Ecosystem Services 41 (2020) 101057

Contents lists available at ScienceDirect

Ecosystem Services

journal homepage: www.elsevier.com/locate/ecoser

Connecting air quality regulating ecosystem services with beneficiaries through quantitative serviceshed analysis

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ARTICLE INFO

Keywords:
Air quality regulation
Serviceshed
Atmospheric transport
Ecosystem service valuation
Spatial modeling
Ecosystem service mapping

ABSTRACT

In response to the growth of ecosystem services research, many concepts have emerged to understand how we connect ecosystem services with the human populations whom receive the benefits. Servicesheds are one of these emerging concepts and can be qualitatively described as the areas which provide ecosystem services to specific beneficiaries. Previous research lacks the use of mathematical, spatially-explicit models to connect beneficiaries with the ecosystem services that are provided to them by neighboring ecosystems. Working with an atmospheric dispersion model, CALPUFF, this research focuses on air quality regulating ecosystem services and specifically, dry deposition of gaseous pollutants. Multiple quantitative, reproducible, and spatially-explicit definitions of the serviceshed concept are proposed. The various definitions are dependent on the model's results for concentration and dry deposition values. To discuss the application of these quantitative serviceshed definitions, a case study is conducted for a biodiesel manufacturing site in Cincinnati, OH. The results of the proposed serviceshed definitions yield different and complimentary information for the air quality regulation services. The results of these spatially-explicit definitions yield maps with serviceshed boundaries, which can inform ecosystem restoration and management decisions.

1. Introduction

From clean air to water to food provision, humanity relies on a multitude of ecosystem services for its well-being. Ecosystem service research has been growing rapidly since the release of the Millennium Ecosystem Assessment (MA), a project carried out from 2001 to 2005 (Schirpke et al., 2014; Ash et al., 2010). Introduced as a concept to promote sustainability and understand the many services which ecosystems provide benefiting humans, the MA categorized the services into four categories: supporting, provisioning, regulating, and cultural (Ash et al., 2010). Approaching sustainability from a breadth of ecosystem services enables an understanding of the trade-offs between services as we act to increase the capacity, or supply, of these services. However, within ecosystem services literature, there is still debate on which services should be assessed and how to conduct an assessment (Grêt-Regamey et al., 2017; Martínez-Harms and Balvanera, 2012). Further, Boerema et al. suggests a possible lack of agreement on what constitutes an ecosystem service after conducting a systematic review of 405 peer-reviewed papers (Boerema et al., 2017).

In application of ecosystem service assessment, there exists an inconsistency among mapping methods and the scales at which they are conducted; although, a majority are conducted at a regional scale (Grêt-Regamey et al., 2017; Martínez-Harms and Balvanera, 2012; Crossman et al., 2013). Ecosystem service mapping is simply the spatially-explicit valuation of ecosystem service production. Depending on the service being considered, ecosystem service mapping relies on different sources of data. Fortunately, larger and more complete data sets and tools, like "EnviroAtlas" (Pickard et al., 2015) have become available as ecosystem service mapping has been mandated by various government agencies in the EU and U.S. (European Commission, 2011; PCAST, 2011). Despite availability, it can be challenging to find a broad collection of ecosystem service valuation tools because many of them cannot be found using 'ecosystem services' as keywords (Grêt-Regamey et al., 2017).

Understanding the benefits of ecosystem services to mankind requires the ability to connect a given service to the population it benefits. Identifying beneficiaries is often disregarded from ecosystem service assessments (Schirpke et al., 2014); however, it has been identified as a research need to understand the many dynamic interactions that occur between ecosystems and human populations (Anton et al., 2010).

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https://doi.org/10.1016/j.ecoser.2019.101057
Received 12 April 2019; Received in revised form 5 December 2019; Accepted 8 December 2019
2212-0416/

Understanding ecosystem services and the scale at which the services are delivered to various beneficiaries increases our understanding for better land management, restoration and conservation methods. Of the current ecosystem assessments which do aim to identify beneficiaries, most do so qualitatively (Schirpke et al., 2014) or on a loosely-assigned scale (Burkhard et al., 2012) and lack the spatially-explicit data required for mapping these beneficiaries (Anton et al., 2010). Often, ecosystem service assessments that do map beneficiaries do so for a specific area of land, such as a national park or other protected land area (Schirpke et al., 2014). However, the reverse application lacks in literature, focusing on a specific beneficiary and connecting them to the land that provides its ecosystem services. With this type of application, the beneficiary can be defined and different scales of human activity or community can be chosen such as a single household, a manufacturing facility, a city, a county, etc.

A past literature review was conducted to identify research needs and knowledge gaps necessary to address as we incorporate ecosystem service concepts and data into policy and decision-making. Specifically, it acknowledged the need for spatially-explicit models which identify both locations of ecosystem service production and the beneficiaries of those services, while also quantifying and understanding the flow of services between them (Anton et al., 2010).

Current research that satisfies this need is the concept of watersheds. By definition, a watershed is "an area of land in which all of the incoming precipitation drains to the same place" (Edwards et al., 2015). Also referred to as drainage basin, the watershed has historically been accepted as the appropriate scale for natural resource development and conservation decisions (Knetsch and Hart, 1961). It is the serviceshed of the water provisioning ecosystem service and is defined by geographic characteristics and the beneficiaries within the area that benefit from the water provisioning. The research in this field has developed large data sets that outline the boundaries of watersheds across the globe, including a U.S. national data model of hierarchical hydrologic units maintained by the USGS, the Watershed Boundary Set (USGS et al., 2013).

To connect beneficiaries with the production location of other ecosystem services (other than water provisioning), the scale of interaction or "serviceshed" needs to be defined. The concept of serviceshed is echoed throughout ecosystem service literature using the term "service production area" (Fisher et al., 2009), "service providing areas" (SPA) (Syrbe and Walz, 2012; Burkhard and Maes, 2017), or "service-providing unit" (SPU) (Castro et al., 2014; Andersson et al., 2015; Luck et al., 2003). The common definition of serviceshed reads "the areas that provide specific ecosystem services to specific beneficiaries" (Tallis et al., 2012). The concept of serviceshed goes further than ecosystem mapping as the connection between ecosystem service areas and beneficiaries must be determined.

Our literature review reveals different qualitative and few quantitative definitions of servicesheds or similar concepts, varying with characteristics such as spatial, temporal and accessibility dynamics. Most commonly, servicesheds are qualitatively labeled as the types of land which provide the services (Syrbe and Walz, 2012) or described with a scale-related term such as local, regional, or scalable (Andersson et al., 2015) with no further quantitative, or spatially varying, analysis. Others are determined empirically on the basis of indirect proxies, such as flow routing (Bagstad et al., 2013; Johnson et al., 6016) for hydrological services, maps of resource location and public access maps (UUNU-IHDP & UNEP, 2014) for subsistence water provision and surveys for human-use of various services (Willemen et al., 2013; García-Nieto et al., 2013; Castro et al., 2014).

There is a limited number of exact mathematical methods to define servicesheds (Tallis et al., 2015). One method that has been used in assessments is the use of a "buffer zone" to connect beneficiaries to land or vice versa (Schirpke et al., 2014). The buffer zone simply estimates the transport or delivery of the ecosystem service to exist within a radius around the beneficiary and lacks inclusion of any transport model. Previous work in sustainability analysis and design has included ecosystem service assessment for technological processes by using the same method of the "buffer zone" for air quality regulation (Gopalakrishnan et al., 2016). Other than the crude detail of using a "buffer zone", the serviceshed concept lacks quantitative definition that is reproducible in application to various beneficiaries.

