Vniversitat de València

Doctorado en Desarrollo Local y Cooperación Internacional

NUEVAS HERRAMIENTAS PARA PROMOVER LA REUTILIZACIÓN DEL AGUA REGENERADA: UN ENFOQUE BASADO EN LA ECONOMÍA CIRCULAR Y EL PAGO POR LOS SERVICIOS AMBIENTALES

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ACRÓNIMOS Y ABREVIACIONES

ACM	Acetaminofeno
CBZ	Carbamazepina
DMU	*Decision Making Unit* (unidad de toma de decisión)
EDAR	Estación Depuradora de Aguas Residuales
fsQCA	*Fuzzy set qualitative comparative analysis*
HOSP	Número de hospitales
IBP	Ibuprofeno
INCLEV	*Income level* (Nivel de renta)
MEC	*Measured effluent concentration* (concentración medida en el efluente)
NAP	Naproxeno
NURHOM	Número de residencias de la tercera edad
PNEC	*Predicted no-effect concentration* (concentración esperada sin efecto)
POPAG	*Population ageing* (Índice de envejecimiento)
PPCPs	*Pharmaceutical and Personal Care Products* (productos farmacéuticos y de cuidado personal)
PSA	Pago por Servicios Ambientales
TMP	Trimetoprima
SE	Servicios Ecosistémicos
WATCON	*Water Consumption* (Consumo de agua)

AGRADECIMIENTOS

Me gustaría dedicar unas palabras a todas aquellas personas que me han acompaño durante la elaboración de la presente tesis doctoral.

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Una tesis doctoral, una experiencia de vida.

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Autorización para la presentación de la tesis doctoral

Departament d'Economia Aplicada

Valencia, 16 de septiembre de 2021

Francesc Hernández Sancho, Coordinador del Grupo de Economía del Agua y Catedrático de Economía Aplicada de la Universidad de Valencia,

hace constar que:

Como director de la tesis doctoral de ÁGUEDA BELLVER DOMINGO, con NIF 22598809-K, titulada "*Nuevas herramientas para promover la reutilización del agua regenerada: un enfoque basado en la economía circular y el pago por servicios ambientales*", inscrita en el Programa de Doctorado "Desarrollo Local y Cooperación Internacional" de la Universidad de Valencia, autorizo a presentar dicha tesis mediante la modalidad de compendio de artículos, constituida por las siguientes publicaciones:

1. **Bellver-Domingo, A.**, Hernández-Sancho, F., and Molinos-Senante, M. (2016). A review of Payment for Ecosystem Services for the economic internalization of environmental externalities: A water perspective. Geoforum, 70, 115-118.
2. **Bellver-Domingo, A.**, Fuentes, R., and Hernández-Sancho, F. (2017). Shadow prices of emerging pollutants in wastewater treatment plants: Quantification of environmental externalities. Journal of Environmental Management, 203, 439-447.
3. **Bellver-Domingo, A.**, Maldonado-Devis, M., Hernández-Sancho, F., Carmona, E., Picó, Y. (2019). Identification of effective parameters for anti-inflammatory concentration in València City's wastewater using fuzzy-set qualitative comparative analysis. Science of the Total Environment, 663, 110-124.

Acreditando que dicha tesis cumple con los requisitos formales al uso y presenta unos contenidos completos, fundamentados y acordes con la normativa que regula los estudios de doctorado y que se ha hecho un uso ético de la información utilizada en el proceso de investigación.

Atentamente,

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han sido publicadas en tres revistas científicas JCR de alto impacto, como son *Geoforum*, *Journal of Environmental Management* y *Science of the Total Environment*, donde Geoforum es de segundo cuartil y *Journal of Environmental Management* y *Science of the Total Environment* son de primer cuartil; con un factor de impacto de 3,901, 6,789 y 7,963, respectivamente.

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la doctoranda es la principal autora de las mismas, y éstas no han sido utilizadas de forma directa o indirecta en otras tesis doctorales.

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PUBLICACIONES QUE CONSTITUYEN EL COMPENDIO DE ARTÍCULOS

Artículo 1


Geoforum

Review

A review of Payment for Ecosystem Services for the economic internalization of environmental externalities: A water perspective

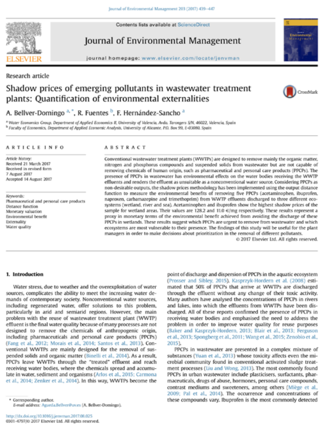
A review of Payment for Ecosystem Services for the economic internalization of environmental externalities: A water perspective

Bellver-Domingo, A., Hernández-Sancho, F., and Molinos-Senante, M.

Geoforum
Volume 70, February 2016, Pages 115-118
Quartile: Q2; Impact Factor: 3.901

https://www.sciencedirect.com/science/article/pii/S0016718515303183

Artículo 2


Journal of Environmental Management

Research article

Shadow prices of emerging pollutants in wastewater treatment plants: Quantification of environmental externalities

Shadow prices of emerging pollutants in wastewater treatment plants: Quantification of environmental externalities

Bellver-Domingo, A., Fuentes, R., and Hernández-Sancho, F.

Journal of Environmental Management
Volume 203, August 2017, Pages: 439-447
Quartile: Q1; Impact Factor: 6.789

https://www.sciencedirect.com/science/article/pii/S0301479717308101

Artículo 3


Science of the Total Environment

Identification of effective parameters for anti-inflammatory concentration in València City's wastewater using fuzzy-set qualitative comparative analysis

Identification of effective parameters for anti-inflammatory concentration in València City's wastewater using fuzzy-set qualitative comparative analysis

Bellver-Domingo, A., Maldonado-Devis, M., Hernández-Sancho, F., Carmona, E., Picó, Y.

Science of the Total Environment
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https://www.sciencedirect.com/science/article/pii/S0048969719304012

ABSTRACT

Wastewater Treatment Plants (WWTPs) are a necessary facility of water cycle that ensure the correct management of wastewater as well as its return to environment. WWTPs has commonly been considered as the "end point" of wastewater, where treated effluent is discharged into receiving water bodies. However, the possibility of using this effluent as a water source in water scarcity areas is becoming a new sustainable option to meet the demand. Water reuse is an effective solution to solve water imbalances, allowing WWTPs to be considered as a non-conventional water source. This situation reinforces their position as key facilities of water cycle whose performance need to be monitored and analysed. According to National Statistical Institute data for 2018, Spain generates almost 14 million m^3/day of wastewater, where only 1,534,000 m^3/day were reused. This imbalance is an opportunity to implement new approaches to use and manage the reclaimed water, as is the case of the circular economy.

Circular economy has the aim to change the approach of products and services, where both the production process of a product and its useful life (including its waste stage) are conceived as circular. Through this approach the use and revaluation of the materials and by-products generated throughout the production system are promoted, avoiding the dependence between economic growth and production processes. Circular economy reduces the supply risk and increases the adaptability of the production and economic systems to imbalances in raw materials stock. The use of this approach in water cycle makes it possible to manage efficiently the available water sources since all water flows generated are considered as a valuable resource. Further measures to encourage water reuse under circular economy approach should be considered in order to include all actors in the decision processes. The paradigm shift of water reuse under circular economy highlights the multidisciplinary approach associated with its implementation. Different points of view must be considered and analysed to implement new management measures that encompass all the factors involved, as carried out in this thesis.

The WWTPs provide an environmental service to humans being and ecosystems through water provision to agricultural and environmental uses, that is WWTPs are responsible of the ecosystem service (ES) of provisioning. Traditionally, ES have been defined as the benefits that an ecosystem brings to society and take part in both the economy and quality of life. However, focusing on the water cycle, the interdependence between water bodies and water regulation and management facilities means that the concept of ES can be applied to WWTPs. Considering the ES of provisioning allows to establish foundations to implement Payment for Ecosystem Services (PES) as new tool to manage water reuse and relationships between the stakeholders involved, as is proposed in the article "*A review of Payment for Ecosystem Services for the economic internalization of the environmental externalities: A water perspective*", which is part of this thesis. This article shows, through a detailed literature search, that PES is an easily adaptable tool to different scales allowing the correction and prevention of environmental impacts related with water consumption.

The conservation and protection of the ES of provisioning requires monitoring the quality of the WWTPs effluent. Current studies have found new types of pollutants, called pharmaceuticals and personal care products (PPCPs), arising from human consumption of both prescription and non-prescription drugs and a wide variety of personal care and cleaning products. Chemical structure of PPCPs makes their removal complicated in WWTPs, causing their discharge into water bodies through effluents. For this reason, the ES of provisioning is damaged, having a negative impact on the quality of effluent and its reuse potential. Removing PPCPs from effluent

provokes a clear environmental benefit, which can be quantified – through monetary valuation methodologies – and included into decision-making processes, in accordance with the requirements of the Water Framework Directive. To obtain the environmental benefit of removing PPCPs from WWTPs effluents, the Shadow Price methodology is implemented, as described in the article "*Shadow prices of emerging pollutants in wastewater treatment plants: Quantification of environmental externalities*". Results obtained show that removing PPCPs has a high environmental benefit, laying the foundations for new management measures (such as PES). In addition, it highlights the importance of preserving the ES of provisioning in areas with serious water imbalances.

The presence of PPCPs in wastewater is related to urban areas so that assessing their influence on the PPCPs concentration has a double advantage. Firstly, it helps to implement new management approaches (such as PES). Secondly, it allows to reinforce the wastewater treatments that are currently being implemented to treat wastewater to address the problem of PPCPs at source. The interdependence between PPCPs and urban areas means that there are several variables that determine their presence in wastewater. Identifying this interdependence provides the basis for the implementation of corrective and preventive measures while, at the same time, allowing the population and the administration to participate actively into decision-making processes. Considering the limited availability of data about the PPCPs concentration in urban areas, the use of methodologies that combine quantitative and qualitative data allows to establish an overview of the relationship between PPCPs and urban variables. The article "*Identification of effective parameters for anti-inflammatory concentration in València City's wastewater using fuzzy-set qualitative comparative analysis*" proposes the use of fuzzy-set qualitative comparative analysis (fsQCA) as a tool to assess and identify the behaviour of urban variables (analysed at district level) regarding the PPCPs detected in the WWTPs analysed. Results obtained show, among other conclusions, that those districts with hospitals have high influence on the PPCPs presence in wastewater. These results support the approach of pollution reduction at source, as well as the suitability of reinforcing the wastewater treatment of hospital greywater before its discharge into the sewerage system.

The approaches and results presented in this thesis are considered as preliminary stages to the design and implementation of PES, where the importance of quantifying the environmental benefit of reducing PPCPs in wastewater and the relationship between urban variables and PPCPs have been highlighted. Considering these preliminary stages in the PES design is a novelty in the literature since they have not been previously analysed because of the pollutants and the approach presented. Through this approach, PES becomes an effective management tool that allows reducing the PPCPs pollution at source, facilitating the WWTPs' performance. This thesis highlights the importance of preserve the ES of provisioning in WWTPs to enhance the water reuse through circular economy approach, using novel methodologies that combine economic, environmental, and social aspects of water management.

RESUMEN

Las Estaciones Depuradoras de Aguas Residuales (EDARs) son una infraestructura necesaria dentro del ciclo del agua y de la gestión de los recursos hídricos, asegurando la correcta gestión de las aguas residuales, así como su vuelta al ecosistema. Comúnmente se ha considerado a la EDAR como el "punto final" del agua residual, donde el agua depurada se descarga en las masas de agua receptoras. Sin embargo, la posibilidad de utilizar ese caudal como fuente de agua en zonas con desequilibrios hídricos se convierte en una opción cada vez más defendida. La reutilización es una solución efectiva ante los desequilibrios hídricos, permitiendo que la EDAR sea considerada como fuente de agua no convencional. Esta situación refuerza su imagen y las posiciona como infraestructuras esenciales dentro del ciclo del agua, y como tal han de ser monitorizadas y analizadas. Según datos del INE para 2018, en España se generaron casi 14 millones de m^3/día de agua residual, de los cuales únicamente se reutilizaron 1.534.000 m^3/día. Esta descompensación en los datos supone una desventaja a la hora de gestionar el ciclo del agua demostrando la necesidad de implementar nuevos enfoques de análisis y gestión que permitan universalizar el uso del agua regenerada, como es el caso de la economía circular.

Esta última busca que tanto el proceso de producción de un producto como su vida útil (incluyendo su etapa de desecho) sean concebidos como circulares con el fin de buscar la utilización y revalorización de los materiales y subproductos generados a lo largo de todo el sistema productivo, al mismo tiempo que se elimina la dependencia entre el crecimiento económico y el proceso productivo. Gracias a la economía circular se cubren los riesgos en el suministro y se aumenta la capacidad de respuesta del sistema productivo y económico ante anomalías y desequilibrios causados en las fuentes de materias primas. El uso de este enfoque en la gestión hídrica permite reforzar y ampliar la gestión del ciclo del agua ya que todas las corrientes de agua generadas son consideradas y gestionadas como un recurso valioso. Por ello deberían plantearse nuevas medidas que fomenten la reutilización bajo este enfoque, con tal de promover e incentivar la participación de todos los actores en el proceso. El cambio de paradigma que supone la reutilización bajo el enfoque de la economía circular pone de manifiesto la multidisciplinariedad asociada a su implementación. Diversos puntos de vista han de ser considerados y analizados con el fin de implementar nuevas medidas de gestión que engloben todos los factores que intervienen en el proceso, tal y como se lleva a cabo en la presente tesis.

Las EDARs prestan un servicio ambiental a los seres humanos y al ecosistema a través de la provisión de agua para uso agrícola y ambiental, es decir, las EDARs son poseedoras del Servicio Ecosistémico (SE) de aprovisionamiento. Tradicionalmente los SE se han definido como los beneficios que un ecosistema aporta a la sociedad y que intervienen en la economía y la calidad de vida. Sin embargo, centrando la atención en el ciclo hidrológico, la interdependencia entre las masas de agua y las infraestructuras de regulación y gestión hídrica hacen que el concepto de SE pueda ser aplicado a las EDARs. En última instancia la consideración del SE de aprovisionamiento permite establecer las bases para la implementación del Pago por los Servicios Ambientales (PSA) como nueva herramienta de gestión de la reutilización y de las relaciones entre los actores implicados, tal y como se propone en el artículo "*A review of Payment for Ecosystem Services for the economic internalization of the environmental externalities: A water perspective*" que forma parte del presente compendio. En esta publicación se muestra, a través de una detallada búsqueda bibliográfica, que el PSA es una herramienta de fácil adaptación a diferentes escalas permitiendo la corrección y prevención de los impactos ambientales asociados a los recursos hídricos.

La protección y conservación del SE de aprovisionamiento necesita de la monitorización y control de la calidad del efluente de las EDARs. Los estudios de laboratorio actuales han encontrado nuevos tipos de contaminantes, llamados productos farmacéuticos y de productos de higiene personal (PPCPs, por sus siglas en inglés), que surgen fruto del consumo humano tanto de medicamentos como de una amplia variedad de químicos para cuidado personal y limpieza. Su estructura química dificulta mucho su eliminación en las EDARs provocando su salida por el efluente y su entrada a las masas de agua. Es por esta razón que el SE de aprovisionamiento se ve dañado, afectando negativamente a la calidad del efluente y a su potencial de reutilización. Eliminar los PPCPs de los efluentes genera un beneficio ambiental evidente, el cual puede ser cuantificado a través de metodologías de valoración monetaria novedosas e incluido en los procesos de toma de decisión de acuerdo con los requerimientos de la Directiva Marco del Agua. Con el objetivo de obtener el beneficio ambiental de eliminar los PPCPs de los efluentes de las EDARs se implementa la metodología de los Precios Sombra, tal y como se recoge en el artículo "*Shadow prices of emerging pollutants in wastewater treatment plants: Quantification of environmental externalities*". Los resultados obtenidos demuestran que la eliminación de los PPCPs conlleva un beneficio ambiental elevado, sentando las bases de nuevas medidas de gestión (como el PSA, comentado anteriormente) y evidenciando la importancia de conservar el SE de aprovisionamiento en zonas con fuertes desequilibrios hídricos.

La presencia de PPCPs en el agua residual está vinculada a las áreas urbanas de tal forma que analizar su influencia sobre la concentración de PPCPs tiene una doble ventaja. Por un lado, ayuda a implementar los nuevos enfoques de gestión (como el PSA) y, por otro, permite reforzar los tratamientos que actualmente se están implementando para depurar el agua residual con el fin de abordar el problema de los PPCPs en origen. La interdependencia entre los PPCPs y las zonas urbanas hace que existan una serie de variables que determinan su mayor o menor presencia en las aguas residuales. Identificar dicha interdependencia sienta las bases para la implementación de medidas correctivas y preventivas, al mismo tiempo que permite que la población y la administración colaboren de forma activa en los procesos de toma de decisión. Teniendo en cuenta la limitada disponibilidad de datos sobre la presencia de PPCPs en zonas urbanas, la utilización de metodologías que combinen datos cuantitativos y cualitativos permite establecer una visión general de la interdependencia entre los PPCPs y las variables urbanas. En el artículo "*Identification of effective parameters for anti-inflammatory concentration in València City's wastewater using fuzzy-set qualitative comparative analysis*" se propone el uso del *Fuzzy-set qualitative comparative analysis* (fsQCA) como herramienta de análisis y obtención de los patrones de comportamiento de las variables urbanas (analizadas a nivel de distrito) con respecto a los PPCPs detectados en las EDARs analizadas. Los patrones de comportamiento obtenidos prueban, entre otras conclusiones, que los distritos con hospitales son los que mayor influencia tienen en la presencia de PPCPs en las aguas residuales. Estas evidencias apoyan el enfoque de disminución de la contaminación en origen, así como la idoneidad de reforzar la depuración de las aguas grises hospitalarias de forma previa a su descarga en el sistema de alcantarillado.

Los enfoques y resultados presentados en este compendio se consideran como las etapas previas al diseño e implementación de un PSA, donde se remarca la importancia de cuantificar el beneficio ambiental de reducir la concentración de PPCPs en las aguas residuales y la interrelación de las variables urbanas que afectan a su presencia. La consideración de estas etapas previas en el diseño del PSA son una novedad dentro de la literatura ya que no han sido abarcadas previamente, debido tanto a la novedad de los contaminantes analizados como al contexto de implementación aquí presentado. A través de este planteamiento, el PSA se convierte en una herramienta de gestión que permite implementar acciones de reducción de la contaminación en origen con el fin de reducir la presión a la que están sometidas las EDARs a la hora de eliminar todos los contaminantes presentes en el agua residual. La presente tesis destaca la importancia de proteger el SE de aprovisionamiento en las EDARs como forma de potenciar la reutilización a través de enfoques y metodologías novedosas que combinan los aspectos económicos, ambientales y sociales de la gestión del agua dentro del marco de la economía circular.

RESUM

Les Estacions Depuradores d'Aigües Residuals (EDARs) són infraestructures necessàries per al cicle de l'aigua i la gestió dels recursos hídrics, assegurant la correcta gestió de les aigües residuals i el seu abocament a l'ecosistema. En general, s'ha considerat l'EDAR com el "punt final" de l'aigua residual, on l'aigua depurada s'aboca a les masses d'aigua receptores, malgrat que aquest cabal pot ser utilitzat com a font d'aigua en aquelles zones que pateixen desequilibris hídrics. La reutilització és una solució efectiva front als desequilibris hídrics que permet que l'EDAR es considere com una font d'aigua no convencional. Aquesta situació reforça la seua imatge i la posiciona com una infraestructura essencial dins del cicle de l'aigua, raó per la qual han de ser monitoritzades i analitzades. Segons les dades de l'INE per a l'any 2018, a Espanya es generaren quasi 14 milions de m^3/dia d'aigua residual, dels quals sols es varen reutilitzar 1.534.000 m^3/dia. Aquesta diferència és un inconvenient a l'hora de gestionar el cicle de l'aigua, demostrant la necessitat d'implementar nous enfocaments d'anàlisi i gestió que universalitzen l'ús d'aigua regenerada, com és el cas de l'economia circular.

Aquesta última busca que tant el procés de producció d'un producte com la seua vida útil (inclouen l'etapa de rebuig) siguen concebudes com circular amb l'objectiu de buscar la utilització i revaloració del materials y subproductes generats al llarg de tot el sistema productiu, al mateix temps que s'elimina la dependència entre el creixement econòmic i el procés productiu. Gràcies a l'economia circular es cobreixen els riscos en el subministrament i s'augmenta la capacitat de resposta del sistema productiu i econòmic davant d'anomalies i desequilibris causats a les fonts de matèries primeres. La utilització d'aquest enfocament en la gestió hídrica permet reforçar i ampliar la gestió del cicle de l'aigua degut a que totes les corrents d'aigua generades són considerades i gestionades com un recurs valuós. Per això han de plantejar-se noves mesures que fomenten la reutilització baix aquest enfocament, aconseguint promoure i incentivar la participació de tots els actors en el procés. El canvi de paradigma que suposa la reutilització i l'economia circular revela l'enfocament multidisciplinari associat a la seua implementació. Diversos punts de vista han de ser considerats i analitzats amb l'objectiu d'implementar noves mesures de gestió que incloguen a tots els actors, tal com es proposa en aquesta tesis.

Les EDARs presten un servei ambiental als éssers humans i a l'ecosistema a través de la provisió d'aigua per a us agrícola i ambiental, és a dir, les EDARs posseeixen el Servei Ecosistèmic (SE) d'aprovisionament. Tradicionalment els SE s'han definit com els beneficis que un ecosistema aporta a la societat i que, al mateix temps, intervenen a l'economia i la qualitat de vida. Però centrant l'atenció al cicle hidrològic, la interdependència entre les masses d'aigua i les infraestructures de regulació i gestió hídrica fan que el concepte de SE puga ser aplicat a les EDARs. En última instància, la consideració del SE d'aprovisionament permet establir les bases per a la implementació del Pagament per Serveis Ambientals (PSA) com a nova ferramenta de gestió de la reutilització i de les relacions entre els actors implicats, tal com es proposa a l'article "*A review of Payment for Ecosystem Services for the economic internalization of the environmental externalities: A water perspective*" que forma part d'aquest compendi. Aquesta publicació mostra, gràcies a una detallada recerca bibliogràfica, que el PSA és una ferramenta de fàcil adaptació a diferents escales permetent la correcció i prevenció dels impactes ambientals associats al recursos hídrics.

La protecció i conservació del SE d'aprovisionament necessita la monitorització de la qualitat de l'efluent de les EDARs. Els estudis de laboratori actuals han trobat nous tipus de contaminants

anomenats productes farmacèutics i productes d'higiene personal (PPCPs, per les seues sigles en anglès), que s'originen degut al consum humà de medicaments i d'una amplia varietat de productes químics per a la cura personal i la neteja. La seua estructura química és complexa i dificulta la seua eliminació a les EDARs, provocant que siguen abocats pels efluents i arriben a les masses d'aigua. Aquest situació danya el SE d'aprovisionament de les EDARs, afectant negativament a la qualitat de l'efluent i a la seua potencialitat per a ser reutilitzat. Per tant, l'eliminació dels PPCPs genera un benefici ambiental evident, el qual pot ser quantificat a través de metodologies innovadores de valoració monetària i, al mateix temps, pot ser inclòs als processos de presa de decisió seguint els requeriments de la Directiva Marc de l'Aigua. Amb l'objectiu d'obtenir el benefici ambiental d'eliminar els PPCPs del efluents de les EDARs, s'implementa la metodologia dels Preus Ombra, tal com es recull a l'article "*Shadow prices of emerging pollutants in wastewater treatment plants: Quantification of environmental externalities*". Els resultats mostren que l'eliminació dels PPCPs comporta un benefici ambiental elevat, establint les bases de noves mesures de gestió (com el PSA) i evidenciant la importància de conservar el SE d'aprovisionament en aquelles zones amb forts desequilibris hídrics.

La presència de PPCPs a l'aigua residual està vinculada a les zones urbanes, de tal forma que analitzar la seua influència sobre la concentració de PPCPs té un doble avantatge. Per una banda ajuda a implementar nous enfocaments de gestió (com el PSA) i, per altra banda, permet reforçar els tractaments que actualment s'estan implementant per a depurar l'aigua residual amb l'objectiu de fer front al problema dels PPCPs des de l'origen. La interdependència entre els PPCPs i les zones urbanes provoquen l'existència de diferent variables que determinen la seua presència a les aigües residuals. Identificar eixa interdependència estableix les bases para la implementació de mesures correctives i preventives, al mateix temps que permet que la població i l'administració col·laboren de forma efectiva en el procediments de presa de decisions. Considerant la limitada disponibilitat de dades sobre PPCPs en zones urbanes, la utilització de metodologies que combinen dades qualitatives i quantitatives permet establir una visió general de la interdependència entre els PPCPs i les variables urbanes. A l'article "*Identification of effective parameters for anti-inflammatory concentration in València City's wastewater using fuzzy-set qualitative comparative analysis"* es proposa la utilització del *Fuzzy-set qualitative comparative analysis* (fsQCA) com a ferramenta d'anàlisi i obtenció dels patrons de comportament de les variables urbanes en relació amb els PPCPs detectats a les EDARs considerant els districtes de la ciutat de València com a zona d'estudi. Els resultat obtinguts proven que els districtes amb hospitals influeixen de forma significativa en la presència de PPCPs a les aigües residuals. Aquestes evidències donen suport a l'enfocament de la disminució de la contaminació en origen, així com la idoneïtat de reforçar la depuració de les aigües grises i negres hospitalàries prèviament a la seua descàrrega al sistema de clavegueram.

L'enfocament i els resultats presentats en aquest compendi es consideren com les etapes prèvies al disseny i implementació d'un PSA, on es remarca la importància de quantificar el benefici ambiental de reduir els PPCPs a les aigües residuals i la necessitat d'identificar la interacció entre les variables urbanes que afecten a la seua presència. La consideració de aquestes etapes prèvies al disseny del PSA són una novetat a la literatura ja que no han sigut considerades degut tant a la novetat dels contaminants analitzats com al context d'implementació ací presentat. A través d'aquest plantejament, el PSA es converteix en una ferramenta de gestió que permet implementar accions de reducció de la contaminació en origen per tal de reduir la pressió a la qual estan sotmeses les EDARs a l'hora d'eliminar tots els contaminants presents a l'aigua residual. La present tesi destaca la importància de protegir els SE d'aprovisionament a les EDARs com a forma de potenciar la reutilització gràcies a enfocaments i metodologies innovadores que combinen els aspectes econòmics, ambientals i socials de la gestió de l'aigua dins del marc de l'economia circular.

DESARROLLO DE LA TESIS DOCTORAL

1. Introducción

La situación actual de creciente estrés hídrico en muchas áreas territoriales especialmente del área mediterránea obliga a cambiar los enfoques tradicionales de gestión del agua por formas novedosas de aprovechamiento de los recursos. Es en este cambio de paradigma donde entran en juego dos conceptos esenciales: la economía circular y la reutilización del agua. El primero de ellos está ganando protagonismo debido al incremento en el uso de los recursos naturales disponibles debido al rápido crecimiento demográfico y económico. De forma general, hablar de economía circular implica que el flujo de materiales y residuos se vuelve circular, buscando su utilización y revalorización a lo largo de todo el sistema productivo. De este modo, la economía circular cubre los riesgos en el suministro de recursos y materiales, aumentando la capacidad de respuesta del sistema de producción ante anomalías y carencias en las fuentes de materias primas. La implementación de nuevas opciones de gestión de los recursos hídricos basadas en la economía circular repercute positivamente no solo en los procesos productivos, sino en el ecosistema y en la sociedad (Comisión Europea 2018).

La reutilización del agua consiste en darle utilidad al efluente de las Estaciones Depuradoras de Aguas Residuales (EDARs), disminuyendo la presión sobre las fuentes de agua convencionales (ríos y acuíferos). La EDAR pasa a ser una fuente de agua no convencional cuyo efluente puede ser usado para fines agrícolas y ambientales. Esta revalorización del efluente entra dentro del concepto de economía circular anteriormente comentado, permitiendo cerrar el ciclo urbano del agua asegurando la monitorización de su calidad. Desde el punto de vista ambiental, el impacto positivo de la reutilización en la reducción de la presión sobre los recursos de agua convencionales es evidente. Por ello habría que considerar los llamados Servicios Ecosistémicos (SE) derivados de la reutilización, ya que las EDARs están prestando un servicio ambiental a los seres humanos y al ecosistema a través de la provisión de agua.

Tradicionalmente los SE han sido definidos como los beneficios que un ecosistema aporta a la sociedad y que mejoran la salud, economía y la calidad de vida (MEA 2005). Dentro de la tipología de SE, los más estudiados son de tipo cultural, hídrico y forestal (Quintas-Soriano et al. 2016), tanto a nivel global como a nivel regional/local (Perez-Verdin et al. 2016). Centrando la atención en el ciclo hidrológico, la interdependencia entre las masas de agua y las infraestructuras de regulación y gestión hídrica hace que el concepto de SE pueda ser aplicado a las EDARs, tal y como se propone en esta tesis.

Los llamados SE hídricos pueden ser desagregados en cinco grandes grupos: (i) aprovisionamiento, (ii) regulación, (iii) formación de suelo, (iv) capacidad natural de tratamiento y (v) producción de alimentos (MEA 2005). Son numerosos los autores que han abordado el estudio de estos SE hídricos (Martín-López et al. 2011, Remme et al. 2015, Bark et al. 2016, Dennedy-Frank et al. 2016, Tesfaye et al. 2016, Watson et al. 2016, Mokondoko et al. 2016) poniéndose de manifiesto la necesidad de su protección, tanto desde el punto de vista del aprovechamiento humano como desde una perspectiva de conservación a largo plazo del ecosistema. Atendiendo a los criterios establecidos por *Millenium Ecosystem Assessment* (MEA 2005), la reutilización del efluente de las EDARs se clasificaría como SE de aprovisionamiento. Es decir, las EDARs se convierten en proveedoras de agua regenerada permitiendo cambiar la concepción que se tenía sobre la depuración como etapa final del ciclo urbano del agua, siguiendo así los principios de la economía circular. La reutilización cambia el paradigma clásico que la literatura establece para los SE, ya que éste evoluciona de la protección y conservación de los SE que están íntegramente en el ecosistema (bosques, zonas de captación de acuíferos) a la protección y conservación de los SE que están directamente relacionados con la intervención humana en el medio ambiente (como es el caso de las EDARs como fuente de agua).

En esta tesis se considera que el cambio de paradigma es necesario debido a diversos factores: (i) la fuerte influencia del ser humano en el ciclo del agua (infraestructuras, sobreexplotación…), (ii) el contexto climático y socioeconómico obliga a utilizar fuentes de agua no convencionales para satisfacer la demanda y (iii) las EDARs se convierten en esas fuentes de agua no convencional. Por ello, el concepto de SE de aprovisionamiento es perfectamente aplicable, siendo de gran relevancia dentro del contexto socioeconómico y ambiental.

La reutilización del agua regenerada requiere la implementación de acciones de monitorización de su calidad ya que es un proceso que implica la reintroducción del agua en el ecosistema, ya sea de forma directa o indirecta. Por esta razón la calidad del efluente de las EDARs es una variable esencial que puede condicionar la propia viabilidad de la reutilización (Simons et al. 2015). El desarrollo tecnológico actual permite la instalación de tecnologías capaces de alcanzar una buena calidad del agua regenerada. Sin embargo, el factor económico puede ser un obstáculo para su implementación debido al marcado carácter ambiental de los proyectos de reutilización (Molinos-Senante et al. 2013). De la combinación del punto de vista económico y ambiental surge el concepto de externalidades ambientales, cuya importancia aparece recogida en la Directiva Marco del Agua (*2000/60/EC of the European Parliament and of the Council of 23 October 2000 establishing a framework for Community action in the field of water policy*). Esta Directiva remarca la necesidad de internalizar las externalidades ambientales en los procesos de toma de decisión, de forma que la importancia ambiental de los proyectos de reutilización quede recogida en los análisis de viabilidad económica.

