step in market analysis, the competing solutions or products need to be identified, in the following referred to as ‘benchmarks’. To do so, at least one application or solution of the assessed product should be defined (*e.g.* methanol, high temperature resistant material, or cancer treatment, small scale energy storage). Furthermore, the currently established competing solutions and their user groups (*e.g.* chemical producer, machine manufacturer, doctors/patients,

households), should be listed. The needs of these user groups are then identified and clustered into the categories essential, desirable and useful. Essential needs are the minimum requirements so that the user has a benefit from the product or in other words, if the product does not fulfil the essential needs, users will not consider it as solutions for the application in focus. Desirable needs are the requirements that are currently not completely matched by existing benchmarks, fulfilling these better than competing products will give a strong market advantage in terms of volume or price. Useful needs can be described as nice-to-have aspects to a product, not providing a strong market advantage in general, but potentially in very distinct niche markets.¹⁰⁹ The needs can be identified by literature review, expert interviews or user group interviews. However, involving potential customers at early product development stages is a major challenge.^{28,109,110} Once the needs are identified, the assessed product and benchmarks are compared by the amount to which they fulfill the identified needs.

As a second step in market analysis, sales price and sales volume of the product can be derived from the benchmark analysis. If the product is a perfect substitute, meaning that it has an identical structure or function, which is generally the case for the product type base chemicals/commodities (*e.g.* hydrogen from syngas vs. hydrogen from electrolysis), the price and volumes can be directly derived from the benchmark prices and volumes of the market in focus. Additional information such as regional limitation (*e.g.* China) or addressable market segment (*e.g.* high-performance), as well as market growth or trends in user needs (*e.g.* bio-based) can be added to the analysis. If the product is not a perfect substitute and exhibits a different structure or function, the price and volume identification requires the additional step of relating its performance to the price-performance ratio in the market. This is especially important for the product groups microstructures, active pharmaceutical ingredients and devices.

If a more detailed cost comparison is required by the assessment goal, the benchmark's COGS should be analyzed. Benchmark costs are estimated bottom-up following the cost estimation methods proposed in chapter 3 or top-down by subtracting a margin from the benchmark price. Top-down tends to be quicker because margins are more easily estimated than the exact process and conditions under which the product is produced by a competitor.

Market analysis and scenario definition are closely intertwined: Market analysis maps conditions under which production is economically viable with respect to location, time and market segment. Important parameters in scenario definition are construction time, timing and value of subsequent investments, project life span, salvage value at liquidation, interest rates (debt/liability and equity), depreciation type and time, income taxes and inflation^{37,111}.

5 Profitability analysis

Profitability analysis leads to decisions about spending money on RD&D activities. Spending money for a specific purpose is covered by the definition of an investment¹¹². In this contribution, profitability indicators are specified as calculated values of investments, representing monetary gains or losses in comparison to an alternative investment.

Profitability analysis is done with indicators that show if, how much and when money can be earned with an economic activity.⁵⁴ Profitability indicators depend on development progress because cost estimation depends on development progress and cost estimates are a fundamental part of profitability indicators. As data availability increases cost estimates become more accurate and market understanding improves. The indicators of profitability analysis become more and more accurate as RD&D progresses.

Profitability indicators are separated into two categories: static and dynamic.¹¹³ Static indicators do not consider time dependence; they consider only one period or an average of

multiple periods. The general alternative investment for static calculations is no investment at all. Dynamic indicators account for time preferences of cash flows. The general alternative investment for dynamic calculations is an investment on the capital market with the same risk profile.

For the chemical industry costs are typically calculated for a period of one year and are often allocated to the amount of product(s) produced in the same period,¹¹⁴ leading to parameters with the dimension 'value per mass'. In general, static indicators are quick to calculate but only provide a first indication if an investment is profitable. Dynamic calculation should be done as soon as product definition is accurate enough for the prediction of future revenues. This is usually the case with completion of advanced laboratory or miniplant research (TRL 5) and planning of pilot trials. At TRL 9 (production phase) the plant is complete and running; profitability is then no longer estimated but checked by calculation of already performed activities (VI, accounting).

Profitability indicators for each TRL are described below. The recommended indicators fit the advance in scenario definition and market analysis as well as the accuracy of estimated cost. The general idea of the profitability indicators suggested here is this simple equation: the profit is the difference of revenue and cost. This difference is in the core of every indicator presented.