To contribute towards the voids in the serviceshed concept, this research will focus on quantifying the serviceshed concept with a reproducible method and creating spatially-explicit results that include the heterogeneity of ecosystem service supply and demand. To do this, we will focus on the ecosystem service of air quality regulation, specifically land cover dry deposition, and apply atmospheric transport models to create spatially-explicit maps of air quality regulation service production, provided to a given point source. Dry deposition is the removal of air pollutants from the atmosphere in dry weather through surface adsorption (Nowak and Crane, 1998).

The transport of molecules throughout the atmosphere has been studied through dispersion modeling for decades with some of the earliest literature written in the 1930s exploring how smoke and gases spread from chimneys (Bosanquet and Pearson, 1936). Dispersion modeling has developed over the years resulting in many distinct models which can be applied to many different chemical source types and modeling in varying dimension, scale, and distribution. Models can be developed for application ranging from local to global scales and can include or exclude different modeling features such as wet and dry deposition or geographical features such as diffusion close to large bodies of water, urban areas, or major elevation changes (Yadigaroglu and Munera, 1987). In literature, applications range from modeling the dispersion of traffic-related NO_x and PM_{10} for one county (Nordling et al., 2008) or finding PM_{10} concentration levels from sources across all of Europe (Kiesewetter et al., 2015). Choosing the right model for a given application requires understanding of the case-specific needs for accuracy and inclusion of the main channels of transport or conversion.

Our approach will incorporate an EPA-approved atmospheric dispersion model, CALPUFF, and present mathematical equations based on the results of concentration and ecosystem deposition. Some of the equations will include optimization methods and constraint equations that rely on neighborhood algorithms, such as the Von Neumann neighborhood commonly used in cellular automation. In quantifying the serviceshed concept for air quality regulation, multiple definitions surfaced and yielded a variety of results, with each definition yielding unique information. Thus, we analyze a variety of proposed mathematical definitions of servicesheds for the ecosystem service of air quality regulation, apply them to a case study, and discuss their implications in terms of location, scale, shape and intra-annual dynamics. Each of these definitions yields a quantitative understanding of an appropriate scale at which to study and manage the ecosystems serving a given beneficiary, satisfying another research need identified in the previously mentioned literature review (Anton et al., 2010).

2. Method and models

2.1. Atmospheric transport and ecosystem service modeling

In the United States, the Clean Air Act requires the Environmental Protection Agency (EPA) to identify models which are approved to be used in the Prevention of Significant Deterioration (PSD) program. The full list of recommended models was most recently updated in 2017 and is found in Appendix A of the Guideline on Air Quality Models (legally know as Appendix W to 40 CFR Part 51) (Environmental Protection Agency, 2017). In 2003, the CALPUFF modeling system was recommended as the preferred model for long-range transport (Environmental Protection Agency, 2003), but was removed from the list in 2017. It was not replaced with another long-range transport model but was suggested to be used as a screening technique for long-range assessments of PSD increments in consultation with the

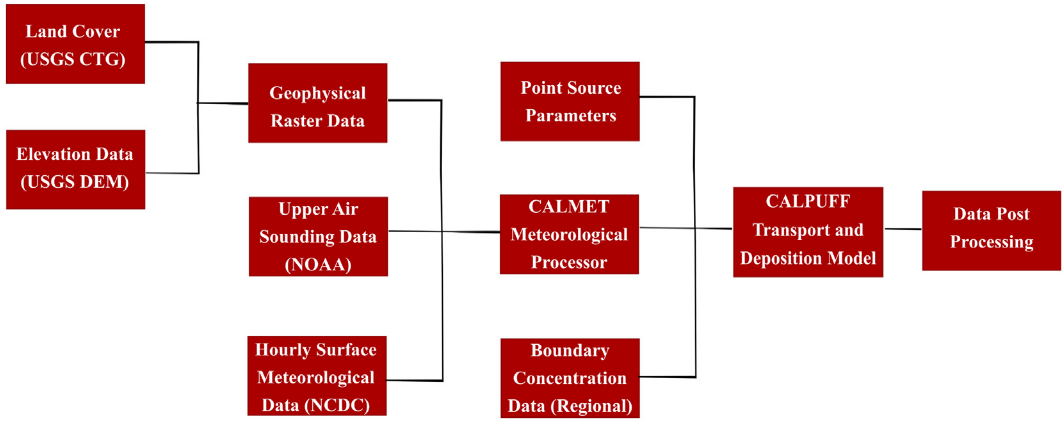

Fig. 1. Data and Modeling System Process Flow for Atmospheric Transport and Dry Deposition. USGS: United States Geological Survey, CTG: Composite Theme Grid (format), DEM: Digital Elevation Model, NOAA: National Oceanic and Atmospheric Administration, NCDC: National Climatic Data Center.

appropriate reviewing authority (Environmental Protection Agency, 2017). We chose to use the CALPUFF modeling system because it can calculate dry deposition surface characteristics with the same resolution as the input land cover data and incorporate the long term dynamics of atmospheric conditions above the simulation domain. This allowed us to utilize higher resolution of land cover and meteorology data for more realistic dry deposition calculations in this study of servicesheds.

CALPUFF can model the interactions between technological and ecological systems simultaneously using a three-dimensional non-steady state Gaussian puff model to apply geological, meteorological, and land cover data to a conservation of mass equation (Scire et al., 2000). The modeling system reveals spatial data of pollutant concentration and dry deposition imposed by a given source(s) onto a receptor grid modelled to user specification.

The process flow of our application of the CALPUFF modeling system is found in Fig. 1. This application is specific to our case study because the source and inclusion of various input data is based on user preference or availability for a particular location. The two main models of the CALPUFF modeling system are CALMET and CALPUFF. The CALMET model creates a 3-dimensional matrix of data storing meteorological and geophysical data such as wind speed, temperature, pressure, elevation, land cover, leaf area index, anthropogenic heat flux, and other variables. Some data only apply to the surface such as elevation or land cover, whereas other data vary along the z-axis such as air temperature and pressure. The CALPUFF model is the main Gaussian puff transport model which uses the CALMET output files along with information about the emission source and background concentration. The background concentration, if chosen to be included, is modeled as a series of boundary point sources. The benefits and limitations of including background concentration data will be discussed further in **Beneficiary vs. Regional Ecosystem Service**.

In order to run CALMET, many data preprocessors must be used to project data onto the selected region of interest. In the pre-processing stage, a 121 × 121 receptor grid with 0.25 km spacing was created, centering the point source of interest. Each receptor is a spatial point where the model will calculate its results for chemical concentration and dry deposition. This creates quite a large modeling region (30 km × 30 km) and calculates data for 14,641 points along the surface for every time step in the model. For other applications, it may be appropriate to use a smaller grid or a more granular resolution to decrease computing time. Along the z-axis, we created 5 vertical layers. The surface layer includes the "puff" or volume between 0 and 20 meters and is the level at which the final results are reported. The ceiling of the model is limited to 1000 meters. The data sets found in Fig. 1 were projected onto the grid area such as: the United States Geological Survey (USGS) Composite Theme Grid data (USGS CTG) (United States Geological Survey, 2018a), the USGS Digital Elevation Model data (USGS DEM) (United States Geological Survey, 2018b), Standard Hourly Surface Data from the National Climatic Data Center (NCDC) (National Climatic Data Center, 2016), and upper air sounding data from the Radiosonde Database produced by Earth's Research Systems Laboratory (ESRL) and operated by the National Oceanic and Atmospheric Administration (NOAA) (Earth's Research Systems Laboratory, 2016).