Una de las externalidades ambientales que actualmente requiere una gran atención es la presencia de contaminantes emergentes en los efluentes de las EDARs. Esta tipología de contaminantes – también conocidos como compuestos farmacéuticos y de higiene personal (PPCPs por sus siglas en inglés) – son compuestos químicos de origen antrópico que alteran los procesos biológicos de los organismos acuáticos, generando graves impactos ambientales a largo plazo (Petrie et al. 2015). Concretamente, el trabajo de Kasprzyk-Hordern et al. (2008) determina que el 50% de los PPCPs que llegan a las EDARs son vertidos por el efluente sin cambios en su actividad tóxica. Esta situación pone de manifiesto la necesidad de actuar sobre los PPCPs, así como el desarrollo de nuevas formas de gestión que permitan minimizar su impacto ambiental. La presencia de PPCPs en las EDARs está siendo ampliamente documentada en la literatura (Baker and Kasprzyk-Hordern 2013, Binelli et al. 2014, Zenobio et al. 2015, Campo et al. 2016, Andrés-Costa et al. 2017), así como sus consecuencias sobre los organismos acuáticos, lo cuales tienen bioacumulación de PPCPs en sus cuerpos (Liu y Wong 2013, Zenker et al. 2014, Subedi et al. 2014, Arlos et al. 2015). Desde un punto de vista químico, la estructura de los PPCPs los convierte en compuestos persistentes con capacidad de ser adsorbidos por las partículas de materia orgánica en suspensión generando conjugados que favorecen su acumulación (Hedgespeth et al. 2012, Liu y Wong 2013, Yargeau et al. 2014). Esta situación es la responsable de que, en numerosas ocasiones, la concentración de PPCPs que se detecta en el efluente sea mayor que la detectada en el influente, ya que fruto de los procesos fisicoquímicos de las EDARs los conjugados se rompen y los PPCPs se liberan (Pothitou y Voutsa 2008).

El impacto de la exposición y bioacumulación de PPCPs en los organismos acuáticos se muestra de diferentes maneras. Los efectos más comunes son los procesos de disrupción endocrina y el desarrollo de genes de resistencia a los antibióticos en las bacterias (Azzouz y Ballesteros 2013).

En el caso de la disrupción endocrina, la literatura demuestra que los PPCPs influyen en el desarrollo embrionario y en la capacidad reproductiva de los organismos acuáticos (Pennington et al. 2015). Estas afecciones provocan, en algunos de los casos, que los órganos reproductores masculinos muestren signos de feminización (intersex) y se impidan los procesos de reproducción (Niemuth y Klaper 2015). Cabe destacar el trabajo de Woodling et al. (2006), el cual demostró la existencia de intersex en las aguas superficiales de Estados Unidos que recibían efluentes de las EDARs urbanas. El resultado de estas alteraciones hormonales es la reducción del tamaño poblacional, repercutiendo directamente en el equilibrio del ecosistema.

En lo que respecta a la resistencia a los antibióticos, el problema es grave ya que tiene consecuencias directas sobre las actividades económicas y sobre la población, aumentando el impacto de las infecciones sobre las cosechas y el ganado. Solo el 30% de la dosis de antibióticos consumida es metabolizada por el cuerpo humano, de tal forma que el 70% restante llega a la EDAR manteniendo su actividad (Rizzo et al. 2013). Los antibióticos llegan al medio ambiente a través del efluente de las EDARs, el cual está siendo vertido al medio o bien se reutiliza para cultivo o para fines ambientales (Becerra-Castro et al. 2015). La generación de genes de resistencia a los antibióticos es un proceso silencioso cuya prevención pasa por monitorizar y eliminar los antibióticos presentes en las aguas residuales, asegurando la idoneidad de las EDARs como fuente de agua. Estos hallazgos ponen de manifiesto la relación entre los PPCPs vertidos a través del efluente y las alteraciones biológicas en los organismos acuáticos (Esteban et al. 2014), permitiendo que los PPCPs actúen como indicadores de la contaminación antropogénica de las masas de agua (Van Stempvoort et al. 2013).

La detección de los PPCPs en las EDARs supone un nuevo reto en la gestión hídrica, ya que estos compuestos no están regulados en la legislación actual. Esta situación abre un nuevo horizonte en la gestión del ciclo del agua, donde los PPCPs se convierten en los contaminantes prioritarios que han de ser eliminados para asegurar la calidad del efluente. Reducir la presencia de PPCPs supone una mejora en la calidad del agua depurada y la potenciación de la reutilización como opción de futuro. Teniendo en cuenta que los efectos de los PPCPs son considerados como externalidades ambientales, la internalización de su impacto ambiental en los procesos de toma de decisiones es prioritaria. Esta internalización demandada por la Directiva Marco del Agua se consigue a través de la implementación de metodologías de cuantificación del beneficio ambiental.

Tal y como se ha comentado, los PPCPs generan las externalidades ambientales en las que se ha centrado el presente trabajo y afectan negativamente al SE de aprovisionamiento prestado por las EDARs. Esta consideración es una novedad dentro del campo de la gestión del ciclo urbano del agua, permitiendo desarrollar diferentes enfoques metodológicos y acciones de gestión innovadoras con el fin de promover la implementación de la economía circular. La importancia de las metodologías de valoración del beneficio ambiental radica en que permiten cuantificar el valor de las externalidades ambientales, las cuales carecen de mercado, en unidades monetarias (Gómez-Baggethun y Muradian 2015) y, al mismo tiempo, contribuyen al mantenimiento del equilibrio del ecosistema (Bark et al. 2016). Por lo tanto, se puede afirmar que los SE representan las nuevas unidades de análisis para implementar las metodologías de valoración monetaria (Sutton y Anderson 2016). Desde el punto de vista de la gestión ambiental, ese valor monetario se convierte en el valor de referencia de cara al mantenimiento óptimo de los SE analizados y la utilidad del efluente de las EDARs como fuente de agua no convencional.

Existen diferentes metodologías de valoración del beneficio ambiental, todas ellas ampliamente recogidas en la literatura (Gren 2013, Kallis et al. 2013, Doherty et al. 2014, Jiang et al. 2015, Rupérez-Moreno et al. 2015, Madani y Khaleghi 2015, Remme et al. 2015, Ahtiainen et al. 2015, Garcia et al. 2016, Ezebilo 2016, Chaikumbung et al. 2016, Momblanch et al. 2016, Franzén et al. 2016). Estos trabajos utilizan los métodos clásicos de valoración (valoración contingente y coste del viaje) basados en la opinión que tiene el usuario del SE, obteniendo su valor a partir de sus decisiones y su disposición a pagar/a ser compensado. Sin embargo, este enfoque no se ajusta a la situación planteada en esta tesis, ya que la presencia de PPCPs en el efluente de las EDARs no es fácilmente perceptible por los usuarios finales del agua. Por ello, en esta tesis se propone el uso de la metodología de los precios sombra (Färe et al. 1989) con el fin de cuantificar el beneficio ambiental de eliminar los PPCPs del efluente de las EDARs.

Según este enfoque, las EDARs representan procesos productivos de agua limpia (output deseado), en cuyo efluente se pueden encontrar contaminantes que no han podido ser eliminados (outputs no deseados). En este contexto se enmarca la utilización de los precios sombra como metodología para calcular el coste ambiental evitado al reducir la concentración de PPCPs en las EDARs. Los precios sombra han sido comúnmente aplicados a los procesos industriales, permitiendo obtener el valor monetario de las externalidades ambientales asociadas al propio proceso productivo (Coggins y Swinton 1996, Reig-Martínez et al. 2001, Färe et al. 2005, Färe et al. 2006, Wei et al. 2013, Zhou et al. 2015). Sin embargo, su marco de aplicación se ha ido ampliando hacia las EDARs, ya que éstas son consideradas como procesos productores de agua, donde los PPCPs se convierten en los outputs no deseados de la corriente de agua depurada (output deseado).

La literatura recoge la implementación de la metodología de los precios sombra en EDARs para obtener el valor monetario tanto del nitrógeno y del fósforo (Molinos-Senante et al. 2010, Molinos-Senante et al. 2011, Bellver-Domingo y Hernández-Sancho 2017), como del CO_2 (Molinos-Senante, Hernández-Sancho, Sala-Garrido, y Cirelli 2013, Molinos-Senante et al. 2015). Sin embargo, la utilización de los precios sombra para obtener el valor monetario de los PPCPs eliminados es una línea de investigación novedosa y cuyo creciente interés ya se manifiesta en la literatura (Molinos-Senante et al. 2013, Bellver-Domingo et al. 2018). Gracias a la aplicación de las metodologías de valoración monetaria se consigue una ventaja significativa a la hora de diseñar e implementar medidas concretas de gestión de los SE. El valor monetario obtenido puede ser incluido en los análisis coste-beneficio (Bark et al. 2016) de forma que se evalúa la viabilidad del proyecto bajo diferentes escenarios (Busch et al. 2012). Este paso supone la internalización de las externalidades ambientales y la elaboración de medidas de gestión eficientes que permiten cambiar el comportamiento de los actores implicados, así como potenciar la conservación de los SE a largo plazo (Kumar et al. 2014).

El origen de los PPCPs debe ser identificado como parte del proceso de valorar el beneficio ambiental de eliminarlos y de potenciación de la reutilización. Debido al consumo generalizado por parte de la población, la presencia de PPCPs en el agua residual tiene un marcado origen urbano. Esto hace que existan una serie de variables que determinan su mayor o menor presencia en las aguas residuales urbanas. Identificar la relación empírica entre los PPCPs y estas variables resulta complicado por diversos factores, como por ejemplo la heterogeneidad en la composición del agua residual, la amplia variedad de PPCPs que actualmente se utilizan y la limitada disponibilidad de los datos. Estos factores son limitantes a la hora de implementar enfoques cuantitativos. Pese a esta restricción, identificar la relación entre las variables urbanas y la presencia de PPCPs en las aguas residuales servirá de base para el diseño e implementación de nuevas formas de gestión hídrica dentro del marco de la economía circular.

Como respuesta a estas dificultades se plantea el uso de métodos cualitativos basados en el análisis de conjuntos. Estas metodologías permiten identificar los patrones de conducta que explicarían la presencia de la variable analizada (en este caso los PPCPs en agua residual). Concretamente en esta tesis se propone el uso del *fuzzy set qualitative comparative analysis* (fsQCA). El fsQCA es una extensión del análisis comparativo cualitativo (QCA) – desarrollado por Charles Ragin (1987) – el cual obtiene los patrones de comportamiento entre las variables analizadas y la hipótesis de partida que se pretende explicar (Roig-Tierno et al. 2016). Implementar el fsQCA permite hacer explícitas las relaciones entre las variables y, al mismo tiempo, identifica qué situaciones son las causantes del problema que se está analizando (Mendel y Korjani 2013). Como ventaja adicional, el fsQCA puede utilizarse con muestras pequeñas y medianas, las cuales no pueden ser analizadas con las metodologías cuantitativas clásicas (Schneider y Wagemann 2009, Kraus et al. 2017).

La utilización del fsQCA está consolidada en numerosos sectores como: (i) *negocios* (Leischnig y Kasper-Brauer 2015, Roig-Tierno et al. 2016, De Villiers 2017, Beynon et al. 2017), (ii) *educación* (Mendel y Korjani 2012, Schneider, Carsten y Makszin 2014, Martí-Parreño et al. 2018), (iii) *salud* (Chuang et al. 2012, Dill et al. 2014, Wind et al. 2016, Haynes et al. 2017, Paykani et al. 2018), (iv) *industria* (Meuer et al. 2015, Backes-Gellner et al. 2016, Boratyńska 2016, Adame-Sánchez et al. 2018). Sin embargo, la implementación del fsQCA en el ámbito de los recursos hídricos no está tan extendida, destacan los trabajos de (i) Kunz et al. (2015), donde se analizan las condiciones que afectan a la reutilización del agua residual en el sector industrial de Australia; (ii) Llopis-Albert et al. (2018), donde se aborda el nivel de satisfacción que tiene la población con los procesos de participación pública asociados a la gestión de recursos hídricos; (iii) Pahl-Wostl y Knieper (2014), el cual estudia la capacidad que tienen distintos sistemas de gestión de agua para hacer frente a la influencia del cambio climático; (iv) Jiang et al. (2017), donde se busca identificar las causas del bajo porcentaje de agua reutilizada en las provincias de China que sufren estrés hídrico; y (v) Kirchherr et al. (2016), donde se analizan las condiciones que generan protestas en contra de la construcción de embalses como forma de gestión hídrica para incrementar la oferta. Por lo tanto, la utilización del fsQCA en el contexto de esta tesis es una novedad en el ámbito de la gestión hídrica, permitiendo a los tomadores de decisiones conocer el comportamiento de los PPCPs. Al mismo tiempo, el fsQCA propuesto refuerza los procesos de tratamiento del agua residual y fomenta el uso de enfoques de reducción de la contaminación en origen.

La implementación de nuevas medidas de gestión en el ámbito de los PPCPs y de la reutilización debe considerar a todos los actores implicados, ya sean responsables de la contaminación o se vean afectados por ella. Estas medidas de gestión podrían ser diseñadas para adaptarse a contextos locales donde se pretenda abordar un problema concreto con repercusión en el normal desarrollo de las actividades económicas de la población. Por esta razón y teniendo en cuenta la importancia de promover la reutilización dentro del marco de la economía circular, se plantea el uso del Pago por los Servicios Ambientales (PSA) como nueva herramienta de gestión hídrica dirigida a reducir los PPCPs en los efluentes de las EDARs. El PSA es una herramienta cuyo objetivo es la internalización de las externalidades ambientales a través de un incentivo económico que cambia la forma en la que los actores interactúan con los SE, asegurando su conservación a medio y largo plazo. Además, se caracteriza por una gran flexibilidad a la hora de adaptarse a las condiciones ambientales, políticas, sociales y económicas de la región en la cual se va a implementar (Kaczan et al. 2013). De este modo se puede considerar el PSA como una transferencia de recursos entre los actores sociales a través de incentivos económicos que priorizan el uso sostenible de los SE y su conservación a largo plazo (Garbach et al. 2012, Ishihara et al. 2017).

El concepto de PSA nació con el doble objetivo de conseguir cambios efectivos en la gestión de los SE y la reducción del nivel de pobreza de la población provocado por las condiciones económicas de las regiones de Sudamérica donde surgió (Schomers y Matzdorf 2013, Markova-Nenova y Wätzold 2017, Ola et al. 2019). En el caso de los SE hídricos, la literatura centra su atención en los PSA basados en la gestión forestal fruto del tipo de aprovechamiento económico de los SE (Diswandi 2017). Estos trabajos demuestran la vinculación entre las prácticas forestales y la dinámica de las masas de agua tanto superficiales como subterráneas (Nguyen et al. 2013, Martin-Ortega et al. 2013, Jourdain et al. 2014, Young y de Bakker 2014, Mokondoko et al. 2016, Da Ponte et al. 2017). Sin embargo, basar los SE hídricos en la regulación de la gestión forestal no es aplicable a todas las áreas que sufren alteraciones en sus ciclos del agua. Un ejemplo son los países del área mediterránea, los cuales sufren graves problemas de sequía cuyo origen no está vinculado a la gestión inadecuada de sus masas forestales ya que, en muchos de los casos, ni siquiera existen (Fripp 2014). Es por esta razón que el diseño de un PSA para el área mediterránea debe ajustarse a las amenazas e impactos ambientales que provocan las áreas urbanas y las actividades económicas sobre los SE hídricos.

Tal y como se ha comentado, el PSA es un instrumento de gestión ambiental que se caracteriza por una fácil adaptación a diferentes escalas, permitiendo la corrección y prevención de diversos impactos ambientales (Smith et al. 2013). Es decir, el PSA es capaz de llegar al usuario local y a sus interacciones con los SE, así como a los grandes contaminadores (empresas y procesos de extracción y producción), si bien es cierto que la actividad de estos últimos viene regulada por el aparato normativo de cada país debido al fuerte impacto ambiental que tienen sus acciones. Estos instrumentos legislativos de carácter ambiental regulan el nivel de contaminación que se puede generar y qué empresas, sectores productivos, países, etc. pueden emitirla. Sin embargo, la regulación ambiental lleva asociada un cierto nivel de incertidumbre relacionado con el valor o nivel de contaminación en el cual se fijan tanto las regulaciones como las penalizaciones (Sterner y Coria 2012). Un claro ejemplo es la presencia de PPCPs en las aguas residuales urbanas, la cual no es ajena a esta incertidumbre debido a la inexistencia de un marco regulador que establezca tanto los criterios y umbrales de contaminación, como la escala de análisis en la cual se han de centrar las acciones preventivas y correctivas. Es por esta razón que la utilización del PSA como instrumento de regulación y disminución de la presencia de PPCPs se convierte en una opción eficaz y eficiente para conseguir que la población internalice los impactos ambientales de la presencia de PPCPs en las aguas residuales urbanas y que asuma la necesidad de eliminarlos para fomentar la reutilización y la economía circular.

El PSA tiene como fundamento incentivar económicamente la buena gestión de los SE en lugar de penalizar la contaminación, tal y como hacen la mayoría de los instrumentos legislativos actuales. Bajo este enfoque, los pagos realizados a través del PSA centrado en los PPCPs buscan recompensar la gestión correcta de los SE de aprovisionamiento gracias a que los actores implicados son incentivados a implementar un cambio efectivo en sus acciones, lo cual tiene un impacto positivo sobre la calidad del efluente de las EDARs. Esto permite ir más allá de los requerimientos legales en cuanto a calidad y conservación de ecosistemas hídricos (Dunn 2011).

El aparato normativo y el PSA no son herramientas excluyentes sino complementarias, ambas pueden ser implementadas en un territorio facilitando el flujo de información y la participación de todos los actores directa o indirectamente relacionados con los SE analizados. La literatura sobre PSA remarca que uno de los pilares para el éxito a largo plazo de un PSA es la robustez del sistema político-administrativo dentro del cual se implementa. Un sistema político-administrativo desarrollado implica la existencia de instrumentos dedicados a la gestión de los aspectos legales, sociales y ambientales de los ecosistemas con el fin de proteger la salud pública (Schomers et al. 2015). Bajo este contexto, el PSA se fundamenta en esos instrumentos legales para resguardar los derechos y deberes de los actores involucrados, al mismo tiempo que sirve de herramienta para gestionar aquellos aspectos de los SE de aprovisionamiento con mayor nivel de detalle (Louka 2006). La complementariedad del PSA y los instrumentos legales existentes permite actuar de forma holística y con una mayor velocidad de adaptación a los cambios socioeconómicos y ambientales (Sterner y Coria 2012).

Teniendo en cuenta estos aspectos, el marco teórico-práctico que se plantea en esta tesis se recoge en la Figura *1*. Este marco refleja la importancia de la economía circular y la reutilización del agua tratada desde el punto de vista ambiental, económico y de gestión hídrica con el fin de diseñar un esquema PSA que actúe como herramienta efectiva para la implementación de la reutilización a escala local (Artículo 1). La situación de estrés hídrico del área mediterránea, agravada por los efectos del cambio climático, genera fuertes desequilibrios entre la demanda y el volumen de agua disponible. Teniendo en cuenta los principios de la economía circular, la reutilización del efluente de las EDARs (considerado como SE de aprovisionamiento) se convierte en la solución a estos desequilibrios en el régimen hídrico. Para llevar a cabo esta reutilización es necesario garantizar la calidad del efluente y minimizar el riesgo de impacto ambiental. Sin embargo, se ha detectado la presencia de PPCPs en los efluentes de las EDARs los cuales generan un impacto directo sobre el ecosistema, reduciendo la potencialidad de la reutilización. Por lo tanto, si los PPCPs afectan directamente a la reutilización y la EDAR es considerada como fuente de agua no convencional (SE de aprovisionamiento), esta tesis aborda dos cuestiones relevantes:

- Artículo 2: ¿Se puede valorar el beneficio ambiental de eliminar los PPCPs del agua residual? En este caso entra en juego el punto de vista económico, el cual permite implementar metodologías de valoración que ayudan a representar el impacto ambiental a través de unidades monetarias. La ventaja del valor obtenido es que puede ser internalizarlo en los procesos de toma de decisiones, al mismo tiempo que muestra la importancia que tiene el SE analizado en un lenguaje que puede ser entendido por toda la población.
- Artículo 3: ¿Se pueden identificar los factores responsables de la presencia de PPCPs en las zonas urbanas? Las nuevas metodologías de análisis que identifican la interrelación entre las variables analizadas permiten abordar la novedad de los PPCPs como contaminantes de origen urbano e implementar nuevas estrategias para la gestión hídrica que ayuden a reducir la contaminación en origen.

Cabe señalar el carácter novedoso del marco teórico-práctico propuesto, ya que cambia el enfoque común que los SE poseen en la literatura. Se pasa de proteger y conservar los SE que se desarrollan íntegramente en el ecosistema (bosques, zonas de captación de acuíferos) a SE que se interrelacionan con la sociedad y su intervención en el medio ambiente (EDARs como nueva fuente de agua). En esta tesis se considera que el cambio de paradigma es necesario ante la confluencia de diversos factores: (i) el fuerte impacto del ser humano en el ciclo del agua (infraestructuras y sobreexplotación), (ii) la influencia del contexto climático y socioeconómico que obliga a utilizar fuentes de agua no convencionales para satisfacer la demanda y (iii) las EDARs dejan de ser consideradas como el punto final del ciclo urbano del agua y pasan a ser nuevas fuentes de agua. Es precisamente este punto el que refuerza que a las EDARs se les aplique el concepto de SE de aprovisionamiento. Es decir, la EDAR provee un SE esencial dentro del contexto socioeconómico y ambiental anteriormente comentado, ayudando a disminuir la presión sobre las masas de agua convencionales. Todo este marco conceptual se integra a la perfección en los fundamentos teóricos de la economía circular. Por lo tanto, el PSA y la gestión de los recursos hídricos están estrechamente ligados, reforzando al mismo tiempo la idoneidad de la economía circular como herramienta integradora.

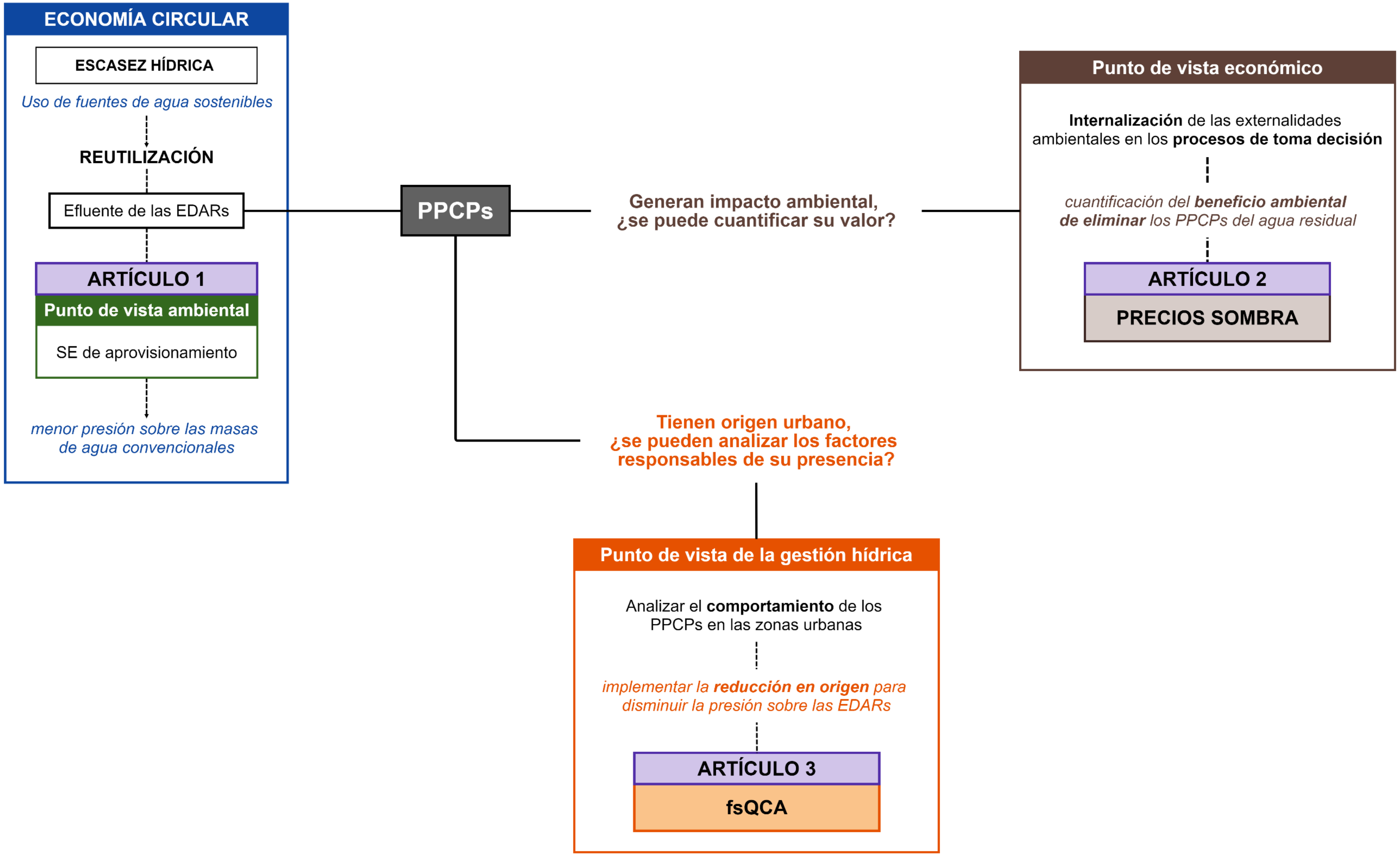


Figura 1. Marco conceptual de la tesis. Fuente: elaboración propia.

2. Objetivos

El objetivo general de la presente tesis es analizar la importancia de las EDARs como fuentes de agua no convencional, así como la potencialidad que tiene el PSA como nueva forma de gestión destinada a reducir la presencia de PPCPs las aguas residuales, fomentando la conexión entre todos los actores implicados. Dentro del objetivo principal pueden diferenciarse los siguientes objetivos específicos:

- Identificar y delimitar los elementos que forman parte del proceso de diseño de un PSA asociado a la reutilización, los cuales serán analizados en el resto de los artículos incluidos en el presente compendio (Artículo 1).
- Valorar el beneficio ambiental de eliminar los PPCPs del efluente de las EDARs a través de la implementación de la metodología de los precios sombra (Artículo 2).
- Analizar el comportamiento de los PPCPs en las zonas urbanas para reforzar el tratamiento del agua residual en origen gracias a la implementación de la metodología fsQCA (Artículo 3).

3. Metodología

La legislación en materia de recursos hídricos y medio ambiente pone de manifiesto la importancia de la valoración monetaria como forma de internalización de las externalidades ambientales generadas. Una muestra de ello es la Directiva Marco del Agua, la cual remarca la necesidad de abordar la gestión sostenible de los recursos hídricos desde un punto de vista holístico asegurando la conservación de las masas de agua. Asimismo, otro de los pilares para conseguir la gestión sostenible de los recursos hídricos es el estudio del origen de las externalidades ambientales y su dinámica dentro del ciclo del agua. De esta forma se pueden implementar nuevos enfoques de gestión basados en la reducción de la contaminación en origen como forma de disminuir la presión sobre las EDARs.

El ARTÍCULO 1, *A review of Payment for Ecosystem Services for the economic internalization of environmental externalities: A water perspective*, lleva a cabo una revisión bibliográfica sobre los SE hídricos, así como del PSA como herramienta efectiva para la gestión del agua. Este paso ha sido fundamental para identificar el estado del arte y los aspectos más relevantes que han de ser considerados a la hora de diseñar un PSA. Concretamente, la metodología aplicada en este artículo se ha dividido en tres fases:

- Fase 1. Definición del problema/hipótesis. Tal y como se ha comentado en la sección anterior, el objetivo general de la presente tesis es analizar la importancia de las EDARs como fuentes de agua no convencional, así como la potencialidad que tiene el PSA como nueva forma de gestión destinada a reducir la presencia de PPCPs en las aguas residuales. La definición de este objetivo ha permitido concretar las palabras clave para la búsqueda bibliográfica (Fase 2) y, al mismo tiempo, ha servido como orientación a la hora de seleccionar, organizar y analizar las fuentes cuya información se ajusta a los criterios establecidos (Fase 3).

- Fase 2. Búsqueda de información. Esta etapa se ha llevado a cabo a través de las plataformas *Scopus* y *ScienceDirect*, usando como palabras clave *water*, *ecosystem services*, *payment for ecosystem services* y *water management*. Los resultados de búsqueda obtenidos se han analizado y filtrado en función del año de publicación y su relevancia dentro de la temática analizada. De esta forma, las fuentes esenciales fueron identificadas, y partiendo de ellas, se seleccionaron los artículos científicos que analizan los SE hídricos y el diseño del PSA con el fin de describir el estado del arte necesario para la presente tesis.

- Fase 3. Organización y análisis de la información. Esta etapa consiste en la lectura y el análisis de las fuentes seleccionadas con el fin de identificar los aspectos claves de la hipótesis inicial, así como los fundamentos teórico-prácticos de las metodologías utilizadas. Al mismo tiempo esta etapa ha permitido definir la contribución y la novedad que el enfoque de PSA propuesto hace a la literatura.

En el ARTÍCULO 2, *Shadow prices of emerging pollutants in wastewater treatment plants: Quantification of environmental externalities*, se calculan los precios sombra considerando el modelo desarrollado por Färe et al. (1993). Este modelo se basa en las funciones distancia que representan la tecnología de producción y, al mismo tiempo, permite modelar la generación simultánea de varios outputs. Esta metodología busca maximizar la producción del output deseado evitando la generación del output no deseado (Wei et al. 2013), de tal forma que los precios sombra caracterizan la relación entre el proceso productivo y la tecnología empleada (Hernández-Sancho et al. 2010).

La metodología parte de un conjunto de inputs $X = (x_1, \dots, x_N)$ y de outputs $U = (u_1, \dots, u_M)$ que forman un conjunto de producción $P(x) = \{u \in \Re_+^M : x \text{ produce } u\}$. Al mismo tiempo se considera que existe disponibilidad débil de los outputs ya que se contemplan una serie de limitaciones a la generación de los outputs no deseados del proceso de producción. La metodología propuesta por Färe et al. (1993) considera el uso de la función distancia y la función de ingresos para estimar el valor monetario de los outputs no deseados. Gracias a estas funciones se consigue relacionar la cantidad de output no deseado producida con los datos económicos del proceso de producción, de tal forma que la fórmula del precio sombra (r'_m) se recoge en la Ecuación 1 (para más información sobre la obtención de la fórmula consular el Anexo C → ARTÍCULO 2: *Shadow prices of emerging pollutants in wastewater treatment plants: Quantification of environmental externalities*).

$$r'_m = r_m^0 \frac{\partial D_0(x,u) / \partial u'_m}{\partial D_0(x,u) / \partial u_m} \qquad (1)$$

Donde m es el output deseado cuyo precio de mercado es r_m^0.

Las funciones distancia involucradas en el análisis pueden ser calculadas de diversos modos, pero el más habitual es mediante la programación lineal no paramétrica y determinística (no estocástica). Entre sus ventajas está la de no suponer ninguna forma funcional de la función de producción y adaptarse a procesos en los que se empleen múltiples inputs para generar diversos outputs simultáneamente. Como inconvenientes destacables están el hecho de no contemplar desviaciones en los niveles de producción de carácter meramente aleatorio y no poder ofrecer pruebas de significatividad para los parámetros estimados. Siguiendo el enfoque de Färe et al. (1993) se procede a parametrizar la función distancia como una función translog, la cual se muestra en la Ecuación 2.

$$\begin{aligned} \ln D_0(x,u) = {} & \alpha_0 + \sum_{m=1}^{M} \alpha_m \ln u_m + \sum_{n=1}^{N} \beta_n \ln x_n \\ & + \frac{1}{2} \sum_{m=1}^{M} \sum_{m'=1}^{M} \alpha_{mm'} (\ln u_m)(\ln u_{m'}) \\ & + \frac{1}{2} \sum_{n=1}^{N} \sum_{n'=1}^{N} \beta_{nn'} (\ln x_n)(\ln x_{n'}) \\ & + \sum_{n=1}^{N} \sum_{m=1}^{M} \gamma_{nm} (\ln x_n)(\ln u_m) \end{aligned} \qquad (2)$$

Para calcular los parámetros de la función distancia (α, β, γ) se resuelve el programa lineal recogido en la Ecuación 3 sujeto a una serie de restricciones las cuales se recogen con detalle en el Anexo A: Restricciones asociadas al proceso de programación lineal de la metodología de los precios sombra aplicada en el ARTÍCULO 2.

$$Max \sum_{k=1}^{K} [\ln D_0 \left(x^k, u^k\right)] - \ln(1) \tag{3}$$

donde $k = 1, \dots, K$ representa el número de unidades de producción incluidas en el análisis (en el caso analizado las EDARs), siendo los primeros i outputs deseables y los restantes $(i + 1, \dots, M)$ no deseados (PPCPs).

