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Tool for Searching USEPA's TMDL Reports Repository to Analyze TMDL Modeling State of the Practice

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Abstract: Total maximum daily load (TMDL) reports archived in the USEPA database can provide useful guidance for the development of new TMDLs and watershed management plans by aiding the selection process for the most appropriate modeling tool. The database contains more than 70,000 individual documents; therefore, a rapid screening tool is needed to elicit information about previous modeling studies that might help guide stakeholders and regulators in dealing with the TMDL application at hand, save time, and lead to a more cost-effective regulatory outcome. The paper introduces a smart web-based software tool for TMDL report selection based on different water management criteria. The tool uses an automated search method based on frequency of common water body impairments and models to categorize and select TMDL reports. Additionally, this tool provides better insight on the relationship between the modeling tools used and the impairments they address. This tool has proven useful in reviewing the state of integrated modeling (IM), applications of remote sensing (RS), application of basic versus mechanistic modeling, margin of safety (MOS) assessment, and the state of practice regarding relationships among impairments, models, and regions where TMDLs for various pollutants are being developed. Despite limitations on direct access to all TMDLs developed and reported to the EPA by the user, the tool can be improved over time to derive a better understanding of the relationships between these impairments, data, and the TMDL development process. Although the MOS is not directly quantified in the current version of the TRS tool, this feature may be incorporated in future updates.

Introduction

The Clean Water Act (CWA) (33 U.S.C. §1251 et seq.) is the primary legislative driver that forces responsible parties—states, territories, and tribes—to develop plans and remediate or maintain the nation's water bodies. To remediate water bodies that are not meeting their designated use, total maximum daily loads (TMDLs) have been developed based on the carrying capacity of the water body. TMDLs are intended to be part of a

comprehensive watershed strategy to restore designated uses (DUs) and should foster collaboration and coordination with all major stakeholders responsible for and impacted by water quality in the watershed. The carrying capacity of the water body for a particular pollutant, a key component for the TMDL development, can be estimated using analytical tools or numerical models based on the hydrochemistry of the natural system and the availability of monitoring data used to calibrate and validate these decision support tools. It is not widely appreciated that the choice of model or analytical tool can affect the estimates of the pollutant assimilative capacity of the receiving water being regulated—which in turn affects acceptable pollutant loading and load allocation (Chapra 2003; ASCE TMDL Analysis and Modeling Task Committee 2017). The standard methodology used in development of TMDLs calculates acceptable pollutant loads and pollutant load allocations, taking into account both point and nonpoint source discharges to the water body under consideration and applying appropriate low-flow hydrology (for sediments, the limiting condition may be high flow) criteria and factors of safety. However, in some watersheds or drainage basins for which there is no dominant point or nonpoint source, the standard TMDL development methodology can lead to suboptimal recommendations. Similarly, the standard criteria guiding model selection may also lead to poor choices. Under these circumstances, a screening tool that allows rapid review of TMDLs developed for the same pollutant in the region, but under varied watershed characteristics such as different flow regimes, water quality conditions, and type of impairment addressed, can have great utility.

Previously published TMDL reports can provide useful information for the development of new TMDLs. These reports can promote deeper understanding of the relationships among data, model(s), and impairment(s), providing beneficial knowledge for critically assessing current practices that are typically simulated in models used for TMDL development. However, the number of TMDL documents (>70,000 at the time of writing this paper) and the lack of a consistent structure in the reports make it hard to gainfully use these reports. TMDL reports rarely follow a defined format, making it difficult and laborious to elicit essential information from these reports in an automated manner. However, the information in these TMDL reports can be accessed using natural language processing and other artificial intelligence algorithms that can be built into a TMDL model selection decision support system (DSS). This DSS could provide a mechanism for planners and consultants to support choices and assumptions typically made during the TMDL development process.

This paper reviews the state of practice of TMDL modeling by analyzing published TMDLs contained in a repository supported by the USEPA known as the Assessment and Total Maximum Daily Load Tracking and Implementation System (ATTAINS). The ATTAINS system at the time of writing this paper contains over 70,000 documents. To review all documents in the repository related to these published TMDLs was not realistic. Hence, an independent database based on all documents in the USEPA ATTAINS repository was created by mining the text for terms that might have been related to TMDL modeling using the relative frequency of a term in the report to assess the relevance and potential utility of the report. A web-based software tool called the TMDL Report Selection (TRS) tool can be used to identify a subset of relevant case studies that might help an analyst choose between candidate TMDL models and glean methodological insights that might be applied to the TMDL at hand.