The input USGS land cover data uses 38 land use categories to classify land across the entire United States and stores the information in a gridded cell dataset. The geophysical pre-processors convert these 38 land use categories into 14 different output types and stores the data as a matrix, the surface layer of the 3D model created in the CALMET Processor. The dataset includes information for "leaf-on" and "leaf-off" characterizations of each land cover type, yielding insight to seasonal variations. The main geophysical pre-processor calculates surface parameters based on the land use data. It first overlaps the resolution of the land use dataset with the resolution of the user-specified model and calculates the fraction of land-use for each receptor. The surface characteristics are determined using default parameter values associated with the land classifications and calculated using an arithmetically-weighted average based on land use fraction for all variables, except surface roughness. Surface roughness is logarithmically weighted. This data becomes the geophysical gridded data, or raster, for variables such as bowen ratio, leaf area index, anthropogenic heat flux, albedo, and surface roughness. These factors are all used as inputs for the sequestration calculation and have various impacts on chemical diffusion. The elevation data is also added to the raster through the geophysical pre-processing.

The preprocessors for the surface meteorological data takes information from the surface, provided as an interpolation of data from the two closest weather stations, to create an input surface meteorological data file compatible with CALMET. The surface meteorological data is measured on an hourly basis. Upper air sounding data provides meteorological information along the z-axis, enabling atmospheric effects away from the surface to be considered in the model. The upper air sounding data is measured at 12-h intervals and is also preprocessed for compatibility with CALMET. All meteorological data used was recorded in 2016. All of the preprocessors use the same receptor grid to ensure that all of the data are projected onto the same space for calculation and visualization.

As shown in Fig. 1, the geophysical and meteorological data are all processed through CALMET, which calculates and stores all the data in the three-dimensional meteorological model. This data includes a simulated wind and temperature field at every time step defined in the model. The model created for the later-introduced case study calculates at a time step of one hour and spans across the entire year of 2016. To run CALPUFF, the CALMET output file is needed along with other input data such as the emission point data, including: stack height, temperature, diameter, emission velocity and emission rate. If the background concentration is to be modeled as well, then a boundary condition is created around the receptor grid with a user-inputted number of point sources and set concentration along the boundary. With the additional data, CALPUFF simulates the chemical dispersion and dry deposition across the time and space defined for the model. After CALPUFF is executed, the final step is data post-processing, which enables specified-time averaged data of concentration and dry deposition over all the receptors, and also enables the visualization of data using software such as ARCGIS (Environmental Systems Research Institute, 2011). For the purposes of this research, the annual and seasonal averages included data for every hour in the set. The seasons were defined using 3-month intervals as follows: Winter included January through March, Spring included April through June, Summer included July through September, and Fall included October through December. Although the calculation is computed with a time step of 1 h, it is important to note that the variation in land cover is only based on the "leaf on-leaf off" periods.

The CALPUFF model results that we are interested in are the concentration and dry deposition flux at each given receptor point (Scire et al., 2000). The ground-level concentration, C, at a given receptor, for a given time step is calculated as,

$$C = \frac{Q}{2\pi\sigma_x\sigma_y} g\, exp\left(\frac{-d_a^2}{2\sigma_x^2}\right) exp\left(\frac{-d_c^2}{2\sigma_y^2}\right) \tag{1}$$

where, Q is the pollutant mass in the puff, σ_x is the standard deviation of the Gaussian distribution in the direction of the wind, σ_y is the standard deviation of the Gaussian distribution in the direction of the cross-wind, g is the height of the plume, d_a is the distance from the puff center to the receptor in the direction of the wind, and d_c is the distance from the puff center to the receptor in the direction of the cross-wind. The height of the puff used in Eq. (1) is calculated as,

$$g = \frac{2}{(2\pi)^{\frac{1}{2}}\sigma_z} \sum_{n=-\infty}^{\infty} exp\left[\frac{-(H_e + 2nh)^2}{2\sigma_z^2}\right] \tag{2}$$

where, σ_z is the standard deviation of the Gaussian distribution in the vertical direction, H_e is the effective height above the ground of the puff center, and h is the mixed-layer height. For puffs within the convective boundary layer, this summation typically reduces to a uniformly mixed limit of $\frac{1}{h}$. This equation shows the third dimension of the Gaussian distribution.

To quantify the air quality regulation ecosystem service, the dry deposition flux, F, is then determined using the following equation,

$$F = v_d\, C \tag{3}$$

where, C is the concentration from Eq. (1) and v_d is the deposition velocity, which is based on a series of three resistances: atmospheric layer, deposition layer, and canopy layer. The canopy layer resistance is a function of the Leaf Area Index (LAI) and the ground or water resistance of the ecosystem, implying that direct surface deposition can occur on land cover with no leaf area. The LAI is a dimensionless characterization of plant canopies which quantifies the amount of leaf area available per ground level surface area. In areas with high LAI values and significant vegetation, the canopy resistance decreases with increased LAI and decreases the impact of surface resistance. However, in areas with meager vegetation, the surface resistance can play a larger impact on the deposition calculation. It is also important to note that only pollutants below the mixing height can deposit onto the surface. The boundary layer that determines the mixing height is also calculated within the model. A full description of the transport and deposition model can be found in the User's Guide for the CALPUFF Dispersion Model (Scire et al., 2000).

This model only includes concentration sources introduced in the creation of the model. This is important to remember, especially because the dry deposition flux (Eq. (3)) is directly dependent on the concentration calculated in the model. Therefore, if background concentration is left out of the model, the deposition of the land cover is highly underestimated. This calculation also assumes that the concentration threshold, the concentration at which the ecosystem begins to degrade, is never reached.

2.2. Beneficiary vs. Regional Ecosystem Service

As previously noted, atmospheric modeling can be used for many applications. For defining servicesheds, we found two different applications of the model were important for mapping ecosystem services and connecting them with the beneficiary. The first application excludes the background concentration, or regional concentration, and only includes the point source of interest within the model domain. We will define this simulation setup as the Beneficiary Model. The second application, which we will define as the Regional Model, includes the background concentration within the model as a set of point sources along the boundary of the model surface area. Since the flux is dependent on the resulting concentration at each receptor per Eq. (3), these two models yield two scenarios and two types of ecosystem services.

In the context of the serviceshed framework, we will consider the beneficiary as a pollution source (point source, area source, volume source, etc.), where the serviceshed reveals the areas which remove pollution from that source. This framework assumes that human activity relies on ecosystem services for air pollution quality and the pollutants removed benefit humans within the serviceshed; however, the serviceshed is directly tied to a particular activity, or region of activity (a pollution source). For example, the application in the **Case Study** section defines a manufacturing site as the beneficiary.