En el ARTÍCULO 3, *Identification of effective parameters for anti-inflammatory concentration in València City's wastewater using fuzzy-set qualitative comparative analysis*, se utiliza el método fsQCA para analizar los patrones de interacción entre las variables que afectan a la hipótesis de partida. El método fsQCA tiene su origen en el análisis cualitativo comparativo (QCA), el cual fue desarrollado por Charles Ragin a finales de los ochenta (Ragin 1987). La potencialidad del fsQCA es que busca identificar qué variables explican el problema que se está analizando, por lo que en primer lugar se define la hipótesis de partida y, posteriormente, se buscan las variables que le afectan con el fin de identificar la interrelación existente entre esas variables. Este planteamiento permite que el fsQCA considere tanto variables cualitativas como cuantitativas, identificando su comportamiento de forma conjunta (González et al. 2012). Este hecho es lo que diferencia al fsQCA del enfoque clásico, el cual busca cuantificar el valor de cada una de las variables con el fin de implementar metodologías analíticas que modelicen el comportamiento de las variables (Figura 2).

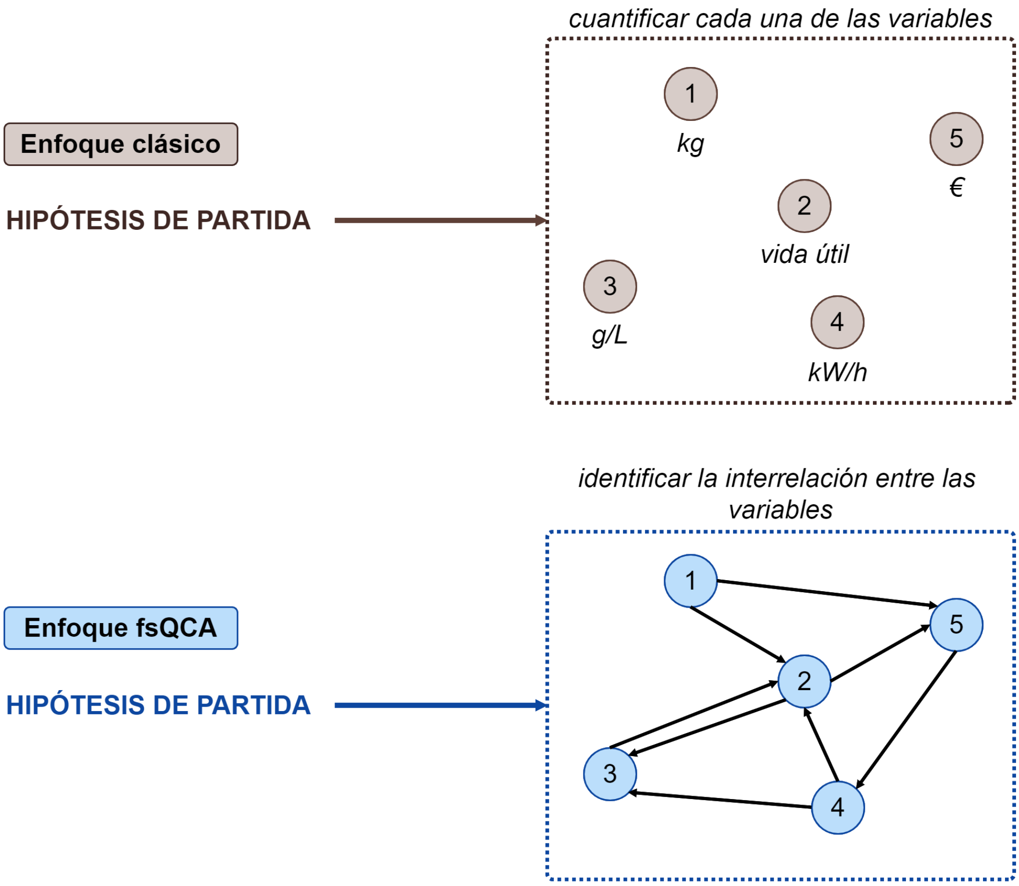


Figura 2. Enfoque clásico vs enfoque del fsQCA. Fuente: elaboración propia.

Para conocer las bases de la aproximación metodológica aquí planteada se deben tener en cuenta el concepto de causalidad y el de conjunto:

- La causalidad se define como la relación entre la causa y el efecto que genera un proceso determinado, donde no es extraño que a un mismo efecto le correspondan multitud de causas (causalidad compleja).
- El conjunto se define como el ente matemático donde los elementos que lo forman tienen una propiedad común. Por lo tanto, un conjunto actúa como frontera que define los límites de inclusión y exclusión de las variables analizadas, donde dichos límites reciben el nombre de grados de pertenencia.

Es importante señalar que los resultados que se obtienen no prueban las relaciones causales, sino que revelan los patrones de asociación y apoyan la existencia de relaciones causales entre las variables. Es decir, esta metodología permite modelizar la relación causa-efecto entre las variables y el problema que se está analizando. Sin embargo, pueden existir otras variables que no se hayan podido identificar que también afecten al problema analizado. Es por esta razón que el fsQCA permite demostrar de forma efectiva las relaciones entre las variables basándose en la lógica booleana, es decir, utilizando signos y letras para representarlas.

Las combinaciones causales que se obtienen con la aplicación del fsQCA muestran la relación entre las variables expresada a través de signos, letras y números ya que se basan en la lógica booleana y en el álgebra difusa, por esta razón reciben el nombre de “recetas” (De Villiers 2017). Tal y como se ha comentado anteriormente, las variables se agrupan en conjuntos en función de la tipología y características de cada una de ellas. En el caso del fsQCA estos conjuntos son difusos, ya que no se puede especificar categóricamente si la variable está dentro o fuera del conjunto, pudiendo pertenecer al conjunto de forma parcial (Schneider y Wagemann 2012). De este modo los límites del conjunto son una gradación entre 0 y 1, donde 0 indica la no pertenencia al conjunto y 1 la plena pertenencia al conjunto (Pappas et al. 2016). Por ejemplo, en el caso del conjunto “personas mayores”, la variable “personas de 60 años” tiene un grado de pertenencia al conjunto es de 0,8 indicando que la variable pertenece al conjunto, pero no de forma plena (Figura 3). Es decir, no son consideradas personas jóvenes, pero tampoco están incluidas en una franja de edad superior a los 70 años. Con este ejemplo se pretende mostrar que los conjuntos difusos y los grados de pertenencia ayudan a identificar los matices de aquellas variables que no pueden ser clasificadas categóricamente dentro de un conjunto.

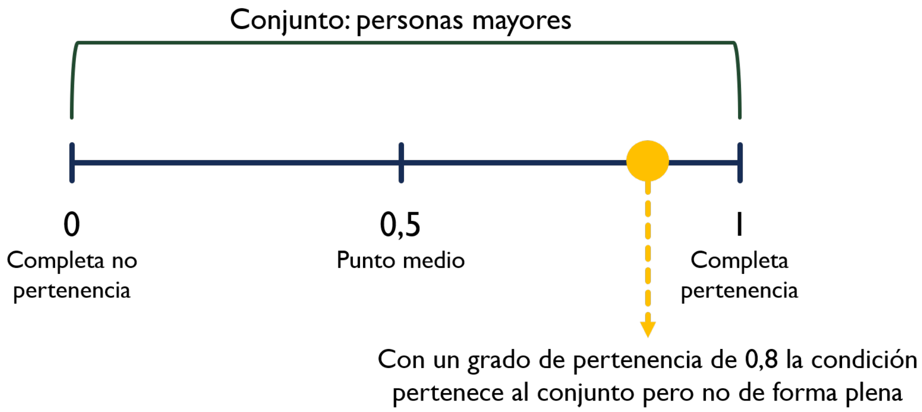


Figura 3. Grados de pertenencia al conjunto para la variable "personas de 60 años". Fuente: elaboración propia.

Como etapa previa a la utilización del fsQCA es necesario un proceso de calibración de los datos con el objetivo de establecer los conjuntos y los grados de pertenencia. Para este proceso deben definirse de forma detallada todas las variables que se van a analizar, así como definir cuáles serán los límites de los conjuntos: pertenencia, no pertenencia y punto medio; siendo necesaria una profunda revisión bibliográfica que corrobore los umbrales seleccionados (Ragin 2006). El detalle del proceso de calibración se encuentra recogido en el ANEXO C → ARTÍCULO 3: *Identification of effective parameters for anti-inflammatory concentration in València City's wastewater using fuzzy-set qualitative comparative analysis*. Una vez finalizada la calibración, la información de cada variable se introduce en el software[1] que aplica el algoritmo del fsQCA, el cual se basa en el algoritmo de Quine-McCluskey[2], obteniendo las combinaciones causales o recetas que explican los patrones de interacción entre las variables (Marx et al. 2014). El software provee tres tipos de soluciones: (i) compleja, es la más completa porque incluye todas las combinaciones causales posibles, (ii) parsimoniosa, es una versión simplificada de la solución compleja, la cual incluye las condiciones esenciales para explicar las combinaciones causales y (iii) intermedia, la cual es una versión intermedia entre las dos soluciones anteriores. Esta última compara las situaciones en las que se produce ausencia y presencia de la hipótesis de partida con el fin de corroborar la interrelación entre las variables y la hipótesis y, generalmente, coincide con la solución compleja (Pappas et al. 2017).

[1] El software está disponible en varias plataformas: (i) web del fsQCA – Universidad de Arizona (http://www.u.arizona.edu/~cragin/fsQCA/software.shtml) o (ii) paquetes en R (https://cran.r-project.org/web/packages/QCA/index.html).
[2] Es un algoritmo de minimización de las funciones Booleanas con múltiples variables (Duşa 2007, Jain et al. 2008).

4. Principales resultados

La presente tesis profundiza sobre la interconexión que existe entre los aspectos ambientales y sociales de la gestión del agua, además de analizar su impacto sobre el equilibrio tanto del medio ambiente como del sistema socioeconómico. Este análisis se centra en tres pilares metodológicos fundamentales (Figura 4): la información bibliográfica, la metodología de los Precios Sombra como forma de valoración del beneficio ambiental y el fsQCA como herramienta para conocer el comportamiento de los PPCPs en zonas urbanas. Estos tres elementos han sido analizados a través de los artículos que forman parte del presente compendio. Los resultados obtenidos se consideran como parte integrante de un todo, cuya finalidad es mostrar el carácter multidisciplinar de las externalidades ambientales en la gestión del agua y la necesidad de implementar diferentes metodologías para conseguir diseñar nuevas medidas de gestión basadas en la sostenibilidad y la economía circular.

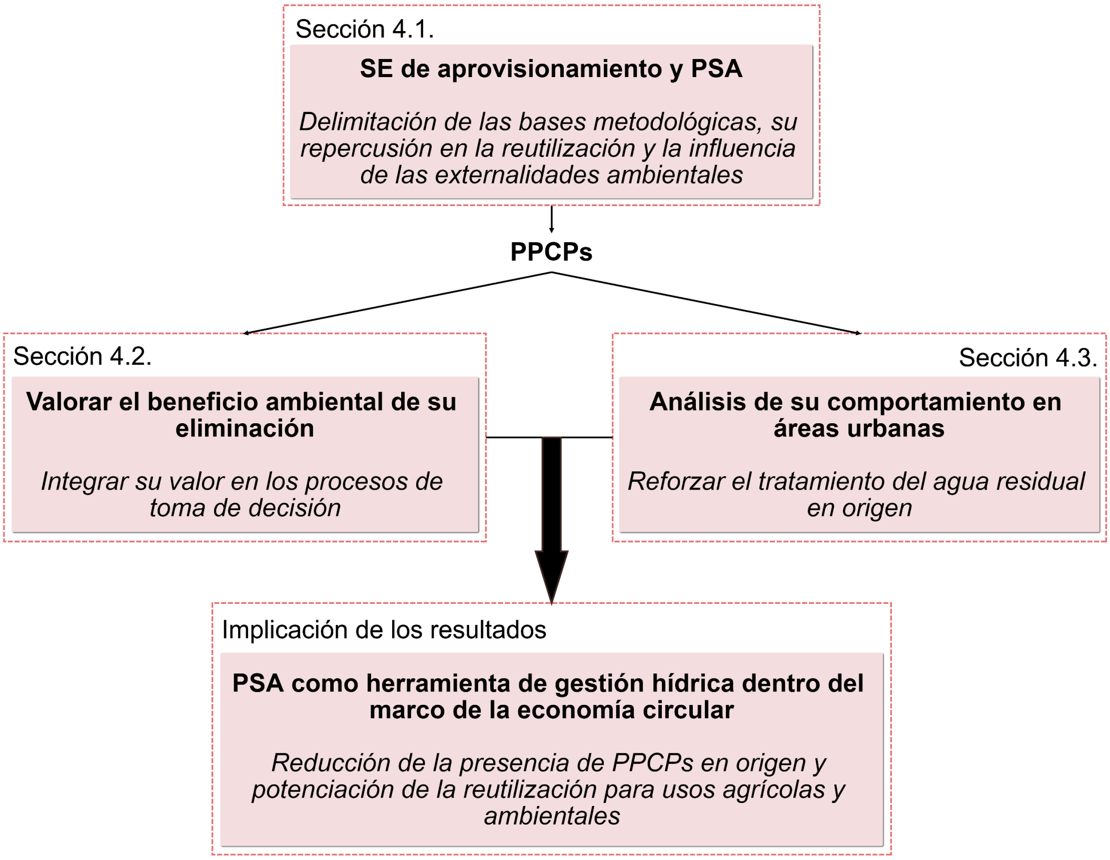


Figura 4. Representación de la interrelación de los resultados obtenidos en los artículos que forman parte del presente compendio. Fuente: elaboración propia.

4.1. Planteamiento del PSA como herramienta de gestión de los recursos hídricos disponibles

Este artículo se centra en la búsqueda de la información esencial sobre SE y PSA con tal de identificar los puntos clave que han de ser considerados para su diseño y, al mismo tiempo, permite determinar las metodologías que analizan la importancia de los PPCPs en la gestión hídrica y en la reutilización (las cuales han sido implementadas en los artículos posteriores). Tal y como se ha mencionado con anterioridad, los SE son los beneficios que la población obtiene de los ecosistemas, si bien es cierto que cabe destacar que el concepto de SE va más allá, considerando también su propia naturaleza ecológica la cual debe ser conservada con tal de asegurar el equilibrio ecológico (Boyd y Banzhaf 2007). Una cuestión recurrente es cuándo surge un SE y, según la literatura, ello sucede cuando aparece un interés por el ecosistema de forma que se crea una vinculación entre éste y la satisfacción de una necesidad humana (Balvanera et al. 2012). De esta forma, las necesidades de la sociedad se convierten en una parte central de los SE y su análisis, otorgando mayor notoriedad a los procesos de toma de decisiones y a la internalización de las externalidades ambientales (Lauf et al. 2014). En el caso de los SE hídricos, la situación es más compleja ya que el acceso al agua ha de ser garantizado por las administraciones públicas, pero la escasez hídrica y la contaminación de las masas de agua ocasiona problemas en los SE que éstas generan. Es por esta razón que la identificación de los contaminantes y su origen es clave para conservar los SE de aprovisionamiento, reforzando a la reutilización como eje fundamental del ciclo del agua (Schomers y Matzdorf 2013).

Según Muradian et al. (2010), lo más importante es el carácter público de los SE y la internalización de las externalidades ambientales. Por esta razón, el análisis y la monitorización de los SE permite diseñar incentivos para la gestión de los ecosistemas al mismo tiempo que se consigue cambiar el comportamiento individual o colectivo con el fin de evitar el daño ambiental y la degradación de los ecosistemas. Estos incentivos son uno de los pilares fundamentales del PSA, cuya ventaja es gestionar los SE de forma que se asegure su continuidad a largo plazo, así como la satisfacción de las necesidades humanas (Garbach et al. 2012). Los SE están fuertemente ligados al territorio (Lockie 2013, Mombo et al. 2014), por lo que el diseño de un PSA permitirá ajustar la gestión a las necesidades concretas de esa zona. Éste es otro de los puntos fuertes del PSA, una escala de aplicación más específica permite conocer las interacciones sociales que existen entre los actores y el medio ambiente, lo cual se traduce en la elaboración de acuerdos concretos de gestión de los SE y ejecución de los procesos de monitoreo efectivos (Tognetti et al. 2003, Chen et al. 2012).

La literatura destaca que un PSA ha de cumplir con las propiedades de condicionalidad y adicionalidad, las cuales han de ser tenidas en cuenta en el proceso de diseño e implementación. La condicionalidad es una propiedad por la cual se demuestra la existencia de una relación causa-efecto entre la aplicación del PSA y la provisión del SE analizado. Gracias a la condicionalidad se fomenta el desarrollo de métodos capaces de monitorizar el impacto que el PSA tiene en la conservación (Barnaud y Antona 2014), como es la elaboración de indicadores basados en el cálculo del beneficio ambiental de eliminar los PPCPs. Kroeger (2013) ha identificado una serie de preguntas que se han de plantear para elaborar el plan de monitoreo que cumple con la condicionalidad. Estas preguntas se recogen en la columna de la izquierda de la Tabla 1, mientras que han sido respondidas en la columna de la derecha según el enfoque analizado en la presente tesis.

Tabla 1. Cuestiones para considerar en un plan de monitoreo adaptadas al enfoque propuesto en la presente tesis.

Preguntas planteadas por Kroeger (2013)	Respuestas según el enfoque analizado en la presente tesis
¿La intervención sobre el medio ambiente provoca cambios reales y específicos sobre el ecosistema?	La eliminación de los PPCPs reducirá su concentración en el efluente y, por lo tanto, la cantidad de PPCPs que llegará al ecosistema.
¿La intervención sobre el SE es específica? Es decir, si la acción llevada a cabo realmente mejora la provisión del SE o por el contrario no le afecta en absoluto.	La eliminación de los PPCPs sí que mejorará la provisión del SE de aprovisionamiento ya que actualmente no están siendo eliminados, por lo que estos contaminantes llegan al ecosistema y provocan efectos graves sobre los organismos acuáticos. Esta situación disminuye la potencialidad de la reutilización y afecta al equilibrio hídrico del ecosistema.
¿Los beneficios que genera la medida son cuantificables y suficientes?	Si que son cuantificables tanto desde el punto de vista ambiental como económico. En esta tesis se propone la valoración monetaria del beneficio ambiental de eliminar los PPCPs, lo cual permite estimar su importancia ambiental y la necesidad de abordar este problema. Por otro lado, desde el punto de vista económico, considerar la EDAR como fuente de agua no convencional permite hacer frente a la escasez hídrica e implementar la economía circular de forma efectiva dentro del ciclo del agua. Esta situación reducirá los gastos de abastecimiento y energía en el ámbito agrícola y ambiental, ya que el agua regenerada permitirá satisfacer su demanda de agua.

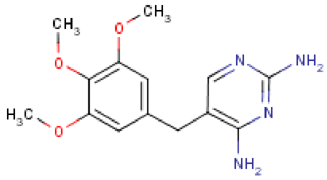
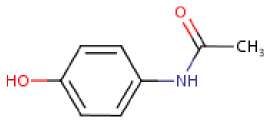
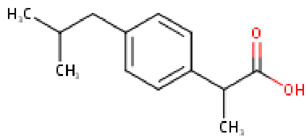
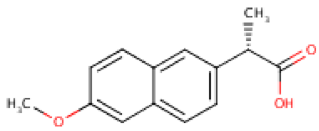
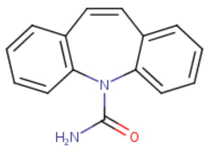
Por lo que respecta a la adicionalidad, ésta es una propiedad del PSA que recoge la ganancia en la prestación del SE que se produce en comparación con la línea de base (Goldman-Benner et al. 2012). Gracias a la adicionalidad se garantiza el correcto funcionamiento del PSA, ya que se mejora la provisión del SE al producirse un cambio real en su calidad. En el caso del enfoque analizado en la presente tesis, la adicionalidad supondría la eliminación de los PPCPs del agua residual de forma que el SE de aprovisionamiento tendrá mayor calidad. La ganancia en la prestación del SE es evidente ya que la línea de base existente no considera la eliminación de los PPCPs ante la ausencia de legislación al respecto. De tal forma que, gracias a esta propiedad se consigue asegurar la efectividad del PSA como herramienta de gestión hídrica en el contexto de las aguas residuales urbanas, la reutilización y la economía circular.

Pese a que la relación del ser humano con los recursos naturales es cambiante su bienestar está ligado al medio ambiente a través de los SE (Greiner y Stanley 2013). El PSA, junto con el resto de las metodologías que se implementan en la presente tesis, permiten internalizar las externalidades ambientales dentro de los procesos de toma de decisiones, convirtiendo a los SE en uno de los pilares fundamentales de la gestión hídrica y la reutilización. El PSA permite reforzar y maximizar el valor presente de los SE con el fin de fomentar su conservación y la interrelación de los actores sociales tanto a corto como a largo plazo, subsanando el daño ambiental que se está produciendo (Roumasset y Wada 2013).

4.2. Valoración del beneficio ambiental de eliminar los PPCPs presentes en el agua residual a través de la metodología de los Precios Sombra

La presencia de los PPCPs en las EDARs está adquiriendo mayor protagonismo en la literatura, si bien es cierto que la novedad en su detección y la ausencia de legislación que regule su presencia provoca que sea complejo acceder a estadísticas sobre PPCPs. Por esta razón se ha elaborado una base de datos a partir de fuentes bibliográficas con el fin de poder valorar el beneficio ambiental de eliminar los PPCPs del agua residual. Se han considerado los cinco PPCPs comúnmente detectados a nivel mundial y cuya presencia es detectada en la mayoría de los trabajos analíticos (Dai et al. 2015, Gros et al. 2017): ibuprofeno (IBP), carbamazepina (CBZ), trimetoprima (TMP), acetaminofeno (ACM) y naproxeno (NAP). Sus características químicas están recogidas en la Tabla 2.

Tabla 2. Características de los PPCPs analizados (HSDB 2014).

PPCPs	Fórmula	log K_{ow}	Clase	Estructura
Trimetoprima	$C_{14}H_{18}N_4O_3$	0,91	Antibiótico	
Acetaminofén	$C_8H_9NO_2$	0,46	Analgésico	
Ibuprofeno	$C_{13}H_{18}O_2$	3,97	Antiinflamatorio	
Naproxeno	$C_{14}H_{14}O_3$	3,18	Analgésico	
Carbamazepina	$C_{15}H_{12}N_2O$	2,45	Antiepiléptico	

logKow = Coeficiente de reparto octanol-agua. Este valor mide la solubilidad de los PPCPs en el agua. Si el valor el alto, la sustancia es hidrófoba y tiene afinidad por los lípidos, por lo que es propensa a adsorberse en sedimentos y organismos. Si el valor es bajo, la sustancia es hidrófila, y tiene afinidad por el agua (Pal et al. 2010).

Se han considerado 24 EDARs de diferentes países con homogeneidad tanto en el número de habitantes equivalentes como en la tecnología de tratamiento, basada en un proceso convencional de fangos activos. Estos datos están recogidos en la Tabla 3, donde se incluyen las fuentes consultadas para cada una de las EDARs. Como parte de los requerimientos metodológicos de la implementación de los Precios Sombra es necesario conocer los costes de inversión y los costes de operación y mantenimiento de las instalaciones. En este caso se han obtenido a través de las funciones de coste para fangos activos recogidas en el trabajo de Guo et al. (2014). El coste de inversión medio para la muestra es de 32,4 millones de €, mientras que el valor medio de los costes de operación y mantenimiento se cuantifica en 25,9 millones de €.

Tabla 3. Características principales de las EDARs consideradas en la base de datos.

EDAR	País	Habitantes equivalentes	Caudal (m^3/día)	Fuente
Torroella de Montgrí	España	11.385	16.500	(Rodriguez-Mozaz et al. 2015)
Cilfynydd	Reino Unido	111.000	36.160	(Kasprzyk-Hordern et al. 2009)
Coslech		30.000	19.750	
Castellón de la Plana	España	265.000	36.000	(Gracia-Lor et al. 2012)
Taipei	Taiwán	227.250	210.000	(Lin et al. 2009)
Lausanne	Suiza	220.000	95.000	(Margot et al. 2013)
Coimbra	Portugal	213.000	N/A	(Santos et al. 2013)
Sena Centro	Francia	90.000	240.000	(Mailler et al. 2015)
Ioannina ciudad	Grecia	100.000	25.276	(Kosma et al. 2010, Kosma et al. 2014)
Arta		38.000	115.000	
Preveza		25.000	7.000	
Agrinio		90.000	14.000	
Grevena		20.000	4.000	
Kozani		70.400	10.000	
Veroia		45.000	9.800	
Alcalá de Henares	España	374.090	74.818	(Rosal et al. 2010)
Wayne Hill	EE. UU.	N/A	227.000	(Yang et al. 2011)
Howdon	Reino Unido	N/A	230.000	(Roberts y Thomas 2006)
Nápoles	Italia	840.000	181.000	(Castiglioni et al. 2006)
Latina		45.000	19.000	
Cuneo		140.000	31.000	
Cagliari		270.000	86.700	
Varese Lago		110.000	40.000	
Varese Olona		120.000	23.000	

Las concentraciones identificadas de los 5 PPCPs analizados se recogen en la Tabla 4. Es importante destacar que la CBZ sigue un comportamiento anómalo ya que la concentración en el efluente es mayor que la concentración en el influente. Esto se debe a la unión de la CBZ con la materia orgánica en suspensión formando un conjugado donde la CBZ queda atrapada en su interior. Cuando el conjugado se rompe debido al proceso de tratamiento del agua residual, la CBZ se libera y provoca el aumento de concentración en el efluente (Luo et al. 2014).

Tabla 4. Concentración de los PPCPs seleccionados en el influente y en el efluente de las EDARs (ng/L).

	Trimetoprima		Acetaminofén		Ibuprofeno		Naproxeno		Carbamazepina	
EDAR	Influente	Efluente	Influente	Efluente	Influente	Efluente	Influente	Efluente	Influente	Efluente
Torroella de Montgrí	118,5	19	208.601	24,5	26.011	3.527,5	982	280,2	230	440,5
Cilfynydd	2.192	1.152	211.380	11.733	1.681	263	838	370	1.694	2.499
Coslech	2.925	876	178.116	353	2.294	143	1.173	170	950	826
Castellón de la Plana	100	90	55.100	9.245,4	14.600	1.980	1.320	130	1.863,4	212
Taipei	36,3	3,1	13.046,2	2.189,1	9.322	2.045	138,6	39,5	219,5	153,5
Lausanne	235	158	51.438	7,9	4.101	952	697	380	482	461
Coimba	124	167	2.463	96,1	1.596	119	741	303	433,8	49,4
Sena Centro	64	4	5.870	1.030,0	951	432	154	52	215	41,0
Ioannina ciudad	132,1	59,8	2.872,5	91,6	2.633,4	301,2	230,3	57,3	98,8	119,9
Arta	23,1	11,6	8.313,2	195,7	177	24	544,4	128	59,7	211,9
Preveza	16,2	8	293	192,3	279,9	77,5	1.814	170,7	21,8	57,7
Agrinio	16,7	8,3	139,9	51,8	56,5	31,3	324,6	58,8	95,4	61,7
Grevena	158,5	13,4	20.600	900	12.500	1.500	1.500	500	800	900
Kozani	33,7	2,8	4.184,9	209,7	1.041,9	412,2	574,5	23	83,8	76,6
Veroia	22,9	10	30.353,6	368,7	1.021	395,9	1.583,7	534	38,9	110,5
Alcalá de Henares	104	99	23.202	3.893,1	2.687	135	2.363	923	129	117
Wayne Hill	610	10	80.000	50	11.000	10	123,2	35,2	230	1
Howdon	258,7	270,3	27.341	20	23.161,3	3.063,3	169,4	48,3	253	28,8
Nápoles	31,5	15,8	11.344,5	267,1	566,2	129,9	742,9	174,7	55,7	129,9
Latina	3,3	1,7	1.190,9	28	30,3	7	78	18,3	3	7
Cuneo	5,4	2,7	1.943	45,7	94,4	21,7	127,2	29,9	9,3	21,7
Cagliari	15,1	7,6	5.434,1	127,9	182	41,8	355,9	83,7	17,9	41,8
Varese Lago	7	3,5	2.507,1	59	74,1	17	164,2	38,6	7,3	17
Varese Olona	4	2	1.441,6	33,9	80,9	18,6	94,4	22,2	8,0	18,6

Los resultados de la implementación de la metodología de los Precios Sombra se encuentran recogidos en la Tabla 5. Se ha obtenido el precio sombra de cada uno de los PPCPs analizados con respecto al ecosistema en el cual se vierte el efluente de las EDARs (humedal, río y mar), según el trabajo de Hernández-Sancho et al. (2010). En dicho artículo se demuestra que existe un precio de referencia para el agua depurada en función del ecosistema en el cual se vierte el efluente, concretamente 0,9 €/m^3 para los humedales, 0,7 €/m^3 para el río y 0,1 €/m^3 para el mar. Analizando los resultados obtenidos para los tres escenarios propuestos, se observa que el precio sombra de los PPCPs asociado a los efluentes vertidos en humedales es mayor. Esto se debe a que los humedales son un ecosistema con una menor tasa de renovación de las aguas, de forma que si un contaminante llega tarda más tiempo en degradarse. Esa baja tasa de renovación también provoca que los organismos estén más tiempo expuestos a las sustancias contaminantes, generando problemas ambientales a corto, medio y largo plazo. El siguiente escenario en importancia es el río, donde los precios sombra reflejan que el vertido del efluente en ese ecosistema ha de ser monitorizado. Por último, el escenario cuyo impacto ambiental sería menor es el mar, donde el vertido del efluente está condicionado por la elevada capacidad de dilución que posee.

Tabla 5. Precio sombra de los PPCPs analizados (€/mg) para los diferentes escenarios propuestos.

	TMP	ACM	IBP	NAP	CBZ
Humedal	0,4	128,2	11	3,4	0,6
Río	0,3	99,7	8,5	2,6	0,5
Mar	0,041	14,2	1,2	0,4	0,1

En función de los resultados obtenidos en los tres escenarios (Tabla 5), el orden de prioridad de los PPCPs analizados es ACM > IBP > NAP > CBZ > TMP. Pese a que existen estudios como el de Kumar y Xagoraraki (2010) donde se establece un ranking de prioridad de PPCPs en función de su presencia y sus efectos ecológicos y sobre la salud, el orden de prioridad propuesto en nuestro estudio surge a partir de una valoración monetaria de los PPCPs mediante una metodología objetiva. Esta diferencia es relevante a la hora de contextualizar a los PPCPs dentro del ámbito de la toma de decisiones, en tanto que permite conocer qué valor monetario tiene la externalidad (en este caso los PPCPs). Yendo un paso más allá, el orden de relevancia propuesto coincide con la literatura de análisis de riesgo sobre organismos acuáticos en contacto directo con vertidos de aguas residuales, porque es en las aguas residuales donde se espera que los valores de riesgo toxicológico sean mayores (Gros et al. 2010). Para ello se ha llevado cabo una revisión bibliográfica donde se han analizado 82 artículos (disponibles en el Anexo B: Listado de artículos utilizados para la evaluación del riesgo toxicológico de los PPCPs analizados en el ARTÍCULO 2) que llevan a cabo un análisis de riesgo toxicológico de PPCPs en organismos acuáticos que están en contacto con aguas residuales. Este análisis de riesgo se lleva a cabo mediante un cociente entre la concentración medida en el efluente (MEC) y la concentración prevista sin efecto (PNEC). Si el cociente entre ambos es mayor o igual que 1 existe riesgo significativo para los organismos acuáticos; mientras que si el cociente es menor o igual a 0,1 el riesgo para los organismos acuáticos es mínimo (Chen et al. 2016).