The general interpretation of most of these indicators in the subsequent TEA phase is: A positive indication is given if the value is above zero or meets the required target value; when comparing alternatives, the higher value is favored. Indicators differing from that rule are explained in more detail. In the efficiency form the threshold value is 1. Furthermore, evaluating uncertainty is part of the interpretation and can only be briefly touched upon here: The uncertainty of an estimate is often given as deviation from a reference estimate and is commonly

shown with error bars. An overall uncertainty can be presumed in very early stages and can be refined with weighted errors in early project progress. Later, uncertainty is examined with uncertainty analyses which show how the uncertainty of input conditions and parameters changes the variation of outputs and sensitivity analyses that examines how a model's outcome variation can be attributed to input information and model structure ¹¹⁵.

Following the interpretation, decision-making is again a very complex process and includes portfolio strategy considerations and other assessment fields.^{27,116} A positive indication given by the interpretation of a profitability indicator does not necessarily imply a positive decision as the error allowances of deciders may differ. Companies' decision rules vary from a very conservative approach that the intervals for estimated selling price and estimates cost must not overlap to a more risk-seeking approach being to opt for an investment even if only cost plus highest error and selling price minus lowest error match.

TRL 1: In TRL 1 ideas for a product group or application do not necessarily have to be translated into reaction schemes. Ideas, as outlined in the description of TRL 1 of this framework, do usually not consist of elements that have costs, thus making cost estimation and subsequent profitability analysis not applicable. Instead of calculations a first qualitative evaluation can be conducted. For example, rankings for multiple criteria can be prepared in comparison to benchmarks or other ideas in concept screenings.^{45,109}

TRL 2: At TRL 2 process development is not started, yet economic considerations can be made based only on the stoichiometry of the reaction. The revenue (products' value, Π_p) results from the products' percentages in the mass balance and their market prices. The educts' cost (material cost, Π_{mat}) is determined in the same way. In addition, the theoretical energy cost of the reaction (Π_{en}) contribution can be roughly estimated as indicated in section 3.3.

The obtained specific gross margin ($\Pi_p - (\Pi_{mat} + \Pi_{en})$; see also ⁴⁷ (excluding energy cost)) is proposed to be normalized in early TRLs to cost for the following reason: in early stages, the focus is on concept comparison and deciding which pathway is favored. In this context, the interpretation of normalized values is simplified as a larger number of normalized values can be more easily displayed in a single figure. Absolute values of possible investments gain more interest when narrowing down alternative process concepts to only a few. The previous thought yields the ‘relative gross profit’ (P_{gr} , I , eq. 5) as a dimensionless figure that provides information about how efficient the economic activity will be (*cf.* ¹¹⁷). This indicator is also used in its efficiency form⁵² or as its inverse (*cf.* ¹¹⁸, (including all cost items)).

$$I \quad \text{relative gross profit} \quad P_{gr} = \frac{\Pi_p - (\Pi_{mat} + \Pi_{en})}{\Pi_{mat} + \Pi_{en}} \quad \text{eq. 5}$$

For some products, R&D can aim at a wide range of applications, for example nanoparticle surface modification technology can be used for information technology hardware or medical devices. While this does not directly affect cost estimation, it increases effort for market analysis and profitability calculation. The revenue prospects of such products are composed of the multiple possible target markets, *i.e.* the sum of all applications’ sales volumes times their associated sales prices. In relative calculation, the product can be seen as separate products which are either treated as different technology options (each entailing their own profitability calculation) or treated as multiple products resulting from one process whose shares reflect their projected sales volumes or market sizes.

TRL 3: After starting process development, process cost (all OpEx, Π_{op}) and CapEx can be included in the calculation, as it is explained in sections 3.3 and 3.5. In this step capital expenditure is not yet discounted but divided by the project life time or recovery period (n) and

capacity (K)¹¹⁴. At this point, first market studies and similar plants serve as an orientation for rough capacity planning. Technical feasibility considerations must not contradict this capacity. The relative gross profit (I) is updated with all cost items to the ‘relative profit’ (P_{rel} , II , eq. 6).

$$II \quad \text{relative profit} \quad P_{rel} = \frac{\Pi_p - \Pi_{op} - \frac{CapEx}{n * K}}{\Pi_{op} + \frac{CapEx}{n * K}} \quad \text{eq. 6}$$

Practitioners, especially in companies where absolute numbers are important for strategy considerations, may prefer the difference, called ‘specific profit’ (P_{spec} , III , eq. 7 *cf.* ²⁰, “static cost benefit assessment”), over the normalized form for a rough comparison with established products and deriving cost increments.

