Towards transparent and consistent exchange of knowledge for improved microbiological food safety ☆

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Predictive microbial modelling and quantitative microbiological risk assessment, two important and complementary areas within the food safety community, are generating a variety of scientific knowledge (experimental data and mathematical models) and resources (databases and software tools) for the exploitation of this knowledge. However, the application and reusability of this knowledge is still hampered as the access to this knowledge and the exchange of information between databases and software tools are currently difficult and time consuming. To facilitate transparent and consistent knowledge access and exchange new tools and community resources are needed. These resources will promote the creation of a public microbiological food safety knowledge repository encompassing available data and models. However, essential components are currently missing, such as open data formats supported by different software tools and consistent rules for knowledge annotation. The knowledge repository would be a user friendly tool to benefit different users within the microbiological food safety community, especially users like risk assessors and managers, model developers and research scientists working in the private sector (e.g. food industries, consultancy companies), research institutes or food authorities.

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Introduction

Microbiological food safety is a major challenge for the increasingly globalized food sector [1]. Therefore, the microbiological food safety community (including people working within food authorities, food industries, consultancy companies and food research institutes) has invested great research efforts in the fields of predictive microbial modelling [2•] and quantitative microbial risk assessment (QMRA) [3•]. This led to new technologies for obtaining and processing experimental data, open databases to compile and share data, new mathematical models, and software tools capable to generate and apply these models [4,5].

In the present decade, the way of making use of scientific information is changing. Despite of the fact that, there are still some barriers that hamper the open science (e.g. the incentive structures of academic research, which most of the time do not reward efforts to open up the scientific process, fear of ideas being stolen, perception that open science activities are time-consuming, fear of how do you ensure rigorous application of your research, etc. (Open Science Monitor; URL: https://ec.europa.eu/research/openscience/index.cfm?pg=drivers&section=monitor)), we are in an era of open data and open access where sharing of scientific knowledge is of increasing importance. This will increase transparency and facilitate the application and reusability of knowledge.

In the area of microbiological food safety, knowledge includes for example experimental data and mathematical models relevant for predictive microbial modelling and microbial risk assessment. The efficient exchange of this knowledge, for example, between research teams and risk assessor or between risk assessors from different countries, could help to build more pertinent and rapid risk assessment opinions and thus contribute to improvement of microbiological food safety. Therefore, greater efforts are needed to facilitate knowledge exchange between the existing and future resources like software tools and databases.

This paper initially reviews the recent developments in the field of predictive microbial modelling and QMRA,

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focusing mainly on available databases and mathematical models as well as software tools and resources that facilitate the exchange of knowledge. Then this paper, focuses on its main objectives that are firstly, to discuss the recent challenges related to transparency and consistency, deployment and reusability, as well as information exchange between software tools and secondly, to highlight future developments that should be carried out to overcome these current challenges.

Recent developments in predictive microbial modelling

In recent years, predictive microbial modelling has reinforced its position as one of the most promising tools to support microbiological food safety decisions, mainly due to successfully validated models and active software development in this area [2•,6,7]. Predictive microbial models can help to understand the microbial behaviour in food systems depending on different environmental factors, being for example a powerful tool to evaluate the microbial exposure within a quantitative microbial risk assessment [2•].

Predictive microbiology has the potential to become an even more significant element supporting the microbiological safety of food products in the future. New and more accurate models can be generated through new analytical methods that facilitate the fast characterization of relevant environmental factors and pathogens as well as the acquisition of large datasets. As examples of recent advancements, we can highlight the increased adoption of biologically interpretable models that account for new environmental parameters [8–10], models that take into account microbial interaction in food [6,11,12], the introduction of high throughput analytical methods in the domain [13] and the automated acquisition of growth parameter at single cell level by microscopy [14]. Furthermore, next generation sequencing (NGS) techniques will help to explain the observed variability between strains [15].