El análisis de la literatura revela que en el 95% de los artículos el riesgo que se obtiene para el ACM y el IBP es mayor a 1. Esta relevancia coincide con nuestros resultados, ya que el ACM y el IBP son los PPCPs con el valor de precio sombra más alto de toda la muestra en los tres escenarios considerados (humedal: 128,2 €/mg para ACM y 11 €/mg para IBP; río: 99,7 €/mg para ACM y 8,5 €/mg para IBP; mar: 14,2 €/mg para ACM y 1,2 €/mg para IBP). El elevado riesgo toxicológico que destaca la bibliografía consultada se explica por (i) la elevada tasa de consumo de ambos PPCPs (Paíga et al. 2016) – ambos son medicamentos que se consumen tanto bajo prescripción médica como sin prescripción (Ramos et al. 2014) y (ii) por la baja solubilidad que ambos presentan – Jjemba (2006) la cuantifica en valores menores a 0,1 mg/mL. Estos son los factores que determinan la cantidad de tóxico que llega a las EDARs y a las masas de agua receptoras a través del vertido del efluente.

El tercer PPCP en relevancia, teniendo en cuenta el precio sombra obtenido es el NAP. Su precio sombra sigue prácticamente el mismo orden de magnitud entre el humedal y el río (3,4 €/mg y 2,6 €/mg, respectivamente), siendo significativamente menor en el caso del mar (0,4 €/mg). Estos resultados siguen la tendencia de los análisis de riesgo considerados. De los 82 artículos consultados solo en un 7% el NAP tenía un riesgo toxicológico mayor que 1. El comportamiento del NAP en las EDARs está caracterizado por su tendencia a ser adsorbido por la materia orgánica en suspensión debido a su elevado valor de log K_{ow} (Tabla 2). Esto provoca que el destino mayoritario del NAP en las EDARs sean los fangos (Papageorgiou et al. 2016). Pese a esta tendencia, no todo el NAP es eliminado a través de los fangos, sino que una fracción del NAP sale por el efluente de las EDARs, alcanzando las masas de agua (Arlos et al. 2015). Esta fracción del contaminante que permanece en el agua es la responsable de que su precio sombra se sitúe en la zona intermedia del orden de prioridad.

Los PPCPs con menor precio sombra son la CBZ y el TMP. Su precio sombra se aleja significativamente del orden de magnitud del resto de resultados obtenidos. La CBZ muestra un precio sombra similar en los tres escenarios; 0,6 €/mg para humedal, 0,5 €/mg para río y 0,1 €/mg para mar. El 18% de la bibliografía de análisis de riesgo consultada indica que la CBZ tiene un riesgo toxicológico mayor que 1. La CBZ tiene una tasa de eliminación muy baja, concretamente del 3 – 20% (Aymerich et al. 2016) y una fuerte tendencia a crear conjugados con la materia orgánica en suspensión, tal y como se ha comentado anteriormente. El estudio de Zemann et al. (2014) cuantifica que la vida media de la CBZ en el agua residual es de 100 días, incluso superior dependiendo del tipo de tecnología de tratamiento que utilice la EDAR, siendo más susceptibles a su acumulación los reactores de fangos activados (Chen et al. 2015). Estas condiciones convierten a la CBZ en un PPCP persistente y de difícil eliminación de las EDARs (Arlos et al. 2015). La TMP es el PPCP con menor precio sombra de toda la muestra, debido a su baja concentración en comparación con el resto de PPCPs analizados. Asimismo, la revisión bibliográfica avala el precio sombra obtenido, donde sólo el 5% de los 82 artículos consultados obtienen que el riesgo toxicológico de la TMP es mayor que 1, demostrando su bajo impacto ambiental.

Los resultados obtenidos demuestran que el mayor beneficio ambiental de la eliminación de los PPCPs se produce en los humedales. Esto remarca la necesidad de que el agua depurada que llega a estos ecosistemas tenga una calidad adecuada. Hay que tener en cuenta la importancia de la reutilización y el uso del efluente como caudal ambiental, entrando en contacto con el ecosistema. La existencia de PPCPs en los efluentes obliga a buscar nuevas formas de gestión para evitar que los ecosistemas reciban PPCPs, fortaleciendo a la EDAR como fuente de agua no convencional. El hecho de que el beneficio ambiental de eliminar los PPCPs en los humedales sea mayor significa que la eliminación de la ACM, IBP, NAP, CBZ y TMP es muy positiva para ese ecosistema. Los resultados indican que la prioridad en la toma de decisiones debe ir dirigida a los ecosistemas más vulnerables, los cuales se ven fuertemente influenciados por los efluentes de las EDARs. La relevancia de estos resultados es significativa, ya que sirven como justificación de las futuras inversiones en mejoras del proceso de tratamiento en las EDARs (tratamiento terciario).

La cuantificación del beneficio ambiental de eliminar los PPCPs es un enfoque innovador y necesario dentro de la gestión de las aguas residuales urbanas, ya que actualmente no existe legislación que regule su presencia en aguas. Por esta razón este trabajo pone de manifiesto la importancia ambiental, social y económica que tienen estos contaminantes en la potenciación de la reutilización y la economía circular. La obtención del beneficio ambiental en unidades monetarias permite incluir este valor en los procesos de toma de decisiones y en los estudios de viabilidad. Asimismo, el precio sombra puede ser considerado como punto de partida para el diseño de medidas de gestión, como el PSA propuesto en esta tesis, ayudando a internalizar las externalidades ambientales y la concienciación social. Los resultados obtenidos, así como la revisión bibliográfica sobre el análisis de riesgo toxicológico demuestran la robustez de la metodología de los precios sombra como herramienta de valoración del beneficio ambiental de eliminar los PPCPs de los efluentes de las EDARs.

4.3. Identificación de los parámetros que afectan a la presencia de PPCPs en las aguas residuales de la ciudad de València usando la metodología fsQCA

Este trabajo centra su atención en la ciudad de València debido a su cercanía al Parque Natural de l'Albufera (humedal costero) y a la influencia que las EDARs ejercen sobre dicho humedal. La presencia de PPCPs en los efluentes y su uso como caudal ambiental y de riego hace que estos compuestos lleguen a l'Albufera y a los cultivos. Por esta razón es necesario conocer qué variables urbanas influyen en la presencia de PPCPs en las aguas residuales con el fin de establecer medidas de prevención en origen que ayuden a gestionar la reutilización y el ciclo integral del agua. Desde el punto de vista administrativo, la ciudad de València se divide en 19 distritos (Figura 5) que se han tomado como unidades de análisis, de los cuales se ha considerado la siguiente información: (i) concentración de PPCPs, (ii) envejecimiento de la población (iii) consumo de agua, (iv) hospitales, (v) residencias de la tercera edad y (vi) nivel de renta. Los datos se corresponden al año 2013, ya que en ese año se realizó el muestreo y análisis de los PPCPs.

Figura 5. Distritos de la ciudad de Valencia establecidos en la sesión plenaria de enero de 2003 (BSVC 2017).

La hipótesis planteada en este trabajo busca dar respuesta a la pregunta *"¿cuáles son los factores responsables de la presencia de PPCPs en las aguas residuales urbanas?"* Es evidente que los PPCPs detectados en el influente de las EDARs tienen una relación directa con los compuestos excretados por la población a las aguas residuales urbanas. De todos los PPCPs detectados actualmente destaca el caso de los antiinflamatorios, los cuales están recibiendo mayor atención por la comunidad científica debido a su consumo generalizado y a sus efectos tóxicos sobre los organismos acuáticos (Bound y Voulvoulis 2004, Mehinto et al. 2010, Laquaz et al. 2018). Considerando la hipótesis de partida, este trabajo analiza las siguientes variables: el consumo de agua, el envejecimiento de la población, el nivel de renta, el número de hospitales y el número de residencias de la tercera edad. Para la selección de estas variables se ha considerado la disponibilidad de datos en el área de estudio, así como su relación con los PPCPs la cual se ha obtenido de fuentes bibliográficas. En la Tabla 6 se recoge la información disponible y la descripción de cada una de las variables.

Tabla 6. Información disponible y descripción de cada una de las variables consideradas.

Variable	Criterios y caracterización
PPCPs	Los antiinflamatorios son un tipo de PPCPs ampliamente consumido por toda la población tanto en domicilios particulares como en hospitales, lo cual explica su presencia en las aguas residuales urbanas (Escher et al. 2011, Santos et al. 2013). La toxicidad de los antiinflamatorios en los organismos es significativa (Cleuvers 2004, Lee et al. 2011, Mendoza et al. 2015, Schwarz et al. 2017), lo cual justifica la implementación de medidas de monitorización y gestión tanto desde el punto de ambiental como social. Los datos de concentración de PPCPs han sido obtenidos directamente a través de muestreos de campo en los influentes de las dos EDARs que depuran las aguas residuales de la ciudad (Pinedo I y II). Con el fin de implementar la metodología fsQCA se han establecido los siguientes supuestos: (i) los antiinflamatorios no sufren cambios a lo largo de la red de alcantarillado y (ii) el volumen de agua residual que llega a las EDARs es igual al volumen de agua potable consumida.
Consumo de agua (WATCON)	Este trabajo considera que el volumen de agua consumido es igual al volumen de agua residual generado. Los datos de cada uno de los distritos de la ciudad se han obtenido del portal estadístico del Ayuntamiento de València (BSVC 2017). Cabe destacar que los datos de agua consumida se centran únicamente en el consumo doméstico, pero no incluyen el consumo de agua de los hospitales. Teniendo en cuenta la hipótesis de partida y el consumo de PPCPs en los hospitales, se ha calculado el consumo de agua de éstos a través de las modelizaciones publicadas en la literatura. Concretamente, el trabajo de Mendoza et al. (2015) modeliza el consumo en 1.200 L/cama*día.
Índice de envejecimiento (POPAG)	La presencia de medicamentos en las EDARs está asociada a los patrones de consumo de la población (Yin et al. 2017). Conforme avanza la edad de la población también lo hace el consumo de medicamentos (VRG 2012, MHESP 2017), concretamente, los mayores de 65 años consumen una media de entre 5 y 12 tipos diferentes de medicamentos al día (Carrera-Lasfuentes et al. 2013) bien sea bajo prescripción médica o por automedicación (Nicieza-García et al. 2016). En el caso de los antiinflamatorios, la posibilidad de adquirirlos sin receta médica supone que su consumo y su presencia en las aguas residuales urbanas sea significativa (Alexa et al. 2014). Este patrón de consumo justifica la consideración del índice de envejecimiento, cuyos datos se han obtenido del portal estadístico del Ayuntamiento de València (BSVC 2017).
Nivel de renta (INCLEV)	El consumo de PPCPs está relacionado con el nivel de renta de la población (Das et al. 2017, Otto et al. 2018). Los PPCPs adquiridos son de amplio espectro y están destinados a combatir síntomas de enfermedades menores, como es el caso de los antiinflamatorios. Este patrón también está recogido en el estudio de Mukherjee y Kamal (2017), Turek y Owczarek (2014) y Wang et al. (2010). Los datos para la ciudad de València se han obtenido de la oficina de estadística del Ayuntamiento de València (BSVC 2017).
Número de hospitales (HOSP)	Los hospitales consumen grandes cantidades de agua y medicamentos los cuales son excretados por los pacientes y forman una mezcla compleja de diferentes sustancias en sus aguas grises y negras (Ort et al. 2010, Santos et al. 2013). En lo que respecta a esos tipos de aguas, los hospitales no poseen infraestructuras para su tratamiento y son vertidas directamente a la red urbana

	de alcantarillado ya que se consideran similares a las aguas domésticas (Mendoza et al. 2015). Sin embargo, las elevadas concentraciones de medicamentos en esas aguas hacen que los hospitales sean considerados como una de las fuentes principales de PPCPs (Escher et al. 2011, Al Aukidy et al. 2014, Oliveira et al. 2015, Perrodin y Orias 2018). Los datos se han obtenido del portal estadístico del ayuntamiento de València (BSVC 2017), donde se han considerado tanto los hospitales públicos como privados.
Número de residencias de la tercera edad (NURHOM)	Los pacientes de las residencias de la tercera edad sufren diversas patologías cuyos tratamientos implican el consumo de diferentes tipos de medicamentos, entre los que se encuentran los antiinflamatorios (Advinha et al. 2014, Neumann-Podczaska et al. 2016), convirtiendo a las residencias en otra de las fuentes de antiinflamatorios en las aguas residuales urbanas (Escher et al. 2011). Concretamente, el trabajo de Sicras-Mainar et al. (2009) destaca que el 60% de los pacientes de las residencias de la tercera edad consumen antiinflamatorios de forma regular. Por esta razón se ha tenido en cuenta el número de residencias de la tercera edad que hay en cada distrito de la ciudad de València. Al igual que ocurre con los hospitales, no se ha hecho distinción entre residencias de tipo público y privado. Se considera que todas ellas contribuyen a la presencia de antiinflamatorios en el agua residual. Los datos han sido obtenidos del listado telefónico empresarial de la ciudad de València (BDV 2018).

En la Tabla 7 se muestran los resultados obtenidos (combinaciones causales o recetas) para los 19 distritos de la ciudad de València, calculados a través del software fsQCA 2.0 desarrollado por Ragin et al. (2006)[3]. Estas tablas incluyen información sobre: (i) cobertura total y cobertura exclusiva, las cuales analizan en qué grado la hipótesis es explicada como un todo (cobertura total) y en qué grado la hipótesis es explicada por cada uno de los términos de la receta (cobertura exclusiva) (Ragin 2008a); y (ii) consistencia para conocer el grado de consistencia de cada receta (Ragin 2008a).

[3] Disponible en la página web de la Universidad de Arizona (http://www.u.arizona.edu/~cragin/fsQCA/software.shtml).

Tabla 7. Combinaciones causales (recetas) obtenidas para la muestra analizada.

SOLUCIÓN COMPLEJA Umbral de consistencia[a]: 0,99 Cobertura de la solución[b]: 0,65 Consistencia de la solución[c]: 0,99	**Cobertura total**	**Cobertura exclusiva**	**Consistencia**
Receta 1. **POPAG*WATCON*HOSP*NURHOM*~INCLEV** *Distritos con un grado de pertenencia al conjunto (receta) mayor de 0,5: Patraix (0,68;1)*	0,45	0,29	1
Receta 2. **POPAG*WATCON*HOSP*~NURHOM*INCLEV** *Distritos con un grado de pertenencia al conjunto (receta) mayor de 0,5: el Pla del Real (0,82;1)*	0,27	0,15	0,99
Receta 3. **~POPAG*WATCON*HOSP*NURHOM*INCLEV** *Distritos con un grado de pertenencia al conjunto (receta) mayor de 0,5: Campanar (0,54;1)*	0,17	0,04	1
SOLUCIÓN PARSIMONIOSA Umbral de consistencia: 0,99 Cobertura de la solución: 0,91 Consistencia de la solución: 0,99			
Receta 4. **WATCON** *Distritos con un grado de pertenencia al conjunto (receta) mayor de 0,5: Patraix (1;1), Quatre Carreres (1;1), Campanar (0,96;1), el Pla del Real (0,94;1)*	0,91	0,91	0,99

El símbolo ~ significa que la condición ha de estar ausente para que se cumpla la combinación causal obtenida. [a]Umbral de consistencia: las combinaciones causales cuya consistencia esté por debajo del umbral no son incluidas en las recetas finales (Ragin 2006). [b]Cobertura de la solución: indica la proporción de casos que son explicados por la solución (Ragin 2006). [c]Consistencia de la solución: indica la robustez de la solución (Ragin 2006).

La Receta 1 (POPAG*WATCON*HOSP*NURHOM*~INCLEV) es la que tiene resultados más altos de cobertura. Concretamente el valor de cobertura total (0,45) significa que la Receta 1 permite explicar el 45% de los casos que presentan alta concentración de antiinflamatorios. Por otro lado, el valor de cobertura exclusiva (0,29) indica que el 30% de los casos con alta contaminación por antiinflamatorios son explicados exclusivamente por la Receta 1. El valor de consistencia obtenido (1) significa que el 100% de los distritos que presentan la Receta 1 son barrios con alta contaminación por antiinflamatorios. El software del fsQCA permite conocer qué distrito se corresponde con la receta obtenida. En este caso es el distrito de Patraix, en el cual se ubican tres hospitales: Hospital General Universitario – 503 camas, Hospital Dr. Peset Aleixandre – 539 camas y el Hospital Pare Jofré – 125 camas (BSVC 2017). Por otro lado, la influencia de POPAG se evidencia en la distribución por edades de ese distrito. Concretamente, la población total que posee el distrito de Patraix es de 57,629 habitantes, de los cuales el 20% de su población es mayor de 65 años. Concretamente la tasa de mortalidad del distrito es del 8%, un valor bajo que indica el aumento de la esperanza de vida de la población asociada a la mejora de la calidad de vida y el acceso al sistema sanitario (EUROSTAT 2017). El progresivo envejecimiento de la población lleva asociado el consumo de determinados grupos de medicamentos – como es el caso de los antiinflamatorios – para contrarrestar los síntomas de las dolencias que se asocian con la edad (Salech et al. 2016). En relación con POPAG está NURHOM, ya que en el distrito de Patraix hay seis residencias de la tercera edad.

La Receta 2 (POPAG*WATCON*HOSP*~NURHOM*INCLEV) tiene una cobertura total de 0,27 significa que esa receta permite explicar el 27% de los casos que presentan contaminación por antiinflamatorios. Por otro lado, el valor de cobertura exclusiva (0,15) indica que el 15% de los casos con alta contaminación por antiinflamatorios son explicados exclusivamente por la Receta 2. Por lo que respecta a la Receta 3 (~POPAG*WATCON*HOSP*NURHOM*INCLEV), su valor de cobertura total es de 0,17, lo cual indica que esa receta permite explicar el 17% de los casos que presentan contaminación por antiinflamatorios. Su valor de cobertura exclusiva (0,04) indica que el 5% de los casos con alta contaminación por antiinflamatorios son explicados exclusivamente por la Receta 3. Los distritos que responden a estas dos recetas son Pla del Real para la Receta 2 y Campanar para la Receta 3. En ambos distritos existen hospitales cuya presencia influye en la contaminación por antiinflamatorios. Concretamente, en el distrito de Pla del Real (Receta 2) se ubican dos hospitales: Hospital Clínico Universitario – 582 camas y la Clínica Quirón de València – 79 camas (BSVC 2017). Mientras que en el distrito de Campanar se ubican tres hospitales: Hospital Arnau de Vilanova – 296 camas, Instituto Valenciano de Oncología – 140 camas y el Hospital 9 d'Octubre – 300 camas (BSVC 2017). La ausencia de POPAG y NURHOM en ambas recetas se interpreta como una de las situaciones donde la presencia de antiinflamatorios en el agua residual podría suceder. Es decir, que existen distritos donde los PPCPs están presentes, aunque no existan residencias de la tercera edad y el índice de envejecimiento de la población sea bajo.

En la Tabla 7 también se incluye la solución parsimoniosa, esta solución es una versión simplificada de la solución compleja, de tal forma que únicamente incluye las condiciones esenciales que explican las recetas obtenidas. Los resultados obtenidos para la solución parsimoniosa (Receta 4) incluyen una única variable: WATCON. Concretamente el valor de cobertura total para la Receta 4 (0,91) significa que esa receta permite explicar el 91% de los casos que presentan contaminación por antiinflamatorios. Por otro lado, el valor de cobertura exclusiva (0,91) indica que el 91% de los casos con alta contaminación por antiinflamatorios son explicados exclusivamente por la Receta 4. Existen cuatro distritos que cumplen con la Receta 4: Patraix, Campanar, el Pla del Real y Quatre Carreres. Los tres primeros coinciden con los distritos obtenidos para las Recetas 1, 2 y 3, mientras que el distrito de Quatre Carreres únicamente aparece en la Receta 4. Este hecho es destacable ya que solo existe un hospital en ese distrito: el Hospital Universitario y Politécnico de la Fe con 1.284 camas. Al ser la variable WATCON la más importante pone de manifiesto la inclusión del distrito de Quatre Carreres donde se encuentra este hospital, el mayor de toda la ciudad de València y, por lo tanto, un gran consumidor de agua. De esta forma, todas las recetas obtenidas ponen de manifiesto la importancia del consumo de agua y los hospitales en los diferentes distritos para explicar la concentración de PPCPs en las aguas de la ciudad de València.

Como parte del análisis de las variables obtenidas en las recetas, se ha realizado un análisis de necesidad (opción incluida en el software fsQCA) con el fin de conocer qué variables han de estar presentes para que se produzca la hipótesis analizada (Schneider y Wagemann 2012). Tal y como se ha comentado anteriormente, la hipótesis de partida de este trabajo es conocer *"¿cuáles son los factores responsables de la presencia de PPCPs en las aguas residuales urbanas?"*, por ello, a través del análisis de necesidad se conocerán cuáles de ellas han de estar presentes obligatoriamente para que se produzcan concentraciones altas de PPCPs en las aguas residuales urbanas de la ciudad de València. Las variables que forman parte de las recetas obtenidas (Tabla 7) y que han sido sometidas al análisis de necesidad son POPAG, WATCON, HOSP, NURHOM, RENT, ~NURHOM, ~INCLEV y ~POPAG. Los resultados obtenidos (Tabla 8) confirman que WATCON y HOSP son condiciones necesarias para que haya presencia de PPCPs en las aguas residuales, ya que ambas tienen los valores más altos de consistencia y cobertura: 0,91 y 0,99 para WATCON; y 0,85 y 0,79 para HOSP.

Tabla 8. Resultados de los análisis de necesidad para las variables incluidas en las recetas obtenidas.

Variables	Descripción	Consistencia	Cobertura
WATCON	Presencia de elevado consumo de agua	0,91	0,99
HOSP	Presencia de más de un hospital en el distrito	0,85	0,79
POPAG	Presencia de envejecimiento poblacional	0,82	0,31
~INCLEV	Ausencia de niveles altos de renta	0,66	0,31
NURHOM	Presencia de residencias de la tercera edad	0,64	0,38
~NURHOM	Ausencia de residencias de la tercera edad	0,54	0,32
INCLEV	Presencia de altos niveles de renta	0,43	0,36
~POPAG	Ausencia de envejecimiento poblacional	0,29	0,39

El símbolo ~ significa que la condición ha de estar ausente para que se cumpla la combinación causal obtenida.

Estos resultados son significativos en tanto que ponen de manifiesto la relevancia que tienen los hospitales sobre la presencia de PPCPs en las aguas residuales urbanas. En la literatura previa sobre PPCPs y EDARs se ha puesto de manifiesto que las EDARs son los puntos de vertido de los antiinflamatorios al ecosistema. Gracias a los resultados obtenidos se corrobora el hecho de que los hospitales contribuyen a la presencia de antiinflamatorios en las aguas residuales urbanas, y más concretamente influyen en su llegada a las EDARs. En general, las aguas residuales hospitalarias (grises y negras) son vertidas directamente a la red de alcantarillado urbano (Chonova et al. 2018, Wiest et al. 2018). Al no recibir un tratamiento por separado aportan una gran variedad de medicamentos a las aguas residuales urbanas, entre los que se encuentran los antiinflamatorios (Verlicchi et al. 2012, Chonova et al. 2016). La identificación empírica de los hospitales como puntos de vertido de PPCPs permite diseñar futuras acciones de depuración del agua en origen con el objetivo de reducir la presión a la que las EDARs están sometidas y, además, implicar a todos los actores en los procesos de gestión y toma de decisiones.

Siguiendo con el análisis de necesidad del resto de variables, POPAG, NURHOM e INCLEV han de ser tenidas en cuenta (Tabla 8). Éstas están presentes en dos de las tres recetas obtenidas. El análisis de necesidad para la condición POPAG (Recetas 1 y 2) revela que puede ser considerada como una condición necesaria para la presencia de PPCP. Desde un punto de vista poblacional, el envejecimiento de la población es una tendencia al alza, asociada a la mejora de las condiciones de vida de la población, tal y como se recoge en las previsiones de la Unión Europea (EUROSTAT 2017). Estos hallazgos se corresponden con las evidencias encontradas en la literatura, donde se destaca que el envejecimiento de la población implica un mayor consumo de medicamentos tanto recetados como automedicados (Sanwald y Theurl 2017). Sin embargo, existen otras variables cuya presencia no es tan necesaria como las anteriores, es el caso de INCLEV y NURHOM, cuyos valores de consistencia son menores. Estos resultados implican que, aunque su presencia sí que está relacionada con la presencia de PPCPs en las aguas residuales (ya que forman parte de las recetas obtenidas), no es obligado que ambas variables estén presentes para que exista una concentración elevada de antiinflamatorios en las aguas residuales.

Los resultados obtenidos permiten identificar los factores responsables de la presencia de PPCPs en las aguas residuales urbanas. Concretamente, los hospitales, el consumo de agua y el envejecimiento de la población son las principales variables que determinan el vertido de antiinflamatorios a la red de alcantarillado. Este hecho repercute negativamente en la eficiencia de tratamiento de las EDARs al no estar diseñadas para retener estos compuestos, provocando su salida a través del efluente y su llegada a las masas de agua. Como forma de evitar su llegada al medio natural y ayudar a las EDARs en la eliminación de los PPCPs, se recomienda la instalación de unidades de tratamiento de aguas grises y negras en los hospitales como forma de reducir su carga contaminante y, por ende, su impacto ambiental. Es decir, implementar acciones de reducción en origen que conserven los SE de aprovisionamiento de las EDARs y ayuden a reforzar la reutilización como nueva fuente de agua.

5. Conclusiones

La reutilización ayuda a reducir la presión sobre los recursos hídricos disponibles y a cerrar el ciclo del agua, ya que la EDAR deja de ser el punto final del agua residual y se convierte en una nueva fuente de agua. Sin embargo, la presencia de PPCPs en las aguas residuales es un problema real que afecta tanto a la utilidad del efluente como a las masas de agua receptoras. Desde un punto de vista tecnológico, las EDARs no está diseñadas para eliminar los PPCPs, sino que se centran en la reducción de la carga orgánica. Como resultado los PPCPs son vertidos a través de los efluentes y llegan al ecosistema, perjudicando la instauración de la reutilización como herramienta efectiva para reducir la presión sobre los recursos hídricos disponibles. Con el fin de promover la reutilización y la eliminación de los PPCPs en las aguas residuales, esta tesis combina diferentes metodologías que permiten proponer nuevas medidas de actuación, cuantificar el beneficio ambiental de eliminar los PPCPs e identificar la combinación de variables urbanas responsables de su presencia. Gracias a estas metodologías se refuerza el enfoque holístico de la economía circular en el ciclo del agua y permite diseñar nuevas herramientas de gestión ambiental, como el PSA. A continuación, se recogen las conclusiones de cada uno de los artículos que componen el presente compendio, así como las conclusiones generales de la tesis y las futuras líneas de investigación.

ARTÍCULO 1, *A review of Payment for Ecosystem Services for the economic internalization of environmental externalities: A water perspective*.

Los SE permiten entender la relación del ser humano con el medio ambiente de forma que pueda ser abordada de una forma empírica a través del PSA. El PSA permite maximizar el valor presente de los SE con el fin de asegurar su conservación y la interacción entre los actores tanto a corto como a largo plazo, subsanando el daño ambiental que se está produciendo. La revisión bibliográfica que se ha llevado a cabo en este trabajo permite identificar los puntos clave que han de ser considerados para diseñar un PSA y, al mismo tiempo, definir qué aspectos relacionados con la contaminación que se quiere corregir han de ser incluidos. Por un lado, la cuantificación del beneficio ambiental de eliminar la contaminación y, por el otro, la identificación de las variables que intervienen en su presencia. La identificación de ambos aspectos sirve como base del resto de artículos incluidos en el presente compendio.

Las evidencias recogidas en este trabajo muestran que comúnmente se ha considerado al PSA como una herramienta de gestión hídrica en zonas donde la deforestación en cabecera amenaza el volumen de agua almacenado y la integridad de las cuencas hidrográficas. Sin embargo, teniendo en cuenta la hipótesis de partida de la presente tesis, la novedad de este trabajo se centra en proponer el PSA para fortalecer la reutilización del agua en zonas urbanas donde existe riesgo toxicológico por la presencia de PPCPs en el agua residual. Todo ello con el fin de reducir la presión sobre los recursos hídricos y utilizar la economía circular como base para la creación de un nuevo esquema de gestión de las EDARs. Estos resultados cumplen con uno de los objetivos específicos establecidos en la presente tesis, al mismo tiempo que permiten establecer las bases para el cumplimiento del objetivo general de la tesis. Esto se debe a que se identifican los elementos que forman parte del proceso de diseño de un PSA asociado a la reutilización, los cuales serán analizados en el resto de los artículos incluidos en este compendio.

ARTÍCULO 2, *Shadow prices of emerging pollutants in wastewater treatment plants: Quantification of environmental externalities*.

La implementación de la metodología de los precios sombra en el ciclo del agua es un enfoque novedoso, principalmente para la valoración del beneficio ambiental de los PPCPs. Se ha calculado el precio sombra de los PPCPs más comunes en las aguas residuales urbanas (ACM, IBP, NAP, CBZ y TMP) para 24 EDARs seleccionadas con tecnología de tratamiento basada en proceso de fangos activos. Los resultados obtenidos demuestran que los PPCPs con mayor precio sombra (ACM e IBP) son aquellos cuyo valor de riesgo toxicológico es mayor. Mientras que, el resto (NAP, CBZ y TMP) presentan precios sombra menores, así como un valor de riesgo toxicológico menor. La relación entre el precio sombra y el análisis de riesgo toxicológico supone un paso más allá en la interpretación de los resultados. Esta relación demuestra que los precios sombra calculados son coherentes con los hallazgos científicos, aportando robustez al enfoque planteado en esta tesis. Además, esto supone una aportación adicional de esta tesis a la literatura sobre precios sombra, ya que no había sido tenido en cuenta con anterioridad. Gracias a esto se consigue aunar la dimensión ecotoxicológica de los PPCPs con el cálculo de su beneficio ambiental, convirtiendo a la metodología de los precios sombra en un referente a la hora de cuantificar el beneficio ambiental de los PPCPs en agua residual.

Los resultados obtenidos son de gran utilidad para los tomadores de decisiones a la hora de implementar medidas concretas de actuación para reducir la presencia de los PPCPs en las masas de agua, principalmente debido a la ausencia de legislación que regule su presencia. La capacidad de obtener su beneficio ambiental permite que sean incluidos en los análisis de viabilidad económica cumpliendo con los requisitos de inclusión de las externalidades ambientales exigidos en la Directiva Marco de Agua. Además, los resultados permiten identificar a los humedales como los ecosistemas más amenazados por la presencia de PPCPs, fruto de su baja tasa de renovación del agua y su ecotoxicidad. Estos resultados cumplen con uno de los objetivos específicos establecidos en la presente tesis, al mismo tiempo que permiten establecer las bases para el cumplimiento del objetivo general de la tesis. Ello se debe a que el beneficio ambiental alcanzado sirve de referencia a la hora de proponer un PSA, conociendo su importancia expresada en unidades monetarias fácilmente incorporable en su proceso de diseño.

ARTÍCULO 3, *Identification of effective parameters for anti-inflammatory concentration in València City's wastewater using fuzzy-set qualitative comparative analysis*.

La problemática de los PPCPs en las aguas residuales es generalmente abordada desde el análisis de su presencia y concentración en el agua residual, o bien analizando su toxicidad en las masas de agua influenciadas por las EDARs. Sin embargo, la novedad del enfoque propuesto en este trabajo es identificar qué combinación de factores es la responsable de la presencia de PPCPs en las aguas residuales urbanas de la ciudad de València. Partiendo de los datos disponibles y la información bibliográfica, se propone el uso de la metodología fsQCA para analizar las variables seleccionadas (WATCON, POPAG, INCLEV, HOSP y NURHOM) y conocer las interrelaciones existentes. Gracias a la metodología fsQCA se obtiene la combinación de variables que permiten explicar el comportamiento de las variables analizadas con respecto a la hipótesis de partida planteada.