The **Beneficiary Model** only considers emissions from the point source and shows direct, undiluted chemical transport from the point source. This model yields spatial connection between point source and local ecosystem services. However, it only simulates a fraction of the dry deposition provided by local ecosystems, driven by levels of higher regional concentration. This reveals the idea that a given local ecosystem will have limited direct interaction with the air pollution emitted from a nearby point source. The ecosystem services associated with this model will be referred to as beneficiary ecosystem service.

The **Regional Model** considers the accumulated emissions that exist for a given area and shows the full capacity of the dry deposition ecosystem service provided by the surface within the model. However, regional concentration is often much larger than the contribution from one single source because it considers an accumulation of all sources within range of the limits of chemical dispersion. This causes the impacts of direct dispersion from the point source to be diluted as the background concentration becomes the main contributor of chemical source and is dispersed based on the wind field across the model, instead of focusing on flow from the point source. This creates a disconnection between the ecosystem service and beneficiary, which is the main purpose of quantifying the serviceshed. Ecosystem services associated with this model will be referred to as regional ecosystem service (See Table 1).

2.3. Serviceshed definitions

In approaching quantitative definition of servicesheds, three concepts surfaced from the available data. The dispersion model yielded spatial and time dependent results of concentrations and deposition rates at every receptor site along the geographical surface. The first two concepts simply focus on the data of concentration and deposition separately and propose definitions accordingly. The third concept compares the 'supply' of ecological deposition provided by neighboring land with the 'demand' imposed by the operation of the manufacturing site. This definition uses the resulting deposition rates of land area and the

Table 1
Advantage and Disadvantage of Beneficiary and Regional Model Scenarios.

	Advantage	Disadvantage
Beneficiary Model	Concentration results show impact of transport from the point source (see Fig. 3)	Ecosystem service valuation is highly underestimated
Regional Model	More realistic ecosystem service valuation	The contribution of the point source contribution is diluted by accumulated regional concentration (Fig. 3)

emission rate, initially defined as a point source parameter in the model for comparison.

For the first two concepts, the area within the serviceshed is defined by the set of receptors which have a concentration or deposition rate greater than a defined fraction of the maximum value. The maximum concentration value, C_{max} can be determined with the following equation,

$$C_{max} = \max_{\substack{x \in [1..M],\ y \in [1..N] \\ t \in [1..Y]}} C_{x,y,t} \tag{4}$$

where, x and y represent the spatial coordinates of the receptor grid, time step, t, is the time step of resulting concentration data collected, which is not necessarily the same time step used in the CALPUFF calculations. The variable Y represents the total number of time steps for the resulting data. Therefore, C_{max} is the maximum value of concentration found across all modeled receptors and all discrete time steps determined for the serviceshed analysis.

Using the value of C_{max}, we defined the serviceshed based on concentration, Ξ_C, as,

$$\Xi_C(t) \equiv \{(x, y)\}\ s.\ t.\ \ C_{x,y}(t) > \alpha_C\, C_{max} \tag{5}$$

where α_C is a user-defined parameter bounded from (0,1). The serviceshed is then defined, for time step t, as the set of all receptors that have a concentration or flux value greater than α_C multiplied by the maximum value of concentration.

Similar to Eq. (4), the maximum dry deposition flux value, F_{max} can be calculated as,

$$F_{max} = \max_{\substack{x \in [1..M],\ y \in [1..N] \\ t \in [1..Y]}} F_{x,y,t} \tag{6}$$

where, x, y, and t represent space and time similar to Eq. (4). Then, the serviceshed based on dry deposition, Ξ_F, can be calculated as follows,

$$\Xi_F(t) \equiv \{(x, y)\}\ s.\ t.\ \ F_{x,y}(t) > \alpha_F\, F_{max} \tag{7}$$

where α_F has the same properties as α_C.

Because these models of transport and deposition are dynamic and a discrete function of time, it is important that the definition of serviceshed is also a discrete function of time, such as a seasonal or annual serviceshed. It was previously mentioned that the modeling time step was 1 h. However, the discrete time step of the serviceshed analysis (t in Eqs. (4)–(7)) can range anywhere from the high-resolution modeling time step to the lowest resolution of the entire model's duration. In this case study, the modeling time step is one hour and the model duration is one year. The serviceshed analyses were conducted as an annual average serviceshed using only one time step and also as a seasonal average which used four time steps. For any case, the time step should be determined with respect to the application of desired analysis. For most cases, seasonal or monthly variation probably yields high enough temporal resolution.

For the third concept and serviceshed definition, a comparison between 'supply' and 'demand' of ecosystem services was quantified. This serviceshed definition is similar to the concept of ecological footprints (Mancini et al., 2018), which express environmental impacts in units of land area required to provide related resources.However, the footprint concept does not include the spatial and location-specific information that this serviceshed definition provides. This definition identifies a set of points, where the sum of their deposition rates is approximately equal to a fraction of the pollution rate. However, this definition creates an under-determined system as there are many combinations of receptors which will give the desired sum and an additional formulation is needed. This optimization problem can be defined and constrained based on user-preference for the problem. The under-determined system is defined as,

$$\Xi_{SD}(t) \equiv \{(x, y)\}\ s.\ t.\ \sum_{x,y} F_{x,y}(t) A_{x,y} \approx \alpha_{SD}\, P_{rate} \tag{8}$$

where Ξ_{SD} is the serviceshed based on supply and demand, $F_{x,y}(t)$ is the deposition flux value of a given receptor with x, y coordinates at time t, $A_{x,y}$ is the area allocated to the receptor at (x,y), α_{SD} is a set parameter bounded from (0,1), and P_{rate} is the rate of total pollution leaving the stack(s) defined in the transport model. Since the CALPUFF model uses a grid with even spacing between x and y for all points, the spatial resolution of $A_{x,y}$ is constant for every coordinate (x,y) and is equal to the spatial resolution of the receptor grid.

Determining which receptors are used in the set to determine the serviceshed can be done in different ways. This paper will present two formulations used in the case study and describe a couple other possible methods.

First, we must return to the concept of the regional versus beneficiary models and understand how the comparison of ecosystem supply, or deposition flux rate, will compare with the demand, emission rate. Using only the beneficiary model, we know that the deposition rate of the ecosystems will be underestimated compared to the actual capability of the land cover, driven by the higher accumulated concentration of the region. Therefore, the parameter α_{SD} should be adjusted to meet the need of the region. One way to adjust this parameter is to compare results between the average or peak concentration from the beneficiary model with the measured background concentration used in the regional model. This could lend insight into the order of magnitude difference between the two models.