TMDL Analysis and Modeling

The range of models available for use in TMDL analysis is large, ranging from simple mass balance formulations (mostly empirical modeling) to complex, fully distributed, numerical models (physically based mechanistic modeling) (ASCE TMDL Analysis and Modeling Task Committee 2017). Scaling issues, the granularity of the natural system being simulated, and the data required for model calibration and validation introduce further complexity. Best practice dictates that independent data sets be used for the model calibration and validation exercises. However, every TMDL is unique and although the TMDL methodology is designed to standardize analysis to the extent possible, exceptions will invariably occur. Understanding the watershed characteristics is crucial in selecting the adequate model or analysis tool to be used for the development of a TMDL. However, model selection will also depend on other factors such as data collection methodology implemented, model integration framework, calibration data availability, and margin of safety (MOS) factor to be used to develop the TMDL.

Model Integration and Model Integration Frameworks

An evolving area of activity in support of TMDL modeling is the use of integrated models (IMs) and the development of techniques to link models at runtime that provide a more comprehensive and realistic simulation of water quality than would be possible with a water quality model alone. This has allowed greater use of wellaccepted, established models for TMDL analysis rather than the more typical spreadsheet and other simple models that, being less physically based, rely on empirical relationships and assumptions. A comprehensive review of the principles of integrated modeling, the use of modeling frameworks, and model linkages was provided by Laniak et al. (2013).

Integrated environmental modeling (IEM) has been defined as a "set of interdependent science-based components (models, data, and assessment methods) that together form the basis for constructing an appropriate modeling system" (USEPA 2008). A major goal of software for integrated modeling is to ensure soundness of results and maximize model reuse. The coupling or linking of model components requires attention to model granularity—setting appropriate boundary conditions between one model and model components. The relationship between modeling components can use a formal framework that defines the data structures and software interfaces for moving information from one model or module to another or informal protocols. A number of popular modeling frameworks have been developed over the last decade (Laniak et al. 2013). Castronova and Goodall (2010) and Lloyd et al. (2011) have summarized a variety of these IEM frameworks, including Earth System Modeling Framework (ESMF) (Hill et al. 2004) and Community System Dynamic Modeling System (CSDMS) (Peckham et al. 2013), Open Modelling Interface (OpenMI) (Moore and Tindall 2005), System for Environmental and Agriculture Modeling Linking European Science and Society (SEAMLESS) (Van Ittersum et al. 2008), and Object Modeling System (OMS) (Ahuja et al. 2005; David et al. 2002). These frameworks have in common a set of protocols that attempt to address the interoperability issues that are legion when unlike models must be made to communicate to solve a particular problems or TMDL planning goal. There is no universal set of protocols that works for all instances of linked or coupled models—hence, interoperability issues usually must be resolved for every combination of science component and modeling infrastructure (Laniak et al. 2013). Another group creating solutions with an increased emphasis on interoperability issues includes the Consortium of Universities for the Advancement of Hydrologic Science (CUASHI) (Maidment et al. 2004). Integrated modeling will be of increased importance to TMDL modeling as problems become more complex and greater simulation accuracy and capabilities are expected from TMDL project analysts.

Geographic Information Systems and Remote Sensing

The spatial diversity and lack of observation in many natural systems modeled for TMDLs make a strong case for integration of geographic information systems (GISs) and remote sensing into TMDL modeling; examples of this integration appear among the TMDL models described in the case studies section of this paper. The USEPA better assessment science integrating point and nonpoint sources (BASINS) TMDL modeling approach and framework was the first successful public-domain product that sought to integrate environmental data, analysis tools, and watershed and water quality models using GIS, allowing spatial information to be displayed as maps, tables, or graphics (USEPA 2004). These GIS capabilities also allow the user to perform spatial analysis of landscape information and graphically display relationships among data (Jensen and Jensen 2017). BASINS allowed synthesis of the land use, point source discharges, and water supply withdrawals at a scale chosen by the user. Toolboxes within ArcGIS, the software platform used by BASINS, allow the importation of maps with different projections and conversion to a common spatial projection. This is especially useful when compiling information about a new watershed using online resources such as ArcGIS-Online. This archive contains thousands of published maps and map overlays from around the US that can be mined for information about a candidate watershed for TMDL development.