Los resultados obtenidos demuestran que WATCON, HOSP y POPAG son las variables que tienen mayor influencia sobre la presencia de PPCPs en el agua residual. Este hecho repercute negativamente en la eficiencia de tratamiento de las EDARs al no estar diseñadas para retener estos compuestos, provocando su salida a través del efluente y su llegada a las masas de agua. Como forma de evitar su llegada al medio natural y ayudar a las EDARs en la eliminación de los PPCPs, se recomienda la instalación de unidades de tratamiento de aguas grises y negras en los hospitales como forma de reducir su carga contaminante y, por ende, su impacto ambiental. Es decir, implementar acciones de reducción de la contaminación en origen que conserven los SE de aprovisionamiento de las EDARs y ayuden a reforzar la reutilización como nueva fuente de agua.

Desde un punto de vista metodológico, se refuerza la utilidad del fsQCA como herramienta complementaria a los análisis de laboratorio, ayudando a explicar el comportamiento de las variables y contribuyendo al diseño e implementación de medidas de gestión hídrica novedosas, como el PSA propuesto en la presente tesis. Estos resultados cumplen con uno de los objetivos específicos establecidos en la presente tesis, al mismo tiempo que permiten establecer las bases para el cumplimiento del objetivo general de la tesis. Ello se debe a la identificación del origen y el comportamiento de los PPCPs en las zonas urbanas para reforzar el tratamiento del agua residual en origen gracias al fsQCA.

Conclusiones generales de la presente tesis y líneas futuras de investigación

Esta tesis analiza los aspectos relacionados con la reutilización, la calidad del agua, el beneficio ambiental de reducir la contaminación y la identificación de las variables urbanas que contribuyen a la misma. Los resultados obtenidos se muestran en los artículos que forman parte del presente compendio, permitiendo alcanzar un mayor nivel de detalle en el diseño del PSA. Por lo tanto, la novedad de esta tesis es doble: (i) la consideración de las EDARs como proveedoras del SE de aprovisionamiento (fuentes de agua no convencional), y (ii) el análisis del beneficio ambiental de eliminar los PPCPs y la identificación de las variables urbanas que afectan a su presencia como pilares en el diseño de un futuro PSA centrado en reducir los PPCPs en origen. Estos aspectos resultan esenciales para conseguir que el PSA recoja la realidad del daño ambiental que se está generando, así como la importancia que tiene la conservación de los recursos hídricos. Esta tesis pone de manifiesto la relevancia de considerar los SE que surgen de la intervención humana en el medio ambiente creando nuevas oportunidades para el abastecimiento de agua. Las EDARs son fuentes potenciales de agua cuyo caudal es necesario para mantener el equilibrio del ciclo hidrológico. La economía circular abre una puerta muy importante a la hora de apoyar las propuestas de reutilización para abastecer la demanda de los usos agrícola y ambiental.

Gracias al PSA, y a las evidencias empíricas recogidas en esta tesis, se busca crear un vínculo institucional entre los actores implicados para reducir la contaminación en origen y fomentar la reutilización. Desde un punto de vista legislativo, la ausencia de un marco regulador para los PPCPs y la existencia de procedimientos ya establecidos en el territorio no debe impedir la implementación de otras formas de gestión novedosas, como el PSA. En este caso se busca establecer una estrategia conjunta de gestión hídrica centrada en la reutilización y la reducción de la presión sobre los recursos hídricos a través de la eliminación de los PPCPs en origen, reduciendo la presión que sufren las EDARs. De esta forma se cumple con el objetivo general de la presente tesis de analizar la importancia de las EDARs como fuentes de agua no convencional, así como la potencialidad que tiene el PSA como nueva forma de gestión destinada a reducir la presencia de PPCPs en las aguas residuales, fomentando la conexión entre todos los actores implicados. Al mismo tiempo se abren nuevas líneas de investigación futuras orientadas a la implementación del PSA en un área de estudio real, así como el estudio del impacto de la disminución de los PPCPs sobre las EDARs y la reutilización. Todo ello dirigido a proponer planes de reutilización efectivos en el sector agrícola y la conservación del caudal como base de los espacios hídricos protegidos.

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ANEXOS

Anexo A: Restricciones asociadas al proceso de programación lineal de la metodología de los precios sombra aplicada en el ARTÍCULO 2

La programación lineal se utiliza para estimar los parámetros (α, β, γ) de la función distancia, con el din de minimizar la suma de las desviaciones entre la frontera y la función obtenida para cada unidad (Färe, Rolf et al., 1993; Hernández-Sancho et al., 2010), tal y como se recoge en la Eq. A.1.

$$Max \sum_{k=1}^{K} [\ln D_0 \left(x^k, u^k\right)] - \ln(1) \qquad \text{Eq. A.1}$$

Esta ecuación está sujeta a una serie de restricciones (véase ecuaciones A.1.1, A.1.2, A.1.3, A.1.4 y A.1.5) que han de ser tenidas en cuenta la hora de establecer los parámetros de la programación lineal:

$$\ln D_0 \left(x^k, u^k\right) \leq 0, \;\; \forall k = 1, \dots, K \qquad \text{Eq. A.1.1}$$

$$\frac{\partial D_0 \left(x^k, u^k\right)}{\partial \ln u_m^k} \geq 0, \qquad \forall k = 1, \dots, K.; \; \forall m = 1, \dots, i. \qquad \text{Eq. A.1.2}$$

$$\frac{\partial D_0 \left(x^k, u^k\right)}{\partial \ln u_m^k} \leq 0, \qquad \forall k = 1, \dots, K.; \; \forall m = i+1, \dots, M. \qquad \text{Eq. A.1.3}$$

$$\sum_{m=1}^{M} \alpha_m = 1 \sum_{m'=1}^{M} \alpha_{mm'} = \sum_{m=1}^{M} \gamma_{nm} = 0, \qquad \forall n = 1, \dots, N. \qquad \text{Eq. A.1.4}$$

$$\forall m = 1, \dots, M.$$

$$\alpha_{mm'} = \alpha_{m'm} \qquad \text{Eq. A.1.5}$$

$$\forall m = 1, \dots, M; \forall m, = 1, \dots, M; \beta_{nn'} = \beta_{n'n}, \;\; \forall n = 1, \dots, N; \forall n' = 1, \dots, N$$

donde $k = 1, \dots, K$ representa el número de unidades de producción incluidas en el análisis, i representa los outputs deseados y los restantes $i + 1, \dots, M$ representan los outputs no deseados. Como la función distancia toma valores inferiores o iguales a uno, el $ln\, D_0 \left(x^k, u^k\right)$ será menor o igual a cero y la desviación de la unidad k en relación con la frontera; el $[ln\, D_0 \left(x^k, u^k\right)] - ln(1)$ será menor o igual que cero también. Por ello, al maximizar la función objetivo se busca minimizar la desviación en relación con la frontera de producción, haciéndola lo más próxima posible a cero.

La primera restricción (Eq. A.1.1) implica que las unidades estarán por debajo o justo encima de la frontera de producción. La segunda (Eq. A.1.2), impone que los outputs deseados obtengan precios sombra positivos o nulos, pero nunca negativos. La tercera (Eq. A.1.3), implica que los no deseables tengan valores negativos o nulos, pero nunca positivos. La cuarta restricción (Eq. A.1.4), asegura que exista libre disponibilidad débil de outputs. Finalmente, la quinta restricción (Eq. A.1.5) es una restricción de simetría para los parámetros referidos a pares de inputs y outputs.

Anexo B: Listado de artículos utilizados para la evaluación del riesgo toxicológico de los PPCPs analizados en el ARTÍCULO 2

En este anexo se incluye el listado de artículos utilizados para analizar el riesgo toxicológico al cual están expuestos los organismos acuáticos por entrar en contacto con los PPCPs analizados en el ARTÍCULO 2. Estos artículos han sido utilizados para establecer la relación entre el precio sombra obtenido y los análisis de riesgo toxicológico publicados en la literatura, con el fin de reforzar la utilidad de la metodología de los precios sombra como herramienta efectiva de valoración del beneficio ambiental de eliminar los PPCPs de los efluentes de las EDARs.

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Anexo C: Publicaciones originales

a. ARTÍCULO 1: *A review of Payment for Ecosystem Services for the economic internalization of environmental externalities: A water perspective*

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Review

A review of Payment for Ecosystem Services for the economic internalization of environmental externalities: A water perspective

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ABSTRACT

The allocation of economic value to environmental goods is intended to internalize the socio-economic and environmental costs of policies implemented and thus recognizes the value of the ecosystem and the consequences of environmental damage. This entails identifying the costs and benefits of management measures for conservation and of degraded ecosystems. The difficulties of this task are: (i) they are goods that have no market and (ii) there is a need for economic funding for conservation purposes. Payment for Ecosystem Services (PES) seeks to internalize the environmental externalities of human actions, ascribing monetary value to Ecosystem Services (ES) and helping decision-makers to recognize the real value of the loss of ES. Sustainable management is secured within a model of integrated resource management (a combination of economic, social, environmental, political and cultural spheres). PES breaks with the classical view of environmental protection (based on direct regulation to prevent, correct and punish harmful behaviour). This review focuses on concrete aspects of the sustainable management of ES related to water, examining the possibility of implementing PES for water ES, using mainly the Pigouvian approach. It considers the importance of developing PES schemes at the hydric level in response to the need for management of resources, while ensuring the supply for current uses and demand while being attentive to social and environmental dimensions.

Contents

1. Introduction

The current state of technology has distorted people's relationship with the environment, as the standard argument is that if there is an environmental problem then the scientific community and technological solutions are able to fix it. However, management of ecosystem goods and services is feasible through a multidisciplinary approach (i.e., taking into account environmental, economic, social and political aspects). The use of Payment for Ecosystem Services (PES) is proposed to internalize environmental externalities generated daily. The starting point is viewed as the need to estimate the economic value of goods or services to be preserved and/or restored. For our purposes, the PES tools are associated with the hydric sphere to develop the theoretical foundations necessary to allow its implementation in the water management of

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river basins. Guidelines to be followed are framed with a view to achieving the internalization of environmental externalities. Through this literature review we focus on the general methodology and its relation to the hydric sphere (as a way of managing an increasingly scarce and problematic resource), to consider opening up a new way of managing resources by merging economic, social, political and environmental issues.

2. Ecosystem Services (ES) and internalization of environmental externalities

The Millennium Ecosystem Assessment (MEA, 2003) is defined as: "*the benefits people obtain from ecosystems. These include provisioning services such as food, water; regulating services such as regulation of floods, drought, land degradation, and disease; supporting services such as soil formation and nutrient cycling; and cultural services such as recreational, spiritual, religious and other nonmaterial benefits*" (2003: 3). Valuation of environmental goods through ES means valuing the natural capital (Lauf et al., 2014). However, market failure is responsible for creating environmental externalities as a result of inappropriate incentives for ES management; hence, the ability to modify ES quality is not considered within the decision-making process (Adhikari and Boag, 2013). Water is a public good and its degradation becomes an externality that is not taken into account because there is no market value imputed; governments and businesses are unable to internalize the value of such ES degradation (Schomers and Matzdorf, 2013). What are the ES provided by water resources? (i) water supply and aquifer recharge; (ii) regulation of water flows; (iii) regulation of nutrients; (iv) soil formation; (v) treatment capacity; (vi) biological control; and (vii) food production (Baker et al., 2013; Helfenstein and Kienast, 2014). As noted, these are vital for maintaining balance in the ecosystem; and therefore we reiterate the importance of knowledge based on the interrelationships between different ecosystems. According to Fregoso (2006), water ES "*appear in the hydrological cycle, as a result of the ecosystem's capacity to store water and thus keep water supply available for society benefit*" (2006: 30).

3. Managing the environment via Payment for Ecosystem Services (PES)

PES, according to Wunder (2005), is "*a voluntary transaction where a well-defined ES (or a land-use likely to secure that service) is being 'bought' by a (minimum one) ES buyer from a (minimum one) ES provider, if and only if the ES provider secures ES provision (conditionality)*" (2005: 3). PES aims to encourage a change in the management and use of ES and achieve effective conservation financing. As a result, PES can prevent overexploitation of ES and would avoid the need for the recovery of damaged ES. PES undertakes a preventive approach thanks to adapting ES use to population needs (Garbach et al., 2012). PES are designed for guarantee economic welfare through the internalization of environmental externalities; using pricing mechanism is better form for achieve it (Mombo et al., 2014). Economic instruments are important tools to achieve environmental targets thanks to their ability for changing provider behaviour. Under this approach, PES schemes become a complementary tool of command and control measures (Young and de Bakker, 2014). However, this is a highly complex process because the units in which the welfare of a society is expressed do not coincide with the units of measurement for natural parameters (Wallace, 2007). Hence, an ecosystem cannot be reduced to a single assessment process because it is not an isolated system (Fisher et al., 2009; Kallis et al., 2013). The main objectives of PES implementation are: (i) ES maintenance preventing its degradation, (ii) ES restoration (Robert and Stenger, 2013), and (iii) ensuring the continuous supply of the ES (Tacconi, 2012). For the attainment of these objectives, markets have to be created based on the Coase theorem or on the Pigouvian approach.

The Coase theorem establishes that government intervention is not needed for internalizing externalities; PES moves into a private sphere (Coase, 1960). PES schemes based on this principle have only been successfully implemented at the local level, where negotiations between stakeholders are relatively easy. The implementation focus is at the micro level so that stakeholders can agree within the framework of the PES. Furthermore, the price reflected in the agreement should not be considered as representative price of the real market value of the ES (Schomers and Matzdorf, 2013; Tacconi, 2012; Wunder et al., 2008). The Pigouvian approach is better because it emerges when the government is part of the PES design and the implementation is based on the premise that ES are public goods (Shapiro-Garza, 2013). It seeks to encourage a change of management activities to generate positive externalities through the creation of an ES market that establishes contact between target ES providers and beneficiaries; thus the prices arise from the environmental quality standards established by government (Van Hecken et al., 2015). Since government promotes the Pigouvian approach, PES has the greatest magnitude and it has higher transaction costs. For Rawlins and Westby (2013) this is the main PES approach, because ES, such as water are public goods, the only feasible approach in terms of biodiversity conservation and water quality (Wunder et al., 2008). To ensure the future feasibility of PES based on a Pigouvian approach, it is necessary to guarantee the availability of funds for self-maintenance, avoiding dependence on government budgets and turning PES into a more effective conservation tool and maximizing its positive ecological effects on ES. Through the fund, a sustainable source of long-term funding is attained, which *inter alia* covers the costs of monitoring and surveillance, the implementation of measures and payments in kind (Goldman-Benner et al., 2012; Van Hecken and Bastiaensen, 2010). Related to PES implementation for water ES, adoption of a Pigouvian-type approach is proposed. This would manage a resource characterized (in most cases) as a public good, while taking into account the interests of all stakeholders. The result would widen the scope for the development of measures to enable the promotion of communication between the political, social and environmental spheres and the sustainable management of resources within the framework of governance.

PES is subject to transaction costs as it seeks to link the political sphere to the economic, social and environmental spheres. The establishment of a PES scheme is expensive and complex, resulting in the need to identify correctly ES and to quantify, as realistically as possible, the *ex-ante* and *ex-post* costs. The weight of these costs on the PES programme is strong, so it has a direct impact on the field of decision making and also on the design of the measures to be implemented (Barnaud and Antona, 2014). If all the costs could be quantified, PES would be negotiated between the providers and beneficiaries to maximize the benefits gained from resources, assuming that transaction costs are insignificant. However, it is not possible to quantify all the costs. Thus, it might be necessary reduce PES costs to improve its efficiency. Nevertheless, if the costs are reduced, the consequences will be negative for PES operation and for achievement of the initial objectives. If, however, the approach is taken to the opposite extreme, a high value of transaction costs does not ensure the success of the PES programme as it will be difficult to maintain the level of exigency over time (Wunder et al., 2008). This is why institutional strengthening is crucial for determining, managing and distributing all costs appropriately and equitably (Lin and Nakamura, 2012), because an incorrect estimate will have a strong impact on the development and operation of the PES scheme (Wang, 2012).

PES allows the internalization of environmental externalities within economic valuation, so that ES is brought within the dimension of decision-making and the cornerstones to ensure that environmental quality is preserved. PES implementation expects maximization of the present value of an ES to encourage its potential conservation and tries to remedy current damage (Roumasset and Wada, 2013). Many PES schemes have been implemented with the multiple purposes of maintaining the ES, avoiding overexploitation and alleviating poverty in certain communities, especially where ES provision is relatively easy and the opportunity costs of conservation are low (Bremer et al., 2014; Kolinjivadi et al., 2015; Leimona and Lee, 2008; Schomers and Matzdorf, 2013).

However, not everyone agrees; for Adhikari and Boag (2013), Groom and Palmer (2012), García-Amado et al. (2011), and Hegde and Bull (2011), PES schemes were not originally designed to fulfil social objectives and should not be considered the primary method for achieving them, although these authors argue that the flexibility of PES schemes may go a long way towards addressing these social objectives. Nevertheless, the link between PES schemes and poverty alleviation is considered, as it relates to practical approaches that can be adopted using this methodology.

3.1. Payment for Ecosystem Services and water resource management

Payment for Water Ecosystem Services (PWS) is an approach based on the need for water conservation (Fregoso, 2006). PWS involves an integrated management approach towards the water basin (Lin and Nakamura, 2012). This approach aims to provide economic incentives for stakeholders to show their readiness to cooperate in conservation efforts aimed at improving the water ES. Water ES must clearly be defined, establishing the benefits associated with conservation, e.g. improving the quality of drinking water and the redistribution of allocations for different uses (Martin-Ortega et al., 2013). The scale of analysis is thereby reduced until it is focused solely on hydrological services. Ojea et al. (2012) propose a differentiation into the following categories: (i) provision of cultural services; (ii) improved water quality and quantity of the resource available, leading to improvements in the extraction of water for supply; (iii) conservation of ecosystems strongly related to water (such as wetlands, rivers, and lakes); and (iv) mitigation of damage caused by water on which the conservation of forest land and soil structure depends. Much of the literature consulted focuses on the implementation of such PWS schemes to ensure the supply of water to urban settlements, mainly in Latin America, Asia and Africa, where deforestation and irregular handling in water catchment areas because of agricultural practices threaten the maintenance of the aquifer flow (see Bennett et al. (2014), Brouwer et al. (2011), and Fisher et al. (2010)).

The application of this methodology has largely been in South America, where conservation of forest cover upstream is necessary. PWS aims to stop the high rates of deforestation responsible for increased runoff and erosion – increasing the levels of sediment in the water, which reduces quality and complicates the subsequent treatment (Wunder, 2005). Furthermore, the rates of recharge are decreased because of the inability of bare soil to aid water filtration. These issues primarily affect two basic features of ES: water quality and seasonal distribution. A well-known example of this type of PWS is the province of Heredia in Costa Rica. Here, the government obtains the funds necessary for forest recovery from rates that are charged by the water service. Thus, the beneficiaries of the water supply internalize the costs derived for forest recovery in areas of ecological and hydric importance (Fregoso, 2006). The positive aspect of this new enforcement approach is that with the protection of water ES, not only is a quality supply guaranteed, but also it promotes the attainment of secondary benefits, such as the conservation of animal and plant biodiversity (Wünscher et al., 2008), and the linking of ES users with forest resource managers (Fregoso, 2006). New York City had problems with the drinking water treatment due to inadequate management of agricultural pesticides. Water treatment was carried out by natural filtration using the characteristics of the underlying soil; however, farms had caused the contamination of the soil and therefore the degradation and pollution of water sources used for the water supply. To solve this problem, the local government carried out a comparative analysis of the costs and benefits of changing agricultural practices towards more sustainable activities that would reduce the level of contamination in the aquifer. The result was that if farmers were paid to improve their management, the government would benefit at a lower cost and there would be no need for a filtration plant. To implement this measure, a number of consumer tariffs were applied through the water bill to fund the payments to ES providers (Kemkes et al., 2010; Lurie et al., 2013). Another example of a PWS scheme is the bottling company *Vittel* (part of the *Nestlé* group), which began implementing a compensation programme in 1993 focusing on improving practices within the local dairy farming sector, with the aim of preserving the quality of groundwater and reducing the impact on livestock. Farmers were paid by the company to cover opportunity costs associated with changes in farming practices. However, the programme presents a more complex case: not only do the farmers receive cash, but they also receive payments in kind through technical assistance. This aspect, coupled with the fact that the contracts are long-term arrangements (18–30 years) and that the opportunity costs incurred by each farm are studied, has created a solid basis for implementation and established strong bonds of trust among the stakeholders. This case uses a Coase-type approach as it is the company that handles the programme and makes the payments (Wunder et al., 2008).

4. Conclusions

ES are the basis for understanding the economic valuation of environmental goods and services, enabling the application of an economic approach in the environment and expressing this evaluation in language that can be understood by people and institutions. Achieving the objectives discussed in this paper needs the formation of a multidisciplinary team to provide a global view of the environment and understanding of the social dimension. The contexts in which projects are undertaken involve the valuation of water as a relevant environmental asset in today's society.

The PES method implements the internalization of environmental externalities in the process of identifying and adapting ES for economic valuation and obtaining funding for conservation programmes. Thus, PES process makes it possible to gather information on how the positive incentives provided by PES influence relationships between society and the environment, supporting those processes chosen by the diffusion of new practices. With this measure neither the conservation nor the management of ecosystems is perceived as a cost to society but as an investment.

The management of water resources is a complicated issue due to the increased use and demand prevailing today. The approach proposed here serves as a methodological basis for considering the fundamental aspects of PES schemes when applied to water management. These are intended to improve water quality and supply the ever-greater demand while reducing environmental impact.

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b. ARTÍCULO 2: *Shadow prices of emerging pollutants in wastewater treatment plants: Quantification of environmental externalities*

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Research article

Shadow prices of emerging pollutants in wastewater treatment plants: Quantification of environmental externalities

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A B S T R A C T

Conventional wastewater treatment plants (WWTPs) are designed to remove mainly the organic matter, nitrogen and phosphorus compounds and suspended solids from wastewater but are not capable of removing chemicals of human origin, such as pharmaceutical and personal care products (PPCPs). The presence of PPCPs in wastewater has environmental effects on the water bodies receiving the WWTP effluents and renders the effluent as unsuitable as a nonconventional water source. Considering PPCPs as non-desirable outputs, the shadow prices methodology has been implemented using the output distance function to measure the environmental benefits of removing five PPCPs (acetaminophen, ibuprofen, naproxen, carbamazepine and trimethoprim) from WWTP effluents discharged to three different ecosystems (wetland, river and sea). Acetaminophen and ibuprofen show the highest shadow prices of the sample for wetland areas. Their values are 128.2 and 11.0 €/mg respectively. These results represent a proxy in monetary terms of the environmental benefit achieved from avoiding the discharge of these PPCPs in wetlands. These results suggest which PPCPs are urgent to remove from wastewater and which ecosystems are most vulnerable to their presence. The findings of this study will be useful for the plant managers in order to make decisions about prioritization in the removal of different pollutants.

1. Introduction

Water stress, due to weather and the overexploitation of water sources, complicates the ability to meet the increasing water demands of contemporary society. Nonconventional water sources, including regenerated water, offer solutions to this problem, particularly in arid and semiarid regions. However, the main problem with the reuse of wastewater treatment plant (WWTP) effluent is the final water quality because of many processes are not designed to remove the chemicals of anthropogenic origin, including pharmaceuticals and personal care products (PPCPs) (Fang et al., 2012; Morais et al., 2014; Santos et al., 2013). Conventional WWTPs are mainly designed for the removal of suspended solids and organic matter (Binelli et al., 2014). As a result, PPCPs leave WWTPs through the "treated" effluent and reach receiving water bodies, where the chemicals spread and accumulate in water, sediment and organisms (Arlos et al., 2015; Carmona et al., 2014; Zenker et al., 2014). In this way, WWTPs become the point of discharge and dispersion of PPCPs in the aquatic ecosystem (Prosser and Sibley, 2015). Kasprzyk-Hordern et al. (2008) estimated that 50% of PPCPs that arrive at WWTPs are discharged through the effluent without any change of their toxic activity. Many authors have analysed the concentrations of PPCPs in rivers and lakes, into which the effluents from WWTPs have been discharged. All of these reports confirmed the presence of PPCPs in receiving water bodies and emphasised the need to address the problem in order to improve water quality for reuse purposes (Baker and Kasprzyk-Hordern, 2013; Blair et al., 2013; Ferguson et al., 2013; Spongberg et al., 2011; Wang et al., 2015; Zenobio et al., 2015).

PPCPs in wastewater are presented in a complex mixture of substances (Yuan et al., 2013) whose toxicity affects even the microbial community found in conventional activated sludge treatment processes (Liu and Wong, 2013). The most commonly found PPCPs in urban wastewater include plasticisers, surfactants, pharmaceuticals, drugs of abuse, hormones, personal care compounds, contrast mediums and sweeteners, among others (Miège et al., 2009; Pal et al., 2014). The occurrence and concentrations of these compounds vary. Ibuprofen is the most commonly detected

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pharmaceutical because of its frequent worldwide consumption (Fang et al., 2012). Many authors have performed studies to identify the specific PPCPs in wastewater samples, analysed their concentrations and examined different options for their elimination (Al Aukidy et al., 2012; Baker et al., 2012; Blair et al., 2015; Collado et al., 2014; Fernández et al., 2014; Godayol et al., 2015; Kumar et al., 2011; Silva et al., 2014). Although the PPCPs found in wastewater vary depending on the study area, overall, the frequencies with which PPCPs appear are greater than 50% (i.e. more than half of PPCPs are found in all samples analysed). From an environmental perspective, PPCPs in WWTP effluents can be considered as indicators of anthropogenic pollution in water bodies (Van Stempvoort et al., 2013).

One possible way to reduce PPCP levels in water bodies is through tertiary treatment technologies. However, not in all cases WWTPs incorporate tertiary treatment technologies. For example, in Spain only 9% of urban wastewater receives tertiary treatment (AEAS, 2002). This situation makes the presence of PPCPs in the effluent of the WWTPs relevant for water reuse purposes. Hence, it is necessary to quantify overall costs of wastewater treatment processes (including technological improvements in WWTPs) for selecting the proper technology to remove them. Some authors have assessed the efficiency of removing PPCPs by different processes, such as advanced oxidation, ozonisation and activated carbon (Mailler et al., 2016; Rosal et al., 2010; Tang et al., 2014; Zhang and Geißen, 2010). When the characteristics of raw wastewaters that reach the WWTP are known, all of these technologies are able to reduce the PPCP concentration in the effluent substantially (up to 80%). Thus, by monitoring and removing PPCPs, the addition of tertiary treatment to urban WWTPs could be the key step to improving wastewater treatment (Alfonsín et al., 2014). Although technological improvement is the most appropriate solution for improving WWTP effluents, the economic implications of such investments should be considered. The current trend of the economy, in relation to the environment, is to include the environmental externalities within feasibility analysis.

Including environmental externalities in feasibility analysis allows to quantify properly the costs of wastewater treatment. However, determine monetary value of environmental externalities is not an easy process. There are many limitations that must be overcome, like the own complexity of ecosystem and the lack of standard methodology for monetary valuation (Kallis et al., 2013). To begin with, it is required a proper identification of the environmental externalities and environmental goods and services that are being evaluated as well as the selection of the suitable methodology for the valuation purposes (Lamarque et al., 2011). Those environmental goods and services which provide tradable goods are easy to value (as wood production) due to their market value. However not all environmental goods and services have market value. Water quality, for example, is a significant part of ecosystems without market value. Poor water quality means a serious deterioration of ecosystems, including loss of biodiversity. Hence, for achieve a proper assessment of environmental externalities, the monetary valuation of ecosystems should include not only the environmental goods and services with market value but those without this market value. Obtaining the monetary value of these environmental goods and services aims to raise awareness about the importance of an ecosystem, through the calculation of monetary value of a good and ecosystem service that lacks a market (Kallis et al., 2013). Hence, this monetary value is associated with an efficient use of the resource since the managers know its significance (Wallace, 2007). Monetary valuation is associated to a behavioural change in the use and management of environmental goods and services (Kumar et al., 2013). This reasoning is based on taking into account that we are within a market society, where the best way for society to internalize the importance of an environmental good or service is by giving it monetary value (Aznar-Bellver and Estruch-Guitart, 2012). Thanks to the monetary valuation, it is possible to frame the scale of provision of environmental goods and services, helping to delimit the scope in which planning and management processes will be developed (Kumar et al., 2013).

There are a wide range of valuation methods, but the most common of them are summarized below. Stated preference methods (as contingent valuation and choice experiment) use a survey for knowing the willingness to pay of respondents (He et al., 2015; Rupérez-Moreno et al., 2015). Revealed preference methods (as travel cost and hedonic price methods) consider that the monetary value can be obtained from existing markets (Ezebilo, 2016; Zhang et al., 2015). Cost-based methods consider that the damage of ecosystems modify the capacity of ecosystems to regulate the environment (as flood protection). Hence, the monetary value of ecosystems is calculate from the economic cost that would be necessary for recover them (Jackson et al., 2014; Remme et al., 2015; Yao et al., 2016). Benefit transfer methods consider that the monetary value of an ecosystem is the same that the monetary value of other ecosystem located in a different place (Chaikumbung et al., 2016; Madani and Khaleghi, 2015). These methodologies for monetary valuation of ecosystems show the range of option available. In the case of PPCPs in WWTPs effluents, the implementation of previous methodologies would be complicated because PPCPs have no market value.

One methodological option for valuing environmental externalities without market value is the shadow price methodology. This method represents the environmental damage that PPCPs are causing through the discharge of WWTPs effluents into water bodies. According this methodology, production processes generate marketable (desired) outputs as well as nonmarketable byproducts that adversely affect the environment. The shadow price approach is used to calculate the monetary value of PPCPs as non-desirable outputs. The monetary value obtained can be included in the decision-making process during the economic valuation of ecosystem services (Zhou et al., 2014). Molinos-Senante et al. (2013) calculated shadow prices for PPCPs in their analysis of ozonisation processes for eliminating these pollutants from effluents discharged in sensitive and non-sensitive areas. The shadow prices obtained in sensitive areas are 11.06 €/kg (for galaxolide), 13.98 €/kg (for tonalide), 44.46 €/kg (for sulfamethoxazole) 53.47 €/kg (for diclofenac) and 93.76 €/kg (for ethinylestradiol), and results in non-sensitive areas ranged from 8.67 €/kg (for galaxolide), 10.98 €/kg (for tonalide), 34.95 €/kg (for sulfamethoxazole), 42.20 €/kg (for diclofenac) and to 73.73 €/kg (for ethinylestradiol). Overall, the environmental benefit of eliminating PPCPs was greater for sensitive areas, where conservation actions are necessary.

The main aim of this paper is to obtain the monetary value of the environmental externalities associated to PPCPs existing in WWTP effluents, through using the shadow prices methodology. The obtained results can be used as proxy of environmental benefit related to the removal of PPCPs in WWTPs effluents. The secondary objective is to analyse the relationship between the shadow prices of PPCPs and the results of toxicological risk assessments in the literature. It has been sought to confirm the connection between the shadow price methodology and the degree of environmental impact showed by the selected PPCPs. This paper contributes to the literature of valuing environmental externalities calculating the monetary value of removal the PPCPs in the effluent of wastewater treatment processes; which could be included in feasibility analyses and decision-making processes.

2. Methodology

The shadow price methodology has been used following the approach of Färe et al. (1993). This approach uses distance functions to represent the technology of production processes, allowing identify the relationship between inputs and outputs. Specifically, distance functions measure the difference between the efficiency of a WWTP and its efficiency frontier of reference, given by the set of WWTPs with highest efficiency from a specified input level (Hernández-Sancho et al., 2010). This methodology seeks to maximise the production of the desired outputs and at the same time to avoid the generation of non-desirable output (Wei et al., 2013), in the context of available technology (Hernández-Sancho et al., 2010).

