ULTIMATE
WATER SMART INDUSTRIAL SYMBIOSIS

Deliverable 5.4:

Report on customizable WSIS contracts and financing schemes

WP5 | Explore new business models and arrangements

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List of Acronyms

Acronym	Full Title	Acronym	Full Title
BIS	Bank of International Settlements	GAR	Green Asset Ratio
CE	Circular Economy	GhG	Greenhouse Gas
CEAP	Circular Economy Action Plan	IS	Industrial Symbiosis
CEF	Circular Economy Finance	KPI	Key Performance Indicator
ChL	Chemical Leasing	LCA	Life Cycle Analysis
CSR	Corporate and Social Responsibility	NCPC	National Cleaner Production Centre
DJSI	Dow Jones Sustainability Index	NFBS	Non-Financial Business Sector
EBA	European Banking Authority	OPL	Objective Pricing Limit
EBRD	European Bank for Reconstruction and Development	PEF	Product Environmental Footprint
EC	European Commission	RES	Renewable Energy Source
ECB	European Central Bank	SEEA	System of Economic-Environmental Accounting
EIB	European Investment Bank	SDG	Sustainable Development Goal
EIF	European Investment Fund	SME	Small-Medium Enterprise
EPR	Extended Producer's Responsibility	SP	Sherwood Plot
ESG	Environment, Society, Governance	TEEB	The Economics of Ecosystems and Biodiversity
ES	Ecosystem Service	UN	United Nations
EU GBS	European Union's Green Bond Standard	UNIDO	United Nations Industrial Development Organization
EU GD	European Green Deal	VAC	Value Added Compound
EU TSF	European Union's Taxonomy of Sustainable Finance	VAC DI	Value Added Compound Dilution Index

Executive Summary

Summary of the Deliverable

The CE has made remarkable technological progress by offering a wide range of alternative engineering solutions. However, a remaining obstacle for its large-scale commercialization is nested at the *financial* level. So far, especially in the EU, CE investments have been designed almost exclusively by institutional financial organizations, such as the EIB [1] and the EBRD [2-5]. However, with the establishment of the EU TSF [6], many private financial institutions gradually enter the field of *tailored* financial instruments to meet the specific needs of CE cases. The present **ULTIMATE Deliverable 5.4 is titled *"Report on customizable WSIS contracts and financing schemes"*** and is part of the **Work Package 5 titled "*Explore new business models and arrangements*"**. In D5.4 we examine qualitatively and quantitatively the potential of *Chemical Leasing (ChL)* contracts as a tailored business model and financial agreement for IS clusters, firstly introduced by the UNIDO in 2004 [7]. In this context, we primarily examine the regulatory international and EU banking framework to assess the direction of tailored CEF instruments. In turn, we construct a quantitative framework for the design and deployment of ChL contracts in relation to the *Sherwood Plot* (SP), as chart depicting the (proportional) relationship between the dilution of a *Value Added Compound* (VAC) in a wastewater matrix and its cost of recovery.

The value-added of the ULTIMATE D5.4 consists in three pillars: **(1)** The benefits deriving from the ULTIMATE consortium synergies that increased the "knowledge stock" by newly created tailored CEF and IS instruments that enrich the global literature background, as well as their pilot testing in other ongoing ULTIMATE works; **(2)** The post-ULTIMATE commercial potential, as the ChL quantitative framework developed can be applied in case studies outside ULTIMATE with *measurable monetary effects* and **(3)** The compatibility of the ChL framework of ULTIMATE D5.4 to existing EU policy directions towards the upscaling of the CE in all EU member-states.

Regarding the first pillar, although these values are constantly reminded across the D5.4 chapters, in brief we may emphasize on the fact that other ULTIMATE works, such as Subtask 2.2.1 on LCA benefits of IS solutions and Subtask 2.2.2 on the SP framework on the measurable economic performance of IS solutions, comprise vital inputs for D5.4. Specifically, as the environmental benefit of IS practices is substantiated at LCA level, the next question is *how these practices could be incorporated in standardized business models and agreements that are economically beneficial for all counterparties*. Regarding the second pillar -and in direct relation to the first- D5.4 answers the question on the measurability of the benefits of such business models and financial arrangements. Hence, D5.4 can be considered as a bridge between background ULTIMATE works and future works concerning pilot testing of exploitation results, such as T5.5 on the marketplace and T5.6 on the Greenfield Assessment of three selected case studies outside the already existing ones. Finally, regarding the third pillar, although CEF instruments such as ChL can be highly innovative and tailored, they should be following the policy guidelines set by both international [7] and EU institutions aiming at the mitigation of environmental impacts and not just the enrichment of the conventional financial instruments with “green” ones. In this context, D5.4 examines in **Chapters 1 and 2** thoroughly the EU institutional background of CEF instruments, ensuring that the ChL framework developed is *compatible* to UN global sustainability directions since the *Rio Earth Summit* (1992) and the establishment of *Agenda 21*, while *compliant* to both EU economic-environmental accounting standards, such as the SEEA [8-10] and the PEF [11-12] as an umbrella of LCA methods, CE and IS plans promoting the EU GD [13-15] and -above all- EBA regulations towards the assessment of “green” portfolios of commercial banks via ESG harmonization [16] and establishment of the GAR [6,17] that are hierarchically imposed by the BIS [18-19] as responsible for the Basel III and IV banking compliance frameworks.

In overall, D5.4 addresses the crucial issue of environmental performance measurement by the commercial financial institutions that can direct massive amounts of capital towards the CE and IS. Although environmental markets have made remarkable progress with carbon markets there are still great limitations for the large-scale commercialization of CEF instruments that extend beyond limiting CO2 emissions. Due to the large heterogeneity of environmentally-aware companies that wish to utilize environmental finance know-how, commercial banks seek reliable and comparable metrics and KPIs for coupling payments to environmental performance as well as tools to facilitate the realization of CEF. The theoretical background of the SP as foundation of VAC recovery cost performance -and the need to sign ChL arrangements is presented in **Chapter 3**. Our quantitative framework in **Chapters 4 and 5** develop an integrated ChL framework based on the SP for recovering VACs, in full compliance and compatibility to the existing EU GD policies, modus operandi and tools.

Regarding the ChL *financial engineering* aspects, D5.4 substantiates that such contracts have the additional role of *quality control* of a VAC’s recovery diluted in a wastewater matrix. Specifically, *provided that all technical specifications of the recovered VAC are satisfied*, ChL optimizes the allocation of VAC recovery costs via industrial *synergies* that minimize the total market cost; hence, motivating industries to collaborate for delivering the VAC at the target dilution level, at the market’s minimum cost and at a profit for them. In this context, a ChL *market typology* is further developed, examining how payoffs tend to be allocated between industries in each one of them. Although ChL agreements can acquire a variety of forms, in D5.4 we examine the two ChL contract types -the *Bilateral* and the *Multilateral*- as the most inclusive for agreements between two or more counterparties. In turn, we analyze three ChL contract *pricing* systems, their *profitability* limits and their fitting potential by market type. Finally, in **Chapter 6** we examine the utilization of Deliverable 5.4 to other ULTIMATE works, while in **Chapter 7** we briefly conclude and discuss research and market extensions at the post-ULTIMATE era.

Disclaimer

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1. Introduction

1.1. Overview of ChL in the CEF context

The transformation of the EU towards the CE is implemented at a growing rate and all related technological progress offers a wide range of alternative engineering solutions. From an institutional point of view the CE has already been put on track. However, the next and most demanding challenge for the large-scale CE commercialization concerns the financial sector. So far, CEF instruments have been designed almost exclusively by institutional banks [1-5]; however, the development of tailored financial instruments to correspond to the specific needs of industrial ecosystems comprises a major challenge for private financial institutions as well, as they seek reliable models and metrics for coupling payments to environmental performance. In short, the major obstacle for the private financial sector to respond to the investment needs of the CE upscaling is the lack of suitable *underlying indices* reflecting the environmental performance of their investments in monetary terms.

D5.4 develops the technical facets of ChL as a tailored CEF instrument, suitable for IS clusters. The current ChL tailoring integrates to the SP [20] as a framework for quantifying the composition of an industry's cost to recover a VAC from wastewater across its increasing dilution (or decreasing concentration) in it. The SP framework was empirically investigated, utilizing data from an ULTIMATE case study concerning polyphenols' (as VAC) recovery from wastewater generated by fresh fruit juice production.

Historically, ChL was primarily introduced in several case studies by the UNIDO [7, 21]. Originally, ChL focused on a product's life-cycle consultation *from the Producer to the User* to achieve its optimal industrial utilization and environmental performance. From an institutional standpoint, ChL is directly related to the EPR principle that constitutes a pillar of the EU's economic transformation towards the CE. In ULTIMATE ChL contracts are further evolved by setting the necessary chemical use conditions by the Producer to the User so that a VAC's recovery from the generated wastewater is maximized and effluents to the environment are minimized.

ChL agreements can take various forms; however, in D5.4 we identify two prevalent ones as their financial engineering building elements can potentially include any other variety of lower or higher contractual complexity: **(1)** the *Bilateral* and **(2)** the *Multilateral* contracts. With a *Bilateral* contract a chemical's *Producer* "leases" the chemical to the *User* that is contractually obliged to use it in a specific way by following designated steps (by the Producer) who has deep knowledge on how the chemical's environmental impacts change across its different commercial uses. In that way, the User will eventually return the wastewater to the Producer that after VAC recovery, water purification and reclamation, it will discharge the residual safely to the environment. If the contract's conditions are not met, the generated wastewater "package" is returned to the User that is burdened with all related costs - as penalty for failing to meet the initial terms of the agreement- for further processing until the contract's terms on the wastewater's composition are eventually met.

The *Multilateral* or *Bus* contract is based on similar principles to the Bilateral one; however including two main differences: **(a)** The chemical's Producer may *sell* the chemical to the User without necessarily leasing it -and hence not having the obligation to consult on or supervise its use- and **(b)** The chemical's User can address to a third party, such as an IS cluster, to *lease* or *outsource* the wastewater management and VAC recovery. In this way, the Multilateral ChL contract with the Producer choosing to sell the chemical concerns an *up to 2-level* set of agreements; the *first* between the User and the IS cluster and the *second* between industries within the IS cluster. The Multilateral contract is applied to a higher number of sequential "end users".

With the above described ChL mechanics, we argue that at the heart of the CE lies IS concerning the concentration of industries into clusters and agglomerations to minimize the economic obstacles of physical geography and maximize the recovery of valuable resources in a business scheme where the wastes of one industry become inputs for another. From this perspective, CEF instruments like ChL can be upscaled in IS closed-loop complex networks with objective function the energy and material flow optimizations. In this context, SP-based performance metrics for ChL can provide structural and flow optimization diagnostics that will keep industries constantly motivated for improving their physical infrastructures towards VAC concentration maximization and recovery cost minimization.

1.2. Outline of D5.4

The Deliverable's structure is presented below:

- **Chapter 1**. Introductory presentation of the ChL elements in the context of CEF.
- **Chapter 2**. Description of the EU institutional shift towards CEF.
- **Chapter 3.** Physical and economic quantitative foundations of VAC recovery and CEF.
- **Chapter 4**. ChL quantitative modelling as a special case of CEF for IS.
- **Chapter 5.** ChL pricing for mutual benefits of collaborating industries recovering a VAC.
- **Chapter 6.** ChL and CEF applications in other ongoing ULTIMATE works.
- **Chapter 7.** ChL and CEF extensions for the post-ULTIMATE era.
- **Chapter 8.** Bibliographical references used for the Deliverable's substantiation.