$$III \quad \text{specific profit} \quad P_{spec} = \Pi_p - \Pi_{op} - \frac{CapEx}{n * K} \quad \text{eq. 7}$$

TRL 4: For the estimation of absolute profit and payback time the annual addressable market sales volume (V) is necessary. Often, the initial market size is calculated as a desired share of the benchmark product’s market in a certain region. Plants can be built with planned over-capacities that consider increasing market sales volume; CapEx is therefore allocated to the produced (and sold) amount of product. The absolute ‘static profit’ (P_{stat} , III , eq. 8) is calculated as the specific profit (III) multiplied by the annual market sales volume and project life time or recovery period (n). As indicated for TRL 3, practitioners may additionally show an updated specific profit (bracketed term in eq. 8) and market potential ($n * V$) separately.

$$IVa \quad \text{static profit} \quad P_{stat} = n * V * \left(\Pi_p - \Pi_{op} - \frac{CapEx}{n * V} \right) \quad \text{eq. 8}$$

The payback time is the time after which an investment is amortized and starting to generate net profit. Only investments with shorter payback time than project life time should be considered. When comparing alternatives, the investment with the shortest payback time is favored. The ‘static payback time’ ($t_{payback,stat}$, *IVb*, eq. 9) is calculated as CapEx divided by the annual profit resulting from plant operation and product selling (*cf.* ^{21,38}, “payout period”; *cf.* ^{19,37,45,48}, “payback period”; *cf.* ^{46,47}, “[simple] pay-back time”; *cf.* ^{44,49}, “payout time [without interest]”). The date from when an economic activity generates net profit is also called ‘break even point’.

$$\begin{array}{ll} \text{IVb} & \text{static payback time} \end{array} \quad t_{payback,stat} = \frac{CapEx}{V * (\Pi_p - \Pi_{op})} \quad \text{eq. 9}$$

Dividing the static profit (*IVa*, eq. 8) excluding CapEx by the initial CapEx committed gives the ‘static return on investment’ (static ROI, *IVc*, eq. 10, cumulated for a specified number of years, n , *cf.* ³⁷) which is a useful indicator when comparing the quality of the utilization of profitability resources. Various definitions of ROI exist, differing in details (*e.g.* which CapEx items to include); often this indicator is calculated for a single or average year of operation (*cf.* ^{21,38,44–49}).

$$\begin{array}{ll} \text{IVc} & \text{static return on investment (ROI)} \end{array} \quad ROI_{stat} = \frac{n * V * (\Pi_p - \Pi_{op})}{CapEx} \quad \text{eq. 10}$$

Differentiating between years of operation requires an understanding of the product and market that corresponds with TRL 5 in the concept of this framework. Multi-period tables are therefore not included in TRL 4 assessment. If future cash flows are known or can be estimated it is advised to include interest as well and directly discount a cash flow table without previous interpretation,¹¹¹ as discussed in the following paragraph.

From TRL 5: Below TRL 5 it is believed that the cost estimation error is larger than the effect of including interest. For example, from TRL 5 the estimation error for capital investment cost is in the same range or smaller than the effect resulting from including interest. The combined error range for all other costs is expected to be similar. In addition, the product definition at TRL 5 is advanced enough to allow for a first description of a complete set of scenario-related parameters, leading to the recommendation of including interest from TRL 5. Moreover, pilot plants (TRL 6) are a critical point of investment for chemical companies in RD&D projects (“valley of death”¹). Before deciding about building a pilot plant the viability of an estimated full-scale plant should be analyzed considering interest. With the conclusion of pilot phase and before entering final engineering multiple scenarios concerning different market entry strategies should be examined in economic calculations including interest.

From TRL 5 simple dynamic indicators are recommended:^{111,116} Future cash flows are discounted according to the period they occur in with the corresponding assumed interest rate(s). The ‘net present value’ (*NPV*, *Va*, eq. 11, *cf.* ^{19,20,45–49,56}) is the sum of all discounted cash flows (*cf.* ^{21,36–38,116}, “net present worth”). It depicts the amount of money that an investment is worth in period zero. Similarly, cash flows can be compounded to a “net future worth (or net terminal value)”^{36,116} which depicts the value of an investment at a certain point in future time.

$$Va \quad \text{net present value (NPV)} \quad NPV = \sum_{t=0}^n \frac{V_t * (\Pi_p - \Pi_{op})_t - CapEx_t}{(1 + i)^t} \quad \text{eq. 11}$$

