Research Article

Identification of Specific Pollutants and Derivation of Environmental Quality Standards in Turkey

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Abstract

Specific pollutants are defined as the substances posing a risk on national or river basin level due to being discharged in serious amount according to Water Framework Directive (2000/60/EC) and control of them in surface waters is ensured by the implementation of environmental quality standards (EQS). As a candidate for EU membership, Turkey, has conducted studies on determination of specific pollutants between 2011 and 2015. In this scope, firstly, list of candidate pollutants were prepared based on the field studies, questionnaires and literature surveys. Different prioritization methods were then applied for candidate chemicals considering hazard characteristics, exposure levels and production/use patterns of the substances. Finally, 117 point sourced and 133 non-point sourced specific pollutants were designated with their national EQSs.

Key words: *specific pollutants, environmental quality standards, prioritization, hazard characteristics*

Öz

Su Çerçeve Direktifi'ne göre, belirli kirleticiler, sulara önemli miktarda deşarj edilmeleri sebebiyle ulusal veya nehir havzası ölçeğinde risk teşkil eden maddeler olup bu maddelerin yerüstü sularındaki kontrolü çevresel kalite standartlarının (ÇKS) uygulanması ile sağlanmaktadır. AB üyeliği için aday ülke konumundaki Türkiye'de, belirli kirleticilerin ortaya konulmasına yönelik 2011-2015 yılları arasında çalışmalar yürütülmüştür. Bu kapsamda, ilk olarak, saha çalışmaları, anketler ve literatür araştırmalarından faydalanılarak aday kirletici listesi oluşturulmuştur. Çalışmanın devamında, maddelerin tehlike özellikleri, maruziyet seviyeleri ve üretim/kullanım biçimleri dikkate alınarak aday kirleticiler için farklı önceliklendirme metotları uygulanmıştır. Neticede, 117 noktasal kaynaklı ve 133 yayılı kaynaklı belirli kirletici ile bu kirleticilere ilişkin ulusal ÇKS değerleri ortaya konulmuştur.

Anahtar sözcükler: *: belirli kirleticiler, çevresel kalite standartları, önceliklendirme, tehlike özellikleri*

Introduction

Hazardous substances in surface waters are the chemicals having a property of toxicity, persistency and bio-accumulation. Industrial chemicals, personal care products, pesticides, pharmaceuticals, detergents and metals are some of the hazardous substance groups commonly used in daily life.

According to Water Framework Directive (2000/60/EC), hazardous substances can be either priority substances or specific pollutants. Priority substances are defined as the substances posing a significant risk for water environment which also including priority hazardous substances among them (Directive 2000/60/EC; Directive 2013/39/EU) and recently reviewed by the Directive 2013/39/EU on EU level. Specific pollutants, on the other hand, are the substances posing a risk on national or river basin level due to being discharged in serious amount and they are designated by Member States on a country basis. Control of priority substances and specific pollutants in surface waters are ensured by the implementation of their environmental quality standards (EQS), concentrations in water, sediment or biota which should not be exceeded in order to protect human health and the environment.

As a candidate for EU membership, Turkey, has conducted the scientific studies on the surface water management of hazardous pollutants between the years of 2011-2015 by considering the abovementioned issues. Within the scope of these studies, efforts were being made on the determination of river basin specific pollutants in surface water resources, monitoring of these substances in receiving water bodies and wastewaters, and setting EQSs for them.

In this paper, specific information is provided on the prioritization of chemicals and selection of national specific pollutants and derivation of EQSs.

Method

Prioritization of chemicals

First step of the identification of specific pollutants was the constitution of the list of candidate chemicals. This list was prepared based on the field studies in the pilot regions, questionnaires, literature surveys and the list of chemicals produced or imported more than 1 tons annually in Turkey. Second step was the screening and prioritization of chemicals in the candidate list. In this stage, Combined Monitoring and Modeling Based Priority Setting (COMMPS) and Total Hazard Score (THS) methodologies were applied.

COMMPS methodology.