Given a set of inputs $X = (x_1,\ldots,x_N)$, set of outputs $U = (u_1,\ldots,u_M)$ and production set $P(x) = \{u \in \Re_+^M : x \text{ can produce } u\}$, the reference technology is assumed to satisfy the conditions proposed by Färe et al. (1988). An output distance function is defined by Shephard (1970) as:

$$D_0\ (x,u) = inf\{\theta : (u/\theta)\in P(x)\} \tag{1}$$

satisfying that $\in P(x)\ <=> D_0\ (x,u) \leq 1$. Price vector has been defined as $r = (r_1,\ldots,r_M)$ of outputs with $r \neq 0$. Given r, the revenue function is defined as:

$$R(x,r) = sup_u\ \{ru : D_0\ (x,u) \leq 1\} \tag{2}$$

Under the assumption that the functions $D_0\ (x,u)$ and $R(x,r)$ are distinguishable, according to Shephard (1970), it is possible to show that:

$$\nabla_u D_0\ (x,u) = r^*(x,u) \tag{3}$$

It has been denoted $r^*(x,u)$ as the maximum income achievable through the price output vector $\nabla_u D_0\ (x,u)$). To obtain the shadow prices of non-desirable outputs, it has been assumed that the shadow price of a desired output is the same value as its market price, which is the observed output price of the *mth* output $= r_m$, where r_m is the *mth* desired output shadow price. Hence, all m ≠ m' will have the shadow price formula (Färe et al., 1993):

$$r'_m = r_m^0 \frac{\partial D_0(x,u)/\partial u'_m}{\partial D_0(x,u)/\partial u_m} \tag{4}$$

where m is the desired output with a market price of r_m.

Färe et al. (1993) used optimisation of a translog function, which estimates a distance function whose aim is to maximise production of the desired output. The translog function is defined by:

$$\begin{aligned}\ln D_0\ (x,u) = {} & \alpha_0 + \sum_{m=1}^{M} \alpha_m\ \ln u_m\ + \sum_{n=1}^{N} \beta_n\ \ln x_n + \frac{1}{2}\sum_{m=1}^{M} \\ & \times \sum_{m'=1}^{M} \alpha_{mm'}\ (\ln u_m\ )(\ln u_{m'}) + \frac{1}{2}\sum_{n=1}^{N} \\ & \times \sum_{n'=1}^{N} \beta_{nn'}\ (\ln x_n\ )(\ln x_{n'}) + \sum_{n=1}^{N} \\ & \times \sum_{m=1}^{M} \gamma_{nm}\ (\ln x_n\ )(\ln u_m\ )\end{aligned} \tag{5}$$

Linear programming is used to estimate parameters (α, β, γ) of the distance function, with the goal of minimising the sum of deviations between the function built for each unit and the frontier (Färe et al., 1993; Hernández-Sancho et al., 2010), as follows:

$$Max \sum_{k=1}^{K}\left[\ln D_0\left(x^k, u^k\right)\right] - \ln(1) \tag{6}$$

s.t. :

$$\ln D_0\left(x^k, u^k\right) \leq 0, \quad \forall k = 1,\ldots,K \tag{6.a}$$

$$\frac{\partial D_0\left(x^k, u^k\right)}{\partial \ln u_m^k} \geq 0, \quad \forall k = 1,\ldots,K.;\ \forall m = 1,\ldots,i. \tag{6.b}$$

$$\frac{\partial D_0\left(x^k, u^k\right)}{\partial \ln u_m^k} \leq 0, \quad \forall k = 1,\ldots,K.;\ \forall m = i+1,\ldots,M. \tag{6.c}$$

$$\sum_{m=1}^{M} \alpha_m = 1 \sum_{m'=1}^{M} \alpha_{mm'} = \sum_{m=1}^{M} \gamma_{nm} = 0, \quad \forall n = 1,\ldots,N.; \quad \forall m = 1,\ldots,M. \tag{6.d}$$

$$\alpha_{mm'} = \alpha_{m'm}, \forall m = 1,\ldots,M;\ \forall m, = 1,\ldots,M; \beta_{nn'} = \beta_{n'n}, \quad \forall n = 1,\ldots,N; \quad \forall n' = 1,\ldots,N \tag{6.e}$$

where $k = 1,\ldots,K$ represents the number of production units included in the analysis; i is the desired output; and the remaining $i+1,\ldots,M$ are the non-desirable outputs.

As the distance function takes values less than or equal to one, $\ln D_0\ (x^k,u^k)$ will be less than or equal to zero, and the deviation of the k unit relative to the production frontier, $[\ln D_0\ (x^k,u^k)] - \ln(1)$, will be less than or equal to zero. Therefore, maximising the objective function means minimising the deviation relative to the production frontier, i.e., as close to zero as possible.

The first restriction, given by Equation (6.a), implies that the units should be below or forming part of the production frontier. The second restriction (6.b) establishes that the desired outputs should have positive or zero, but not negative, shadow prices. Restriction (6.c) establishes that the non-desirable outputs should have negative or null, but not positive, shadow prices. The fourth restriction (6.d) ensures that there is free availability of outputs. Finally, restriction (6.e) is a symmetry restriction for parameters that refer to pairs of inputs and outputs.

3. Sample description

A database by compiling 12 international research papers analysing the presence of PPCPs in 24 WWTPs has been constructed. For homogeneity, it has been required that all WWTPs use the same wastewater treatment technology (activated sludge). Characteristics of the WWTPs are shown in Table 1. The shadow price methodology requires cost data of the analysed sample; in our case, these data correspond to the costs of activated sludge treatment. It has been calculated the capital costs and the operation and maintenance costs using the cost functions for activated sludge treatment provided by Guo et al. (2014). The average of the capital costs for our sample was 32.4 million € (M€), and the average of the operation and maintenance costs was 25.9 M€. These results are in the same order of magnitude that costs obtained for activated sludge treatments in the literature, as the study of De Gisi et al. (2015).

Table 1
Characteristics of WWTPs used as database.

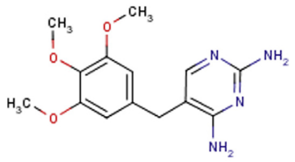
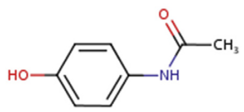
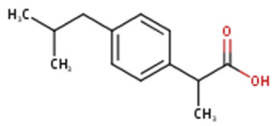
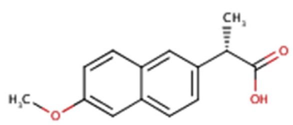
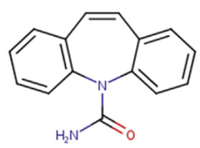
WWTP	Country	Population equivalent	Average flow (m^3/day)	Source
Torroella de Montgrí	Spain	11,385	16,500	(Rodriguez-Mozaz et al., 2015)
Cilfynydd	United Kingdom	111,000	36,160	(Kasprzyk-Hordern et al., 2009)
Coslech		30,000	19,750	
Castellón de la Plana	Spain	265,000	36,000	(Gracia-Lor et al., 2012)
Taipei	Taiwan	227,250	210,000	(Lin et al., 2009)
Lausanne	Switzerland	220,000	95,000	(Margot et al., 2013)
Coimbra	Portugal	213,000	N/A	(Santos et al., 2013)
Sena Centro	France	90,000	240,000	(Mailler et al., 2015)
Ioannina city	Greece	100,000	25,276	(Kosma et al., 2010; Kosma et al., 2014)
Arta		38,000	115,000	
Preveza		25,000	7000	
Agrinio		90,000	14,000	
Grevena		20,000	4000	
Kozani		70,400	10,000	
Veroia		45,000	9800	
Alcalá de Henares	Spain	374,090	74,818	(Rosal et al., 2010)
Wayne Hill	USA	N/A	227,000	(Yang et al., 2011)
Howdon	United Kingdom	N/A	230,000	(Roberts and Thomas, 2006)
Naples	Italy	840,000	181,000	(Castiglioni et al., 2006)
Latina		45,000	19,000	
Cuneo		140,000	31,000	
Cagliari		270,000	86,700	
Varese Lago		110,000	40,000	
Varese Olona		120,000	23,000	

N/A: data not available.

Five PPCPs with the highest detection frequency in WWTPs which have been considered are ibuprofen (IBP), carbamazepine (CBZ) and trimethoprim (TMP) are detected 100% of the time, while acetaminophen (ACM) and naproxen (NAP) are detected around 90% of the time (Dai et al., 2015; Gros et al., 2017; Matamoros et al., 2009). Chemical characteristics of the PPCPs are shown in Table 2.

Concentrations of the selected PPCPs for the 24 WWTPs are shown in Table 3. The concentration of CBZ in effluent is often

Table 2
Main characteristics of analysed PPCPs (HSDB, 2014).

PPCPs	Formula	log K_{ow}	Function	Molecular structure
Trimethoprim	$C_{14}H_{18}N_4O_3$	0.91	Antibiotic	
Acetaminophen	$C_8H_9NO_2$	0.46	Analgesic	
Ibuprofen	$C_{13}H_{18}O_2$	3.97	Anti-inflammatory	
Naproxen	$C_{14}H_{14}O_3$	3.18	Analgesic	
Carbamazepine	$C_{15}H_{12}N_2O$	2.45	Antiepileptic	

logKow = Octanol-water partition coefficient. This value measures the solubility of PPCPs in water. If the value is high, PPCP is hydrophobic and it has affinity for lipids, so it tends to be adsorbed to sediments and organisms). If the value is low, PPCPS is hydrophilic and has an affinity for water (is stable within aqueous solution) (Pal et al., 2010).

Table 3
Concentration of selected PPCPs both influent and effluent in our sample (ng/L).

WWTP	TMP		ACM		IBP		NAP		CBZ	
	Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent
Torroella de Montgrí	119	19	208,601	25	26,011	3528	982	280	230	441
Cilfynydd	2192	1152	211,380	11,733	1681	263	838	370	1694	2499
Coslech	2925	876	178,116	353	2294	143	1173	170	950	826
Castellón de la Plana	100	90	55,100	9245	14,600	1980	1320	130	1863	212
Taipei	36	3	13,046	2189	9322	2045	139	40	220	154
Lausanne	235	158	51,438	8	4101	952	697	380	482	461
Coimba	124	167	2463	96	1596	119	741	303	434	49
Sena Centro	64	4	5870	1030	951	432	154	52	215	41
Ioannina city	132	60	2873	92	2633	301	230	57	99	120
Arta	23	12	8313	196	177	24	544	128	60	212
Preveza	16	8	293	192	280	78	1814	171	22	58
Agrinio	17	8	140	52	57	31	325	59	95	62
Grevena	159	13	20,600	900	12,500	1500	1500	500	800	900
Kozani	34	3	4185	210	1042	412	574	23	84	77
Veroia	23	10	30,354	369	1021	396	1584	534	39	111
Alcalá de Henares	104	99	23,202	3893	2687	135	2363	923	129	117
Wayne Hill	610	10	80,000	50	11,000	10	123	35	230	1
Howdon	259	270	27,341	20	23,161	3063	169	48	253	29
Naples	32	16	11,345	267	566	130	743	174	56	130
Latina	3	2	1191	28	30	7	78	18	3	7
Cuneo	5	3	1943	46	94	22	127	30	9	22
Cagliari	15	8	5434	128	182	42	356	84	18	42
Varese Lago	7	4	2507	59	74	17	164	39	7	17
Varese Olona	4	2	1442	34	81	19	94	22	8	19

greater than the concentration in influent due to conjugate formation between CBZ and suspended organic matter. When these conjugates break down during the wastewater treatment process, CBZ is released, which causes the concentration of CBZ in the effluent to increase (Luo et al., 2014).

4. Results and discussion

Results of the implementation of the shadow price methodology for the three proposed ecosystems are presented in Table 4. As references to obtain the shadow prices of PPCPs in each ecosystem, it has been used the reference prices for treated wastewater effluents provided by Hernández-Sancho et al. (2010): 0.9 €/m^3 for wetlands, 0.7 €/m^3 for rivers and 0.1 €/m^3 for sea. Among the analysed scenarios, wetland showed the highest shadow prices of PPCPs, followed by river and sea. Environmental costs that would be avoided in wetlands if the effluent did not contain PPCPs were quantified as 0.4, 128.2, 11.0, 3.4 and 0.6 €/mg for TMP, ACM, IBP, NAP and CBZ, respectively. The impact of PPCPs discharge into the sea was mitigated by the sea's high dilution capacity compared to wetlands or rivers. When the effluent reaches the receiving water body, both volumes of water are mixed; so that the larger volume of water in the ecosystem means a lower PPCP concentration within the receiving water body (Acevedo-Merino et al., 2005). From an environmental point of view, the impact of PPCPs in sea ecosystems will be lower than the effects in wetlands, since the volume of water that the sea has is larger than the existing in a wetland.

According to the results obtained in the three ecosystems (Table 4), the priority for removing PPCPs should be ACM > IBP > NAP > CBZ > TMP. Kumar and Xagoraraki (2010) and others have established priority rankings of PPCPs according to their occurrence and ecological and health effects. The order of priority proposed in our study arises from a monetary valuation of the environmental externalities (i.e. PPCPs) through the shadow price methodology. The difference between priority orders is relevant from the context of decision-making processes. Hence, the shadow prices obtained here have been quantified the monetary value of this PPCPs, which are considered as an indicators of anthropogenic pollution in water bodies. This starting point allows to frame the subsequent decision-making process and adapt the results to the management measures that will be implement later for guarantee water ecosystems quality.

Table 4
Shadow prices results for PPCPs sample (€/mg) for the three ecosystems proposed.

	TMP	ACM	IBP	NAP	CBZ
Wetland	0.4	128.2	11.0	3.4	0.6
River	0.3	99.7	8.5	2.6	0.5
Sea	0.041	14.2	1.2	0.4	0.1

Our prioritisation has been compared to findings from 82 articles (available in the Supplementary Online Data), which performed toxicological risk analyses for aquatic organisms in direct contact with WWTP effluents (Gros et al., 2010). The value of the toxicological risk to aquatic organisms was calculated as the ratio of the measured effluent concentration to the predicted no-effect concentration. The risk was considered high if the ratio was greater than or equal to 1, and the risk was minimal if the ratio was less than or equal to 0.1 (Chen et al., 2016).

In 95% of the 82 analysed articles, the toxicological risks of ACM and IBP were high (ratio > 1). Similarly, in our results, ACM and IBP were the PPCPs with the highest shadow prices for the three analysed ecosystems (wetland: 128.2 €/mg for ACM and 11 €/mg for IBP; river: 99.7 €/mg for ACM and 8.5 €/mg for IBP; sea: 14.2 €/mg for ACM and 1.2 €/mg for IBP). The high toxicological risks of these PPCPs can be explained by their high consumption rates (Paíga et al., 2016) as nonprescription drugs (Ramos et al., 2014) and their low solubility (<0.1 mg/ml) (Jjemba, 2006). These are the two main factors that determine the amounts of ACM and IBP that arrive at the WWTPs and receiving water bodies through effluent discharges.

NAP was the third-most-relevant PPCP. Its shadow price was of the same order of magnitude for wetland and river (3.4 €/mg and 2.6 €/mg, respectively), but the shadow price for sea was significantly lower (0.4 €/mg). Our NAP shadow prices followed the trend of the results of the risk analysis literature. Of the 82 articles consulted, only 7% reported a high toxicological risk (ratio > 1) for NAP. In WWTPs, NAP tends to be adsorbed by suspended organic matter due to its high log K_{ow} value (Table 2), which causes most of the NAP to be reached to sludge (Durán-Álvarez et al., 2012; Papageorgiou et al., 2016). However, a fraction of the NAP remains in the wastewater and leaves the WWTP through the effluent. According to Huber et al. (2016), NAP is susceptible to photodegradation by contact with sunlight, which reduces its half-life in surface waters but also generates toxic byproducts that provoke serious health problems in aquatic organisms (Ebele et al., 2017). Furthermore, photodegradation does not completely eliminate NAP from water bodies that receive WWTP effluents (Arlos et al., 2015). This trend is responsible for its shadow price being placed in the middle of our priority order.

PPCPs with the lowest shadow prices were CBZ and TMP. Their shadow prices were significantly different in order of magnitude from those of the other PPCPs. CBZ showed a similar shadow price in all three scenarios (0.6 €/mg for wetland, 0.5 €/mg for river and 0.1 €/mg for sea). Only 18% of analysed studies found a high toxicological risk of CBZ. A greater percentage of articles reported a high toxicological risk for CBZ than for NAP, due to the fact that CBZ directly affects aquatic organisms and causes serious problems in their biological functions. CBZ has a very low rate of removal from water (3–20%) (Aymerich et al., 2016) and a strong tendency to create conjugates with organic matter in suspension. Zemann et al. (2014) reported a CBZ half-life in wastewater of 100 days. The half-life may even be higher depending on the type of treatment technology used by the WWTP, as CBZ is more susceptible to accumulation with activated sludge reactors (Chen et al., 2015)). Overall, CBZ is a persistent PPCP that is difficult to remove from WWTPs (Arlos et al., 2015; Chen et al., 2015). However, the shadow prices of CBZ were significantly lower than those of ACM and IBP, due to the different consumption rates (and, therefore, WWTP influent concentrations) of the PPCPs.

Among the analysed PPCPs, TMP had the lowest shadow prices, which were nearly the same for wetland (0.4 €/mg) and river (0.3 €/mg) and were very low in sea (0.041 €/mg). The environmental cost avoided by not spilling TMP into the sea through WWTP effluent was almost zero. One reason for the low shadow price of TMP is its relatively low concentration. According to Yan et al. (2014), TMP has a wide range of elimination rates in WWTPs (17–86%), although the lower elimination rates are more common and elimination rates near 80% are rarely achieved for TMP. The literature review highlights the low toxicity risk of TMP; only 5% of the 82 articles (see Supplementary Online Data) reported a high toxicological risk of TMP.

The shadow prices reported here are estimates, in monetary units, of the environmental costs that would be avoided by removing PPCPs from the WWTP effluents. Considering the shadow prices (Table 4), the average volumes of treated wastewater in the samples and the amount of contaminants that WWTPs can eliminate with current technologies (Table 3), it has been calculated the environmental benefits (in millions of €/year) that would be achieved by eliminating the PPCPs from the effluents of the sample WWTPs (Table 5).

Table 5
Environmental benefit (M€/year) of PPCPs analysed for the three scenarios proposed.

	TMP	ACM	IBP	NAP	CBZ
Wetland	1.9	135,920	1277	47.8	3.1
River	1.4	105,716	933.2	37.2	2.4
Sea	0.2	15,102	141.9	5.3	0.3

M€: millions of €/year.

The results show that the greatest environmental benefit of eliminating PPCPs from WWTP effluent occurs in wetlands, highlighting the need for treated wastewater to be of adequate quality before reaching this ecosystem. In many cases, WWTP effluent is used as a maintenance flow in wetlands to preserve their natural conditions. Therefore, the effluent directly affects this ecosystem. PPCPs must be eliminated from the effluent reaching wetlands because this ecosystem does not have the dilution capacity of the sea (where the environmental benefit of PPCP elimination was lowest). The low water flow in wetlands means that PPCPs are accumulated in water, sediment and biota. PPCPs are designed to be stable compounds that work at very low concentrations. As a result, their toxic activity remains unchanged when they go through WWTPs and reach the wetlands (Galus et al., 2013; Postigo et al., 2010). Similarly, nitrogen and phosphorus must be removed from WWTP effluents that are released to wetlands. It wants to avoid eutrophication problems, toxicological risks associated with PPCPs and long-term effects of these compounds on the ecosystem. Elimination of ACM, IBP, NAP, CBZ and TMP would have very positive results for wetlands and rivers. The priority in decision-making processes should be aimed towards these two ecosystems, which are highly influenced by WWTP effluents, especially from highly urbanised areas. Our results are highly relevant because they justify future investments in technological improvements of WWTPs (i.e. tertiary treatment). Results shown in Table 5 could be included as external benefits in feasibility analyses.

The sample WWTPs only use activated sludge treatment. There are no tertiary treatment technologies that minimise the presence of the analysed PPCPs in the used sample. Extensive literature has analysed tertiary treatment technologies and their ability to eliminate PPCPs. It is important to taking into account that the removal of PPCPs through tertiary treatment technologies increases the cost of wastewater treatment. The costs associated with the technological improvements in WWTPs are a serious constraint to the reuse options of effluents (Schröder et al., 2016). Hence, shadow prices could be used to internalize the environmental externalities related to PPCPs and their removal into decision-making processes and achieving the proper assessment of overall WWTP costs. There is currently no consensus about which technology is suitable for this purpose. The choice depends on the quality of the raw wastewater (WWTP influent) and the design characteristics of the WWTP (Michael et al., 2013; Radjenović et al., 2009). Activated carbon, ozonation, advanced oxidation processes and membrane processes, which are capable of oxidising and retaining PPCPs, are the most frequently analysed tertiary treatment technologies in the literature (Luo et al., 2014). However, like all technologies, these treatments have distinct advantages and disadvantages related to their retention percentages and the generation of byproducts, whose levels of toxicity may be greater than those of the original PPCPs (Mohapatra et al., 2014).

The recent publication of Directive 2013/39/EU of the European Parliament and Council of 12 August 2013 amending Directives 2000/60/EC and 2008/105/EC as regards priority substances in the field of water policy constitutes an important step forward with respect to the Water Framework Directive. However, none of the PPCPs analysed in our study appear on the list of priority substances (European Parliament, 2013). The lack of regulatory legislation concerning the concentration of PPCPs in treated wastewater is another disadvantage to take into account. At present, efforts to mitigate the presence of PPCPs in water bodies are voluntary initiatives, and economic costs are a barrier to implementation.

This study sheds light on the quantification of the environmental benefit in monetary units, which could be included in decision-making processes regarding technological improvements of WWTPs. Specifically, the shadow price methodology is a way to calculate the monetary value of environmental externalities which lack of market value. Implementation costs of the methodology are lower than those of other methodologies, such as contingent valuation. Shadow prices provide decision makers with estimates of the environmental costs of having PPCPs in WWTP effluents. These prices allow PPCPs to be prioritised for the implementation of environmental conservation measures. From a holistic point of view environmental externalities need to be vertically and horizontally integrated within environmental policies; without forgetting the relevance of presence of stakeholders within that process (Schleyer et al., 2015). Therefore, economic valuation of environmental externalities can be integrated into governance processes; whose institutions encourage interaction among political and social actors to manage their interests with respect to ecosystems exploitation and conservation, so that decisions will take for achieve long-term conservation (Loft et al., 2015).

Economic value of PPCPs may be included within a feasibility analysis - like cost-benefit analysis (Bark et al., 2016) - to assess the feasibility of different management measures analysed under different scenarios (Busch et al., 2012). Final result will be the design of technological improvement in those WWTPs whose effluent have been discharged into sensitive areas, such as wetlands or rivers through the internalisation of environmental externalities. This line of analysis will be continued in our future research work applying a multi-criteria method as used in De Feo et al. (2013). Shadow prices obtained in this study and the bibliographic review of toxicological risk analysis demonstrate the robustness and consistency of our results. The obtained shadow prices follow the trend of the literature findings in quality issues and demonstrate that the shadow price methodology is able to quantify the environmental cost that is avoided by removing PPCPs from WWTP effluents.

5. Conclusions

Environmental benefit of removing ibuprofen, carbamazepine, trimethoprim, acetaminophen and naproxen in effluents discharged from WWTPs has been calculated. Using shadow prices methodology, it has been quantified the environmental cost that could be avoided if these PPCPs were not discharged into water ecosystems. The results shown here contribute to current literature about how shadow prices can be used to quantify the monetary value of environmental externalities of wastewater treatment processes. Specifically, our study is innovative in terms of the application of shadow prices methodology to calculate the cost of not removing PPCPs of WWTPs effluent that can be discharged into environmental-sensitive areas (such as wetlands and rivers). The shadow prices approach is useful to quantify the cost of water pollution in areas where the wastewater effluent is discharged. It has been discussed if there is a relationship between the toxicological risk assessment published in the literature and our shadow prices results. The literature review confirms that PPCPs with higher shadow price (acetaminophen and ibuprofen) have a higher toxicological risk. This study is innovative to highlight the relationship between the shadow price methodology and toxicological risk assessment.

Quantifying environmental benefits, via shadow prices approach, has allowed us to highlight that exists positive effects on the improvement of wastewater treated quality (reducing PPCPs). From methodological point of view, a monetary valuation of the externalities of wastewater treatment process has been accomplished. This environmental benefit can be used to justify investments in technical improvements in WWTPs, specifically new technologies that achieve better quality in wastewater effluent. The current need to implement concrete measures to reduce the presence of PPCPs in water bodies makes our results a benchmark for decision-makers. Shadow price methodology enabled us to identify wetlands as the ecosystems that are most threatened by PPCPs. The environmental benefits of removing PPCPs from WWTP effluents were the highest for wetlands for all five analysed PPCPs. These results open a wide range of possibilities, all with the ultimate objective of allowing an integrated management of water resources, minimising environmental impacts and enhancing the reuse of treated water.

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Appendix A. Supplementary data

Supplementary data related to this article can be found at http://dx.doi.org/10.1016/j.jenvman.2017.08.025.

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c. ARTÍCULO 3: *Identification of effective parameters for anti-inflammatory concentration in València City's wastewater using fuzzy-set qualitative comparative analysis*

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Identification of effective parameters for anti-inflammatory concentration in València City's wastewater using fuzzy-set qualitative comparative analysis

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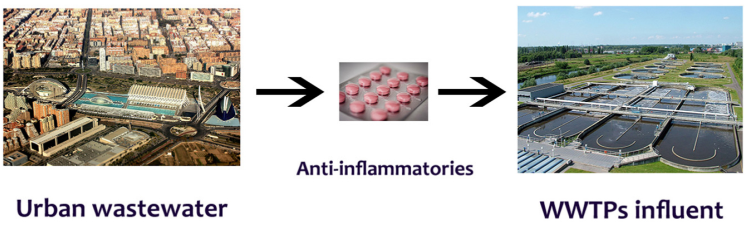
H I G H L I G H T S

- Preventive measures are essential to reduce anti-inflammatories in WWTPs effluents.
- Urban variables are responsible for the anti-inflammatories discharge in wastewaters.
- fsQCA is used to obtain recipes that explain the presence of anti-inflammatories in wastewaters.
- Water consumption, hospitals and population ageing are main responsible of anti-inflammatories pollution.

G R A P H I C A L   A B S T R A C T



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The current literature about pharmaceutical and personal care compounds (PPCPs) focuses on identifying their concentration and toxicological risk both in surface water and in wastewater. However, the influence of urban areas (population ageing, income level, hospitals and others) has not yet been analysed. Knowing how a population (and its facilities) affects PPCPs' presence in wastewater is important to identify the conditions that are responsible for their presence. In this work, the influence of water consumption, population ageing, income level, hospitals and nursing homes on the anti-inflammatory concentration have been analysed. To fill the gap between the quantitative data on PPCPs' concentration and the qualitative reasoning of the influence of urban areas on the anti-inflammatory concentration, the use of fuzzy-set qualitative comparative analysis (fsQCA) is proposed. The fsQCA results are presented as recipes that show the different causal combinations of conditions that explain the presence of anti-inflammatories in wastewater. Using fsQCA for urban wastewater management with the aim of explaining the presence of anti-inflammatories in wastewater treatment plants (WWTPs) is a novelty in the literature. The results obtained here show the influence of water consumption (WATCON), hospitals (HOSP) and population ageing (POPAG) as the main conditions for the anti-inflammatory concentration in Valèncian wastewater. Specifically, these conditions are present in all the recipes obtained with consistency of 99%. Through the results obtained, it would be possible to identify that HOSP are the main facilities that discharge anti-inflammatories into urban wastewater. Hence, the necessity of preventive measures to avoid the anti-inflammatory discharge into water bodies has been showed. Furthermore, under a methodological point of view, this work highlights the eligibility of fsQCA as a wastewater cycle management tool.

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1. Introduction

Water stress hampers the water management in densely inhabited areas with an arid or semi-arid climate. Currently regenerated water has been a non-conventional water source for irrigation and environmental purposes. This trend reduces the strain on water resources available for urban water supply. Thanks to reuse a double benefit is obtained: to close the water cycle and to reduce the strain on water bodies. Under this approach the circular economy and long-term sustainability are promoted (WWAP, 2017). Water reuse needs that effluent of wastewater treatment plants (WWTPs) is of high quality since it has been reintroduced into the ecosystem. However, the presence of pharmaceutical and personal care compounds (PPCPs) in effluents of WWTPs compromise the safety of effluent (Teijon et al., 2010). Current WWTPs are mainly designed for removing organic matter, suspended solids, nitrogen and phosphorus (Binelli et al., 2014; Tchobanoglous et al., 2003). However, WWTPs are not designed for removing PPCPs, which leaving the WWTPs through the effluents and they arrive to water bodies (Vazquez-Roig et al., 2012).

The presence of PPCPs in rivers and lakes that receive effluent from urban WWTPs is highly recognized in the literature (Blair et al., 2013; Carmona et al., 2014; Ferguson et al., 2013; Sui et al., 2011; Wang et al., 2015; Yang et al., 2017; Zemann et al., 2014; Zenobio et al., 2015). Hence, WWTPs are considered as discharge points of PPCPs into water ecosystems (Bellver-Domingo et al., 2017; Prosser and Sibley, 2015). This situation provokes long-term environmental impacts on the aquatic organisms exposed to this effluent (Arlos et al., 2015; Subedi et al., 2014; Zenker et al., 2014). Specifically, in the Section 2.2.1 the toxicological effects of PPCPs have been detailed. Taking into account both the presence of PPCPs in the ecosystem and the human origin of these PPCPs, there are two issues to consider: (i) humans' continued consumption of PPCPs and (ii) the inability of WWTPs to remove them from wastewater. Being aware of WWTPs' discharge points of PPCP pollution, it is possible to apply preventive and corrective measures to reduce the concentrations of PPCPs in effluent and ensure the sustainability of both the effluent quality for reuse and the water bodies (Bellver-Domingo et al., 2017).

The presence of PPCPs in urban wastewater is caused by human consumption of these substances. This means that there are different variables (also called conditions) that determine their concentration in urban wastewater. Identifying the empirical relationship between the conditions and the PPCPs is difficult for different reasons, such as the heterogeneity in wastewater composition, the wide variety of PPCPs currently being used and the limited availability of data. For these reasons, quantitative approaches cannot be applied. In response to this situation, the qualitative methodologies based on set analysis can be used. This type of methodology allows the identification of the patterns that explain the presence of the analysed variable (also called the outcome). One type of qualitative methodology is fuzzy-set comparative analysis (fsQCA), which is used in this work.

fsQCA is an extension of qualitative comparative analysis (QCA) – developed by Charles Ragin (1987) in its work "The comparative method; moving beyond qualitative and quantitative strategies". QCA is based on Boolean logic, allowing the establishment of comparison patterns between the conditions and the outcome (Roig-Tierno et al., 2016). Thanks to this, the relationship between conditions and outcome are made explicit (Mendel and Korjani, 2013; Roggero, 2015). fsQCA is used with small and medium-sized samples, which cannot be analysed under the classical quantitative methodologies (Kraus et al., 2017; Schneider and Wagemann, 2009). The applicability of fsQCA is reflected in the large number of areas in which it has been applied: (i) business (Beynon et al., 2017; De Villiers, 2017), (ii) education (Martí-Parreño et al., 2018; Schneider and Makszin, 2014), (iii) health (Haynes et al., 2017; Paykani et al., 2018; Wind et al., 2016) and (iv) industry (Adame-Sánchez et al., 2018; Andreas et al., 2017; Backes-Gellner et al., 2016; Boratyńska, 2016). The use of fsQCA in water studies has been less widespread. It is possible to highlight the works of: (i) Kunz et al. (2015), who analysed the conditions that affect industrial water reuse in Australia; (ii) Llopis-Albert et al. (2018), who analysed the satisfaction level of the population with public participation processes regarding water resource management; (iii) Pahl-Wostl and Knieper (2014), who investigated the capacity of water management systems to deal with climate change; and (iv) Jiang et al. (2017), who determined the causes of the low percentage of water reuse in China despite water stress.