The ‘dynamic payback time’ ($t_{payback,dyn}$, *III*, eq. 12) is the first period (t_{min}) in which the sum of all past discounted cash flows is zero or positive (*cf.* ³⁸, “payout period with interest”; *cf.* ^{19,45}, “discounted payback period”; *cf.* ⁴⁹, “payout time with interest”) and is interpreted as described for *IVb*.

$$Vb \quad \text{dynamic payback time} \quad t_{\text{payback,dyn}} = t_{\text{min}} \text{ for } (NPV \geq 0) \quad \text{eq. 12}$$

Analog to the static ROI (IVc , eq. 10), a dynamic ROI (Vc , eq. 13) can be calculated including interest. It is popular for comparing the relations of investments' earnings to their initial investments. Including interest, it is calculated as the ratio of all discounted cash flows resulting from plant operation and product selling to all discounted cash flows associated with the initial spending.

$$Vc \quad \text{dynamic return on investment (ROI)} \quad ROI_{\text{dyn}} = \frac{\sum_{t=0}^n \frac{V_t * (\Pi_p - \Pi_{op})_t}{(1+i)^t}}{\sum_{t=0}^n \frac{CapEx_t}{(1+i)^t}} \quad \text{eq. 13}$$

The internal 'rate of return' (IRR, Vd , eq. 14) is the interest rate that leads to an NPV of zero (*cf.* ^{19,20,38}; *cf.* ⁴⁴⁻⁴⁹, "discounted[-]cash[-]flow rate of return"; *cf.* ¹¹⁶, "true rate of return"). A positive indication is given if the value is higher than the market interest rate or exceeds a certain value. The IRR is a good measure when comparing how well capital is spent in different projects; it should however only be shown together with an NPV, as it does not reveal absolute profits.

$$Vd \quad \text{Internal rate of return (IRR)} \quad IRR = i \text{ for } (NPV = 0) \quad \text{eq. 14}$$

From TRL 6 it is advised to account for different interest rates for different cost items. Moreover, it should be included how CapEx is financed; it is for example due in period zero and liability financed over several periods, thus increasing the budget in period zero by the cost that is needed for financing it.

From TRL 7: In addition to refined dynamic indicators, detailed prediction/estimation of future developments should be included in economic simulations (*VI*) from TRL 7. Simulations can be based on discrete events (scenarios) or comprising detailed models based on functions that describe market, cost and scenario parameter behavior. Simulations can for example include depreciation type and time, income taxes and inflation as well as distribution cost, time dependence of cost items like wages, utilities and other or material cost as a function of time if contract price data are available³⁶ and knowledge about customers and competitors as well as organizational resources¹¹⁹. Simulation is done for solving existing and hypothetical problems in manufacturing¹²⁰ and optimizing¹²¹ and can include economic risk analysis^{45,49}. From TRL 8, CapEx items can be updated with actual data of past cash flows.

TRL 9: At TRL 9, economic simulations (*VI*) can be performed for the prediction of economic effects of future production, plant expansions, new plants of the same kind or minor optimizations that are not considered new technology development. Past economic activities are summarized in accounting for cost checks and profit calculations (*VII*).

Table 3 summarizes the recommended profitability indicators explained in the above paragraphs. After qualitative evaluating an idea (TRL 1), specific static indicators are recommended during laboratory research (TRLs 2 and 3). Market sales volume is included as soon as systematic process development is started (TRL 4) to allow for forecasts of absolute profits. Building on more detailed technology and market understanding and before piloting (from TRL 5), a variety of dynamic indicators is at hand; these are refined in the following steps and ultimately lead to complex simulations of future economic activities prior to building a full-scale plant.

Table 3. Profitability indicators in the TRL framework

TRL	1	2	3	4	5	6	7	8	9
Profitability indicator	Qualitative evaluation	<i>I</i>	<i>II</i>	<i>IVa</i>	<i>Va</i>	<i>Va</i>	<i>(Va)</i>	<i>(Va)</i>	<i>(VI)</i>
				<i>IVb</i>	<i>Vb</i>	<i>Vb</i>	<i>(Vb)</i>	<i>(Vb)</i>	
				<i>IVc</i>	<i>Vc</i>	<i>Vc</i>	<i>(Vc)</i>	<i>(Vc)</i>	
				<i>IVd</i>	<i>Vd</i>	<i>Vd</i>	<i>(Vd)</i>	<i>(Vd)</i>	
							<i>VI</i>	<i>VI</i>	