2. EU context of CEF

Chapter 2 presents the ongoing fundamental transition of the EU financial and banking sector at the institutional level. The accurate charting of this shift is of crucial importance as any CEF instrument newly introduced will have to be compatible and compliant to the EU's new "Green" Finance standards. In particular, Chapter 2 examines the two major pillars of this context: **(a)** The institutional change in banking compliance regulations, with emphasis on Basel III and IV guidelines and **(b)** The institutional change towards the establishment of corporate and national integrated economic-environmental accounting at life-cycle level.

2.1. The EU shift towards environmental banking and finance

The EU's institutional transition towards the CE comprises an unprecedented legal shift, being also pivotal to the CEF. CE markets within the EU are currently estimated to have a value between €78,9-84,9·10^9 derived by various sectors [15]. The CE comprises only one of the six pillars of the EU TSF [6] and expands in all economic sectors as well as to all corporate sizes; from SMEs that form more than 98% of all EU businesses [22] to mid-caps and large corporations. The first major applications of the EU TSF concerned the finance of RES units, tethering directly the instruments' yield to the CO2 savings [2-5]. Specifically, in Greece the demand for RES bonds that were issued for renewable energy projects surpassed the supply by more than 4,5 times; for the initially 150·10^6 € asked, 684·10^6 € were offered, while 35% of the initial capital was backed by the EBRD [5], continuing the first "green bond" issuance in Greece by one of the country's 4 systemic banks [2]. These initial steps were further extended in large hydro RES projects, where the "green" bond's underlying index was coupled to ESG profiling and CO2 emissions' reduction by 40% in relation to the benchmark [3]. With the gradual accumulation of environmental finance know-how, such practices are today rapidly adopted by other sectors as well, such as land development [4], where the certified environmental performance and adoption of environmental finance instruments comprise both financial assets and part of "best practices" track. However it should be denoted that the high share of institutional financial organizations in such schemes, demonstrates that the financial sector still needs time to restructure with the motivation of an institutional driver towards large-scale deployment of CEF.

Conventional financial instruments, such as business loans with discount rates reflecting the investment's risk, prove to be structurally insufficient to cope with both the needs of the latest EU version of the SEEA (2012) [10] that identify their origins in 2003 [8-9] with the collaboration of many international organizations. The SEEA aims at establishing full cost-benefit assessments, taking into account the peculiarities of IS clusters and their emerging synergistic business models [15]. However, the current state of the global financial and banking system experiences a top-down institutional paradigm shift towards the incorporation of monetized environmental costs and benefit, imposed by central banks as the highest levels of the financial and banking regulation hierarchy.

Central banks are regulatory institutions that set the foundations of monetary compliance rules and monitor their abidance by commercial banks. Thus, to examine the prospect of CEF schemes within sustainability contexts from central banks that will determine the role of money and the structural directions of environmental finance in the next years is of definitive importance. For instance, the BIS, with its role as "central bank of central banks", identified environmental and climate factors as determinants of the global financial system's future stability. Specifically, the BIS introduced the concept of the "Green Swan" event [18], in analogy to the "Black Swan" concept [23], highlighting the fundamental financial risks able to threaten the foundations of the financial architecture itself by manifesting where least expected. Respectively, the ECB has recently issued a multi-level action plan for the period 2021-2024 on the introduction of environmental protection criteria in the banking system. Besides the purely macroeconomic stability aspects of environmental degradation (leading to the loss of natural capital), one of the most important identified goals is the incorporation of environmental risks in credit ratings for collateral and asset purchases [17]. In addition, the EBA launched an EU-wide pilot exercise on ESG risks that included a proposal for the establishment of GAR under the EU TSF [6, 16]. Practically, this context translates into a fundamental review of credit rating methodologies and an operational “game changer” in the financial sector, as for the first time the criteria extend beyond capital requirements.

Central banks have also begun to fundamentally reassess the role of money itself in the global economy; in some cases tethering it directly with critical natural resources, such as forests in the role of carbon sinks and metabolic networks [24]. In any case, monetary architectures start leaning towards more decentralized and local forms of financial organization; especially if respective business models and financial agreements combine the CE and ecosystems’ conservation. A vehicle for achieving a higher level of consensus for global trade and corporate transactions that include environmental goods and services via the banking system is the reform of the Basel III and the introduction of Basel IV regulatory frameworks [19], towards the establishment of environmental credit ratings that affecting the overall credit rating of a financial instrument’s recipient. Additionally, the “Green Swan” concept has an operational utility besides its epistemological value, as central banks provide themselves with a quantification tool on financial risks’ sources and incorporating environmental performance KPIs to their credit ratings’ evaluations that will orient commercial banks’ portfolios as well. In addition, the EBA introduces ESG risk requirements as well as a GAR assessment for commercial banks according to the EU TSF. The roots of such unprecedented changes can be identified two decades back in the *Stern Review on the Economics of Climate Change* [25].

With central banks at the role of “gravitational monetary centers”, the large-scale commercialization of CEF is currently steered by banking compliance authorities. Respectively, new tailored financial engineering schemes will become an inseparable element of the ongoing paradigm shift. In this context, ChL contracts are introduced as flexible bilateral or multilateral agreements with well-defined rules and quantified performance criteria, filling the gap of resource recovery and ecosystem conservation performance KPIs. Thus, ChL engineering with such underlying indices would allow CE practices to release their full potential for industrial parks, increase the diversity of CF “species” and tailoring options for financial institutions and at the same time completely align to the EU GD. In turn, CEF inventories applied successfully to a small number of counterparties could be engineered to upscale towards more complex structures, such as for whole industrial parks that wish to issue debt for investments on infrastructures that maximize total energy and mass recovery, based on the EU GBS [6].

2.2. The EU shift towards environmental national accounting

Although institutional CEF shifts comprise a pillar for the large-scale market deployment of IS, the monetization of environmental corporate and national accounts’ is the corner stone for the accurate pricing of diminishing reserves of natural resources and ecosystem capacities. By establishing SEEA frameworks, a systematic record of environmental and resource utilization performance becomes a standard practice. Integrated economic-environmental cost-benefit accounting should be coupled to the pricing of natural resource reserves (whether material stocks or carrying capacities) so that a proper “scarcity signal” via the price mechanism can be sent to both producers and consumers. Besides that, no economically meaningful or sufficient investment can be implemented by financial institutions on technical measures of resource use efficiency increase -with the CE and IS being among them- unless the resource prices have sent a prior message for that need. In a few words, whatever is to become a financial investment target must have been accounted for beforehand.

There are numerous methods one can utilize to account for natural resource scarcity; however, the need for SEEA frameworks has been repeatedly substantiated for depicting accurately total resource costs for corporate and national accounts [27-30]. In addition, SEEA frameworks should definitely involve measurements across a resource’s life cycle -from its *Extraction* to its *End of Life* (EoL). To deal with the high heterogeneity of more than 400 LCA methods, the EU has begun establishing the PEF as an umbrella of guidelines for all future LCAs [30-31]. Specifically, the PEF is the dominant candidate in the EU states for assessing accurately environmental value chains at the corporate, international (global trade) and national accounting level, as well as the environmental goods’ costs, revenues and pricing. Environmental accounting has been a fundamental factor for the acceleration of the EU GD as well as the EU TSF as its main vehicle through the establishment of the EU GBS.

Although the SEEA foundations go quite back in time, the first significant collective work was implemented in 2003, under the term *Integrated Environmental and Economic Accounting* [8], with the collaboration of the EC and all major international organizations, in a first attempt to create a manual towards a coherent system for corporate and national environmental cost-benefit accounting. The manual was updated in 2012 into the latest version of the SEEA [10] at the initiative of the EC as a benchmark for environmental and resource efficiency performance and hence for the proper tailoring of CEF instruments that would further select KPIs as *underlying indices*. The identification of the environmental costs and benefits of products or services within a generally acceptable accounting framework would automatically provide financial institutions with the proper information for building all national and corporate *environmental credit profiles* -irrespectively of economic size, national income or corporate turnover (SME, mid-cap or large corporation)- and additionally address the request for accounting transparency and “green washing” prevention. Specifically, for environmental value chains at the corporate level the DJSI [31] is an index that accounts for various dimensions of corporate environmental performance and affects a corporation’s stock value; thus being highly compatible to the SEEA. A critical DJSI dimension directly related to IS and ChL concerns participation in supplier networks that provide recycled materials. As IS clusters are at the core of recycled or recovered materials, a business’ ChL contract with an industry for utilizing recovered materials would increase its DJSI performance.

Specifically, material resource use optimization constitutes the one significant aspect of the CE and sustainability. A complementary aspect for classifying a CEF instrument as eligible for CEF concerns the conservation of ESs’ value. For example, when a VAC is recovered from a wastewater matrix, it is not only the savings of virgin natural resources (that would otherwise be used for the VAC's composition) achieved. As the combined effect of waste discharge and various uncontrolled effluents threatens with severe distortion of the interlocked biogeochemical sequences of ecosystems and degrades their ability to maintain their functions [32], the avoidance of the environmental pollution from waste discharge offers a respective conservation of ecosystem features and bio-capacities. Ecosystem features synergistically manifest a variety of functions with economic value for human societies. Specifically, at the biophysical level, the ability of ecosystems to produce valuable life-supporting and economic services primarily relies on the stability of their biogeochemical metabolic ability and networks. Such indicative services are timber, flood protection, crop pollination, nature-based recreation, a variety of genetic resources for nutritional and pharmaceutical purposes, as well as social and cultural value that have numerous utilizations for humans at a very low cost.

In this context, the TEEB framework could be considered complementary to the SEEA, having been developed in order to put a monetary value into ecosystem services and estimate accurately the environmental damage caused -or saved if financed sustainability projects take place [33]. In line with the TEEB, various works on CEF for the conservation of continental and marine ecosystems have been published [34] for the developed, the developing [35] and the least developed world that may lack even basic financial services [36] but has the opportunity build the foundations environmental finance instruments from the beginning. In fact, in some cases the accounting methodologies have even been incorporated into state legislations. Taking into consideration the local biophysical and social (such as stakeholder interests) features of ecosystems in which industrial activity takes place, it is clear that tailored CE financial engineering -such as ChL- will comprise a very flexible and scale-free vehicle for the implementation of integrated (technological, governance, financial) sustainability policies to release the potential of "symbiotic markets" and be established as mainstream activity for private financial institutions.

3. Theoretical Foundations of CEF

In Chapter 3 we present the theoretical foundations on which we build ChL mechanics. Specifically, the issues we are concerned are: **(1)** An examination of the *ChL origins* and the international pilots introduced and surveyed by the UNIDO; **(2)** The structuring of *ChL mechanics* on the revised foundations of the SP [20], as well as how the market structure can lead to synergistic industrial schemes; **(3)** What are the microeconomic theoretical principles by which ChL works as a *mutually beneficial VAC recovery synergy* and **(4)** The major *ongoing developments of the EU GD and TSF* that inaugurate the large-scale deployment of tailored IS finance instruments from the private sector, continuing the context presented in Chapter 2.