Using the beneficiary model, the simplest way to determine which receptors are used to satisfy Eq. (8) is to include those which have the highest deposition rate, or minimize the land area. This optimization problem can be written as,

$$\begin{aligned} \min_{x,y}\ & \textstyle\sum_{x,y} A_{x,y} \\ \text{s. t.}\ & (x, y) \in \mathbf{U} \\ \textstyle\sum_{x,y} & F_{x,y}(t) A_{x,y} \geqslant \alpha_{SD}\, P_{rate} \end{aligned} \tag{9}$$

where U is defined as the set of feasible points of (x,y), the set within the boundary of the model. Due to the discrete nature of the data, this can be simply solved by ranking all the receptor values by deposition flux and calculating the cumulative sum for each receptor, ranked greatest to least. The point where the cumulative sum exceeds the emission rate determines the boundary point of the serviceshed. All receptor data ranked with greater deposition rates than the boundary point are included in the serviceshed. Now this simple ranking problem only works with the beneficiary model results because of the spatial relationship between the point source and nearby land cover. In the beneficiary model, the concentrations and deposition rates are calculated only from the dispersion of the emissions from the point source. This means that the general trend of resulting values decreases with distance from the point source. If the model boundary is large enough,

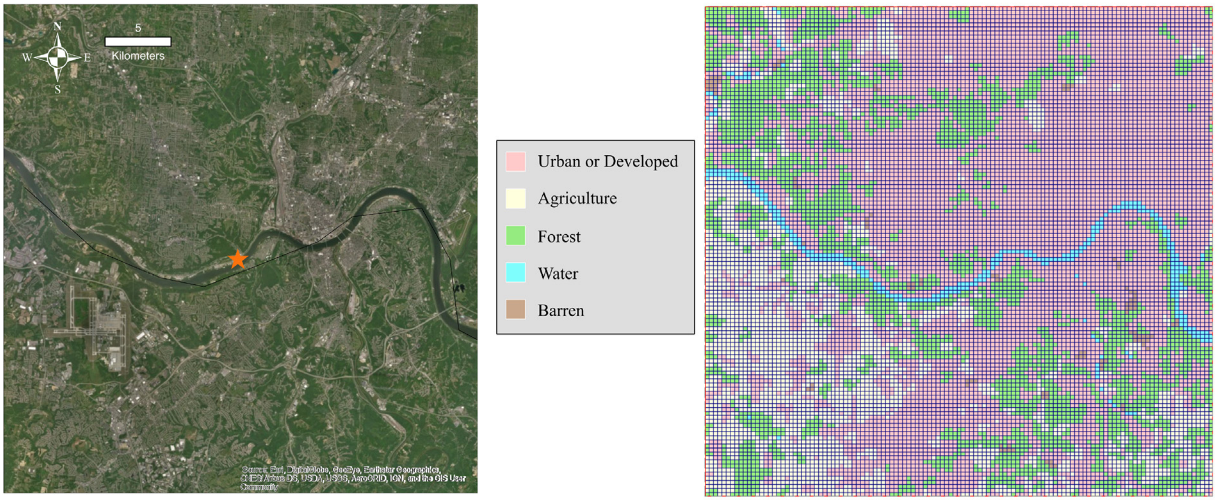

Fig. 2. Case Study Site: Satellite Imagery and Land Use Classifications. Satellite Imagery Source: Esri, DigitalGlobe, GeoEye, i-cubed, USDA FSA, USGS, AEX, Getmapping, Aerogrid, IGN, IGP, swisstopo, and the GIS User Community. Land Use Classifications Source: USGS CTG Land Use Land Cover (United States Geological Survey, 2018a).

the serviceshed will converge within its boundaries. It is important to remember that α_{SD} may need to be a small fraction for the serviceshed to converge within the boundary of the model without interference of the boundary.

Using Eq. (9) with the regional model yields a set of points that may have no relation to the point source. For cases where the background concentration is much higher than the contribution of the point source emissions, the regional model loses the general trend of resulting values decreasing with distance from the point source. As mentioned previously, the model loses the inherent spatial connection between ecosystem service and beneficiary source and needs a separate optimization problem to satisfy the proposed concept of serviceshed.

To address this, we add the following constraint to Eq. (9) when calculating Ξ_{SD} for the regional model: "Ξ has rooted connectivity with the point source". This constraint requires that the serviceshed include the point source and be connected, meaning a path can be made through the serviceshed area between any two points in $\boldsymbol{\Xi}$. Because the receptors create a 2D grid along the surface, the user can decide whether to use a Von Neumann or Moore neighborhood to define connectedness. A Von Neumann neighborhood includes adjacent cells which share at least one side with the point or set and a Moore neighborhood includes the Von Neumann neighborhood along with cells that are diagonal to the point or set (Breukelaar and Bäck, 2005). Using the Von Neumann neighborhood, the rooted connectivity constraint can be written as,

$$I_{(x+1,y)} + I_{(x-1,y)} + I_{(x,y+1)} + I_{(x,y-1)} \geqslant I_{(x,y)} \quad \forall \ (x, y) \in \mathbf{U} \tag{10}$$

where, I is a binary state variable equal to 1 if the cell is included in the set which satisfies the optimization problem in Eq. (9). Essentially, this says that for every cell included in the set, a neighboring cell must also be within the set.

This modified optimization problem can be solved using a greedy algorithm, which iteratively adds the next neighboring receptor with the highest deposition rate to the serviceshed set until the equation is satisfied. Using the regional model data, α_{SD} should be set equal to 1 for comparison of supply and demand of the air quality regulating ecosystem service. Adding a serviceshed definition which uses the regional model provides a metric for absolute sustainability and insight into the scale at which design and decision-making of ecological systems can be approached, satisfying the research need proposed by Anton et al. (2010).

Other ways to determine which receptors define Ξ so that it satisfies Eq. (8) could include constraining the set to a known property line or expanding a radius from the point source until the set satisfies the equation. Depending on the spatial constraint, the problem may not be feasible if not enough points are included in the set to satisfy Eq. (8).

2.4. Case study

To apply the definitions proposed in the previous section, a case study was conducted on a biodiesel manufacturing facility in Cincinnati, OH along the Ohio River. The case study was used to explore multiple quantitative definitions for the air quality regulation ecosystem service, assuming the point source facility as the beneficiary. Thus, the purpose of this case study was to determine the area of surrounding ecosystems which provides air quality regulating services for the technical process. In this example, the ecosystem service was chosen to be dry deposition of the land cover surrounding the manufacturing site. The chemical species selected for the case study was chosen to be SO_2. The servicesheds being explored in this paper are only for SO_2, although the same method could be used for any air pollutant which could be modeled appropriately. The site would have a different serviceshed analysis for each chemical species emitted.

For this application, a full process model was not needed and the point source data parameters were pulled from the EPA's FLIGHT database (United States Environmental Protection Agency, 2016) using a biodiesel production company's self-reported data. The point source parameters used from this data include a stack height of 41.1 m, a stack diameter of 0.6 m, an exit velocity of 17.8 m/s, an exit temperature of 588.7 K, and an emission rate of 0.111 g/s of sulfur dioxide (SO_2). The background concentration for the point source was estimated as a weighted average between the two closest active SO_2 monitoring stations found in Cincinatti, OH and Highland Heights, KY. EPA's Outdoor Air Quality Data can be found using their Interactive Map of Air Quality Monitors. Using the 2016 1-h average SO_2 data, the weighted average yielded a background concentration of 6.55 μg/m^3. The location is considered an urban area and is more likely to have a higher background concentration than a rural location.

Within the boundary of the model, five types of land use were categorized to show spatial heterogeneity of the surrounding surface: urban or developed land, agriculture land, forest land, water, and barren land. The results of these land covers, along with the satellite imagery of the case study location are found in Fig. 2.