6 Conclusions

For profit-oriented stakeholders, a techno-economic assessment is an instrument for evaluating whether or not (and when and how much) an investment generates a positive monetary return. Technical parameters alone cannot help in answering that question; they have to be translated into economic indicators. Depending on the availability of technological data the methods for evaluating economic viability differ and no commonly accepted standard exists for this issue. A systematic framework for techno-economic assessment can assure best exploitation of available data. In addition, it facilitates communication and comparison of assumptions or results between all stakeholders affected by a possible economic activity resulting from an RD&D project. Cost estimation is an example of major importance for the strong dependence of adequate methodology from data availability. Progress in RD&D projects is best monitored by the TRL concept, which describes technological maturity in nine distinct levels; however, there is so far no common understanding of these levels in the chemical industry. A suggestion for TRLs in the chemical industry was made (first key challenge). The suggested TRLs offer a suitable framework for the sorting of cost estimation methods and subsequently profitability indicators (second key challenge). Profitability indicators are recommended as follows: Different static

indicators for earlier development (TRLs 1-4) and inclusion of time (*e.g.* interest in net present values) for later stages (TRLs 5-9).

This framework was demonstrated in a case study in which the selection of CapEx estimation methods was based on an in-depth description of a technology and subsequent TRL rating:⁴² The study revealed that the selection of methods is facilitated following TRL rating, however, methods of one TRL may show great deviations which makes a structural comparison of cost drivers within each method crucial. For CapEx estimation, especially in early to mid TRLs, it was recommended to compare several methods that rely on the same depth of input data (TRL).

A framework for adequate methods of market analysis and scenario description in each TRL might be a useful tool, but is left to future research. It would be beneficial to have methods of other assessment fields (*e.g.* LCA) sorted in the TRL framework in order to extend the here presented TEA framework for profit-oriented to a more holistic framework for the assessment of RD&D projects in the chemical industry.

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Funding

Authors 1 and 2 received funding from the European Institute of Technology (EIT) Climate-KIC

Author 1 received funding from the German Federal Ministry of Education and Research (BMBF)

Acknowledgement

The authors would like to thank Ali Hassan, Michael Schwarze, Johannes Wunderlich and Anne-Christine Haskamp (TU Berlin), Annika Marxen (IASS Potsdam) as well as Christoph Gürtler, Ludger Kaster and Natalia Pieton (Covestro AG) for their fruitful discussions. This work was funded by the European Institute of Technology (EIT) Climate-KIC enCO₂re program and German Federal Ministry of Education and Research (BMBF) FONA3 r+Impuls program.

Supporting information

Table S1. Estimation factors for indirect operational expenditure (indirect OpEx) and general expenses

Nomenclature

TEA	Techno-economic assessment
CCU	Carbon capture and utilization
LCA	Life-cycle assessment
TRL	Technology readiness level
R&D	Research and development
RD&D	Research, development and deployment
COGS	Cost of goods sold
COGM	Cost of goods manufactured
IP	Intellectual property
CapEx	Capital expenditure
OpEx	Operational expenditure
E&U	Energy and utilities

M&S	Marketing and sales
TIC	Total invested capital
FCI	Fixed capital investment
OSBL	Outside battery limits
ISBL	Inside battery limits
DC	Direct cost
EC	Equipment cost
IC	Indirect cost
EARTO	European Association of Research and Technology Organisations
CEPCI	Chemical Engineering Plant Cost Index
AACE	American Association of Cost Engineering

Symbols

Π	cost, price [\$/kg]
P	profit, <i>rel, gr</i> : [1], <i>spec</i> : [\$/kg], <i>stat</i> : [\$]
$CapEx$	capital expenditure [\$]
FCI	fixed capital investment [\$]
EC	equipment cost [\$]
N	number of functional units [1]
pp	characteristic process parameter [various dimensions]
n	project life time or recovery period [a]
K	capacity [kg/a]
a	pre-factor in methods for cost estimation [\$/[various dimensions]]
V	annual market sales volume [kg/a]

<i>t</i>	time period [1]
<i>i</i>	interest rate [1]
<i>b</i>	exponent in methods for cost estimation [1]
<i>ROI</i>	return on investment [1]
<i>NPV</i>	net present value [\$]
<i>IRR</i>	internal rate of return [1]

Indexes

<i>mat</i>	material
<i>op</i>	including all allocated OpEx
<i>p</i>	product(s)
<i>en</i>	energy and utilities
<i>gr</i>	gross
<i>rel</i>	relative
<i>spec</i>	specific
<i>stat</i>	static
<i>dyn</i>	dynamic
<i>min</i>	minimum

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