COMMPS methodology is developed by Fraunhofer Institute of Environmental Chemistry and Ecotoxicology and used for the aim of identifying priority pollutants under the Water Framework Directive (Klein et al., 1999). Both the exposure and the hazards are evaluated in this methodology. The risk score is calculated by the Equation 1:

$$I\_PRIO = I\_EXP \times I\_EFF \tag{1}$$

I_EXP stands for the exposure score of the substances and I_EFF stands for the effect score of the substances.

Two different exposure scores can be calculated by this method. These are modeling based exposure score and the monitoring based exposure score (Şıltu, 2015). Monitoring based exposure score is calculated based on the arithmetic mean of the results in each monitoring station by the Equation 2:

$$I\_EXP\ (\text{substance } i) = \frac{\log(Ci / (Cmin \times 10\text{-}1))}{\log(Cmax / (Cmin \times 10\text{-}1))} * 10 \tag{2}$$

The minimum and maximum values are given in Table 1:

Table 1. Maximum and minimum values used in calculations

	C_{max}	C_{min}	Unit
Organic substances in the water phase	100	0.0001	pg/1
Organic substances in the water phase (maximum likelihood	100	0.0001	pg/1
Metil compaunds in the water phase	200	0.2	pg/1
Organic substances in the sediment	10000	0.01	pg/kg
Metil compaunds in the sediment	2000	6	pg/kg

The modeling based exposure score is calculated based on the emission, degradation and dispersion by using the below equations:

$$I_{\_EXP} = 1{,}37\ (\log(EEXV) + 1{,}301) \qquad (3)$$

$$EEXV = EMISSION \times DISTRIBUTION \times DEGRADATION \qquad (4)$$

I_EXP is normalized such that the range is between 0 and 10. The calculation of each component of this equation is as follows.

$$EMISSION = 0{,}01\times T1 + 0{,}1\times T2 + 0{,}2\times T3 + 1{,}0\times T4 \qquad (5)$$

Table 2. Values used in emission factor calculation

Main use category	**Fraction**
1 Used in closed systems	0.01
2 Use resulting in inclusion in matrix	0.10
3 Non-dispersive use	0.20
4 Wide dispersive use	1.00
Default	1.00

The factor “DISTRIBUTION” represents the fraction of a chemical which partitions at equilibrium into the aquatic compartment and it is calculated by using the Mackay I Model according to the environmental characteristics given in the model (Mackay, 2001). By this model, fugacity (f) of the chemicals in each environmental compartment can be calculated. Fugacity is the tendency of a chemical to escape from a system. The model requires the calculation of fugacity capacity (Z) for each compartment and the fugacity is related to the concentration of the chemical in the environmental compartments.

$$C=Zf \tag{6}$$

$$\text{Air (1) } Z1 = 1/RT \tag{7}$$

$$\text{Water (2) } Z2 = CS\ /VPS \tag{8}$$

$$\text{Soil (3) } Z3 = Z2\ n_3 f_{oc3}\ K_{oc}\ /\ 1000 \tag{9}$$

$$\text{Sediment (4) } Z4 = Z2\ n_4 f_{oc4}\ K_{oc}\ /\ 1000 \tag{10}$$

$$\text{Susp. Solids (5) } Z5 = Z2\ n_5 f_{oc5}\ K_{oc}\ /\ 1000 \tag{11}$$

$$\text{Fish (Biota) (6) } Z6 = Z2\ n_6\ L\ K_{ow}\ /\ 1000 \tag{12}$$

R : Gas constant (8.314 J/mol K)

T : Temperature (K)

Cs : Water solubility (mol/m^3)

VPs : Vapour pressure (Pa)

ni : Density of phase i (kg/m^3)

foci : Mass fraction of organic carbon in phase i

L : Lipid content in fish (0.10)

Koc is derived from Kow according to Mackay model: Koc = 0.41

The environmental characteristics defined in Mackay I Model are given in the table below (Mackay, 2001):

Table 3. Environmental characteristics defined in Mackay I Model

Compartment	**Air**	**Water**	**Soil**	**Sediment**	**Suspended Solids**	**Fish (Biota)**
Volume (m^3)	10^{14}	$2x10^{11}$	$9x10^9$	10^8	10^6	$2x10^5$
Depth (m)	1000	20	0.1	0.01	-	-
Volume (m^2)	$10x10^{10}$	$10x10^9$	$90x10^9$	$10x10^9$	-	-
Fraction oc(f_{oc})	-	0.02	0.02	0.04	0.2	-
Density (kg/m^3)	1.2	2400	2400	2400	1500	1000