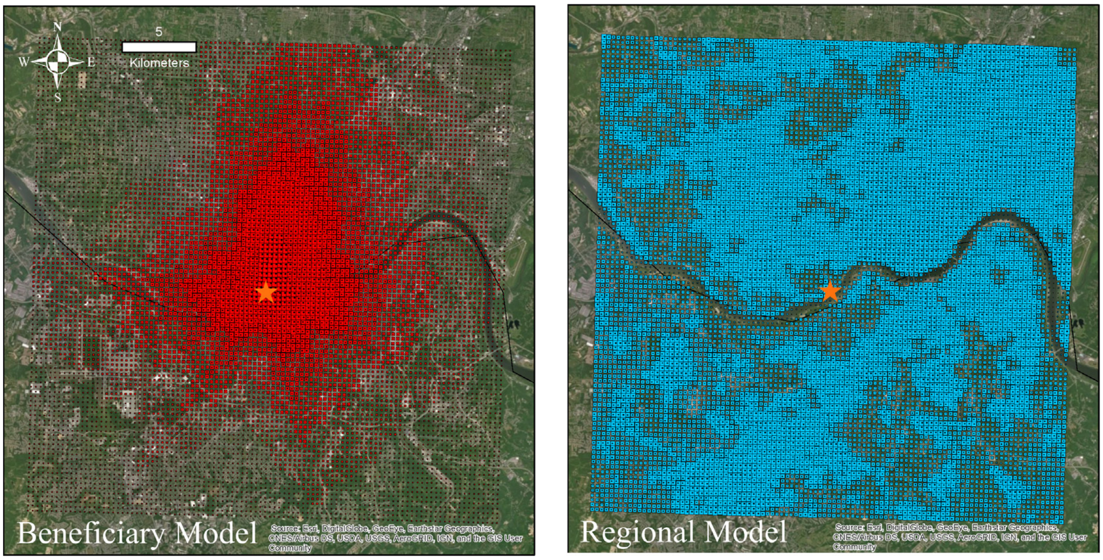

Fig. 3. Concentration Results of Beneficiary and Regional Models: Higher concentrations are shown by larger point size for each receptor, resulting in higher density of color for areas of higher concentration.

3. Results and discussion

The concentration results of the beneficiary and regional models described in the Method and Models section are found in Fig. 3. In the beneficiary model, the minimum and maximum concentrations are 3.57×10^{-4} μg/m^3 and 8.85×10^{-2} μg/m^3, respectively. For the regional model, they were 2.67 μg/m^3 and 6.81 μg/m^3. The results of these two models reveals multiple orders of magnitude in difference of value, and also the difference of range that is seen across the model. The significant difference of concentration values, and inherently deposition values (Eq. (3)), explains the need for using the two different models to understand the properties of serviceshed definitions proposed in Table 2. Also, it is important to note that the beneficiary transportation model naturally shows a tapering of concentration away from the point source, but for the regional model the areas of highest concentration may not be near the point source, especially if emission from other sources in the vicinity of the point source is significant.

The proposed serviceshed definitions were calculated for the biodiesel case study. The results of the annual servicesheds, using annual averages for concentration and deposition values, are shown in Fig. 4. The figure outlines all receptors which satisfy the different definitions given in the Methods and Model section and found in the legend. Due to the resolution of the receptor grid, each receptor represents a 250 m × 250 m area of land. The figure shows four applications of the serviceshed definitions given in Eqs. 5, 7, and 8. For the first two definitions, Ξ_C and Ξ_F, the values of α_C and α_F were set at 0.05. Therefore, the white and yellow outlines show the areas which satisfy a concentration or deposition value greater than 5% of the respective maximum. The light blue outline represents the definition Ξ_{SD} applied to the beneficiary model. For the beneficiary model, the α_{SD} value was assumed to equal 0.01 and used the problem formulation in Eq. (9), minimizing land area without an explicit constraint on connectedness. The light blue outline shows the area which deposits 1% of the biodiesel facility's SO_2 emissions directly, without consideration of background and accumulated concentration of the region. Using the same equation for Ξ_{SD}, the purple outline applies the regional model and assumes α_{SD} equal to 1. To determine the set which satisfies Eq. (8), we added the constraint of rooted connectivity and used the greedy algorithm described in Methods and Models. The purple outline shows the area which deposits 100% of the facility's SO_2 emissions with the full ecological deposition capacity driven by regional and accumulated concentration.

The values of α used in this case study were based on the size of the model. The parameter values used ensured that all the resulting serviceshed boundaries existed within the limits of the model. The value of α_{SD} was set equal to 1 based on the concept of analyzing absolute sustainability, comparing the neighboring ecosystem's ability to mitigate the emissions produced by the point source. The size of the resulting servicesheds vary and to compare all of the definitions using the same modeling region of 30 km × 30 km, the other α parameters were set accordingly.

Due to the modeling data's discrete nature, the resulting servicesheds are characterized, in part, by the resolution of the receptor grid created in the pre-processing stage. In this case study, each receptor was spaced with 250 meters in between. The spatial distribution, or shape and size, of each serviceshed is unique across definitions and reveals different information that can connect the ecosystem service of air quality regulation with the beneficiary of the biodiesel manufacturing site.

The first definition, Ξ_C, shows the range of physical transport of the SO_2 air pollutant from the point source and across the region's ecosystems. The result of this serviceshed depends on many meteorological variables, and in particular, dominant wind direction. From Fig. 4, we see a dominant wind direction pointing north-northeast. Related to concentration by Eq. (3), the resulting serviceshed based on deposition, Ξ_F, yields a much higher dependence on land cover. The yellow outline of the serviceshed based on deposition tends to include the areas close to the point source with green color from the satellite imagery.

Table 2
Summary of Proposed Serviceshed Definitions.

	Transport Model(s)	Based on	Parameter
$\Xi_C(t)$	Beneficiary Model	Physical Transport and Resulting Concentration of Emission Source	α_C
$\Xi_F(t)$	Beneficiary Model	Physical Transport and Ecological Deposition of Emission Source	α_F
$\Xi_{SD}(t)$	Regional Model or Beneficiary Model	Supply and Demand of Ecosystem Service Additional Problem Formulation	α_{SD}

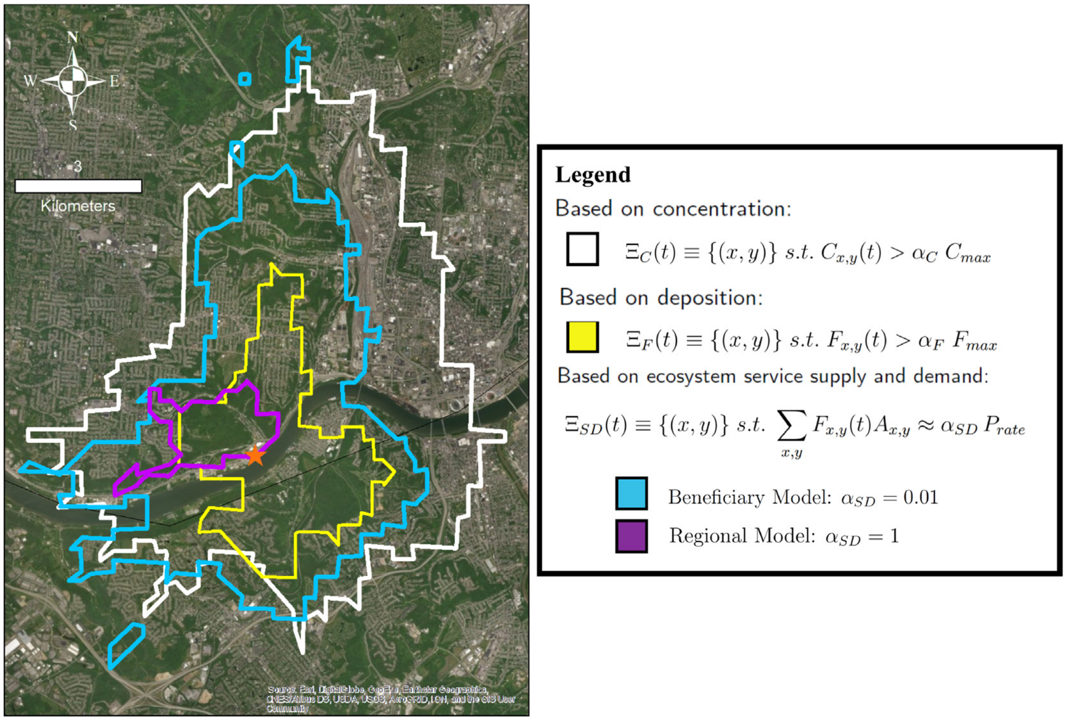

Fig. 4. Annual Servicesheds.