3.1. CEF: The case of Chemical Leasing (ChL)

The ChL philosophy addresses two major issues concerning the transformation towards the CE: **(1)** The increase of chemical compounds' use efficiency via its adaptation to the EPR principle to the business practice of chemical industries, motivating them towards the design of low environmental impact chemicals at life-cycle as well as the provision of consultation for their optimal use and **(2)** The shift

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from the concept of a (purchased) product's *ownership* towards the concept of *renting* a product's properties; in short, that being *turning the owner to a user*. These two elements constitute an integrated view of the ChL business model.

3.1.1. The origins and philosophy of ChL

ChL finds its official origins in 2004, as an innovative business model from UNIDO with the direct support of the Austrian government. In 2007, the German government joined the cause, followed by the Swiss government in 2013 [21]. Initially, the UNIDO ChL program was launched as a pilot with 12 case studies in 8 different countries and 11 different sectors [37] in controlled commercial environments. Since the program's inception, pilot projects have been conducted in close cooperation with NCPCs, including South American, African, East European and Asian countries. Today, the UNIDO records that more than 100 companies worldwide have included ChL in their standard business practice.

The ChL concept was developed to deal with the core issue of how to detach revenues and profitability from the need to maximize the volume of chemical compounds sold, as it was the conventional practice in the chemicals' sector [7, 21]. Besides the profound correlation between the volume of chemicals used to the discharge of wastewater in ecosystems and degradation of their services, an environmental *moral* hazard emerges. Specifically, with the high importance of targeted commercial chemicals, producers tend to underestimate the environmental efficiency during the design phase of their compounds at *life-cycle* level. With this practice, emphasis has been given so far at the *Use* level, while the *End of Life* (EoL) level was heavily underestimated. This has resulted so far to the manufacturing of chemical compounds that are difficult or very costly to neutralize or recover from solid or liquid wastes. With the lack of proper EPR legislation this approach initiated and enhanced a *vicious circle* of unsustainable paths of chemicals' use, crowding out or even cancelling the progress achieved in other vital sectors, such as the accrued energy efficiency increases in the EU [38-39]. Hence, currently the by default *ecological re-design* of chemical compounds comprises a priority chemical engineering aspect accompanying ChL practices at the financial level.

3.1.2. The context of ChL

Since 2004, significant findings have been produced on the utilization of ChL by the UNIDO pilots as well as other case studies. The literature is diversified on these results; for instance, some academic works provide a list and an overall examination of ChL practice successes as well as a hierarchy of the ChL with compatibility and compliance to the EPR principle [40], while other works analytically present the benefits of ChL for industrial processes with traditionally heavy environmental impacts, such as conveyor lubrication in the beverage industry [41]. Complementary to the above, some works attempt to present a basic typology of possible partnerships in ChL agreements [37] along with an introductory presentation of quantified results in specific countries. For instance, partnerships could concern the supply of the equipment for processing the liquid waste after the chemical's use that may belong to the producer or rented from a third party specialized in the field. Respectively, the consultancy on the chemical's optimal use could be outsourced to a third party by the producer and applied to the user. There are numerous possible combinations that can be applied in such agreements that are related to the *cost* *structure* and *ontology* discussed in the ULTIMATE Subtask 2.2.2 and scrutinized in a related published work [20]. Other ChL works introduce a more thorough attempt to combine qualitative and quantitative assessments to create ChL performance KPIs [42] for promoting sustainable chemistry practices that could also be compatible with the philosophy of ESG criteria. Continuing this effort, other works address the issue of quantifying ChL efficiency with energy and mass balances across the life-cycle of a chemical compound [43] also with a view of the relation between the sale price / original cost to its recovery risk. Another category of related works deals with how the social benefits or positive externalities of ChL could be incorporated to standard corporate environmental accounts and CSR reporting [44]. More recently, UNIDO published a report on ChL for cleaning operations [45] where the performance in core ecosystem health variables was assessed. Finally, the most recent works on ChL examine the potential for its improvement [46], along with the design of user-friendly questionnaire models for businesses [47].

3.1.3. Typology and depiction of ChL business agreements

Within the above context, we depict in Figures 1 and 2 below the two basic models examined in our work. The first model concerns the standard *Bilateral* UNIDO scheme, with two counterparties:

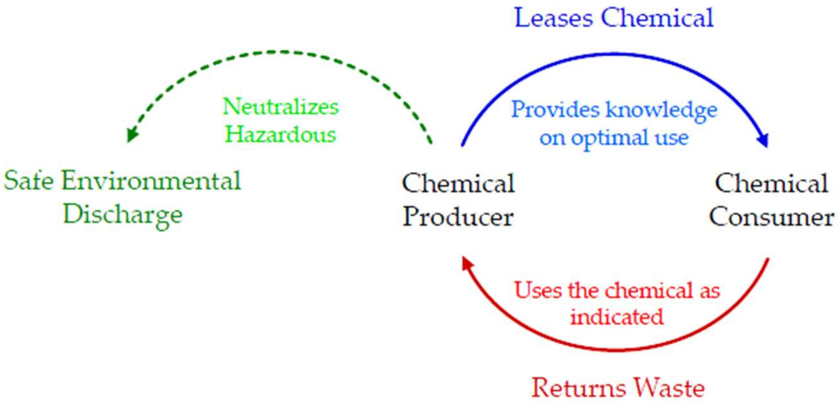

Figure 1: Schematic depiction of the *Bilateral* UNIDO standard ChL model with 1-level agreement.

More analytically, the *Bilateral* ChL model includes collaboration between the chemical’s producer and the user at life-cycle level. Specifically, the producer provides the chemical to the user along with consultation on its optimal utilization in order to minimize its amount and waste discharged in the environment. The point of attention in the standard UNIDO model is the *transfer of know-how* from the producer to the user on the chemical’s optimal use; which binds the producer of dedicating R&D funds on manufacturing *by default* more environmentally-efficient chemicals, as this knowledge will be partially shared with its client. An enhanced version of the Bilateral ChL model (as also depicted in Fig. 1) is the additional element in the agreement where the producer is legally binded to receive the wastes of the user provided that the latter has used the chemical in the designated way. In this way, the agreement is more powerful as it secures the EPR principle application by establishing checks and balances for both counterparties. Specifically, **(a)** The *User* ensures that the producer’s consultation is indeed effective as via the designated use of chemicals the amount, related costs and generated wastes will be minimal and expected, while **(b)** The *Producer* ensures that the User has indeed used the chemicals as it was exactly designated; something that is verifiable from the produced wastes. Once the wastes are the expected ones, the last step of the agreement includes the Producer's responsibility to manage and neutralize hazardous compounds for safe environmental discharge.

In Fig. 2 we generalize the standard model to the *Multilateral/Bus* scheme that is more complex and also includes the Producer's option to sell the chemical. This scheme deals with chemicals' producers that continue their standard business practices but are constrained by the environmental legislation.

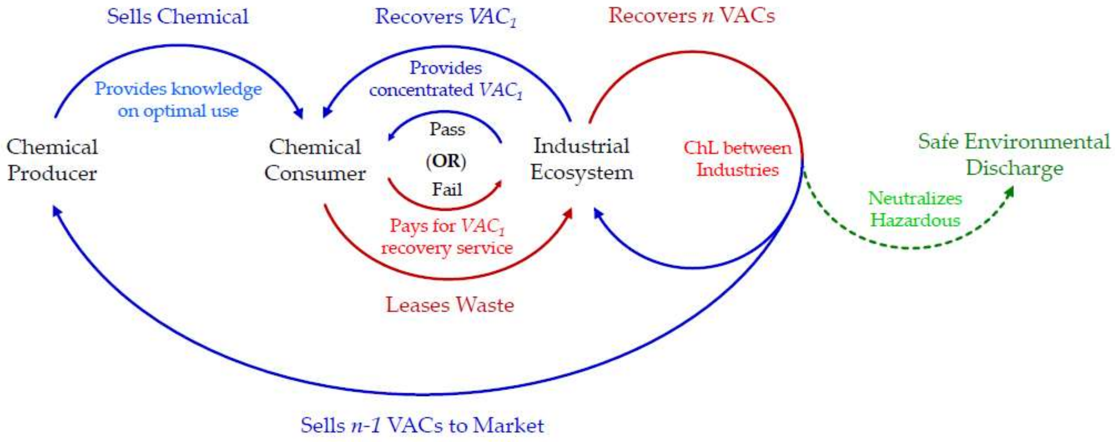

Figure 2: Schematic depiction of the extended *Multilateral/Bus* ChL model with 2-level agreements.

Respectively, the *Multilateral/*Bus ChL model involves a higher complexity of relationships, including both the case of selling chemicals (hence, the User's ownership and responsibility to manage wastes is preserved) and the involvement of third parties that are specialized in recovering VACs from waste matrices. In this case, the main diversification is that the User would seek a specialized third party to outsource (lease) the management of its wastes and minimize its environmental footprint. This agreement would include the payment for the (outsourced) neutralization of wastes along with the service of recovering identified VACs. During this process, several intra-industrial cluster agreements may also take place in order to maximize the number and amount of identified VACs, minimize or eliminate hazardous compounds before safe environmental discharge and sell back to the market any VAC that is not a part of the initial agreement between the chemicals' User and the cluster.

3.1.4. The Sherwood Plot (SP)

An important aspect for implementing a Multilateral/Bus ChL contract is the cost of a VAC's recovery across the processing of a waste matrix. In principle, the SP is a *microeconomic chart*, depicting the relationship between a VAC's *dilution* in a waste matrix and the *Cost of its Recovery* from a single industry. Although the SP could theoretically take any other nonlinear form (monotonic or not), the *linear regression model* -either deriving from a mathematical transformation (e.g. a log-log plot) or from default data- is the most convenient to use, without excluding more complex depictions. Hence, the basic SP form concerning a VAC's recovery cost at every level of its dilution in a waste matrix is:

$$C\left(m_i^{-1}\right)=a_i+b_i\cdot\left(\frac{1}{m_i}\right) \qquad (1)$$

In Eq. (1), for every VAC$_i$ the *cost of its recovery* C_i is a function of the VAC's *dilution* in terms of reverse mass concentration $1/m_i$, parameter a_i concerning *constant costs* (costs that are paid by the industry irrespective of the VAC's recovery volume) and parameter b_i concerning *variable* costs (costs that are proportional to the VAC's dilution level). Alternatively stated, the SP depicts the reverse proportional relationship between VAC dilution and recovery cost in wastewater matrices, due to the increasingly lower statistical probability of finding the VAC within a waste matrix. The SP's rationale can be replicated for the recovery of all types of materials and even generalized for all types of resources, including energy recovery and wastewater reclamation (as it is often a complementary product to VAC recovery). The theoretical framework for working on the cost-benefit analysis of VAC recovery is the SP), as it was restated in [20] and presented in Fig. 3 below:

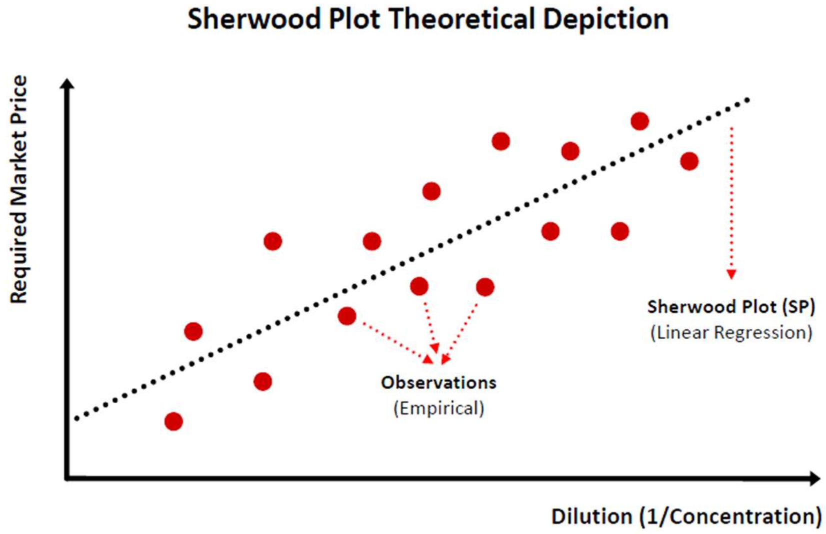

Figure 3: Schematic depiction of the *Sherwood Plot* (SP) on the relation between a VAC's dilution in a wastewater matrix and its cost of recovery from it.