The factor “DEGRADATION” assumed depending on the biodegradability of the substances. The values used are given below:

Table 4. Values used as degradation factor

Biodegradabilty	Fraction
Ready biodegradabilty	0.1
Internet Biodegradabilty	0.5
President	1.0
Default	1.0

The effect score is calculated according to the equation shown below:

$$I\_EFF = EFSd\ (5) + EFSi\ (3) + EFSh \tag{13}$$

Where EFSd stands for the direct aquatic effect score, EFDi for indirect aquatic effect score and EFSh for human health effect score.

$$\text{EFSd (substance i)} = \frac{\log\left(PNEC_i / (10 \times PNEC_{max})\right)}{\log\left(PNEC_{min} / (10 \times PNEC_{max})\right)} \times WF \tag{14}$$

WF Weighting factor for direct effects (5 for organic substances, 8 for metals).

The PNEC values used are:

Table 5. Maximum and minimum PNEC values

	$PNEC_{max}$	$PNEC_{min}$	Unit
Organic substances in the water phase	1	0.000001	mg/l
Organic substances in the sediment (see chap. 5.2)	10	0.000001	mg6kg
Metal compounds in the water phase (see chap. 5.3)	0.1	0.000001	mg/l

EFSi is determined according to the criteria given in Table 6:

Table 6. Criteria of determining indirect aquatic effect score (EFSi)

$logP_{ow}$		Molecular Eight	Bioconcentration Factor (BCF)	Scores
< 3	or	< 700	< 100	0
3 <= log Pow < 4	and	< 700	100 - < 1000	1
4 <= log Pow < 5	and	< 700	1000 - < 10000	2
>= 5	and	< 700	> 10000	3
default (nologPow)	and	< 700	no BCF	3

EFSh is determined according to the criteria given in Table 7:

Table 7. Criteria of human health effect score (EFSh)

Carcinogenicity	Mutagenicity	Effects on Reproduction	Chronic Effects (oral)	Scores
R45	R46	R47,R60 or R61	-	2
R40	R40	R62,R63 or R64	-	1.8
-	no test	no test	R48 in any combination with R23 - R28	1.4
-	-		R48 in any combination with R20 - R22	1.2
-	-	-	R33	1
-	-	-	-	0

The maximum risk score calculated is 100 by COMMPS methodology. There is no cut-off criteria defined for the evaluation of risk scores and this is a shortcoming of the COMMPS methodology (Şıltu, 2015).

THS methodology.

The original methodology is developed in UK to propose an alternative screening tool for the identification of priority pollutants under Water Framework Directive (Daginnus et al., 2011). The methodology consists of both hazard and exposure assessment. However, due the data gaps on environmental levels of chemicals, only hazard assessment was considered in these studies. The equation used for the hazard score calculation is given below:

$$THS = P + B + T + ED \qquad (15)$$

Where P stands for Persistent (no persistence = 0, persistent = 1), B for Bioaccumulative (no bioaccumulation = 0, bioaccumulative = 1), T for Toxic (no toxicity = 0, toxic = 1) and ED for being in the Endocrine Disruptors list Categories 1 and 2 (no ED activity = 0, ED = 1). An additional +1 was added to the total score if the substance fulfilled all the screening criteria or if the substance was classified as vPvB (v= very).

The cutoff values used in the studies are:

$P=1$ if half-life in water > 40 days

$B=1$ if $BCF > 2000$, if $BCF > 5000$ then vB

$T=1$ if $NOEC < 0{,}01$ mg/L or $E(L)C_{50} < 0{,}1$ mg/L

Therefore, the maximum hazard score is 4 which corresponds to a substance classified as PBT or vPvB, while the minimum score is 0.

Derivation of EQSs.

For EQS derivation, detailed literature survey were done to collect acute (i.e. LC50, EC50) and chronic (i.e. NOEC) ecotoxicological data of chemicals for 3 trophic levels (i.e. daphnia magna, algae and fish) and surface water EQSs were calculated by deterministic and/or probabilistic method (ETX 2.0 Software) in line with the procedures given in the Technical Guidance Document No.27 of 2000/60/EC Water Framework Directive (EC, 2011).