Rapidly evolving technologies such as remote sensing (RS), which provides spectral data that can be interpreted to provide data on factors such as land use, evaporation and evapotranspiration, and soil moisture, are being directly supported by some of the more popular TMDL modeling tools such as BASINS (USEPA 2004) and watershed analysis risk management framework (WARMF) (Goldstein 2001; Herr and Chen 2012). However, outside these tools and their customized user interface for data assimilation, there are no standardized protocols for acquisition and processing of imagery. The models used for TMDL development often have no method available to assimilate these data. At present, the popularity of low-cost unmanned aircraft system (UAS) technology and the requirement for functional and compatible imagery processing tools has, de facto, been setting some of these standards. Future work is needed to address this aspect of TMDL modeling.

Other remote sensing tools such as light detection and ranging (LIDAR) and both multispectral and hyperspectral satellite imagery can provide a useful resource to identify vegetation types and determine the areal extent of vegetated areas. The normalized difference vegetation index (NDVI) algorithm applied to multispectral remotely sensed imagery can help separate healthy vegetated areas from bare soil and distinguish between major crop types. Although satellites have been the major provider of multispectral imagery for remote sensing, the rapid proliferation of UAS hardware and downwardspiraling cost of these aircraft and the cameras that attach to them have created new opportunities for the use of GIS and remote sensing technology in TMDL development. It may be reasonable to expect a significant increase in accessible water resource, land use, and derived environmental contamination data from the satellite and aerial platforms. These data often need sophisticated processing before they may be used in the current models.

TMDL Model Calibration and Validation

One of the procedural limitations of TMDL modeling is that TMDLs are often developed whether the supporting data resources are adequate to develop fully calibrated and validated models. Under ideal circumstances, the model selected would be both scientifically appropriate for the particular TMDL approach taken and the available data resources—however, expediency often trumps this principle. Calibration is the process of selecting model parameter values to improve the goodness of fit between simulation model outputs and field measurements. Calibration can be a complex task when models are highly parameterized, and practitioners often resort to popular automated parameter estimation algorithms tools such as PEST (Doherty and Hunt 2010; Doherty and Simmons 2013). The Regularization inversion technique adopted by the PEST tool is capable of achieving unique calibration by making mathematically ill-posed problems tractable as well as substantially decreasing the time and cost associated with the calibration process. Model validation refers to the procedures undertaken to verify that the model is performing as expected and is commonly effected, where time

series datasets of observations are adequate, by splitting the dataset in two, with the earlier subdataset used for calibration and the later subdataset being used for model validation. For complex watershed models, such as Hydrologic Simulation Program Fortran (HSPF), used as the underlying hydrological process simulator for the popular BASINS TMDL decision support system, endorsed by USEPA (2004), linkage to this parameter estimation procedure has been incorporated into the model graphical user interface.

The CWA requires that all TMDLs include a margin of safety. However, a universally accepted method for selecting the MOS has not been developed, thereby creating a source of potential analytical uncertainty (Chapra 2003; Zhang and Yu 2004). The 2001 National Research Council report suggested in its assessment of the TMDL program that the EPA should end its practice of arbitrary selecting the MOS and instead require an uncertainty analysis as the basis for MOS determination (NRC 2001). Dilks and Freedman (2004) have pointed out that the rigorous application of the MOS is inhibited by limited practical experience, absence of policy regarding the degree of protection desired with MOS, and data-poor or high-uncertainty situations that make MOS unsustainable. In practice, an explicit or quantifiable MOS, such as an assignment equivalent to 10% of carrying capacity, is typically used. For an implicit MOS, an assumption of the MOS is made based on poorly articulated management practices.