In addition, the SP is a chart of optimal dilution-cost coordinates for the single industry. According to Fig. 4a we may begin from any initial coordinate of VAC dilution and cost of recovery (X_1,Y_1). By default, this option creates four distinct areas where each has specific microeconomic properties. The boundaries of these areas are determined by the lines $Y=Y_1$ and $X=X_1$ respectively $\forall X,Y\in(0,+\infty)$, with the combination (X_1,Y_1) as their unique intersection point. Each shift from the central coordinate (X_1,Y_1) to any of the four formed areas has a particular microeconomic meaning.

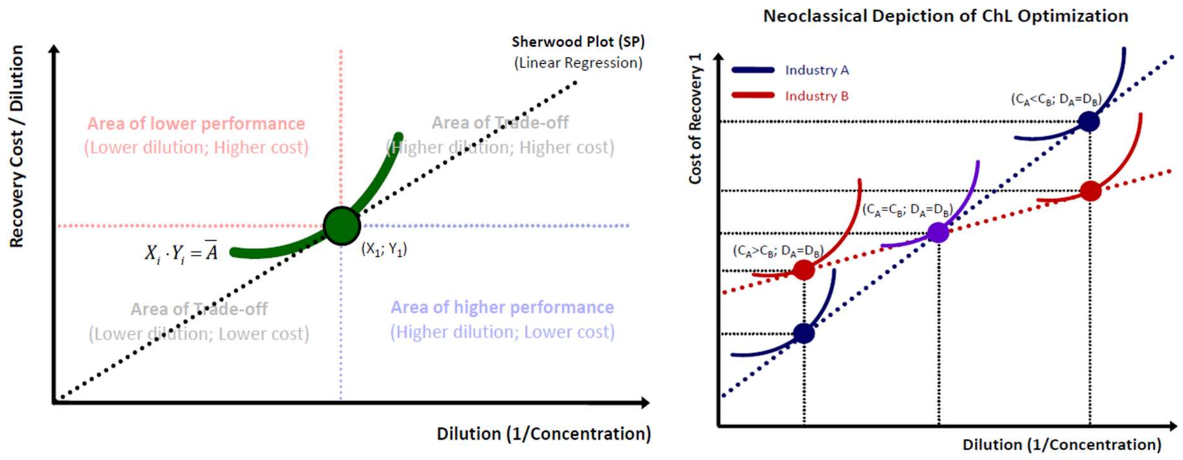

Figure 4: Schematic depiction of **(a)** The SP as a chart of microeconomic optimal dilution-cost points (left) and **(b)** ChL optimization potential along the SPs of two industries (right).

The resultant of each possible dilution-cost coordinate shift can be described with the following options: **(a)** An upward shift across the line $X=X_1$ (hence for $Y^*>Y_1;\ X^*=X_1$) line signifies that the VAC's recovery cost from the waste stream has increased for the same dilution level. A shift to the left across the $Y=Y_1$ line (hence for $Y^*=Y_1$; $X^*<X_1$) signifies the same recovery cost but for lower dilution levels (which at the X_1,Y_1 coordinate depicted a higher dilution level). Any other coordinate falling into these boundaries and in the compartment in between (upper left) signifies relocation towards a *worse by a Pareto criterion performance* in the SP, with higher VAC recovery costs and lower dilutions in relation to X_1,Y_1; **(b)** In contrast, a downward shift across the line $X=X_1$ line ($Y^*<Y_1$; $X^*=X_1$) signifies that the VAC's recovery cost from the waste stream has decreased for the same dilution level. Respectively, a shift to the right across the $Y=Y_1$ line ($Y^*=Y_1$; $X^*>X_1$) signifies the same VAC recovery cost but for higher dilution levels. Any coordinate falling into these boundaries and in the compartment in between (lower right) signifies relocation towards a *better by a Pareto criterion performance* in the SP, with lower VAC recovery costs and lower dilutions in relation to X_1,Y_1; **(c)** For the remaining area in the lower left compartment and **(d)** the upper right compartment, the resultant is indefinitive as all these coordinate sets consist of a trade-off between lower (higher) VAC dilutions and lower (higher) recovery costs. From a microeconomic standpoint, these areas crossed by a SP depict in principle the *reverse proportional relationship* (irrespective of its intensity) between VAC dilution and cost of recovery.

An additional element that a typical SP (whether linear or non-linear) crosses through the trade-off areas (lower left, upper right) is that these compartments are the only ones providing a full chart of *infinite equivalent solutions* to the initial coordinate X_1,Y_1, so that the *per unit* (average) cost remains constant. In general, the benchmark average cost of VAC recovery for a variable dilution level is:

$$C_i \cdot m_i^{-1} = \overline{C} \qquad (2)$$

By Eq. (2) to maintain a constant average cost, the total recovery cost C_i must be increasing across increasing dilution, as depicted in Fig. 4a. Alternatively stated, the ratio between the VAC's average cost of recovery and its total cost of recovery must always depict the dilution level.

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Additionally, according to Fig. 4a a SP is also a sub-chart gathering the subset of *all optimal* dilution-cost coordinates out of *all possible* coordinates formed by *all equivalent per unit cost charts* to which the SP comprises the common tangent. Except for the common coordinate (X_1,Y_1) that depicts a *pivotal equivalent solution*, Fig. 4a presents all other coordinates of the $X_i \cdot Y_i$ chart that are positioned higher than those of the SP for the same segment, depicting higher average recovery costs. Hence, for any set of dilution values X_i, where $\forall X_i \in (0,+\infty)$, the SP comprises the *Pareto optimal* chart of the minimum recovery costs. From a microeconomic view, this comprises also a proof of why in Fig. 4b there is a benefit margin and intra-industry ChL agreement potential in a VAC's recovery between two industries with different SPs except for the point where the SPs intersect (point in purple).

3.2. Macroeconomic upscaling of CEF instruments

Continuing from the microeconomic quantitative foundations of the SP, we describe briefly the necessity of tailored ChL contracts for different (in terms of features) eco-industrial parks. SP-based ChL contracts are more universal as via the necessary descriptive adjustments, they can fit to a variety of eco-efficiency indices, with underlying reference reduced to dilution-cost relationships.

With VAC recovery and ESs markets under establishment and new ChL target groups constantly identified, the various eco-industrial parks under formation are to be guided towards the strategic steps for leveraging CEF instruments. The EU GD comprises a beacon through the realization that with the current financial architecture, massive amounts of funds can be directed to environmental projects for recovering numerous VAC species' that have been identified to embody significant monetary and environmental value. Although this potential is not yet fully identified, strategic use of CEF instruments can achieve more decentralized production of wealth and be targeted towards projects with the highest economic and environmental impact.

In December 2019 the EC set the ambitious target to turn the EU into the first climate-neutral area until 2050, by introducing the EU GD [13]. Numerous actions are to be followed in various sectors, including energy, transport, food systems, construction, biodiversity, ESs valuation, where potential carbon tariffs are to be appointed for member states not curtailing GhG emissions at the rate set. In addition, the EC adopted the new *Circular Economy Action Plan* (CEAP) in March 2020 [14]. It is a main building block of the EU GD and vital element of CEF schemes, while besides the mitigation of environmental pressures the transformation is expected to create new professional specialties along with sustainable growth-related jobs. Finally, on July 14, 2021, the EC adopted a series of legislative proposals on energy efficiency, where heat recovery (as the 2nd ULTIMATE pillar) by industrial ecosystems is part, included in the "Fit for 55" package [48] with the intermediate target of at least 55% net reduction in GHG emissions by 2030.

In addition, significant market reshapes leave no doubt on the new "market attractors" that will draw significant capital to the CE. In November 2019, in line with the ambition behind the EU GD, the EIB declared its transformation to an EU "climate bank" [1], where along with the EIF it committed on delivering the UN SDGs. Specifically, the EIB's decision consists in increasing its level of support to the thematic areas of the EU TSF; which translates in exceeding 50% of its overall lending activity by 2025 and beyond, and thus leverage a €10^{12} of investment by the EIB Group over the decade ahead. Additionally, the EIB Group also sets the conditions to ensure that the rest of its 50% of capital funding is not contradictory to the direct 50% funding; hence paving the way for CEF instruments to dominate the financial engineering applications for at least until 2030. This unprecedented new level of commitment is designed to accelerate the transition to a sustainable CE.

Moreover, the above include an additional commitment for a proposal regarding a just transition due to the fundamental reshape of traditional economic sectors. That consists in limiting the gap of the access to CEF instruments between large enterprises and SMEs; with the latter accounting for 99.8% of all enterprises in the EU-27 NFBS in 2020. Of the total number of SMEs in the EU, 93% is recorded as micro SMEs generating 53% of value added and employing 53% of the total EU's work force [22]. SMEs and micro-SMEs have also been identified as a core target group and "beachhead market" for secondary (recovered) materials' supply.

4. Chemical Leasing (ChL) Modelling

In Chapter 4 we develop the *Multilateral/Bus* ChL stochastic framework that integrates the process of waste matrices arrivals to the optimal allocation of a VAC's recovery based on individual industry SPs. The combined SPs of at least two industries form the *market SP*, depicting the *collective* VAC recovery performance. An exhaustive quantitative analysis of the individual SP along with the VAC recovery market formation process along with market concentration diagnostics and KPIs can be found in a related ULTIMATE-funded paper by Karakatsanis and Makropoulos [20].

4.1. Waste matrices' arrivals: Preparing the data

A significant mathematical SP aspect when VAC dilution is used instead of VAC concentration is the non-constant increases of the fraction $1/m$ across constant decreases of concentration m. This results to a nonlinear $1/m$ growth pattern that follows a pattern of *Harmonic Series* similarly to the decay function of $1/n$ across constant changes of n. Primarily, the use of reverse concentration provides conceptual, graphical and visual SP conveniences as it allows the depiction of the dilution-cost coordinates with increasing values at both axes; beginning from high concentrations (low dilutions) and low recovery costs to lower concentrations (higher dilutions) and high recovery costs. However, in this way when the VAC dilution data (real or simulated) are plotted in relation to their frequencies they yield asymmetrical distributions like the ones presented in Fig. 5a. Whatever the true distribution of the VAC dilutions in a population or sample of n wastewater "packages" may, its true properties will be presented distorted, exactly due to the transformation of concentrations into dilutions; hence, this view needs to be corrected.