During these studies, data sources for the collection of ecotoxicological data of chemical are EPA Ecotox Database, HSDB (Hazardous Substances Data Bank), OECD (The Organization for Economic Co-operation and Development) Database, EU Risk Assessment Reports and material safety data sheets. Thanks to deterministic and probabilistic methods, both annual average (AA-EQS) and maximum allowable (MAC-EQS) EQSs were calculated.

Deterministic method.

In deterministic method, the lowest EC50 or LC50 value is taken and divided by the assessment factor (AF) changing between 1 and 10000 and given in the Technical Guidance Document No.27 of 2000/60/EC Water Framework Directive based on the number of acute toxicological data gathered from the literature. Similarly, the same procedure is followed for the calculation of AA-EQS from the chronic toxicological data considering the lowest NOEC value. In this approach, AF can be thought as the indicator of uncertainties in the available data (Koç Orhon, 2015).

Within the process of derivation of EQS by this method, AF values differ according to the number of data, data type and type of the organisms that data is originated from. The reason is that the difference between the chemical sensitivity of the marine species is much more apparent and there is an uncertainty coming from whether the species living in marine environment are represented in the data set. Therefore, by having higher AF values, EQS values are generally lower and stricter for salt waters compared to the freshwaters (EC, 2011).

In this method, regardless of whether data is combinable or not, AF values are determined separately for fresh and salt waters. In this scope, for MAC-EQS, in the stage of determining AF, Table 3.4, represented in Technical Guidance Document No.27, is used for freshwater while Table 3.5, represented in the Document, is used for salt water (EC, 2011).

Probabilistic method.

Probabilistic method is based on species sensitivity distribution (SSD) modeling in which all reliable toxicity data are ranked and a model fitted. By this method, the threshold level that represents a safe concentration of the substance which thereby protects most organisms (typically 95%), namely hazardous concentration (i.e. HC5), is calculated with the log-normal distribution of data and then this value is divided by the AF ranging between 1 and 5 based on the available toxicological data. This method can be applied if and only the number of available data for 3 trophic levels is equal or greater than 10. ETX 2.0 Software can be used for the EQS calculation by this method (Aldenberg and Jaworska, 2000). This method is more reliable than the deterministic method due to running with lower AF value; therefore; it should be preferred for EQS calculation when there is available sufficient data (Koç Orhon, 2015).

Rationale behind SSD by ETX 2.0 Software:

ETX 2.0 Software uses the method of Aldenberg and Jaworska (2000) for HC5 calculation.

$$\text{Log HC5} = X_m - k \times s \qquad (16)$$

Where:

Xm: mean of log-transformed data

k: extrapolation constant depending on protection level and sample size (according to Aldenberg and Jaworska, 2000)

s: Standard deviation of log-transformed data

$$\text{EQS} = \text{HC5} / \text{AF} \quad (\text{AF: 1-5}) \qquad (17)$$

According to fraction affected (%), there is a table giving the value of k constant based on the number of toxicity data available. Rows are sample size, columns are fraction affected in this table. There are 6 sets of fraction affected as 1%, 2%, 5%, 10%, 25% and 50%. Sample size changes between 2 and infinity. “k” value is independent of the substance involved (Aldenberg and Jaworska, 2000).

According to the Guidance Document, an AF of 5 is used by default but it may be reduced where evidence removes residual uncertainty. The exact value of the AF depends on an evaluation of the uncertainties around the derivation of the HC5. Generally, the number of data used in HC5 derivation is taken as a baseline and different AFs between 1 and 5 are designated depending on the number of available data. In these studies, AFs were determined based on the considerations in Table 8.