TMDL ATTAINS Database

All TMDL plans must be submitted to the USEPA for review and approval or disapproval. If the USEPA decides not to fully approve a TMDL, it will develop what it considers an acceptable TMDL. This process of submitting reports to USEPA has created a repository of all TMDL documents that describes how the TMDL was developed and includes information related to modeling, data collection, use of innovative strategies, stakeholder involvement, and a procedure for dealing with uncertainty. In 2018, 71,397 TMDL documents addressing 75,075 causes of impairment had been submitted to the USEPA. This information is useful to managers and practitioners to plan and scientifically defend their TMDL development process. The fundamental challenge is to develop effective and efficient techniques to guery, summarize, and disseminate the essential relevant information from these documents. The USEPA developed the online system described earlier, known as the Assessment and Total Maximum Daily Load Tracking and Implementation System, for assessing information about the conditions in the nation's surface waters. The ATTAINS web portal is an invaluable resource of information on TMDL reports and documented impairments impacting US waters. However, ATTAINS has a limitation in that it does not explicitly provide information about the modeling tool(s) used for TMDL development.



Fig. 1. Temporal and geographical distribution of the reports captured by the current version of the TRS tool.





TMDL Report Selection Tool

The ATTAINS repository of TMDL reports was used to generate a database of modeling and other information relevant to TMDL development (TMDL-DB). The records retrieved from the ATTAINS repository included information such as links to the report, document type, impairment category, USEPA region, and lead state. These records, however, did not identify the models or analytical techniques used in developing the TMDL reports. The TMDL-DB was populated using about 27,068 unique (singular) TMDLs (identified using an unique TMDL ID) from the ATTAINS repository that represented 76,127 TMDLs developed between 1975 and 2017 (Fig. 1). The model description and other information were retrieved from the TMDL report with text searches based on regular expressions that were designed to recognize variations in the model names. For example, HSPF and Loading Simulation Program C (LSPC) were recognized as same model, and LDC, Load-durationcurve, Load Duration Curve, Flow Duration Curve, Flow-Duration-Curve, and various other combinations were recognized as the same modeling technique (Kumar 2017). The frequency of occurrence of several models, modeling techniques, and other terms associated with modeling for TMDL development was identified using this text searching procedure (Fig. 2) for the reports available within the ATTAINS database. This can help the analyst

in two ways—first by providing an indicator of the popularity of a particular modeling approach and documenting trends, where they exist, of transitions over time from one modeling approach to another. This can occur when a particular TMDL modeling tool is significantly enhanced or upgraded, resulting in a consequent shift in use. This TMDL-DB has been used in this paper to analyze the state of practice of selected TMDL topics, discussed earlier.



Fig. 3. Model frequency statistics supported by the TRS tool. The frequency count of specific models used in TMDL analysis is somewhat similar for many of the familiar models commonly used for TMDL analysis.



Fig. 4. Frequency count of the more common constituents that appear in the text of the TMDL reports in the ATTAINS repository. The Cause Unknown category refers to ATTAINS database queries that do not fall into an established pollutant group.

The TRS tool (version 1.1) is available at https://occviz.com /tmdl/ (Kumar 2017) as a decision support tool to explore and identify relations between impairments and modeling techniques in the TMDL-DB. This tool lets the users select TMDL reports that may be used as case studies based on impairments, modeling techniques, and other characteristics of interest (e.g., use of remote sensing) by presenting a visual representation of the associations between the parameters of interest. These associations are based on the number of reports that contain these descriptors (e.g., impairments, modeling techniques, remote sensing, GIS, etc.), and may not always yield relevant TMDL project examples for the TMDL under development. In addition, the underlying ATTAINS repository used to develop these linkages does not contain the totality of published TMDL reports; hence, quantitative assessment of the prevalence of a modeling technique or impairment using the reporting tool may be biased. Despite these limitations, having ready access to prior TMDL reports has the potential to

save time and budget and possibly lead to selection of the best tool for the problem at hand.

Characteristics of the TRS Tool

Two interactive plots—the chord and matrix graphs—are used to visualize the relationship between impairments, watershed models, receiving water models, and other terms associated with TMD models. A connection is established between any two terms, regardless of categories, when a TMDL report is identified as containing both these terms. For example, if a TMDL report is identified to contain impairment descriptors Sediment and Nutrients and models HSPF and CE-Qual-W2, connections are established between all possible binary pairs of descriptors. A report is marked for attribution to an impairment based on the original data record available from the ATTAINS database. A user-configurable critical frequency is used to mark a report as having used a modeling technique. If the TMDL report has been identified by the text search algorithm to have used the modeling technique name equal to or greater than the critical frequency number, then the report is marked as having used the modeling technique.