Although the definition for deposition flux depends directly on concentration, the difference in land use between the maximum deposition value and the other areas in the model tend to create a wider variance in deposition rate. This causes Ξ_F to have a noticeably smaller land area than Ξ_C, however, the size of both servicesheds is largely determine by the parameter α.

Applying the definitions of Ξ_C and Ξ_F to the regional model with α equal to 5% yields a serviceshed of the entire grid because the regional model has a more constant distribution of concentrations than the beneficiary model. For cases where the point source has a much larger emissions rate and the background concentration is low, this may not be the case. An example of this would be a large SO_2-emitting factory in a rural area.

Using the serviceshed definition based on ecosystem service supply and demand with the beneficiary model reveals similar characteristics to both the results for Ξ_C and Ξ_F. The light blue shape is similar to the white outline with the exception of the urban and developed areas east of the point source. Because the light blue shape is based on an optimization formulation, it picks areas with highest deposition value to create the set of receptors which satisfies Eq. (8). Therefore, the serviceshed is more likely to include areas with forest land cover rather than urban and highly developed areas. This is seen in Fig. 4 by the green of the background satellite imagery of the region that is within the light blue outlines. The serviceshed outlined in light blue also completely contains Ξ_F, the yellow outline, because those are the points of highest deposition value. As long as the definition for Ξ_F provides less total deposition than needed to satisfy Ξ_{SD}, this will be the case. The size of this serviceshed is significantly dependent on the parameter α_{SD} which determines the fraction of emissions that must be deposited by the neighboring ecosystems. The second serviceshed definition, which uses the regional model, results in a shape that is largely determined by the optimization problem formulation. Because our application required rooted connectivity and used a greedy algorithm, the purple outline includes the green areas around the point source which have the highest deposition value. The deposition values resulting from this model may or may not be connected with the beneficiary, or manufacturing site. However, using the regional model shows a significant increase in ecological function, as the serviceshed which has an equal rate ($\alpha_{SD} = 1$) of ecological deposition and manufacturing emission is much smaller than the light blue outline where α_{SD} equals 0.01. Other constraints or problem formulations included in the serviceshed definition Ξ_{SD} can drive different resulting serviceshed shapes and sizes.

Additionally, the results for the average values for each season is shown in Fig. 5, which displays the serviceshed shapes and scales for each seasonal average value. These definitions are included to show the time-dependence of the serviceshed definitions, noted in each serviceshed definition (Eqs. 5, 7,8). The seasons were defined as three month intervals of the year, starting with the winter including January through March. The proposed serviceshed definitions show an explicit dependence on time; however, this dependence is subject to the time interval being explored. With seasonal averages, four different servicesheds can be calculated: t_1, t_2, t_3, t_4; but this number of intervals can be increased or decreased to the minimum or maximum time resolution of the model calculations. For example, the time dependence can be eliminated by looking at the average value across the entire time period of the model, such as the annual average results. Servicesheds can also be calculated at the hourly level since that is the time step used in the model calculations, although an hourly analysis of servicesheds will have little practical use. Therefore, user discretion must be applied to determine appropriate time scales of interest. Unless high-resolution dynamic land-use data is obtained for the area of the model, a seasonal calculation of serviceshed dynamics will typically suffice as a method for understanding the different extremes of winter and summer, or leaves-off and leaves-on. The areas of each serviceshed are found in Table 3.

In comparing the sizes of the serviceshed definitions across seasons, many observations can be made. First, looking at the definitions outlined in blue and purple, we know that these definitions are smaller in the spring and summer than they are in the winter and fall, while the annual average falls in between these values. This makes sense because in the summer and spring, the leaves are on the trees and higher ecological deposition rates occur as a result. Higher deposition of the land area which provides the "supply" side of Eq. (8) will require less land area to satisfy the equation because the emission rate is assumed

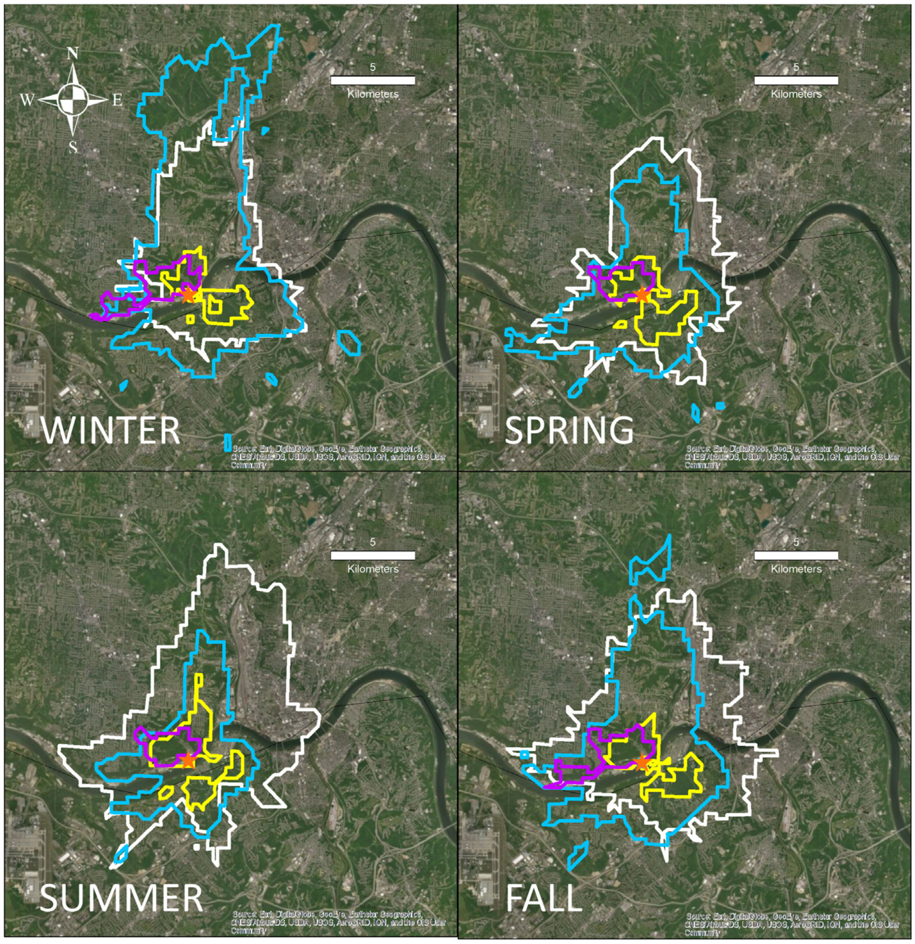

Fig. 5. Serviceshed Definitions by Seasonal Average. Legend found in Fig. 4.