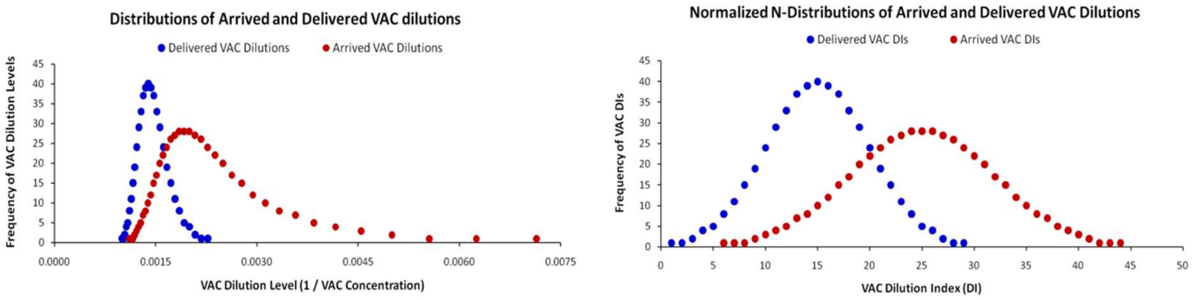

Figure 5: Transformation of **(a)** raw VAC dilution data into **(b)** normalized *VAC Dilution Index* (VAC DI).

In Fig. 5a we present such a distortion example of a perfectly symmetrical Normal Distribution that visualy provides a false impression of a positively skewed Normal Distribution or even a Log-Normal Distribution. Specifically, in Fig. 5a two simulated samples of 500 of VAC dilution observations eachare presented. The first distribution (in red) is the distribution of VAC dilution level frequencies at the arrival to the IS cluster for further processing, while the second distribution (in blue) is the distribution of VAC dilution frequencies at the delivery (after processing and recovering them from wastewater). Both distributions are described by the formula *1/Concentration* (with concentration expressed as mg/L). By keeping the data at that scale, a visual distortion is created, giving the impression of asymmetrical distributions. By correcting the data by simply assigning to each dilution level a constantly increasing VAC *Dilution Index* (DI) (e.g. for dilution 0,001→DI=1; 0,001020→DI=2 etc.) the data are visualy corrected back to resemble the properties of the true distribution. In our simulated case the VAC DI ranges from 1-50 (*DI*∈(0,50)); however one could choose any range according to the desired presentation of frequecy density. With this correction, Fig. 5b depicts a symmetric Normal distribution with Mean=25, Standard Deviation=7, Skewness=0 and Kurtosis=-1,10. With the same rationale, we respectively simulate the distribution of VAC deliveries after processing and dilution reduction with Mean=15, Standard Deviation=5, Skewness=0 and Kurtosis=-0,14, suggesting that at delivery higher cocentrations of the VACs are achieved due to recovery. According to the above, in Fig. 6 we may depict the frequency of VAC dilution levels at the arrival of the *N*=500 simulated samples assuming normality with the above mentioned parameter values.

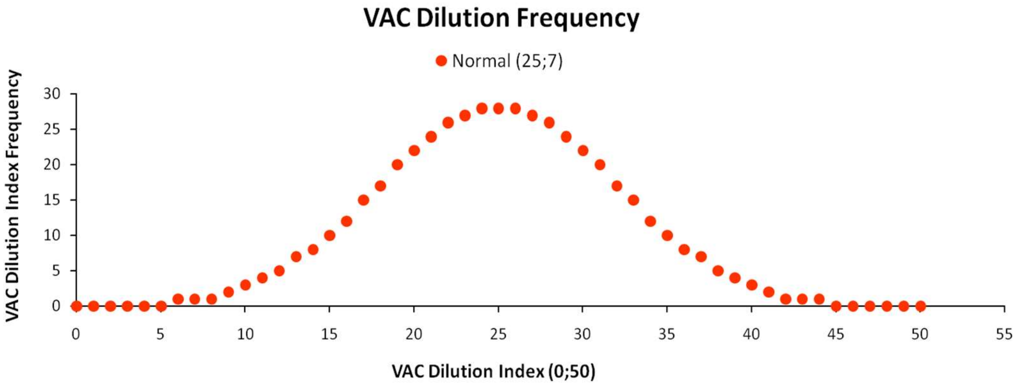

Figure 6: Simulated VAC dilution frequencies that are normally distributed (Mean=25; Standard Deviation=7) across a VAC DI range (0,50).

Of course, in real world cases the distribution of VAC dilution level frequencies could be described by any other distribution as well-symmetrical or asymmetrical. The above simulation assumptions are adopted here for convenience to present the model building purposes in the simplest possible way.

In turn, to compose a VAC's recovery market we need to define some fundamental characteristics of the two individual industries as its elements: *Industry A* and *Industry B*. We have already assumed a difference in their parameters, where specifically $a_{iA}<a_{iB}$ and $b_{iA}>b_{iB}$, according to Eq. (1). We also assume that both industries have linear SPs. Additionally, we assume that both industries have a common *technical limit* and *operational range*; meaning that there is an upper VAC dilution level after which none of the industries can technically achieve its recovery. Both industries can operate (to recover the VAC) in the range between that technical limit and zero VAC dilution, meaning that both industries have exactly the same technical capabilities. With these assumptions, Fig. 7 depicts the formation of the market's VAC recovery SP as a composition of the two individual SPs.

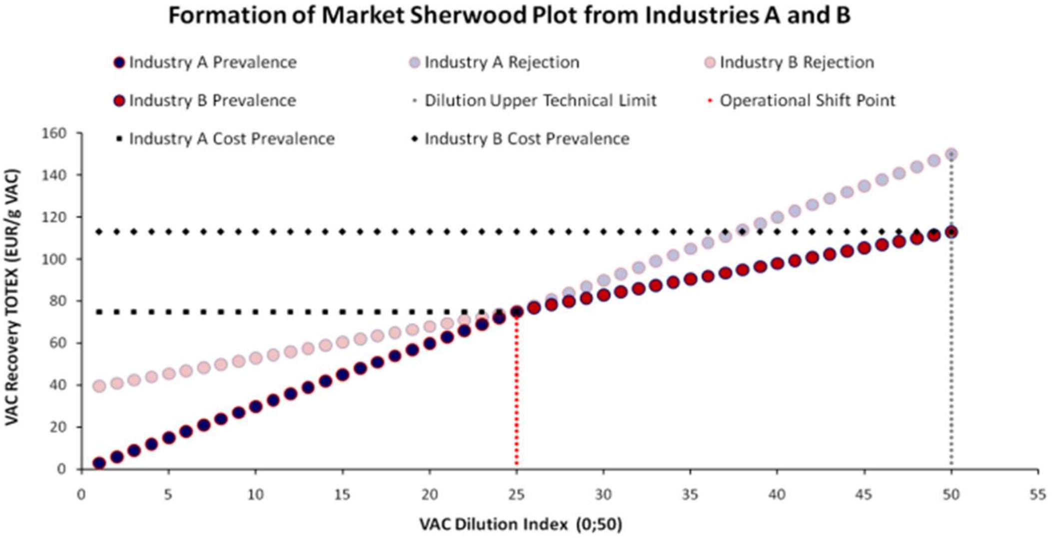

Figure 7: Formation of a VAC recovery *market SP* composed by the minimum cost ($MinC_i$) function.

Based on the above model, as each industry is more cost-efficient at specific domains of the VAC DI range, the market will allocate respectively industry shares by *Cost Prevalence*; that being where the VAC's recovery is achieved at the minimum cost. In our example, *Industry A* as *variable cost intensive* dominates in a range of lower VAC DI values ($DI \in [0,25)$), while *Industry B* as *constant cost intensive* dominates in the domain of higher dilutions ($DI \in (25,50]$). The SPs of the two industries intersect for a VAC DI value =25, at the only dilution level where both industries can recover the VAC at the same cost. This is the *operational shift point*, as across an ascending or descending sorting of the VAC DI, before or after that point, another industry starts to become more cost-efficient and, hence, begins to dominate in the VAC's recovery. In our example, the operational shift concerns the transition of the VAC's recovery from industry *A* to *B*. However, irrespective of these assumptions the total number of operational shift points is relative; depending on the number of industries operating in the VAC DI rage. For convenience, here we assume that the market consists of only two industries.

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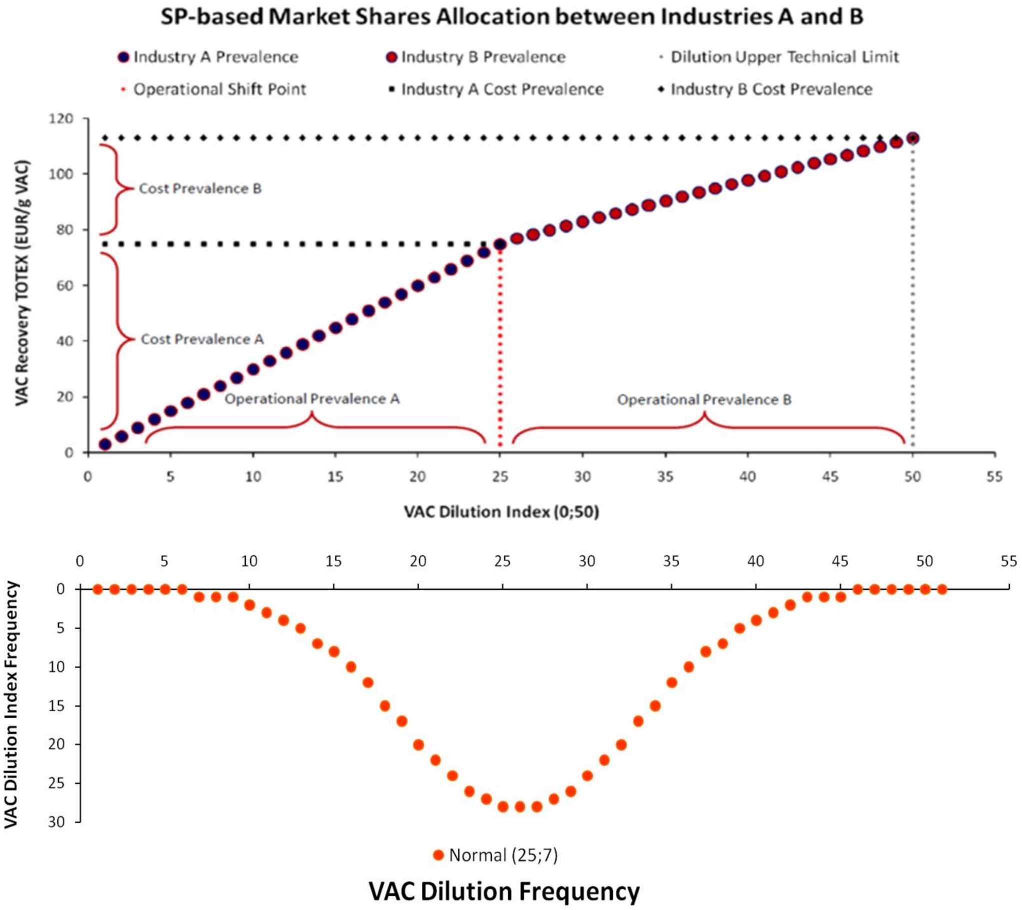

Figure 8: Integrated depiction of the VAC dilution frequencies distribution across the market's SP.