Fig. 5. TRS tool output showing the frequency with which certain models have been used in reports for the eight constituents listed previously: pathogens, oxygen (deficit), nutrients, mercury, ammonia, sediment, turbidity, and pH or acidity.

Use of the TRS Tool

The most-cited models identified using the TRS tool were summarized using a frequency plot (Fig. 3). The plot shows surprising consistency in the number of references to TMDL model reports, with most models falling within the 100–1,000 frequency count on the logarithmic scale of the ordinate axis. Simple, spreadsheet, and mass balance models also score high on frequency count and are all in the 500–5,000 range. The TRS tool provided a similar summary plot of the frequency of pollutant descriptors, including toxic constituents, nutrients, pesticides, sediment, and nuisance biota (Fig. 4). The bulk of the citations are in the 50–500 frequency count, with pathogens and metals (other than mercury) the reports with the highest frequency count (Fig. 5). The Inconclusive category is used to describe those TMDL reports where the modeling approach used could not be determined or did not involve one of the models on the list of models compiled from the ATTAINS database.



Fig. 6. TRS tool user interface shows the chord graphing tool that, when invoked, allows the user to explore connections and relationships between constituents of concern, associated constituents, and TMDL reports that contain references to these constituents of concern. The number of reports can be screened by increasing the frequency count requirement, which can save the user time by selecting those reports with the most use that likely corresponds to the report focus. More than one constituent can be selected with the filter (e.g., mercury and sediment). A section of the matrix is enlarged to show how the various TMDL models selected and the pollutant group to which they are applied are cross-referenced.

Case Studies of TRS Tool Application

The function of the TMDL Report Selection tool (TRS version 1.1) can be seen in Fig. 6. To use the tool, first the user selects the critical frequency using the slider of the user interface. This slider controls how reports are classified with respect to the prevalence of the search parameter in one or more TMDL reports where models were involved. For example, if the selected value for the slider is set to 30, then any model name (and its derivatives or alternates) has to occur a minimum of 30 times in the text of that report for the report to be marked as being used for that TMDL. As the slider is moved to higher numbers, fewer reports are made available in the report table. The slider has no impact on the labeling of watershed impairment. Impairment labels were included in the report metadata provided by the EPA and were assumed to be correctly classified. Clicking on any of the entries on the circumference of the wheel invokes the chord graphing tool that connects constituents of concern with other constituents and shows a connection to those models most commonly associated with the constituents collected in the TMDL reports identified. Clicking the Remove filters button at any time clears all of the filters. A data connections matrix shows below the selection wheel and uses gray shading to show the strength of the relationship between any two table entries on the matrix ordinate and abscissa. Multiple instances of correspondence in the TMDL reports selected show up in darker tones—a black entry on the matrix indicates high correspondence.

Critical frequency (see How to use this app)



Fig. 7. TRS tool output for mercury showing connections to other constituents and models used in prior TMDL reports with a critical frequency of 7.

The TMDL report names, the year completed, region, state, and constituent (pollutant) group identifier all appear in the report table that appears below the matrix. A PDF file of each TMDL is accessible by clicking on the report link under the TMDL ID tab.

Queries Using the TRS Tool: Mercury

Mercury (Hg) is a toxic metal that is found both naturally and as an introduced contaminant in an aquatic environment. Monomethylmercury (MeHg) is the most toxic form, and even very low concentrations can lead to bioaccumulation within the aquatic food web. Hg makes its way into the aquatic ecosystem through one of two major routes: point and nonpoint source discharges or atmospheric deposition. The behavior of Hg depends on numerous chemical, physical, and biological processes that vary in space as a function of the biogeochemical and hydrodynamic environment. Because of its prevalence and threat to lakes and waterways, mercury TMDLs have been conducted in a number of states throughout the United States.



Fig. 8. TRS tool output for salinity showing connections to other constituents and models used in prior TMDL reports.