The aim of this work was to analyse the contribution of the districts of the city of València and urban variables to PPCPs' (anti-inflammatories') presence in urban wastewater that arrives at WWTPs. To achieve this aim, the fsQCA methodology was used. Thanks to fsQCA, it was possible to identify the combination of conditions that is responsible for the anti-inflammatory concentration (outcome) in wastewater. The novelty of this work is the application of fsQCA to a database of anti-inflammatory and population variables that affect the composition of the Valèncian wastewater, disaggregating the data by district level. The influence of urban characteristics on wastewater pollutants had a first approximation in the work of Tjadraatmadja and Diaper (2006). These authors specify that the discharge of pollutants into sewage system is influenced by "*water consumption patterns, frequency and timing of activities responsible for contaminant generation, the characteristics of water consuming appliances used and household products used*." Considering this work, the bases for our approach have been established. Specifically, our approach is novel in the literature for two main reasons: (i) the concentration of anti-inflammatories (a type of PPCP) is considered as the outcome of fsQCA; and (ii) the approach followed focuses on the urban wastewater cycle and WWTPs. Through the use of fsQCA researchers and decision makers would able to identify the combination of conditions that affects of anti-inflammatories concentration in urban wastewater. The combination of conditions will act as starting point for the design of preventive measures and technological improvements for reduce anti-inflammatory presence in the WWTPs effluents. Hence, the negative impact of these substances on the environment would be avoided, favouring, in addition, the water reuse. The study is structured as follows: Section 2 presents a description of fsQCA (Section 2.1), the hypothesis tested (Section 2.2) and the sample (Section 2.3). Section 3 contains the results obtained and a discussion. Finally, Section 4 presents the conclusions reached.

2. Materials and methods

This section includes a description of the methodology (Section 2.1), which includes the calibration process (Section 2.1.1), the hypothesis tested (Section 2.2) and the sample description (Section 2.3), as well as the data and the analytical procedure followed to determine the anti-inflammatory concentrations.

2.1. Description of fsQCA

fsQCA is based on QCA. QCA analyses the patterns of complex causality that involve different conditions in a limited number of cases with a small and medium sample size (Yong and Park, 2017). Each case of the sample is explained through a complex combination of the different conditions analysed. Together with the concept of causality, this allows the outcome to be explained through the different causal combinations obtained – also called recipes (De Villiers, 2017). The consideration of causal combinations means that QCA analyses not only the isolated effect of the conditions but also all the possible interactions that generate the conditions together, leading to the outcome (González et al., 2012).

Both QCA and fsQCA use the principles of Boolean algebra and fuzzy algebra as a way to obtain the recipes (De Villiers, 2017). However, the difference between QCA and fsQCA lies in the use of the logic of propositions that support the set-theoretic relations. Accordingly, it is possible to establish the combination of conditions that is necessary or sufficient to obtain the outcome (Schneider and Wagemann, 2012). The form in which these two approaches represent the information varies between

QCA (also called csQCA) and fsQCA. csQCA is based on dichotomous conditions, which are represented by the values 0 and 1. If the value is 1, the condition belongs to the set. If the value is 0, the condition does not belong to the set. However, not all conditions can be represented as dichotomous conditions. Under this assumption, fsQCA is used. fsQCA represents the set through the range from 0 to 1 (González et al., 2012). This is called a fuzzy set, since it cannot specify whether the condition is inside or outside the set (Ragin, 2008a). In other words, the condition can belong to the set partially – for instance, when the value is 0.5 (Schneider and Wagemann, 2012). Thanks to fuzzy sets, the degree of membership can be defined. The value 1 means that the condition has full set membership, while the value 0 means the opposite situation, that is, non-set membership (Pappas et al., 2016; Yong and Park, 2017).

2.1.1. Calibration process

Successful implementation of fsQCA requires the transformation of the values of the conditions into fuzzy values through the calibration process. Calibration is a prerequisite for implementing fsQCA, which is mainly based on both the previous knowledge of the researcher and the information available in the literature (Ragin, 2006). The most frequently used calibration method is direct calibration, proposed by Ragin (2008a). Specifically, the direct method uses a logistic function to fit the raw data between the three qualitative anchors – also called thresholds (Schneider and Wagemann, 2012) – that define whether the condition is more in or out of the set (Pappas et al., 2016). These three anchors are: (i) full membership (value 1): the cut-off value from which (and above it) the case is in the set; (ii) full nonmembership (value 0): the cut-off value from which (and below it) the case is out of the set; and (iii) the cross-over point (value 0.5): this represents the value with greater ambiguity about whether a condition is in or out of the set (Ragin, 2008a). Specifically, the direct method of calibration quantifies the Napierian logarithm of the odds with regard to the condition's degree of membership of a defined set (González et al., 2012). Following Ragin (2008a), the different metrics used to estimate the direct calibration method are shown in Table 1.

The odds of the full membership results of the transformation of the set membership scores into the odds of full membership are estimated through Eq. (1) (Ragin, 2008a):

$$odds\ of\ membership = \frac{degree\ of\ membership}{(1-degree\ of\ membership)} \tag{1}$$

Having defined the anchor points, the degree of membership is calculated. The Ragin (2008a) procedure was used for this purpose. This procedure establishes the multiplication between the condition value (raw data) and the cross-over point. The result has to be changed into a logarithm value using the values of the log of the odds shown in Table 1. If the result of the multiplication is positive, the ratio of Eq. (2) is used. However, if the result is negative, the ratio of Eq. (3) is used.

$$tranformation = \frac{\log of\ the\ odds * (3.0)}{full\ membership\ value} \tag{2}$$

Table 1
Metrics used to apply the direct method calibration (González et al., 2012; Ragin, 2008a).

	Degree of set membership	Odds of full membership	Log of the odds
Full membership	0.99	99	5.0
Threshold of full membership	0.95	19	3.0
Cross-over point	0.5	1	0
Threshold of full nonmembership	0.05	0.05	−3.0
Full nonmembership	0.01	0.01	−5.0

$$tranformation = \frac{\log of\ the\ odds * (-3.0)}{full-nonmembership\ value} \tag{3}$$

The results of Eqs. (2) and (3) is the log of the odds, which is used in Eq. (4) to obtain the degree of membership. It is important to point out that the results of calibration should not be interpreted as probabilities. The results of Eq. (4) represent the degree of membership that the condition has of the set that has been defined (Ragin, 2008a).

$$degree\ of\ membership = \frac{\exp(\ \log of\ the\ odds)}{1+\ \exp(\ \log of\ the\ odds)} \tag{4}$$

2.1.2. fsQCA software

The degree of membership is the value that the fsQCA software[1] needs to obtain the final recipes. Specifically, the fsQCA software applies a standard analysis based on the Quine–McCluskey algorithm,[2] which produces the recipes. These recipes represent all the different combinations of conditions that produce the same result (outcome). The fsQCA software allows the researcher to analyse the presence or the absence of the outcome, depending on the initial hypothesis (Pappas et al., 2017). Before obtaining the recipes, the fsQCA software provides a truth table. The truth table contains 2^k rows, where k represents the number of causal conditions and each row represents each possible combination (Pappas et al., 2016). In other words, the truth table transforms the values of the degree of membership into all the possible causal combinations (showing the frequencies with which each combination occurs). The results allow a comparison of the results, taking into account the differences and similarities across the cases (pooling similar cases together) and the conditions (Marx et al., 2014). Hence, the truth table includes the total number of causal combinations and the frequency with which they occur in the sample. If the frequency is 0, this causal combination is removed (Rihoux and Ragin, 2009). Furthermore, the causal combinations shown in the truth table have to be consistent. Taking into account the article by Ragin (2006), the consistency value used in this work is 0.75. This value means that all the causal combinations obtained with consistency above 0.75 are considered to be valid for the final recipes (Pappas et al., 2017).

Hence, through the truth table and the Quine–McCluskey algorithm, the fsQCA software obtains the final recipes (final solutions). It is important to clarify the concept of the solution. Following the fsQCA approach, the solution refers to the combination of causal conditions that explains a high number of cases, taking into account the fact that all the combinations are consistent (Marx et al., 2014; Pappas et al., 2017). These recipes are collected in three types of solutions: (i) complex solutions: these are the most complete solutions, which include all the causal combinations; (ii) parsimonious solutions: these are a simplified version of complex solutions, which only include the essential conditions that explain the outcome; and (iii) intermediate solutions: these arise from the counterfactual analysis[3] applied to both solutions: complex and parsimonious (González et al., 2012; Pappas et al., 2017). Furthermore, fsQCA software allows carrying out both the necessity and sufficiency analyses. The necessity analysis shows those situations in which the outcome cannot be achieved without the condition. That is, in fsQCA terms, the necessary condition occurs when the outcome is a subset of the condition (Schneider and Wagemann, 2012). The sufficiency analysis shows those situations in which the outcome occurs if the condition

[1] The software is available on different platforms: (i) the fsQCA website – University of Arizona (http://www.u.arizona.edu/~cragin/fsQCA/software.shtml) or (ii) the R packages (https://cran.r-project.org/web/packages/QCA/index.html).

[2] It is a minimization algorithm for Boolean functions with multiple variables (Duşa, 2007; Jain et al., 2008).

[3] The counterfactual analysis involves comparing the situations in which the presence or absence of the outcome occurs to evaluate whether changes in the outcome are due to the conditions included in the analysis (European Commission, 2014).

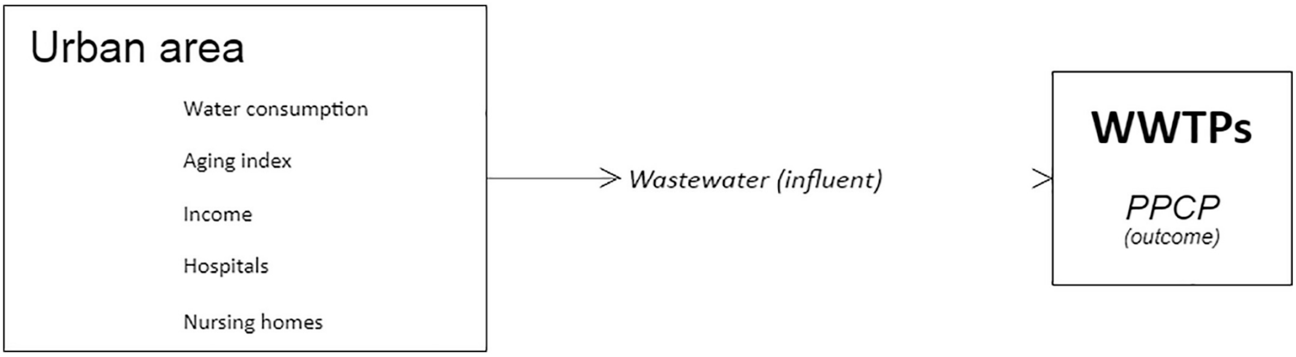


Fig. 1. Graphical representation of the hypothesis tested (own elaboration).

is present, but it is not necessary for the condition to be present for the outcome to occur. In fsQCA terms, the sufficient condition occurs when the condition is a subset of the outcome (Schneider and Wagemann, 2012). Sufficiency analysis is carried out through an XY Plot. The diagonal divides the area into two regions. The area above the diagonal represents the situation in which the condition is a subset of the outcome – that is, the sufficient condition (Schneider and Wagemann, 2012).

2.2. Hypothesis analysed

The hypothesis analysed (Fig. 1) is directly related to the following question: "How does anti-inflammatory pollution occur in urban wastewater?" This work has focused on the influence of urban characteristics on anti-inflammatory concentration due to two main reasons: (i) treated wastewater can be reused for irrigation and environmental purposes (mainly in water-stressed regions – such as València City), (ii) PPCPs discharged through WWTPs effluents have toxic effects on aquatic organisms (which is receiving considerable attention in the literature). Specifically, the characteristics of raw wastewater are influenced by the PPCPs discharged by urban areas. The origin of anti-inflammatories in raw urban wastewater is their widespread consumption. Hence, urban variables, such as water consumption, population ageing, income level, hospitals and nursing homes, could have an influence on the discharge of anti-inflammatories. As a result, the anti-inflammatories in raw wastewater arrive at WWTPs, where they cannot be removed by the current treatment technologies. This situation has a long-term environmental impact, because anti-inflammatory pollution is not covered by law. Hence, the hypothesis considered in this work is to assess the urban conditions (population ageing, drinking water consumption, income level, hospitals and nursing homes) that are responsible for the presence of anti-inflammatories in raw urban wastewater. The response to this question needs to combine the laboratory analysis of anti-inflammatory concentrations in raw wastewater (quantitative assessment) and the relationship between the urban variables that explain anti-inflammatory consumption in urban areas (quantitative assessment). The following sections (Sections 2.2.1, 2.2.2, 2.2.3, 2.2.4, 2.2.5 and 2.2.6) include detailed information about the selection of each condition. The selection has been made taking into account the knowledge of the authors, the published literature and the data availability.

2.2.1. Anti-inflammatory concentration (PPCP – outcome)

Anti-inflammatories are among the most-consumed medicines prescribed to members of the Spanish population, mainly those over the age of 65 (Eiras et al., 2016; Filomena-Paci et al., 2015; Mendoza et al., 2015). This situation, together with the contribution of hospitals, promotes their presence in urban wastewater (Escher et al., 2011; Santos et al., 2013). This widespread growth of anti-inflammatory consumption is the main reason that justifies anti-inflammatories as an fsQCA outcome. Specifically, three anti-inflammatories were selected: (i) naproxen – due to its high environmental impact and the environmental benefit associated with its removal from wastewater, as shown in the work of Bellver-Domingo et al. (2017); (ii) diclofenac – because it is an anti-inflammatory that is highly consumed by the population, either with a prescription or without (Fosbøl et al., 2008; Mijatović et al., 2011); and (iii) flufenamic acid – due to its toxicity for the liver cells of aquatic organisms that have been exposed to it (Nadanaciva et al., 2013) and its widespread presence in surface water influenced by WWTP effluent (Rafqah and Sarakha, 2016). From an environmental point of view, the toxicity of anti-inflammatories in aquatic organisms needs to be taken into account. Laboratory studies have shown that the exposure to anti-inflammatories of brown trout provokes severe problems in the brown trout tissues (Mendoza et al., 2015). The literature has described the toxic effects of anti-inflammatory exposure in different aquatic organisms (Cleuvers, 2004; Lee et al., 2011; Schwarz et al., 2017).

The anti-inflammatory data of València City correspond to the influent data of the selected WWTPs. The laboratory method applied is explained in Section 2.2.1.1. Influent data have previously been used in the literature as the value of anti-inflammatory concentration in raw wastewater (Santos et al., 2013). Two WWTPs treat the wastewater of Valencia City: Pinedo I and Pinedo II. Both receive wastewater that is primarily domestic. Pinedo I, which has a design capacity of 124,800 m^3/day, receives wastewater at an average flow of 94,979 m^3/day. This WWTP serves a population of 339,241. Pinedo II, which has a design capacity of 200,000 m^3/day, receives an average wastewater flow of 208,778 m^3/day and serves a population of 1018,59. Pinedo I and II's treatment includes pre-treatment (thick grating, sieving, sand trap and degreaser), primary treatment (physical–chemical and decantation), secondary treatment (activated sludge for Pinedo I and nitrogen removal in the case of Pinedo II), tertiary treatment (coagulation flocculation and filtration) and disinfection by ultraviolet treatment.

The following assumptions were established for the data: (i) anti-inflammatory concentrations do not suffer any changes in the sewage network and (ii) the volume of wastewater generated is equal to the volume of drinking water consumed. Taking both assumptions into account, the anti-inflammatory concentration (expressed in mg/month) for each district of València City was obtained (see Table 2). For the fsQCA software, the anti-inflammatory was labelled as PPCP. Section 2.2.1.1 includes the laboratory procedure followed to obtain the anti-inflammatory concentration in the influent of both WWTPs considered.

2.2.1.1. Laboratory procedure for anti-inflammatory determination. The analytical standards at purity >99% of the selected pharmaceuticals naproxen, diclofenac and flufenamic acid were from Sigma-Aldrich (Madrid, Spain). All the standards and stock solutions were stored in amber glass vials at −20 °C. Methanol and formic acid were purchased from wwr (Madrid, Spain). Ultrapure water was generated using a

Table 2
Sample description.

Districts	PPCP	POPAG	WATCON	INCLEV	HOSP	NURHOM
Ciutat Vella	36.77	183.35	7.76	30,599	0	11
l'Eixample	1253.22	170.01	264.61	34,852	1	4
Extramurs	68.32	179.38	14.43	24,227	0	6
Campanar	125,537.90	119.71	26,506.84	22,474	3	7
la Saïdia	66.39	185.95	14.02	22,184	0	6
el Pla del Real	112,742.25	159.99	23,805.08	33,663	2	1
l'Olivereta	67.81	180.98	14.32	18,421	0	2
Patraix	199,051.61	141.90	42,028.97	18,513	3	6
Jesús	26,670.76	149.90	5631.43	18,507	1	3
Quatre Carreres	219,021.50	141.65	46,245.53	19,199	1	8
Poblats Maritims	17,642.92	133.00	3725.23	18,140	2	9
Camins al Grau	32,825.91	110.20	6931.06	24,808	1	4
Algirós	52.77	202.03	11.14	22,961	0	5
Benimaclet	40.50	175.43	8.55	22,755	0	2
Rascanya	73.40	108.21	15.50	17,317	0	3
Benicalap	62.58	112.07	13.21	18,811	0	6
Pobles del Nord	9.04	131.63	1.91	20,980	0	5
Pobles de l'Oest	19.78	110.55	4.18	15,189	0	1
Pobles del Sud	28.68	143.64	6.06	19,151	0	7

Milli-Q water purification system from Millipore (Bedford, MA, USA). The GC-50 glass fibre filters with 90 mm and 0.50 μm pores were from Advantec (Minato-ku, Tokyo, Japan). The Strata-X 33U Polymeric Reversed Phase (200 mg/6 mL) was from Phenomenex (Madrid, Spain). 24-h composite samples were collected in both the influent and the effluent simultaneously over seven consecutive days. Once at the laboratory, water samples were filtered through the glass filters and stored at 4 °C for no >24 h. The solid-phase extraction (SPE) was performed according to a previously reported method (Carmona et al., 2014). Briefly, the sample was passed with 400 mbar/hPa of vacuum through the SPE cartridge previously activated with 5 mL of methanol and 5 mL of water; then, the cartridge was washed with 6 mL of water and dried by passing air though it for 15 min. The analytes were eluted with 6 mL of methanol that was evaporated to dryness under a gentle stream of nitrogen and the residue was reconstituted with 1 mL of methanol–water (30:70, v/v).

Naproxen, diclofenac and flufenamic acid were determined using a 1260 Infinity Ultra High-Performance Liquid Chromatograph (UHPLC) coupled to a 6410 Triple Quadrupole Mass Spectrophotometer (MS/MS) from Agilent Technologies (Santa Clara, CA, USA) through an electrospray ionization (ESI) source. The analytes were determined in negative ionization mode. The precursor ion → product ion transitions were 229 → 170 and 229 → 169 for naproxen, 294 → 250 and 294 → 178 for diclofenac and 280 → 236 and 280 → 178 for flufenamic acid. Quantification, based on the peak area ratio, was performed by external calibration. The LODs and LOQs ranged from 0.3 to 1.2 ng L^{-1} and 0.6 to 4 ng L^{-1}, respectively. The matrix effects were from −10% to −35%, the recoveries were from 91% to 102% and the precision as RSDs was always <20%. To avoid false positives and negatives, procedural blanks and spiked control samples were prepared every 10 samples to check any potential contamination occurring during the extraction of samples or any loss of sensitivity or response of the instrument. Solvent blanks containing methanol were injected every 10 samples to monitor the instrumental background. Furthermore, each sample was analysed in triplicate to avoid errors due to sampling processing.

2.2.2. Population ageing (POPAG)

The presence of anti-inflammatories in urban wastewater is associated with the consumption patterns of the population (Sui et al., 2015; Yin et al., 2017). The literature has stated that population members over the age of 65 consume, on average, between 5 and 12 different types of medicines per day (Carrera-Lasfuentes et al., 2013). This medicine consumption includes both prescription medicines and self-medication (Nicieza-García et al., 2016). Considering the consumption of anti-inflammatories, literature shows that self-consumption of anti-inflammatories is mainly carried out by population over the age of 65 to reduce the symptoms of joint pain (Shankar et al., 2002). Specifically, the gradual ageing of the population implies a high consumption level of anti-inflammatories to alleviate the effects of bone and muscular pathologies (MHESP, 2017; SEGG, 2015; VRG, 2012). This behaviour is mainly present in developed countries, such as Spain (Martin-Pérez et al., 2017). The work of Sans et al. (2002) showed that the anti-inflammatory consumption significantly increases from the age of 65 years, because anti-inflammatories can be bought without a prescription. Hence, the population has easy access to them, encouraging self-medication (Alexa et al., 2014). This situation justifies the use of an ageing index as a condition for the fsQCA analysis. The POPAG values were obtained from the Bureau of Statistics of València City Council (BSVC, 2017), as shown in Table 2.

2.2.3. Drinking water consumption (WATCON)

Drinking water consumption data were employed because the analysis focused on the presence of anti-inflammatories in urban wastewater. As discussed earlier in this work, the volume of wastewater generated in València City was considered to be equal to the volume of drinking water consumed. This assumption aimed to model the hypothesis to be tested. It is clear that the reality is otherwise; however, the limited availability of data justifies this assumption. Specifically, the literature has defined wastewater as the sum of domestic, urban and industrial wastewater and storm water (Tchobanoglous et al., 2003). First, the rainfall pattern in València City is characterized by low rainfall due to the Mediterranean climate (BSVC, 2017). Hence, the storm water volume is low and its small influence was not considered. Secondly, industrial wastewater is not characterized by the presence of anti-inflammatories. The composition of industrial wastewater includes a high organic load, oil and greases, heavy metals and various chemicals associated with the typology of the industrial process (Mohd-Udaiyappan et al., 2017). Furthermore, the industrial network is not strong, since València City has an important tourism sector (BSVC, 2017). The values of WATCON were obtained from the Bureau of Statistics of València City Council (BSVC, 2017). It is important to point out that the drinking water volume consumed by hospitals was included. The data from the Bureau of Statistics of València City Council only consider domestic consumption, omitting hospital consumption. Under the hypothesis proposed, hospital water is important. Hence, drinking water consumption data were obtained from the literature, since the authors were unable to access real data. According to Mendoza et al. (2015), hospitals' water consumption is related to the total number of beds. Specifically, Mendoza et al. (2015) quantified the volume consumed as 1200 L bed^{-1} day^{-1}. The final data from WATCON are expressed in m^3/month (see Table 2).

2.2.4. Income level (INCOME)

The literature has clarified the relationship between the income level and the anti-inflammatory consumption (Das et al., 2017). Specifically, a high income level implies high medicine consumption (Otto et al., 2018). The medicines involved are broad spectrum with the aim of combating the symptoms of minor illness, such as anti-inflammatories. This income level–anti-inflammatory consumption pattern has been presented in the works of Mukherjee and Kamal (2017), Turek and Owczarek (2014) and Wang et al. (2010). Table 2 shows the income-level data for each district, expressed as an index by the Bureau of Statistics of València City Council (BSVC, 2017).

2.2.5. Hospitals (HOSP)

Hospitals consume a large quantity of medicines and water, which form a complex mixture of different substances, such as medicines and their metabolites, disinfectants and diagnostic agents, among others. This mixture is discharged directly into the sewage network and arrives at WWTPs (Mendoza et al., 2015; Ort et al., 2010; Santos et al., 2013). Hence, hospitals are considered as hot spots of medicine pollution (Escher et al., 2011; Oliveira et al., 2015). According to Al Aukidy et al. (2014), hospitals are the main source of anti-inflammatories discharging into urban wastewaters. The toxicological risk of hospital wastewater has been proved in the literature (Frédéric and Yves, 2014; Perrodin and Orias, 2018; Yilmaz et al., 2017). These works highlight the need to consider the impact of hospital wastewater on urban wastewater, from both the environmental and the socio-economic point of view (Azuma et al., 2016; Orias and Perrodin, 2013). Table 2 shows the number of hospitals in each district of València City. All types of hospitals were considered, that is, public and private, for two main reasons: (i) the number of beds in public and private hospitals is similar, so the same contribution to the discharge of anti-inflammatories was considered; and (ii) the use of anti-inflammatories is widespread in all hospitals. The values of HOSP were obtained from the Bureau of Statistics of València City Council (BSVC, 2017).

2.2.6. Nursing homes (NURHOM)

Nursing home residents suffer diverse pathologies, the treatments of which imply the consumption of large quantities of medicines (Advinha et al., 2014). Hence, nursing homes can be considered – together with hospitals – as discharging points of anti-inflammatories into urban wastewater (Escher et al., 2011). Chronic pain – mainly muscular and skeletal pain, which is typical in seniors – is alleviated with anti-inflammatories (Neumann-Podczaska et al., 2016). According to Sicras-Mainar et al. (2009), 60% of residents consume anti-inflammatories regularly. For all of these reasons, this work considered the number of nursing homes spread over the districts in València City (see Table 2). As in the case of hospitals, no distinction was made between public and private nursing homes. They all contribute to the discharge of anti-inflammatories into Valèncian wastewater. The values of NURHOM were obtained from the Businesses Directory of València City (BDV, 2018).

2.3. Sample description

The study focuses on València City, in north-eastern Spain, with a population of 787,808 (in 2017). València is close to Albufera Natural Park (a coastal wetland), which has been strongly influenced by the WWTPs that treat Valèncian wastewater. The distribution of the population by age illustrates the gradual ageing of the population, in which the majority group is from 70 to 75 years old (BSVC, 2017). From an administrative point of view, València is divided into 19 districts (see Fig. 2). These districts were considered as units of analysis regarding the following information: (i) anti-inflammatory concentrations, (ii) population ageing, (iii) drinking water consumption, (iv) number of hospitals, (v) number of nursing homes and (vi) income level (see Table 2). All the data are from 2013, since it is the year when the sampling of anti-inflammatories was undertaken (as specified in Section 2.2.1). In this work, the anti-inflammatory concentration of València City corresponds to the influent data of the selected WWTPs. This assumption is in line with the published literature (Jones et al., 2001). Furthermore, the urban variables (population ageing, drinking water consumption and number of hospitals) were obtained from the Bureau of Statistics of València City Council (BSVC, 2017). On the other hand, the number of nursing homes was obtained from the Businesses Directory of València City (BDV, 2018). Following the fsQCA approach, the sample is composed of five elements: the outcome (anti-inflammatory concentration) and four conditions (drinking water consumption, population ageing, income level and number of hospitals and nursing homes).

Fig. 2. Urban districts in València City, which were established in plenary session in January 2003 (BSVC, 2017).

Table 3
Calibration results.

Districts	PPCP	POPAG	WATCON	INCLEV	HOSP	NURHOM
Ciutat Vella	0.04	1.00	0.04	0.96	0.05	0.99
l'Eixample	0.04	1.00	0.05	0.99	0.50	0.32
Extramurs	0.04	1.00	0.04	0.70	0.05	0.68
Campanar	1.00	0.39	0.96	0.54	0.95	0.82
la Saïdia	0.04	1.00	0.04	0.52	0.05	0.68
el Pla del Real	1.00	1.00	0.94	0.99	0.82	0.05
l'Olivereta	0.04	1.00	0.04	0.00	0.05	0.10
Patraix	1.00	0.97	1.00	0.01	0.95	0.68
Jesús	0.41	0.99	0.28	0.01	0.50	0.18
Quatre Carreres	1.00	0.97	1.00	0.01	0.50	0.90
Poblats Maritims	0.21	0.83	0.16	0.00	0.82	0.95
Camins al Grau	0.60	0.22	0.38	0.74	0.50	0.32
Algirós	0.04	1.00	0.04	0.59	0.05	0.50
Benimaclet	0.04	1.00	0.04	0.57	0.05	0.10
Rascanya	0.04	0.19	0.04	0.00	0.05	0.18
Benicalap	0.04	0.25	0.04	0.01	0.05	0.68
Pobles del Nord	0.04	0.79	0.04	0.18	0.05	0.50
Pobles de l'Oest	0.04	0.22	0.04	0.00	0.05	0.05
Pobles del Sud	0.04	0.98	0.04	0.01	0.05	0.82

3. Results and discussion

3.1. Calibration process

All the conditions were calibrated to define the degrees of membership (see Section 2.1 for more information) through the direct calibration method (Ragin, 2008a). The results of this calibration were a set of values ranging between 0.0 and 1.0 – values close to 0 mean non-membership of the set and values close to 1 mean full membership of the set (Maldonado et al., 2015). The thresholds used were based on both the sample characteristics and the knowledge of the authors. The full membership and full non-membership thresholds were determined according to the data range of each condition. For the cross-over point, the average of the sample of each condition was used. This consideration was made for various reasons: (i) this work is the first to apply fsQCA to anti-inflammatory and wastewater data; and (ii) published articles have commonly used the data range to specify the set membership (Schneider and Wagemann, 2012). The results of calibration – the different degrees of membership – are shown in Table 3. The interpretation of the results for the POPAG condition, for instance, is as follows. For the districts Quatre Carreres and Poblats Maritims, the results of the calibration are 0.97 and 0.83, respectively. The calibration method of fsQCA specifies that values close to 1 mean full membership of the set. However, Quatre Carreres's degree of membership of the POPAG set is higher than Poblats Maritims's degree of membership. Hence, both districts belong to the set of POPAG, but Quatre Carreres is slightly more aged. The results in Table 3 are the results produced by the fsQCA software.

3.2. Recipes

The fsQCA software 2.0 – developed by Ragin et al. (2006) – was used to obtain the recipes. As indicated above (Section 2.1.2), the consistency value used in this work was 0.75 (Ragin, 2006). To analyse the hypothesis proposed, two models were tested:

Model 1 (high concentration of anti-inflammatories in Valèncian wastewater):

$$PPCP = f(POPAG, WATCON, HOSP, NURHOM, INCLEV)$$

Model 2 (negation of Model 1, that is, low concentration of anti-inflammatories in Valèncian wastewater):

$$\sim PPCP = f(POPAG, WATCON, HOSP, NURHOM, INCLEV)$$

The results of the truth table for each model are shown in Table 4 (Model 1) and Table 5 (Model 2). Those cases in which the outcome has a value of 1 support the hypothesis proposed. When the values of the outcome are 0, the conditions do not support the hypothesis proposed – although in the row there are conditions with a value of 1 (Thiem and Duşa, 2013).

The recipes obtained for both models are shown in Tables 6 (Model 1) and 7 (Model 2). These tables contain information about: (i) raw and unique coverage, which measures "how much of the outcome is covered (or explained) by each solution term (raw) and by the solution as a whole (unique)" (Ragin, 2008b); and (ii) consistency, which measures "the degree to which solution terms and the solution as a whole are subsets of the outcome" (Ragin, 2008b). As mentioned in Section 2.1.2, the outcome of fsQCA software is composed by three types of solutions: complex, parsimonious and intermediate. In In this case, Tables 6 and 7 do not include the results for the intermediate solution, because it matches the complex solution. Furthermore, the results of the necessity analysis (Table 8) and sufficiency analysis (Fig. 3a, b, c, d and e for Model 1 and Fig. 4a, b and c for Model 2) are included (see Section 2.1.2 for more details).

3.2.1. Results for Model 1

Table 6 shows the results for Model 1. The complex solution, composed by three recipes, has coverage of 0.65. This means that 65% of the districts with a high concentration of anti-inflammatories are explained by the 3 recipes obtained. The Recipe 1 (POPAG*WATCON*HOSP*NURHOM*~INCLEV) has the highest results

Table 4
Truth table for Model 1.

POPAG	WATCON	INCLEV	HOSP	NURHOM	PPCP	Raw consistency[a]	PRI consistency[b]	SYM consistency[c]
1	1	0	1	1	1	1	1	1
0	1	1	1	1	1	1	1	1
1	1	1	1	0	1	0.993464	0.990291	0.990291
1	0	0	1	1	0	0.60989	0.0657894	0.0684931
0	0	0	0	1	0	0.407407	0.0400001	0.0400001
1	0	0	0	1	0	0.27907	0.0176056	0.0176056
1	0	0	0	0	0	0.253304	0.0145349	0.0145349
1	0	1	0	0	0	0.218182	0.0444445	0.0444445
0	0	0	0	0	0	0.216	0.02	0.02
1	0	1	0	1	0	0.172702	0.0294118	0.0294118

[a] Raw consistency: it shows how many cases are covered by each casual combination to total cases (Schneider and Wagemann, 2012).
[b] PRI consistency: proportional reduction in inconsistency, it shows the degree to which the variable is sufficient for the outcome as well as it is sufficient for the negation of the outcome (Schneider and Wagemann, 2012).
[c] SYM consistency: it is a variant of PRI consistency, which is forced to be symmetric. The SYM consistency analyses if it is interesting study both presence and absence of the outcome (Schneider and Wagemann, 2012).