By integrating the market SP and the frequency of VAC arrivals' frequency, we may depict in Fig. 8 the range at which ideally each industry is more cost-efficient at recovering the VAC. In our simulated example, as the market's VAC DI range is allocated in equal parts, with the VAC dilution frequency distribution following the same pattern, the optimal allocation would be respectively for Industry A to recover all VAC arrivals with *VAC DI*∈(0,25) and Industry B to recover all VAC arrivals with *VAC DI*∈(25,50); hence, VAC recoveries to be allocated in exactly equal shares by the two industries.

4.2. Market information and VAC recovery allocation

An important aspect in IS clusters consisting of many industries with different process engineering expertise is the level of information of the *Customer* (here the chemicals' User) on which is the most cost-efficient industry to recover the VAC. In the above simulated example, we connected the SP to a VAC's dilution frequency, where VAC dilutions are described by specific distributions. However, these conditions tell us nothing on *how* the VACs arrive to each industry. If we consider the VAC arrivals as random signals, we can identify two main cases: **(a)** VAC arrivals with *Complete Information*; which is the *customers know in advance* the Cost and Operational Prevalence ranges of both industries and -hence- they know where to optimally assign each VAC recovery package by its DI or **(b)** VAC arrivals with *Incomplete*

Information, where the *customers are a priori unaware* of the industries' ranges of prevalence. In this case, they only see an industrial cluster and are unconcerned to the additional intra-industry arrangements needed to recover the VAC at the minimum cost, as long as they receive it at the agreed concentration.

4.2.1. Complete Information

As mentioned, in this case, customers know in advance the prevalence ranges of both industries. Consequently, they know where to optimally assign each VAC recovery package by its DI. Projected in our numerical example, this would mean that all VACs with *DI*<25 will be assigned directly to Industry A, while all VACs with DI>25 will be assigned to Industry B [for the sake of simplicity we assume that VACs with *DI*=25 are either assigned by the *Uniform Distribution*, with the rationale of a "Fair Dice" (*p* = *1-p* =0,5 for both industries A and B) or that there are no cases of *VAC DI* =25 but only cases of asymptotically approaching it, with values either marginally below or above *DI*=25] as presented in Fig. 9.

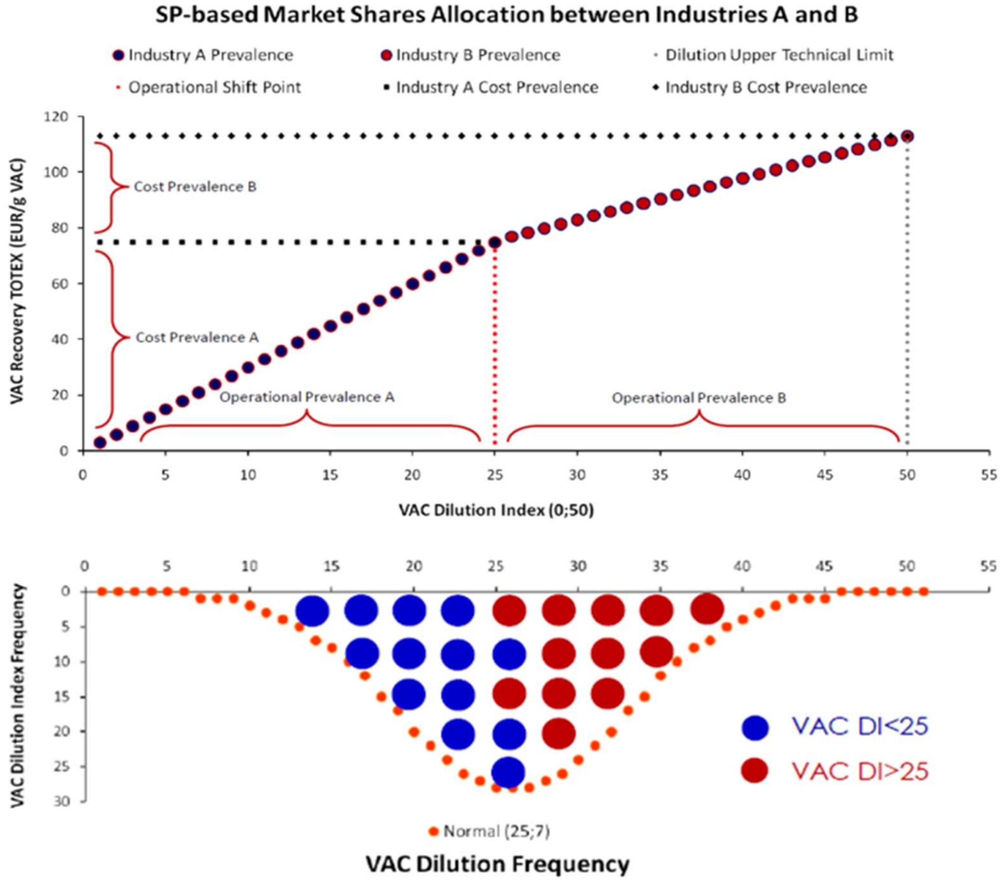

Figure 9: Allocation of VAC arrivals by VAC DI level with *Complete Information* of industries' *Operational* and *Cost Prevalence* ranges.

In the above scheme, the ChL agreement would reduce to a *Bilateral* contract as presented in Fig. 2; involving only the customer and the IS cluster without further need of intra-industry agreements. The physical foundations of such a case could be traced in the existence of advanced sensors and real-time classification infrastructures that are able to handle huge amounts of data via fast and accurate sampling methods accompanied by accurate predictive algorithms on VAC DI distributions.

4.2.2. Incomplete Information

Contrarily to the *Complete Information* case, it is frequent that customers have only partial or even no information on the industries' SPs; thus, are unable to optimally assign VAC recoveries by their DIs directly to the most cost-efficient industries. In short, customers see only a "*black-box" industrial ecosystem* being completely unaware of the *intra-industry* structure. Here, there may also be *partial* or *no* knowledge of the overall VAC DI distribution of a *N*=500 population of wastewater packages but *definitely no knowledge* of each package's VAC DI. In short, while it may be known how the population of *N*=500 packages is distributed in terms of VAC DI, each wastewater package is also a "black box" as far as the VAC's DI contained in it is concerned. With lack of any preference towards a specific industry (e.g. due to marketing or customer relations) that makes them *commercially equal*, customers will rationally choose to assign their wastewater packages according to the only known information; which here is the overall VAC DI distribution. With this pattern, the same number of packages will be initially assigned to each industry (250 in industry A and 250 in Industry B), but this time in a *scrambled* way, as presented in Fig. 10.

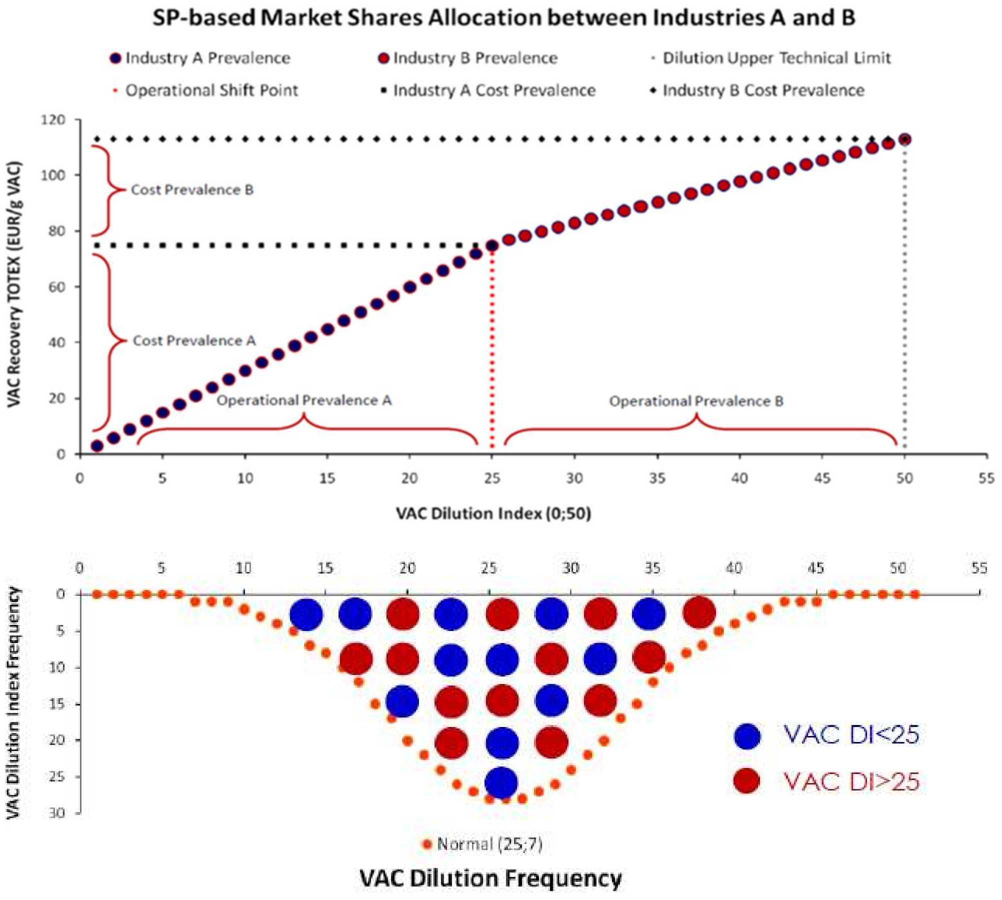

Figure 10: Allocation of VAC arrivals by VAC DI level with *Incomplete Information* of industries' *Operational* and *Cost Prevalence* ranges.

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According to Fig. 10, some VACs with $DI<25$ will be assigned to Industry B that is prevalent for $DI>25$ and vice versa. In such a case, industries have a motivation to collaborate with 2nd level intra-industry ChL contracts and mutually outsource the recovery of VACs with DIs outside their prevalence. In the case of *Incomplete Information*, the initial (by the customer) *fair* assignment of wastewater packages follows a *Galton Board* (GB) process [49]. A GB follows the *Binomial Distribution* that -in turn- for a large sample (such as $N=500$) asymptotically approaches the *Normal Distribution*:

$$P_p(k;n=N;p)=\binom{N}{n}\cdot p^n\cdot q^{n-k} \qquad (3)$$

Eq. (3) describes the stochastic process calculating the probability to have k assignments across a sequence of n independent *Bernoulli Trials*, at a constant *fairness level p* of each separate trial. In overall, 500 wastewater packages arrive at the industrial cluster, with each package containing the VAC at specific DI. The population $N=500$ of wastewater package arrivals follows a binomial process. Assuming no bias towards a specific industry (the industries have equal power in the market; $p=0,5$) the arrivals will preserve the properties of the (Normal) pool's distribution. Hence, for a total number of arrivals $N=500$, spread at a total range of VAC DIs (0,50), 50% percent of the arrived packages will be distributed to the segment (0,25) of the DI range and 50% to the segment (25,50) of the DI range. Alternatively stated, out of a $n=N=500$ fair ($p=0,5$) trials, the most probable outcome is that $k=250$ observations will be assigned to the *VAC DI*∈(0,25) segment and $n-k=250$ observations to the *VAC DI*∈(25,50) segment. Additionally, the *sequence* of arrivals has no impact on the allocation; e.g. in Fig. 10 even if all "blue" packages happen to be the first 250 selected and distributed altogether by the Galton Board and then the 250 "red" packages follow, the asymptotical 50%-50% allocation between the two industries would be still preserved.