User selection of the Mercury tab on the selection wheel of the TRS tool (Fig. 7) shows a connection to studies that involve other metals, as well as TMDL reports where the MOS is invoked. The chord graphing tool in Fig. 7 also

shows minor connections to studies that involve other metals, sediment. pesticides, polychlorinated bi-phenyl (PCB), and other toxic organics. After making the selection, a simple click on the appropriate chord of the graphing tool will freeze the selection. Bold lines are shown in the chord graphing tool that connect mercury with a number of models as well as offering a weak link to the generic spreadsheet tool. The boldest lines, which depict the strength of the connection, connect the mercury chord on the wheel to the models HSPF/LSPC, Generalized Watershed Loading Function (GWLF), Soil and Water Assessment Tool (SWAT), Water Quality Analysis Simulation Program (WASP), BASINS, Universal Soil Loss Equation/Revised Universal Soil Loss Equation (USLE/RUSLE), and the LOAD DURATION analysis. Given the linkage between sediment erosion and mercury export, it is expected that sediment transport models would be chosen in mercury TMDL analyses. Minor connections, shown as thinner colored lines, connect mercury with models Environmental Fluid Dynamics Code (EFDC), Enhanced Stream Water Quality Model/Updated Enhanced Stream Water Quality Model (QUAL2E/QUAL2K), CE-QUAL-W2, and Storm Water Management Model (SWMM). Minor connections also occur to the Mass Balance model tab and the Simple Method modeling technique. The matrix shows the same information derived from the wheel in tabular form with the strongest relationships showing up as black squares and those with weaker connections as various shades of grey that relate to frequency of occurrence in the TMDL report.



Queries Using the TRS Tool: Salinity

Salinity is a common pollutant, especially in the arid, western United States where surface water and groundwater are both elevated in total dissolved solids, precipitation is low and occurs only during winter months, and evapotranspiration rates are high. Salinity is of major concern to irrigated agriculture because elevated soil salinity can reduce crop yields and diminish agricultural productivity in affected areas. User selection of the Salinity/TDS tab on the selection wheel of the TRS tool (Fig. 8) shows strong connections with TMDLs for ammonia and nutrients. Salinity, being a conservative constituent, is a useful parameter in mass balance studies to help validate the fate and transport of nonconservative and reactive constituents such as ammonia and nutrients or phosphate and nitrate-nitrogen. The chord graphing tool in the TRS tool interface shows connections to TMDL models that include Load Duration Models, GWLF, HSPF, QUAL2E, WARMF, Stream Network and Stream Segment Temperature Model Software (SSTEMP), SPREADSHEET, and Curve Number-based models. Of the tools listed, salinity appears to be connected to the load duration curve methodology more than any other modeling tool.

Queries Using the TRS Tool: MOS

As discussed earlier, guidance on the type of MOS (implicit or explicit) and magnitude of MOS is not always readily available from the literature or previous TMDL reports. However, the TRS tool can have utility in assisting users in developing an understanding of the magnitude and type of MOS that have been applied in TMDL models of impairments in the past in those reports where the MOS is discussed. For example, a user may select parameters explicit MOS, pathogens, and HSPF/LSPC (Fig. 9) and analyze the filtered reports for guidance on explicit MOS guantification. Similarly, other gueries can be made to help understand how an implicit MOS has been developed for a TMDL model of a specified water quality impairment. Use of the TRS tool has had utility in identifying MOS reporting and other deficiencies in the ATTAINS database. However, the tool does not directly suggest or quantify the MOS. This may be incorporated in a future update to the TRS tool. Further development of the TRS tool and more widespread adoption of its use could help guide future improvement of this USEPA database resource.

Conclusions

The USEPA database of TMDL reports ATTAINS is an underused resource for TMDL model development. The TRS decision support tool developed by Kumar (2017) is a simple graphical interface that has significant potential to help streamline the process of TMDL model selection, data gathering, and subsequent analysis with the selected modeling tool. The TMDL reports that can be accessed with the help of the tool can also provide insight on the selection of appropriate MOS values based on the prior studies accessed with the TRS tool. Three examples were discussed to familiarize the reader with typical output from the TRS tool and how the chord graph output can be used to show connectivity between previously published TMDL reports and a number of water quality constituents, including the report MOS. The relative weighting of the frequency of model use for these previous TMDLs can give an analyst some level of confidence in the TMDL approach given the popularity of some methodologies over others. Given the increasingly limited public funds available to plan, coordinate, and complete TMDLs, methods such as the one outlined in this paper can go a long way in making the process more efficient and cost effective.

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