Table 8. AF values for probabilistic method

Number of Data	**Fraction**
10-15	5
16-20	4
21-25	3
26-30	2
> 30	1

Results

In the first stage of the studies, candidate chemical list covering nearly 3300 substances were prepared considering the results of field studies and questionnaires in the pilot regions and benefiting from the scientific articles and documents in the literature. Also, the chemicals assigned as specific pollutants in EU countries were assessed in the candidate list. For the point sourced pollutants, production and wastewater treatment processes of pilot urban and industrial facilities were investigated, literature survey was conducted, BREF documents of industrial sectors were studied and national/international legislations were searched. For the identification of diffuse pollutants, lists of pesticides that are in use and prohibited were investigated and questionnaires were made with the distributors of plant protection products in the pilot regions. At the end, inventory of pesticides was established by considering the agricultural production pattern in different river basins.

In order to deal with the chemicals of highest priority among the candidate list, different prioritization methods such as COMMPS and THS were used according to available data on the hazard characteristics, exposure profile and production/use amount of each substance. During the prioritization, COMMPS method was not widely applied since usage and monitoring data are lacking for the chemicals in the list. On the other hand, THS methodology was used for the prioritization of the majority of the substances due to less data requirement and simple way of calculation.

In addition to prioritization scores, results of chemical monitoring studies were taken into consideration for the identification of final specific pollutants, as well. The chemicals detected at significant concentrations in surface waters were also designated as specific pollutants although their prioritization scores were lower. At the end, 117 point sourced and 133 diffuse sourced specific pollutants were determined on national level. Specific pollutant list includes heavy metals, polychlorinated biphenyls, halogenated organics, endocrine disrupters, aromatic hydrocarbons and pesticides.

For these specific pollutants, national EQS values were also calculated by the probabilistic and deterministic methods the details of which are defined in the Technical Guidance Document No.27 of 2000/60/EC Water Framework Directive. Different EQS values were derived for freshwaters and saline waters depending on the acute and chronic toxicological data. In general, for the same specific pollutant, saline water EQSs were found to be more strict compared to the ones of fresh waters. For the calculations, deterministic method was mostly used due to limitation of toxicological data. Acute toxicological data were dominant to chronic toxicological data in literature. This situation has resulted in higher uncertainties in derived AA-EQS values since larger AF values were used to extrapolate to safe concentration.

Discussion and Conclusion

Results of these studies, namely, specific pollutants and their EQSs in freshwaters and saline waters, were adapted to the national legislation called “By-Law on Surface Water Quality” on August 10, 2016. As of this date, these chemicals have been started to monitor in surface waters and quality classification of surface waters has been made by considering their EQSs, as well. In this way, now, it becomes possible to control these pollutants in surface water resources and take necessary precautions in time in order to protect and improve water quality when there is an identified risk of not attaining water quality objectives.

However, the outcomes of these studies demonstrated that there are still important data gaps more specifically on the hazard and exposure profiles, production and use amount and toxicity thresholds of the some chemicals. Monitoring studies were also lacking since most of the chemicals among the candidate specific pollutant list are so-called emerging pollutants and they were not monitored continuously in the surface waters before. Till the next prioritization which should be made after 6 years according to Water Framework Directive (2000/60/EC), the extent of inventory, toxicity and monitoring studies for the chemicals must be enhanced so that more reliable and realistic assessments can be obtained.

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Extended Turkish Abstract
(Genişletilmiş Uzun Türkçe Özet)

Türkiye'de Belirli Kirleticilerin Tespit Edilmesi, Çevresel Kalite Standartlarının Belirlenmesi

2000/60/EC sayılı Su Çerçeve Direktifi (SÇD), yerüstü su kaynaklarının kalitesinin korunması ve sucul ekosistemlerin durumunun iyileştirilmesi hedefine yönelik olarak çevre koruma ve yönetimi konusunda bütünleşik bir yaklaşım getirmektedir. Bu yaklaşımlardan biri de, su kaynakları için risk teşkil eden tehlikeli maddeler için alıcı ortam çevresel kalite standartlarının (ÇKS) belirlenmesi ve uygulamaya alınması şeklindedir.