Two special facets of the adoption of the Binomial Distribution to model the assignment of packages in the two industries are: **(a)** its inability to model the draws from a finite pool of $N=500$ without replacement that changes the next probability and **(b)** the higher analysis of each segment of the DI range. Regarding the first -and most important- aspect, it is rational to assume a continuous flow of wastewater packages by the customers that is equivalent to *sampling with replacement*. Regarding the second aspect, it suffices that each industry is prevalent at a specific segment of the DI range; hence, it can recover the VAC from any package that belongs to its prevalence segment. However, if a higher analysis level is required, the *Multinomial Distribution* can be used instead.

4.3. VAC recovery allocation via ChL

After the examination of how the wastewater packages are initially assigned with the constraint of *Incomplete Information*, the next step is to examine how industries re-allocate the packages in order to optimize the VAC recovery cost efficiency. Wastewater packages that each industry identifies to be outside its cost and operational prevalence range will be chosen to be outsourced to the other up to the VAC DI level where the industry acquires again the cost advantage, as presented in Fig. 11a.

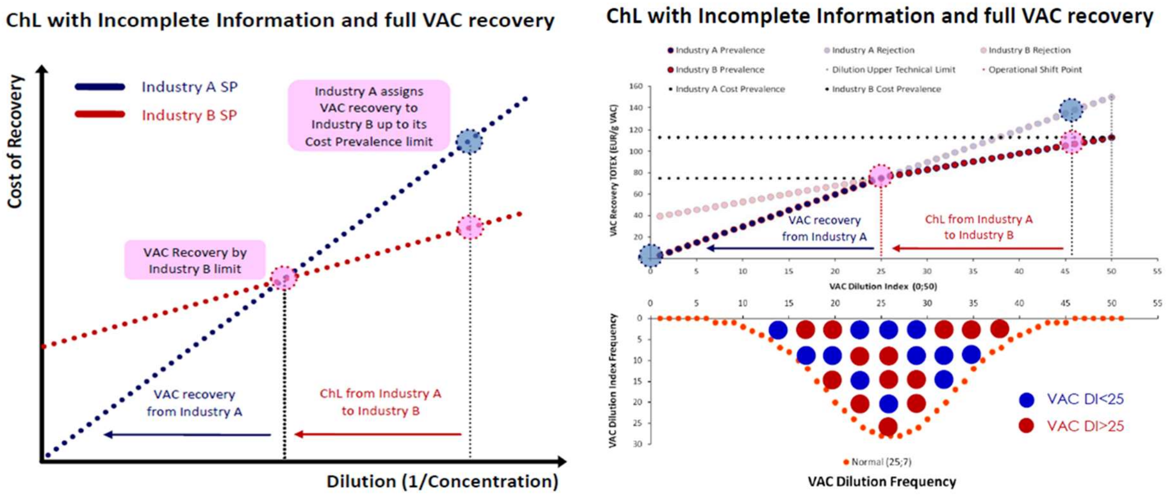

Figure 11: (a) VAC recovery sequence across an intra-industry ChL contract (left) within **(b)** the context of optimizing the VAC recovery allocation from a scrambled distribution of arrivals (right).

As depicted in Fig. 11b, after the initial assignment, Industry A will identify a number of wastewater packages that contain the VAC at a DI level (25,50). Aware of the intra-industry advantages, it knows that at this DI level, Industry B is more cost-efficient at increasing the VAC's concentration up to the *transition point*, where it becomes more prevalent and can continue the VAC's recovery up to 100% concentration. This point is presented in Fig. 11a,b in the intersection of the two industries' SPs for *VAC DI*=25. With the above rationale, as it is presented more analytically in Fig. 11a, the best strategy for Industry A will be to *outsource* or *lease* to Industry B the VAC's concentration increase up to the transition point at *VAC DI*=25, pay it for the service to do so and return it to its own facilities for further processing at the range of *VAC DI*≤25. Respectively, the same rationale will be followed for every wastewater package that will be identified by Industry B to be within the VAC DI range (25,50).

A final question emerging at this point is at what price should these outsourcing/leasing agreements take place -or simply stated- what is the price each industry should charge for the VAC recoveries arriving at it via outsourcing/leasing. The final section of D5.4, deals with the main pricing types of intra-industry ChL financial engineering.

5. ChL Pricing

In Chapter 5 we are finalizing the quantitative framework of CEF with emphasis on ChL agreements tailored for IS. After the examination -in the previous chapter- of the formation of ChL agreements in relation to the SP as a flexible and substantial model for VAC recovery cost performance, we examine three main ChL pricing models that usually take place in intra-industry outsourcing agreements. Specifically, in the next sections, we present: **(1)** The *Fixed* or *Average* (AVG) ChL Pricing, **(2)** The *Variable* or *Capacity* (VAR) ChL Pricing and **(3)** The *Composite* or *Premium* (COMP) ChL Pricing.

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5.1. Fixed ChL Pricing

The *Fixed* or *Average* (AVG) ChL pricing model is the simplest and easily applied for intra-industry agreements, while it comprises the foundation for all other pricing models. Specifically, it sets the foundations, as it provides the *upper* and *lower* pricing limits so that **(a)** the VAC recovery is achieved at the optimal social cost and **(b)** with mutual private benefits for all counterparties engaging in the agreement (Win-Win contracts). The Fixed pricing model is presented in Fig. 12 below.

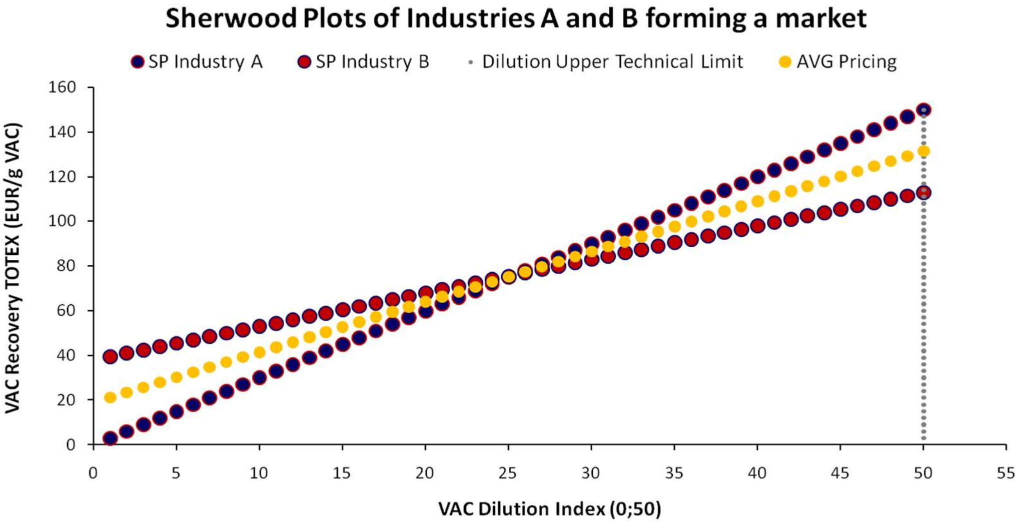

Figure 12: Numerical depiction of the symmetric *Fixed* (AVG) ChL Pricing Model for Industries A, B.

Fig. 12 depicts the two simulated SPs for each industry. Except for their intersection point at *VAC DI* =25, where both achieve the same recovery cost, there is profit margin that is beneficial to both industries across outsourcing/leasing. Specifically, for every *VAC DI*≤25, Industry A is cost prevalent; while for *VAC DI*≥25 Industry B is cost-prevalent. Assuming that we have a case where Industry B has signed a ChL contract with an external customer and holds a wastewater package from which it has to recover a VAC that is found at VAC DI =10, the best strategy will be to sign a 2nd level ChL intra-industry contract that will assign it to Industry A, which will -in turn- return the recovered VAC to Industry B, which will -in turn- deliver it to the external customer.

In this context, the emerging question for Industry A will be *how much to charge for the service of recovering the VAC as part of the outsourcing agreement with Industry B*? The first step for Industry A will be to identify the *objective pricing limits at each VAC DI level*. Specifically, in our numerical example at *VAC DI* =10, the cost of Industry A to recover the VAC is 30 monetary units, while the cost of Industry B is 53 monetary units. That means that Industry A cannot charge any lower price than 30 monetary units as in this case it will be pricing below its own cost -hence will recover the VAC with economic loss- while it cannot price above 53 monetary units as it will be above the cost of Industry B to recover the VAC on its own without outsourcing it. In conclusion, an industry hired to recover a VAC can price its services within a maximum range from just above from its own cost to just below the VAC recovery cost of the second lowest bidding industry. Although in our numerical example the market consists of only two industries, in reality a much higher number of industries is expected to engage in both the VAC recovery and the secondary ChL market with bids following the same rationale in relation to their immediate competitors. Hence, for our special case with two industries, the *Objective Pricing Limits* (OPL) *P* for any pricing model within the SP context is defined by:

$$P\left(m_i^{-1} \mid DI_{im}\right) = Max\left(C_i \mid DI_{im}\right) - Min\left(C_i \mid DI_{im}\right) \qquad (4)$$

Based on the above, the *Fixed* or *Average* (AVG) pricing of two industries that agree to sign an intra-industry ChL agreement for every VAC DI level *m* is described by:

$$P_{AVG}\left(m_i^{-1}\right)_{DIim} = \frac{\left[Max\left(C_i\right) - Min\left(C_i\right)\right]_{D\,Im}}{2} \qquad (5)$$

Eq. (5) describes a state where the two industries agree on pricing their outsourcing services at a constant and predictable level across the whole VAC DI range. According to this type of agreement, each industry prices at *exactly the mean* cost of the OPL at every VAC DI level. Such agreements resemble a long-term mutual commitment that is usually observed in *futures* derivative contracts. Such contracts attempt to eliminate pricing competitions between the counterparties; hence, they reduce pricing variability risks in the IS cluster. In addition, fixed pricing establishes for the secondary ChL market a new market SP that is constant without breaking points (yellow line in Fig. 12).

5.2. Variable ChL Pricing

Having described the general ChL pricing context as well as the first type of pricing such agreements along with the specific motivations of signing counterparties, we may examine the next model that is based on the *Variable* or *Capacity* (VAR) Pricing, as presented in Fig. 13.