Table 3
Total area of each serviceshed definition [ha].

	Ξ_C	Ξ_F	Ξ_{SD} Beneficiary	Ξ_{SD} Regional
Annual	8000	1888	5250	544
Winter	5306	738	8063	713
Spring	6000	950	4550	425
Summer	8600	1075	3413	444
Fall	7256	906	5825	700

constant. It is also important to note that the white and yellow outlines, defined by Ξ_C and Ξ_F are largest for the annual average instead of the seasonal averages, with the exception of Ξ_C outline in the summer. The longer averaging time period causes the distribution of values across all receptors to narrow and also decreases the value of the maximum. This enables the two definitions that compare each receptor to the maximum result to include more receptors, increasing the area of the serviceshed. Across all definitions, there is no exact trend of the ranking of seasons by the size of the resulting servicesheds. For the definitions of Ξ_C and Ξ_F, the servicesheds are both largest in the summer and smallest in the winter. This makes sense because the deposition fluxes are directly related to the resulting concentrations. However, for Ξ_C, the serviceshed is larger in the fall than in the spring, yet for Ξ_F it is the opposite case. Ξ_F is larger in the spring because the leaf area is higher during the "leaf-on" months, which directly relates to increased dry deposition flux. Ξ_C could be larger in the fall for a couple reasons. First, the maximum concentration is lower in the fall, meaning the number of values satisfying the Ξ_C definition may increase. Also, it could be based on meteorological conditions where high wind speeds in the fall could cause the distance of transport of chemicals to be larger. However, seasonal analysis of the various meteorological variables was not conducted. Further, both definitions of Ξ_{SD} are largest in the winter, yet Ξ_{SD} applied to the beneficiary model is smallest in the summer and when applied to the regional model, it is smallest in the spring. Each serviceshed reveals different information, yet all satisfy the broader definition of "areas which provide a specific ecosystem service to the specific beneficiary" (Tallis et al., 2012).

The discussion of this work would be incomplete without consideration of uncertainty. This research does not consider any explicit uncertainty and the case study accuracy relies on previous cross-validation of the CALPUFF modeling system, not on cross-validation of the studies' results. This is not uncommon in the field of ecosystem service quantification. The majority of literature and tools which valuate ecosystem services exclude uncertainty and model validation (Boerema et al., 2017; Grêt-Regamey et al., 2017). Without field measurements and cross-validation, the measure of uncertainty in this modeling research will be unknown. This creates a challenge and potential limitation in translation of research to policy changes for both this serviceshed framework and across ecosystem services research. Further partnership of this framework with a specific field application can help measure impacts and address the issue of uncertainty.

4. Conclusions and future work

This research proposes multiple quantitative definitions of the air quality regulating serviceshed by including spatially-explicit physical transport models with different modeling options to explore the concept of serviceshed mathematically. Although this article provides a specific application for air quality regulation, the quantitative approach to defining servicesheds is a methodology that can and should be applied to other ecosystem services, such as: water quality regulation, nutrient cycling, and pollination for example. The biggest challenge in applying this approach to other ecosystem services is finding proper models which can reveal spatial heterogeneity between the transport of the beneficiary's demand with the supply of the ecosystem service provided. Air quality regulating services were simply chosen as the first application because of the availability of the physical transport models.

In thinking about how these quantitative definitions can be applied to other ecosystem services, it is important to first look at what we can learn from these definitions in regards to air quality regulation. Each serviceshed definition provides a different set of information that can be used to analyze the relationship between an emissions point source and the region around it. From the definition Ξ_C, we reveal the transport range of the given pollutant and the areas that are most impacted by the operation of the biodiesel manufacturing. These areas have the highest concentration that directly transport from the point source. This type of information can be easily converted into health impacts and risks of local communities in these areas. This definition of serviceshed not only helps link ecosystem services to the beneficiary, but also shows the impacts that these demands have on other members and species of the region. From the definition of Ξ_F, results show the land cover which provides the highest rates of ecological deposition. This could be used in spatial planning to understand which areas should avoid land use change, while also considering other excluded areas that could benefit from land use change.

From the definition of Ξ_{SD}, a spatial understanding of what is required for absolute sustainability can be visualized. Absolute sustainability compares the availability of the ecosystems to engage with the demand imposed by various activities. In this case, this sustainability only refers to the specific chemical and process or beneficiary being analyzed. Applying this definition to two different models also shows the differences and implications of beneficiary and regional ecosystem services. For example, if a high emission facility is located in an area with low levels of pollution, land that is associated with the site may have limited direct interaction with the facility's emissions and relatively small levels of regional service due to low background concentration. On the flip side, if a low emission facility is located in an area with higher levels of pollution, the land managed on-site could provide high rates of regional ecosystem service that might exceed the rate of pollution leaving the system.

Using a balance of all four of these serviceshed definitions is important because each definition can reveal a different set of information and all of them connect ecosystem service to beneficiary. Depending on the purpose for analyzing a particular serviceshed, the proper definition, model and parameter can be chosen by the user. Alternatively, calculating all four of the definitions could be helpful to understand the balance of the values associated with concentration, deposition, and the emission rate creating the demand on the ecosystems.

Further research should explore bridging the serviceshed concept with human and ecosystem health impacts, which can help provide more useful information for appropriate values of α used with the different serviceshed definitions. Potentially, values based on health impacts could remove the need for using this parameter altogether and could be based on set concentration value, rather than one relative to the maximum. Additionally, further use of these definitions can help set "best-practice" values for α.

These serviceshed definitions can be further applied to not only one point source, but many point sources like an industrial park, or a regional area source like a city. Moving forward, applications will aim to model multiple beneficiaries and multiple chemical species, revealing overlap or nesting of multiple servicesheds. This information can be useful in determining allocation of different considerations such as payment or ownership of ecosystem services. Generating spatially-explicit maps of a number of local pollution sources can prove to be valuable to both the companies who operate the manufacturing facilities and the neighboring communities as the impacts on the area are better understood. Adding a range of other ecosystem services, serviceshed analysis can generate more effective ecosystem restoration and management scenarios. It may also be beneficial to study long term predictive models which could help understand the change of servicesheds over multiple years, such as, in response to climate change.

In practical application, a spatially explicit and reproducible serviceshed application can be used to improve or complement sustainability and ecosystem service assessments, improve the understanding of stakeholders in land-use decisions, improve the understanding of appropriate design scale in proposed green infrastructure, and possibly show overlapping servicesheds that can be used for allocation methods in impact assessments or PES (Payment for Ecosystem Services) systems. Although this approach is purely analysis, it does provide many opportunities for design synthesis in which we consider how to decrease the impacts provided by the analysis. For example, considering land use change scenarios, how do we minimize Ξ_{SD} or achieve a feasible solution of Ξ_{SD} within a given property line? Quantifying servicesheds and mapping them spatially contributes to the study of ecosystem services by exploring spatial heterogeneity of ecosystem services and bridging theory with application.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

This material is based upon work supported by the National Science Foundation Graduate Research Fellowship under Grant No. DGE-1343012 and by CBET-1804943.

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