ÇKS’ler, su kütlelerinin ekolojik ve kimyasal durum tespiti ve değerlendirilmesi için gerekli araçlar olmakla birlikte su, sediman ve biyota için bağımsız olarak türetilmektedir. SÇD’ye göre, ÇKS’ler öncelikli maddeler ve belirli kirleticiler için oluşturulmaktadır. Öncelikli maddelere ilişkin ÇKS’ler sırasıyla “2008/105/EC sayılı Çevresel Kalite Standartları Direktifi (ÇKSD)” ve “Su Politikası Alanında Öncelikli Maddeler Açısından 2000/60/EC Sayılı Direktifi ve 2008/105/EC Sayılı Direktifi Değiştiren 2013/39/EU Sayılı Direktif” ile Avrupa Birliği (AB) düzeyinde belirlenmiştir. Diğer taraftan, belirli kirleticiler ve bu kirleticilere ilişkin ÇKS’ler ise, SÇD’de verilen muhtemel madde grupları esas alınarak, her bir ülke tarafından kendi endüstriyel ve tarımsal üretim portföyüne bağlı olarak belirlenmektedir. Belirli kirleticiler su kütlesine, kalitesini olumsuz yönde etkileyebilecek miktarda deşarj edilmeleri sebebiyle sucul ortamlar için risk teşkil eden maddeler olarak tanımlanmakta olup, organik ve inorganik maddeler ile konvansiyonel kirleticiler belirli kirletici grupları arasında yer alabilmektedir.

AB üyeliği için aday ülke konumundaki Türkiye’de, kıyı ve geçiş suları dâhil yerüstü su kaynaklarında bulunan tehlikeli maddelerin tespit edilmesi ve bu maddelere ilişkin alıcı ortamda aşılmaması gereken limit değerleri ifade eden ÇKS’lerin geliştirilerek, mevzuata aktarılmak üzere ülkemize özgü noktasal ve yayılı kaynaklı belirli kirleticilerin belirlenmesi çalışmasına altlık oluşturmak maksadıyla 2011-2015 yılları arasında çalışmalar yürütülmüştür. Bu çalışmalar kapsamında, aday kimyasal listesi oluşturulmuş, kimyasallar tehlikelilik özelliklerine göre önceliklendirilmiş, kimyasallara ilişkin çok kapsamlı ve detaylı envanter çalışmaları yürütülmüş, izleme çalışmaları gerçekleştirilmiş ve alıcı ortam kalite standartları geliştirilmiştir.

Noktasal kaynaklı kirliliğin tespitine yönelik olarak, pilot olarak seçilen alanlarda tehlikeli madde kirliliğine neden olan ve kıyı ve geçiş suları ile iç sulara deşarj yapan kentsel ve endüstriyel faaliyetlere ilişkin pilot tesisler belirlenmiştir. Yayılı kaynaklı kirliliğin tespitine yönelik olarak, ülkemizde yasaklı ve izinli pestisitlerin listesi temin edilmiş ve pilot alanlardaki bitki koruma ürünü bayileri ile anket çalışmaları gerçekleştirilmiştir. Aday kimyasal listesi oluşturulurken; pilot tesislere gerçekleştirilen saha çalışmaları verileri, pilot tesislerde kullanılan hammaddeler ve proses sırasında oluşan yan ürünler, endüstriyel sektörlere ilişkin BREF dokümanları ve literatür bilgileri, bitki koruma ürünü bayileri ile gerçekleştirilen anket sonuçları, AB’de belirlenen belirli kirleticiler ile ulusal ve uluslararası mevzuat ve sözleşmelerden yararlanılmıştır. Neticede, yaklaşık 3300 maddeden oluşan aday kimyasal listesi hazırlanmıştır.