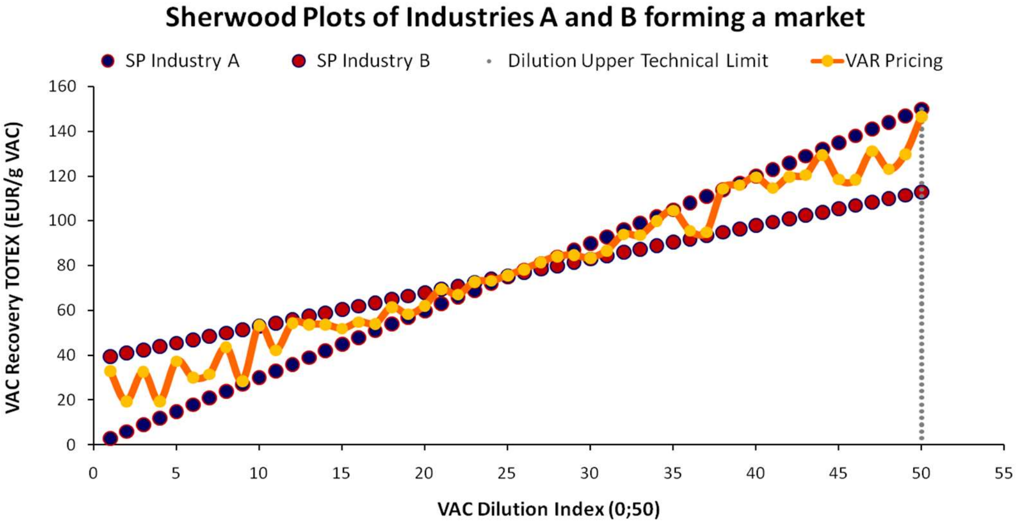

Figure 13: Numerical depiction of the symmetric *Variable* (VAR) ChL Pricing Model for Industries A, B.

As the OPL remains the same, we may see from Fig. 13 that contrarily to the fixed pricing model, VAR pricing is fluctuating at every VAC DI level for both industries, with no other reference value than the OPL. Such pricing model could be perceived as *ad-hoc* pricing and is usually adopted by industries that have limited VAC processing capacity that is easily exhausted across a continuous assignment of wastewater packages (containing the VAC), as described by the Binomial Distribution in Chapter 4. Such industries may be using small compact units that can be easily disassembled and transferred to another geographical location like small modular sewer-mining units [50-51] for treating wastewater of small municipalities. However, such units have rather limited capacities of wastewater processing and VAC recovery volumes or they require additional modules to achieve economies of scale. The *Variable* or *Capacity* (VAR) pricing of two industries that sign an intra-industry ChL agreement for every VAC DI level *m* is described by:

$$P_{VAR}\left(m_i^{-1}\right)_{D\,Im} = a(t)\cdot\left[Max\left(C_i\right)\right]_{D\,Im} + \left[1-a(t)\right]\cdot\left[Min\left(C_i\right)\right]_{D\,Im} \qquad 0<a<1\forall DI_m,t \quad (6)$$

According to Eq. (6), the OPL range that is consumed for pricing depends exclusively on the unit's occupied (%) capacity to recover the VAC at every time step (*t*). For instance, if the unit signs an intra-industry contract for a VAC's recovery that will consume 70% of its operating capacity, it will charge for its services an additional 70% of the OPL as cap above its basic SP cost. Hence, irrespective of the VAC DI at which the unit operates, it will use the OPL at the specific VAC DI only as benchmark to estimate the additional realistic charge above its basic cost.

5.3. Composite ChL Pricing

Finally, we examine the third and last ChL pricing model that is in essence a synthesis of the above mentioned pricing schemes. As presented in Fig. 14, this pricing model is the *Composite* or *Premium* as it aims at maximizing profit via reducing the lower pricing limits quite above the lower OPL bound and maximizing the utilization of the residual capacity towards the OPL upper bound.

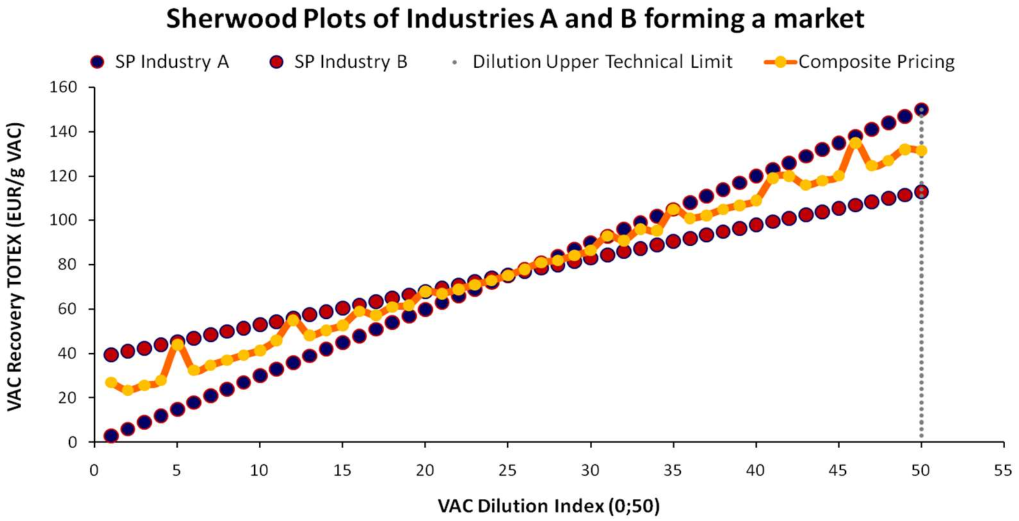

Figure 14: Numerical depiction of the symmetric *Composite* (COMP) ChL Pricing Model for Industries A, B.

The *Composite* or *Premium* (COMP) pricing of two industries that agree to sign an intra-industry ChL agreement for every VAC DI level *m* is described by:

$$P_{COMP}\left(m_i^{-1}\right)_{D\,Im} = Max\left[P_{AVG}\left(m_i^{-1}\right); P_{VAR}\left(m_i^{-1}\right)\right]_{D\,Im} \qquad \forall DI_m,t \quad (7)$$

According to Eq. (7), the industry will simply seek to price its services at each time step at maximum value between the fixed and the variable pricing. This is generally an aggressive pricing policy (that is also why we introduce the title "Premium") and is usually adopted by industries that have significant presence and dominance in the market -possibly being market leaders- either in terms of share or control; thus, they consider themselves to be unaffected by similar retaliating pricing tactics by their competitors as the per cent impact to their revenue and profitability will be lower in comparison.

6. CEF integration to other ULTIMATE works

Besides the original work implemented in D5.4, a concern of high priority was to chart the maximum integration to other ULTIMATE works via theoretical extensions and empirical applications of the ChL concept to the tasks of other Work Packages (WPs). Although we can identify potential applications in all ULTIMATE WPs and Tasks, we record analytically the ongoing cases where the D5.4 has been selected to be tested. These cases are:

- **WP2:** The ChL concept concerns an extension of Subtask 2.2.2 titled “*Utilize costs and benefits of WSIS solutions to optimize industrial ecosystem pathways*”, where ChL provides answers on the link of the SP’s basic dilution-recovery cost relation for individual industrial process and the (cost) ontology mapping of opportunities at the local and regional scale, to optimize industrial ecosystem paths (identifying hidden “intermediate” conversion opportunities) in a way that ensures that the required investments are attractive for CE investments.
- **WP5:** The applications of D5.4 concerns two main Tasks:
    - **Task 5.5:** ChL contracts can be incorporated as an additional special know-how feature to the “*Marketplace for Water, Energy and Materials in a WSIS*”, as well as complementary economic element to the technical know-how library.
    - **Task 5.6:** ChL contracts will be examined in the “*Greenfield assessment for replication*” in order to identify from June 2023 to March 2024 the potential of applying ULTIMATE findings in three selected case studies beyond the nine existing ones from the beginning of the project. This is an ongoing work and the NTUA team has already identified the application potential in one of the three selected case studies that is *KYKLOPAS Estates and Olive Oil Mill* with multiple energy and material flows. In addition, two technology providers (Case Study 4, Nafplion, Greece; Case Study 6, Karmiel/Shafdan, Israel) have been identified to promote both the technical solution and the ChL contract model.

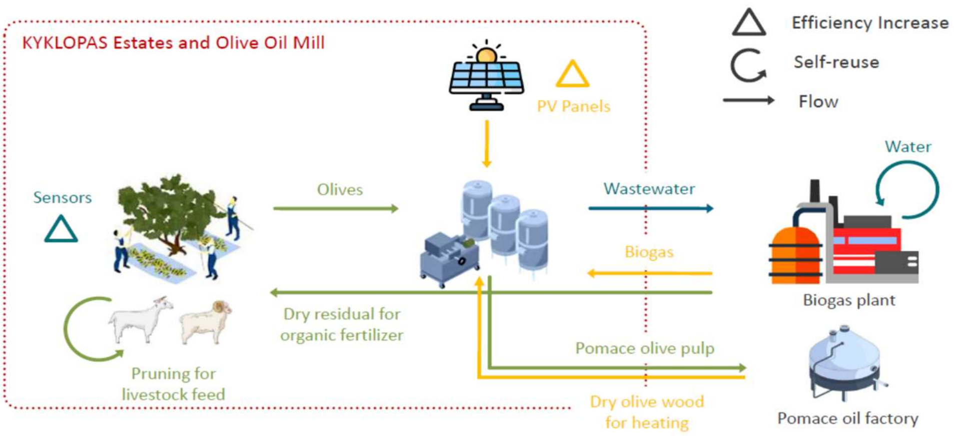

Figure 15: Basic depiction of the KYKLOPAS Estates and Olive Oil Mill's energy, water and other material flows.

7. Conclusions and Discussion

In this deliverable we presented the theoretical foundations and basic quantitative mechanics of Chemical Leasing (ChL) as an integral part of Circular Economy Finance (CEF), specially tailored for Industrial Symbiosis (IS) clusters. ChL contracts can take numerous forms, while CEF itself can be classified in numerous species by sector of application that may be more or less compatible to the EU TSF. As new CEF instruments suitable for private financial institutions that seek the suitable metrics to deploy the full potential of the Circular Economy (CE) and IS emerge constantly, a first discussion will concern the adaptability of the EU TSF to evaluate, classify their applicability for each of its six pillars and eventually incorporate them as standardized commercial finance tools.

A second discussion concerns the selection of most representative metrics depicting accurately the integrated economic and environmental performance of CE and IS practices. In particular, as the CE is at the core of scientific discussion on the future sustainability of the EU's economic system via energy conservation and materials' reuse, it should be able to measure in a standardized way the mitigation of natural resource depletion and ecosystems' degradation as two global environmental pressures.

In this context, the third discussion concerns the field of ChL financial engineering itself and is the performance-based pricing of environmental benefits deriving from IS cluster synergies. Although this research field remains highly uncharted, it holds a very rich field for exploring crucial market and competition aspects of IS clusters, such as the effect of market concentration or the existence of leading/dominant industry on the allocation and optimization of energy and material flows in the network, as well as of the achievement of economies of scale. Although these special issues concern the post-ULTIMATE commercial exploitation era, we will have the opportunity to acquire some first findings across the application in ULTIMATE's Task 5.6 (see Chapter 6).

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