Table 5
Truth table for Model 2.

POPAG	WATCON	INCLEV	HOSP	NURHOM	PPCP	Raw consistency[a]	PRI consistency[b]	SYM consistency[c]
1	0	0	0	0	1	0.988987	0.985465	0.985465
1	0	0	0	1	1	0.98708	0.982394	0.982394
0	0	0	0	0	1	0.984	0.98	0.98
0	0	0	0	1	1	0.975309	0.96	0.96
1	0	1	0	1	1	0.97493	0.970588	0.970588
1	0	1	0	0	1	0.963636	0.955556	0.955555
1	0	0	1	1	1	0.956044	0.894737	0.931507
0	1	1	1	1	0	0.410526	0	0
1	1	0	1	1	0	0.389961	0	0
1	1	1	1	0	0	0.333333	0.00970878	0.00970878

[a] Raw consistency: it shows how many cases are covered by each casual combination to total cases (Schneider and Wagemann, 2012).
[b] PRI consistency: proportional reduction in inconsistency, it shows the degree to which the variable is sufficient for the outcome as well as it is sufficient for the negation of the outcome (Schneider and Wagemann, 2012).
[c] SYM consistency: it is a variant of PRI consistency, which is forced to be symmetric. The SYM consistency analyses if it is interesting study both presence and absence of the outcome (Schneider and Wagemann, 2012).

Table 6
Results of fsQCA for Model 1.

	Raw coverage	Unique coverage	Consistency
Complex solution			
Consistency cutoff[a]: 0.99			
Solution coverage[b]: 0.65			
Solution consistency[c]: 0.99			
Recipe 1. POPAG*WATCON*HOSP*NURHOM*~INCLEV	0.45	0.29	1
*Cases with >0.5 membership in term POPAG*WATCON*HOSP*NURHOM*~INCLEV: Patraix (0.68, 1)*			
Recipe 2. POPAG*WATCON*HOSP*~NURHOM*INCLEV	0.27	0.15	0.99
*Cases with >0.5 membership in term POPAG*WATCON*HOSP*~NURHOM*INCLEV: elPladelReal (0.82, 1)*			
Recipe 3. ~POPAG*WATCON*HOSP*NURHOM*INCLEV	0.17	0.04	1
*Cases with >0.5 membership in term ~POPAG*WATCON*HOSP*NURHOM*INCLEV: Campanar (0.54, 1)*			
Parsimonious solution			
Consistency cutoff: 0.993			
Solution coverage: 0.912			
Solution consistency: 0.998			
Recipe 4. WATCON	0.91	0.91	0.99
Cases with >0.5 membership in term WATCON: Patraix (1, 1), QuatreCarreres (1, 1), Campanar (0.96, 1), elPladelReal (0.94, 1)			

[a] Consistency cutoff: the causal combinations whose value is under consistency cutoff value are not considered in the final recipe (Ragin, 2006).
[b] Solution coverage: it shows the proportion of cases – with the interested result – that are explained by the recipe (Ragin, 2006).
[c] Solution consistency: it shows the proportion of cases included in the recipe who present the interested result (Ragin, 2006).

Table 7
Results of fsQCA for Model 2.

	Raw coverage	Unique coverage	Consistency
Complex solution			
Consistency cutoff[a]: 0.96			
Solution coverage[b]: 0.93			
Solution consistency[c]: 0.99			
Recipe 5. ~WATCON*~HOSP*~INCLEV	0.62	0.17	0.99
Cases with >0.5 membership in term ~WATCON~HOSP*~INCLEV: l'Olivereta (0.95, 0.96), Rascanya (0.95, 0.96), Benicalap (0.95, 0.96), Poblesdel'Oest (0.95, 0.96), PoblesdelSud (0.95, 0.96), PoblesdelNord (0.82, 0.96)*			
Recipe 6. POPAG*~WATCON*~HOSP	0.71	0.27	0.99
Cases with >0.5 membership in term POPAG~WATCON*~HOSP: CiutatVella (0.95, 0.96), Extramurs (0.95, 0.96), laSaïdia (0.95, 0.96), l'Olivereta (0.95, 0.96), Algirós (0.95, 0.96), Benimaclet (0.95, 0.96), PoblesdelSud (0.95, 0.96), PoblesdelNord (0.79, 0.96)*			
Recipe 7. POPAG*~WATCON*NURHOM*~INCLEV	0.33	0.05	0.98
Cases with >0.5 membership in term POPAG~WATCON*NURHOM*~INCLEV: PoblatsMaritims (0.83, 0.79), PoblesdelSud (0.82, 0.96)*			
Parsimonious solution			
Consistency cutoff: 0.96			
Solution coverage: 0.99			
Solution consistency: 0.96			
Recipe 8. ~WATCON	0.99	0.99	0.96
Cases with >0.5 membership in term ~WATCON: CiutatVella (0.96, 0.96), Extramurs (0.96, 0.96), laSaïdia (0.96, 0.96), l'Olivereta (0.96, 0.96), Algirós (0.96, 0.96), Benimaclet (0.96, 0.96), Rascanya (0.96, 0.96), Benicalap (0.96, 0.96), PoblesdelNord (0.96, 0.96), Poblesdel'Oest (0.96, 0.96), PoblesdelSud (0.96, 0.96), l'Eixample (0.95, 0.96), PoblatsMaritims (0.84, 0.79), Jesús (0.72, 0.59), CaminsalGrau (0.62, 0.4)			

[a] Consistency cutoff: the causal combinations whose value is under consistency cutoff value are not considered in the final recipe (Ragin, 2006).
[b] Solution coverage: it shows the proportion of cases – with the interested result – that are explained by the recipe (Ragin, 2006).
[c] Solution consistency: it shows the proportion of cases included in the recipe who present the interested result (Ragin, 2006).

Table 8
Necessary conditions analysis for the both models analysed (ranked).

	Description	Consistency	Coverage
Conditions of Model 1			
WATCON	Presence of high water consumption	0.91	0.99
HOSP	Presence of more than one hospital in the district	0.85	0.79
POPAG	Presence of population ageing	0.82	0.31
~INCLEV	Absence of high income level	0.66	0.31
NURHOM	Presence of nursing homes	0.64	0.38
~NURHOM	Absence of nursing homes	0.54	0.32
INCLEV	Presence of high income level	0.43	0.36
~POPAG	Absence of population ageing	0.29	0.39
Conditions of Model 2			
~WATCON	Absence of high water consumption	0.99	0.96
~HOSP	Absence of hospitals in the district	0.90	0.93
POPAG	Presence of population ageing	0.81	0.73
~INCLEV	Absence of high income level	0.67	0.73
NURHOM	Presence of nursing homes	0.52	0.72

of coverage. Specifically, its raw coverage value (0.45) means that Recipe 1 explains 45% of the districts that discharge a high quantity of anti-inflammatories. The unique coverage value (0.29) means that 30% of the districts with high contamination by anti-inflammatories are explained exclusively by Recipe 1. Finally, the consistency obtained (1) means that 100% of the districts that match Recipe 1 are districts with high anti-inflammatory discharge. The fsQCA software allows us to determine which district matches each recipe. For Recipe 1, it is the district of *Patraix* (southwest of València – Fig. 2). The main conditions presents for Recipe 1 and hence also *Patraix* district are (all the conditions will be explained in detail in the following paragraphs): (i) HOSP. Patraix district contains 3 hospitals: *Hospital General Universitario* – 503 beds, *Hospital Dr. Peset Aelixandre* – 539 beds and *Hospital Pare Jofré* – 125 beds (BSVC, 2017). (ii) POPAG. The influence of POPAG is evident in the age distribution of *Patraix* district. Specifically, the total population consists of 57,629 inhabitants, of whom 20% are over 65 years of age. Furthermore, the mortality rate is low (8%), showing that there is a high life expectancy related to both the improvement of the quality of life and the access to the health system (EUROSTAT, 2017). (iii) NURHOM - in *Patraix* district there are 6 nursing homes. (iv) ~INCLEV. The ~ means the absence of a high income level, which contradicts the literature survey carried out previously (Section 2.2.4). This literature survey argued that access to medicines is higher among people with a high income level. However, anti-inflammatories are medicines that are easy to access at an affordable price. Under these conditions, the consumption of anti-inflammatories has become widespread. Hence, it can be concluded that a low income level (taking into account the economic conditions of each urban area) does not necessarily stop the consumption of anti-inflammatories. Through the sufficiency analysis (Fig. 3b), it is observed that there is practically the same number of districts above and below the line; that is, the condition of ~INCLEV is a sufficient condition for the outcome in some districts but not in others. In both situations, it is not necessary that ~INCLEV to be present, so there is a high concentration of anti-inflammatories in Valèncian wastewaters.

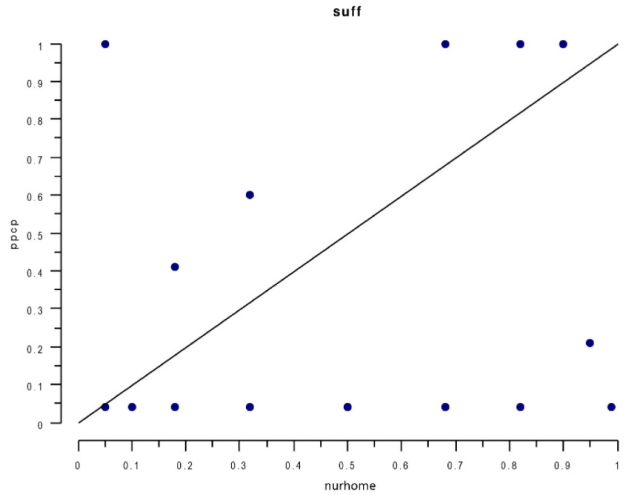
Recipes 2 (POPAG*WATCON*HOSP*~NURHOM*INCLEV) and 3 (~POPAG*WATCON*HOSP*NURHOM*INCLEV) have low values of consistency. Specifically, Recipe 2's raw coverage value (0.27) means that it explains 27% of the districts that contribute to the discharge of anti-inflammatories. Furthermore, the unique coverage value (0.15) means that 15% of the districts with high contamination by anti-inflammatories are explained exclusively by Recipe 2. Meanwhile, the raw coverage value of Recipe 3 (0.17) means that it explains 17% of the districts that contribute to the discharge of anti-inflammatories. Furthermore, the unique coverage value (0.04) means that 5% of the districts with high contamination by anti-inflammatories are explained exclusively by Recipe 3. The districts obtained for each recipe are *Pla del Real* (the centre of València – Fig. 2) for Recipe 2 and *Campanar* (northwest of València – Fig. 2) for Recipe 3. In both districts, there are hospitals, the presence of which is a necessary condition for the outcome, as mentioned previously. Specifically, in *Pla del Real* district (Recipe 2), there are 2 hospitals: *Hospital Clínico Universitario* – 582 beds and *Clínica Quirón de València* – 79 beds (BSVC, 2017). In Campanar district, there are 3 hospitals: *Hospital Arnau de Vilanova* – 296 beds, *Instituto Valenciano de Oncología* – 140 beds and *Hospital 9 de Octubre* – 300 beds (BSVC, 2017). Analysing Recipes 2 and 3, two conditions are absent: ~NURHOM and ~POPAG, respectively. Their absence is related to the data and calibration thresholds established (Table 2): (i) for ~NURHOM there is only 1 nursing home in the whole district; and (ii) in the case of ~POPAG, the value of ageing index is the lowest of the sample.

Following paragraphs analyse in-deep the conditions that take part in the recipes of the complex solution: POPAG, WATCON, HOSP, NURHOM, INCLEV, ~NURHOM, ~INCLEV and ~POPAG. The complex solution consistency (0.99) means that 99% of the districts that have high anti-inflammatory pollution have this combination of conditions. Considering the recipes 1, 2 and 3, WATCON and HOSP are the conditions that are present in all of them. The necessity analysis (Table 8) confirms that WATCON and HOSP are necessary conditions for the outcome, since they have the highest values of consistency and coverage: 0.91 and 0.99 for WATCON, and 0.85 and 0.79 for HOSP. The presence of PPCP in wastewater only occurs if WATCON and HOSP are present. These results are significant, since they show the relevance of HOSP (and the high water consumption) to the presence of anti-inflammatories in València City's wastewater. The previously published literature about PPCPs and WWTPs (see Section 2.2.1 for more information) has highlighted that WWTPs are hot spots of anti-inflammatory discharge into surface water bodies. The results obtained here emphasize that the presence of hospitals in urban areas contributes significantly to anti-inflammatory concentrations in urban wastewater. This is in line with the fact that, in study area, hospital wastewater is not treated before being discharged into the sewage system. Literature supports the results obtained due to previous studies highlight the high presence of anti-inflammatories in hospitals wastewaters and its influence in urban wastewaters (Chonova et al., 2018; Wiest et al., 2018).

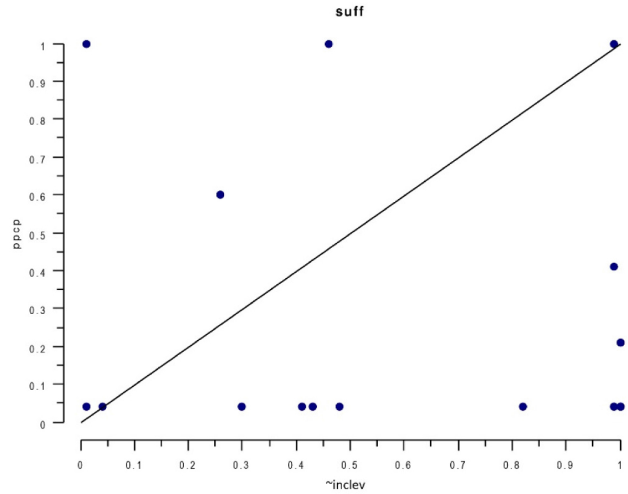
Following the analysis of complex solution (Model 1 – Table 6), the conditions POPAG, NURHOM and INCLEV have to be taken into consideration. Specifically, the necessity analysis for POPAG condition (Table 8) – Recipes 1 and 2 – shows that POPAG can be considered as a necessary condition for the outcome (consistency = 0.82 and coverage = 0.31). Hence, the POPAG in the districts analysed is also partly responsible for the presence of anti-inflammatories in València City's wastewater. The population ageing is an increasing trend associated with the improvement of people's living conditions (EUROSTAT, 2017; Kim et al., 2016). With an older population, the purchase of medicines is greater, whether they are prescription medicines or self-medication (Salech et al., 2016; Sanwald and Theurl, 2017). These findings correspond to the evidence obtained in this study.

The necessity analysis for INCLEV (Table 8) – Recipes 2 and 3 – shows that, despite INCLEV being present in both recipes, it is not a necessary condition for the outcome. This is due to its low consistency and coverage values (0.43 and 0.36, respectively). However, the sufficiency analysis (Fig. 3d) shows that almost half of the districts (the blue points on the plot) are above the line. This means that, for almost half of the

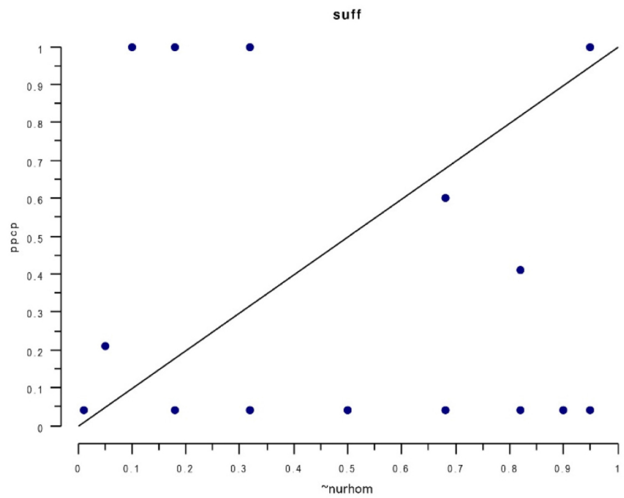
Fig. 3. a. Sufficiency analysis for PPCP and NURHOM (Model 1). b. Sufficiency analysis for PPCP and ~INCLEV (Model 1). c. Sufficiency analysis for PPCP and ~NURHOM (Model 1). d. Sufficiency analysis for PPCP and INCLEV (Model 1). e. Sufficiency analysis for PPCP and ~POPAG (Model 1). (For interpretation of the references to color in this figure, the reader is referred to the web version of this article.)



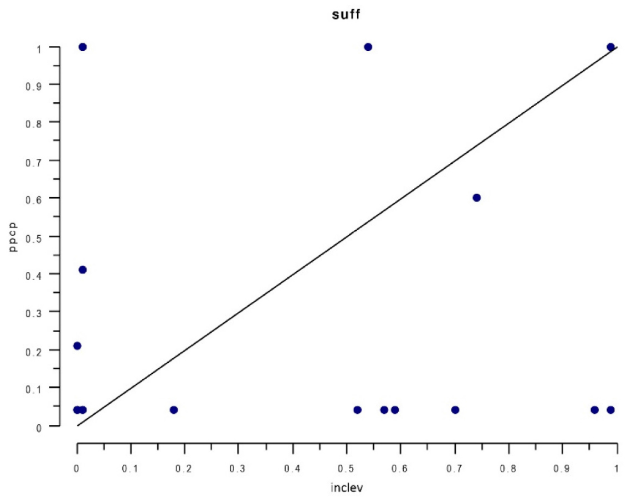
a. Sufficiency analysis for PPCP and NURHOM (Model 1).



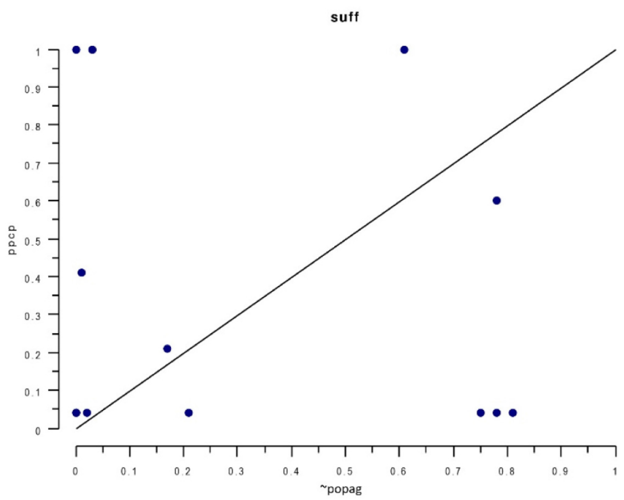
b. Sufficiency analysis for PPCP and ~INCLEV (Model 1).



c. Sufficiency analysis for PPCP and ~NURHOM (Model 1).



d. Sufficiency analysis for PPCP and INCLEV (Model 1).

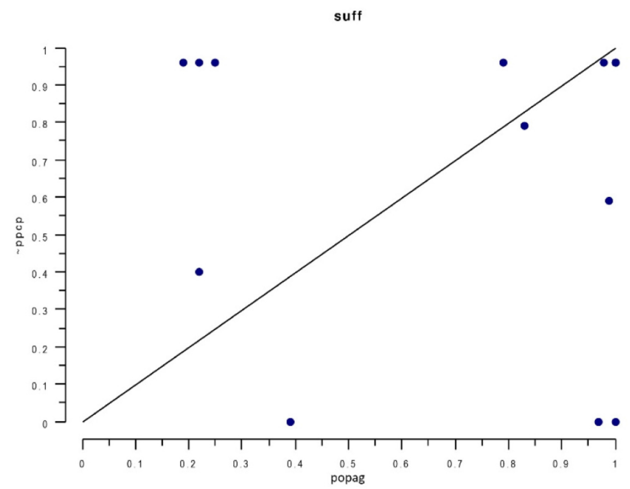


e. Sufficiency analysis for PPCP and ~POPAG (Model 1).

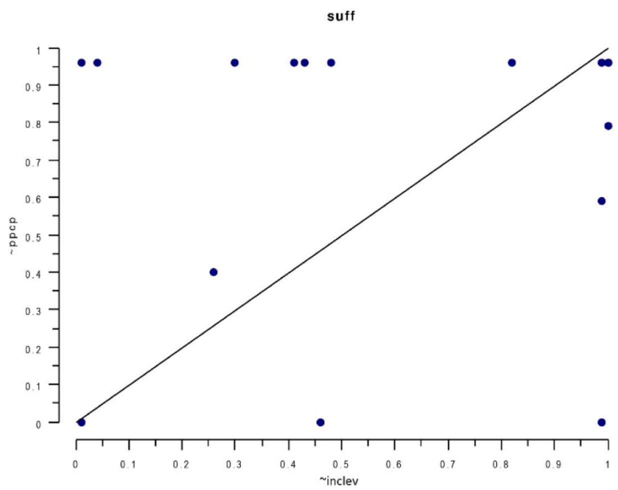
districts, the presence of INCLEV is sufficient for the outcome to occur. However, it is not a requirement that INCLEV is present for the outcome to occur. The results of the sufficiency analysis are in line with the published literature, in which a high income level has been related to high consumption of anti-inflammatories (Nielsen et al., 2003; Sanwald and Theurl, 2017). Specifically, Otto et al. (2018) highlight that the income level is one of the factors that most affects the consumption of anti-inflammatories in urban areas.

In the case of NURHOM (Recipes 1 and 3), the necessity analysis (Table 8) shows that it is not a necessary condition for the outcome. Its consistency value is less than the consistency value of the first three conditions analysed (WATCON, HOSP and POPAG). This means that – although the presence of NURHOM is related to the anti-inflammatory consumption – NURHOM is not as important as WATCON, HOSP and POPAG. The sufficiency analysis for NURHOM (Fig. 3a) shows that the majority of the districts are blow the line and only six are above the line. This means that there are some districts in which NURHOM is a sufficient condition for the outcome. However, it is not a requirement that NURHOM is present for the outcome to occur. Obviously, the influence of NURHOM on the outcome needs to be considered. The work of Stein et al. (2001) highlighted the recurrent use of anti-inflammatories in nursing homes to relieve the symptoms of the residents. This means that there is a relationship between NURHOM and POPAG. The gradual ageing of the population, along with other socio-economic causes – such as the increasing incorporation of women into the workplace – provokes an increase in the number of older people who live in nursing homes (Ayuso-Gutiérrez et al., 2010). The Valencian statistical data with regard to the dependent population (over 64 years old) reflect that increase. Specifically, in 1975, the value was 18% of the population being dependent, while in 2017 the value was practically 30% (INE, 2018). Hence, the progressive ageing of the population together with the increase in the dependent population aged over 64 years are indicators of the importance that nursing homes currently have (Luppa et al., 2010; Rodriguez-Blazquez et al., 2012). These findings highlight the importance of taking into account the influence of nursing homes on the concentration of anti-inflammatories in urban wastewater.

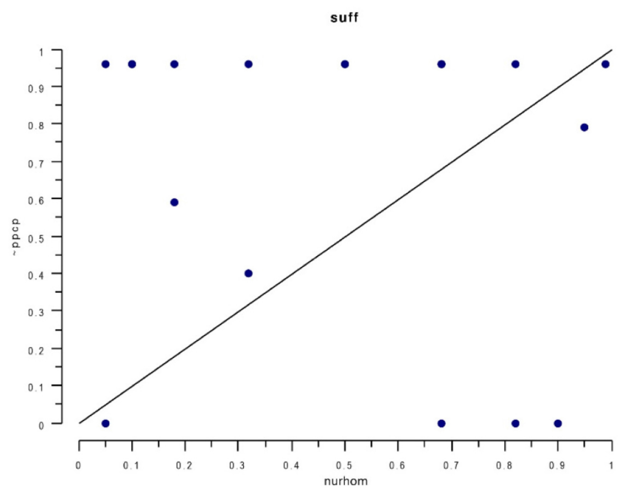
Finally, Table 6 also includes the parsimonious solution. As mentioned previously, the parsimonious solution is a simplified version of the complex solution. Hence, it only includes all of those conditions that the fsQCA software identifies as being essential (see Section 2.1.2 for more information). The result of the parsimonious solution (Recipe



a. Sufficiency analysis for ~PPCP and POPAG (Model 2).



b. Sufficiency analysis for ~PPCP and ~INCLEV (Model 2).



c. Sufficiency analysis for ~PPCP and NURHOM (Model 2).

Fig. 4. a. Sufficiency analysis for ~PPCP and POPAG (Model 2). b. Sufficiency analysis for ~PPCP and ~INCLEV (Model 2). c. Sufficiency analysis for ~PPCP and NURHOM (Model 2).

4) is composed of only one condition: WATCON. Specifically, its raw coverage value (0.91) means that Recipe 4 explains 91% of the districts that contribute to the discharge of anti-inflammatories. Furthermore, the unique coverage value (0.91) means that 91% of the districts with high contamination by anti-inflammatories are explained exclusively by Recipe 4. The necessity analysis (Table 8) shows that WATCON is the condition with the highest values of consistency and coverage. Recipe 4 is composed of four districts: *Patraix*, *Campanar*, *el Pla del Real* and *Quatre Carreres*. The first three districts are in line with the results obtained for Recipes 1, 2 and 3, whereas the district of *Quatre Carreres* appears for the first time. It is significant that, in the parsimonious solution, *Quatre Carreres* district appears for different reasons. First, Table 2 shows that, in *Quatre Carreres* district, there is only 1 hospital. Under calibration thresholds considered, if there is 1 hospital in the district the condition is close to the non-membership threshold. For that reason, this district would remain outside the recipes of the complex solution. However, analysing the data in detail, the hospital is the *Hospital Universitario y Politécnico de la Fe*, with 1284 beds, and currently it is the largest hospital in València City. Hence, it is significant that *Quatre Carreres* district appears in the parsimonious solution, because WATCON is a necessary condition for the outcome. That is, the behaviour of all hospitals and their influence on PPCP have been taken into account.

3.2.2. Results for Model 2

The results for Model 2 are shown in Table 7. The complex solution, which is composed by 3 recipes, has coverage of 0.93. It means that the 93% of the districts with low concentration of anti-inflammatories are explained by the 3 recipes obtained. Specifically, the conditions included in the recipes are ~WATCON, ~HOSP, ~INCLEV, POPAG and NURHOM. The complex solution consistency (0.99) means that the 99% of the districts that do not contribute to high anti-inflammatory pollution have this combination of conditions. From the complex solution, it can be observed that ~WATCON is present in all of them. The necessity analysis (Table 8) confirms that ~WATCON is a necessary condition for that the outcome (~PPCP) to occur. Specifically, ~WATCON has the highest values of consistency (0.99) and coverage (0.96). On the other hand, the necessity analysis also shows that ~HOSP is a necessary condition for a low concentration of anti-inflammatories in the urban wastewater of València. It is clear that there will always be anti-inflammatories in urban wastewater, because their consumption is widespread. However, these values of concentration are not comparable to the influence of hospitals on the anti-inflammatory concentration in urban wastewater.

The analysis of the complex solution results for Model 2 shows that ~INCLEV is present in two of the three recipes (Recipe 5 and 7). The condition ~INCLEV (low income level in the district) present in Recipes 5 and 7 has a relationship with the low anti-inflammatory consumption, as has been discussed above. Hence, the low consumption of anti-inflammatories provokes a low discharge into urban wastewater. This trend is in line with the literature assumptions, such as those in the work of Luppa et al. (2010). Luppa et al.'s (2010) study also highlighted the relationship between a low income level and an increasing number of nursing home admissions. Hence, according to Luppa et al.'s findings, it is reasonable that the NURHOM condition appears in Recipe 7. The sufficiency analysis (Fig. 4a, b and c) supports the findings for Model 2. That is, in the majority of the districts, POPAG, ~INCLEV and NURHOM are sufficient conditions for a low concentration of anti-inflammatories in Valencian wastewater (~PPCP).

The parsimonious solution of Model 2 (Recipe 8 included in Table 7) is composed of only 1 condition: ~WATCON. Specifically, its raw coverage value (0.99) means that Recipe 8 explains 99% of the districts that do not contribute to the discharge of anti-inflammatories. Furthermore, the unique coverage value (0.99) means that 99% of the districts with low discharge of anti-inflammatories are explained exclusively by Recipe 8. These findings are in line with the necessity analysis (Table 8), in which ~WATCON has the highest values. There are 15 districts that are included in Recipe 8: *Ciutat Vella*, *Extramurs*, *la Saïdia*, *l'Olivereta*, *Algirós*, *Benimaclet*, *Rascanya*, *Benicalap*, *Pobles del Nord*, *Pobles de l'Oest*, *Pobles del Sud*, *l'Eixample*, *Poblats Maritims*, *Jesús* and *Camins al Grau*. These districts are those that have low water consumption, mainly due to the absence of hospitals in them (Table 2).

All the results obtained (Tables 6 and 7) are relevant to the current literature about PPCPs and WWTPs, because the relationship between urban areas and PPCPs in wastewater has been proved. The effluent of WWTPs has the potential to be used as a water source for irrigation and environmental purposes. Knowing how the population (and its facilities) affects PPCPs' presence in wastewater is important to identify the conditions that are responsible for their presence. An urban area without hospitals and nursing homes does not have the same PPCP presence in wastewater as an urban area like València City. Hence, the WWTP performance will be different because of the lower presence of PPCPs in wastewater. From the scientific point of view, this statement is obvious. However, to justify preventive investments in wastewater treatment, it is necessary to prove that relationship. Through fsQCA, recipes for the anti-inflammatory pattern in València City wastewater were obtained. The presence of hospitals is the main phenomenon responsible for the discharge of anti-inflammatories into sewage system, followed by the number of nursing homes and population ageing. The continuous discharge of anti-inflammatories and the inability of the WWTPs' technology to remove these anti-inflammatories have a negative impact on the receiving water bodies, specifically their high toxicological effect on exposed aquatic organisms (Bound and Voulvoulis, 2004; Laquaz et al., 2018; Mehinto et al., 2010). For all of these reasons, and considering the implementation of preventive measures, it would be advisable for hospitals would to perform pre-treatment to reduce the quantity of anti-inflammatories (and other medicines) in wastewater. The approach proposed in this work is unable to suggest a specific technology for the pre-treatment of hospitals wastewater. This is the next step in our research, analysing in detail the different technologies available for each situation. Future preventive measures applied on hospitals wastewaters will be an improvement of wastewater management in urban areas. This would reduce the impact that hospital wastewater has on WWTPs and increase the quality of treated wastewater (Chonova et al., 2016), promoting its reuse. Authors are aware that the removing of PPCPs 100% could not be feasible under an economic point of view. Despite this situation, the environmental benefit of removing PPCPs of wastewater (which were reused for irrigation and environmental purposes) needs to be considered. Hence, preventive measures (such as pre-treatment in hospitals) and technological improvements in WWTPs will allow to reduce the concentration of PPCPs in effluents.

4. Conclusions

The presence of PPCPs in wastewater is becoming increasingly important due to both, the reuse of wastewater for agricultural and environmental purposes and the toxicological risk of PPCPs. Reuse water in water-stressed areas (such as València City) is an essential part of water cycle and removing PPCPs from wastewater has become a necessity. The aim of this work was to identify the patterns related to the presence of anti-inflammatories in urban wastewater of València City. The assessment of the patterns that explain the presence of anti-inflammatories in Valèncian wastewater was conducted at the district level. This approach is a novelty because it has not been considered in the literature published about PPCPs and fsQCA. Five conditions were analysed: WATCON, POPAG, INCLEV, HOSP and NURHOM. Considering the literature published, the data availability and the use of both quantitative and qualitative data, the fsQCA methodology was implemented. Through fsQCA, recipes that explain the anti-inflammatory patterns in urban wastewater were obtained.

The results are composed by eight recipes which WATCON, HOSP and POPAG are the conditions that have a strong influence on the presence of anti-inflammatories in Valèncian wastewater. All these conditions are present in the recipes obtained with consistency of 99%. The recipes obtained allow the identification of those districts with high discharge of anti-inflammatories and the reasons of the high discharge. Hence, these districts can be considered as hot spots of anti-inflammatory discharge. From decision makers' point of view, different measures can be implemented to reduce the concentrations of anti-inflammatories in urban wastewater. One of these measures could be the installation of wastewater treatment equipment in hospitals (as a pre-treatment before the discharge to sewage system). Thanks to that pre-treatment, the toxicological risk of hospital wastewater would be reduced. As a result, the wastewater that arrives at WWTPs would have a lower anti-inflammatory concentration and the effluent obtained would have a better quality – facilitating wastewater treatment and enhancing wastewater reuse.

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