Çalışmanın devamında, aday kimyasal listesindeki maddeler risk derecelerine göre önceliklendirme çalışmasına tabii tutulmuştur. Önceliklendirme yapılırken, kimyasala ilişkin üretim verisinin mevcut olup olmamasına bağlı olarak 2 farklı yöntem kullanılmıştır. Kimyasala ilişkin üretim verisinin mevcut olması halinde Birleşik İzleme-Bazlı ve Model Bazlı Önceliklendirme Prosedürü (COMMPS), üretim verisinin mevcut olmaması halinde ise Toplam Tehlike Skoru (TTS) metodu kullanılmıştır. COMMPS metodu AB’de SÇD “Öncelikli Maddeler Listesi” oluşturulurken uygulanan önceliklendirme metodu olup, bu yöntemde 5 kademeli bir seçim sistemi uygulanmaktadır. Bunlar sırasıyla; aday listenin belirlenmesi, maruziyet skorunun (I_EXP: maruziyet indeksi) hesaplanması (izleme ve modelleme bazlı), etki skorunun (I_EFF: etki indeksi) hesaplanması, risk bazlı skorun hesaplanması ve öncelikli kirleticilerin belirlenmesidir. TTS metodunda kimyasalların tehlikeliliklerine ilişkin değerlendirme yapılmakta olup neticede bir tehlike skoru hesaplanmaktadır. Tehlike skoru; kimyasalın kalıcı (P), toksik (T), birikim potansiyeli (B) ve endokrin bozucu (ED) olup olmadığı dikkate alınarak hesaplanmaktadır. Söz konusu her bir değerlendirme kriteri için ilgili sınır değer aşılmışsa skor ‘1’, aşılmamışsa ‘0’ olarak alınmaktadır. Bir madde eğer çok dirençli ve çok biyoakümülatif (vPvB) olarak sınıflandırılıyorsa, toplam skora ‘1” eklenmektedir.

COMMPS ve TTS metotları ile yapılan önceliklendirme sonuçları ile pilot alanlarda gerçekleştirilen izleme sonuçlarının birlikte değerlendirilmesi neticesinde 117 noktasal kaynaklı ve 133 yayılı kaynaklı olmak üzere toplamda 250 adet belirli kirletici ortaya konulmuştur. Bu aşamada, bir kimyasal izleme çalışmalarında önemli konsantrasyonlarda tespit edilmişse, önceliklendirme skoru çok yüksek olmasa da uzman görüşü ile belirli kirletici listesine dâhil edilmiştir.

Belirli kirleticiler için tatlı ve tuzlu sularda yıllık ortalama ve maksimum ÇKS’lerin (YO-ÇKS, MAK-ÇKS) belirlenmesi maksadıyla, literatürden elde edilen ve kalite değerlendirmesinden geçen farklı taksonomik gruplara ilişkin güvenilir ve ilgili akut ve kronik toksisite verileri bir araya getirilmiş ve ekstrapolasyon yöntemleri ile kalite standartları hesaplanmıştır. Hesaplama sırasında, veri sayısı ve türüne bağlı olarak kullanılan yöntem değişiklik göstermiştir. ÇKS geliştirilirken, 2011 yılında SÇD için Ortak Uygulama Stratejisi kapsamında “Çevresel Kalite Standartlarının Belirlenmesine İlişkin Teknik Rehber Doküman”, kısa adıyla “27 No’lu Rehber Doküman”dan faydalanılmış ve “deterministik” ve “probabilistik” olmak üzere 2 temel metot kullanılmıştır. Deterministik metot, ekotoksikolojik veri sayısının kısıtlı olması durumunda kalite standardı belirlemede kullanılan bir yöntem olup, Rehber Dokümana göre ekotoksikolojik veri sayısının 10’dan az olması halinde bu metot ile ÇKS türetilmiştir. Deterministik metot kapsamında güvenilir en düşük toksisite verisi baz alınarak bu veriye 1 ila 10000 arasında değişen bir değerlendirme faktörü (DF) uygulanmış ve bu şekilde elde edilen değer ÇKS olarak belirlenmiştir. Diğer taraftan, ekotoksikolojik veri sayısının 10 ve üzerinde olması halinde probabilistik metot kullanılmıştır. Probabilistik metot, ÇKS belirleme yöntemi olarak türlerin hassasiyet dağılımı (SSD) modelini esas almakta olup, kimyasala ilişkin tüm güvenilir toksisite verileri sıralanarak model çalıştırılmakta ve bu sayede kısaca HC5 olarak da bilinen söz konusu kimyasala karşı türlerin %95’i için koruma sağlayabilecek konsantrasyon eşiği belirlenmektedir. Bu yöntemle elde edilen tehlike eşik değeri, deterministik metoda kıyasla daha küçük aralıkta seyreden ve eldeki veri sayısına bağlı olarak 1-5 arasında değişen bir DF’ye bölünmüş ve bu sayede modelde hesaba katılamayan diğer belirsizlikler de dikkate alınarak ÇKS değerleri hesaplanmıştır.