Besides, there is novelty in predictive microbial modelling itself. For example, in the last years new predictive microbial models have been developed considering different factors like, the structural characteristics of the food matrix [16] and the cross-protection between different stresses [17]. In addition, the modelling approach followed in those studies that consider the inter-strain variability of the same microbial species has changed with respect to previous studies [18,19]. Latter developments in predictive modelling approaches have also resulted in new model equations [20], stochastic models [6,21,22] and models considering dynamic conditions [23].

The application of available data and predictive microbial models by the microbiological food safety community has been greatly facilitated by the development of new software tools that provide easy access to data and models

from this domain. A review of the available tools has been generated by Tenenhaus-Aziza and Ellouze in 2013 [4]. However, since that study, new software tools for predictive microbial modelling were developed by the scientific community, including the R packages nlsMicrobio (F Baty *et al.*, nlsMicrobio: Nonlinear regression in predictive microbiology, URL: https://rdrr.io/cran/nlsMicrobio) and Bioinactivation SE/core [24], and the modular Food Safety Knowledge Lab (FSK-Lab) (Food Safety Knowledge Lab; URL: https://foodrisklabs.bfr.bund.de/fsk-lab/). Furthermore, new initiatives like STARTEC (Decision Support Tools to ensure safe, tasty & nutritious Advanced Ready-To-Eat foods for healthy and vulnerable Consumers; URL: http://www.startec-eu.info/) and SOPHY (Development of a SOftware tool for Prediction of ready-to-eat food product sHelf life, quality and safetY; URL: http://sophy-project.eu/) also emerged, aiming at developing new software tools for the application of predictive microbial models. A regularly updated catalogue of tools is available online (Tools for Predictive Microbial Modelling and QMRA; URL: https://foodrisklabs.bfr.bund.de/rakip/). In addition, a community driven search engine named 'openFSMR' (M Filter *et al.*, 9th International Conference on Predictive Modelling in Food, 8–12th September, Rio de Janeiro, Brazil. Accession Number: 2015009A4CS) has been created to facilitate the comparison of available models within the different tools (openFSMR; URL: https://foodrisklabs.bfr.bund.de/openfsmr/).

Recent developments in the QMRA

Since the 1990s, a series of political and technical factors have stimulated adoption of the risk analysis framework as the basis for international food safety decisions [25,26]. Since then, an increasing number of QMRA models are developed by scientists and risk assessment bodies for guiding risk management options [3•].

Different modelling techniques and modelling objectives are being explored within the QMRA area. QMRA were first developed for food and waterborne bacteria and protozoa, recently new research and data on viruses allow QMRA for these hazards as well [27–29]. The incorporation of omics technology into QMRA has been discussed for some time [30,31]. Most of the studies in this area have focused on the use of whole genome sequencing (WGS) in the hazard identification step of QMRA [3•]. However, achievements in the exposure assessment step are still limited, and a rare example is the study by Njage and Buys [32] that includes the potential of gene transfer between strains into the exposure to *Escherichia coli* due to the consumption of lettuce.

Risk-benefit assessments (RBA) are the most recent risk-based method that has the potential to integrate approaches of chemical and microbiological risk assessment and the nutritional aspects of food consumption. To

date, most of the RBA integrate chemical and nutritional assessments, and generally, microbial risk is seldom assessed and rarely in a quantitative way [33]. Recent examples are the studies of Berjia *et al.* [34] that integrated microbiological risks and nutritional benefits in cold smoked salmon and Boué *et al.* [35] that integrated microbiological and chemical risks with nutritional benefits in infant feeding. Recently, Guillier *et al.* [36] discussed the importance of another integrative approach to assess a more global overview of food safety concepts by combining sustainability, economy and microbial food safety. An example of economy and risk analysis is the work of Van Wagenberg *et al.* [37] on the cost effectiveness of interventions to control *Campylobacter* on broiler farms.

A QMRA should be documented fully and systematically in a transparent manner, and be available to all interested parties, such as risk assessors, risk managers, consumers, industry and the scientific community [38]. Here, QMRA software tools can be useful. However, the number of software tools intended to QMRA is far less than those aimed at predictive microbial models [4]. Many of the QMRA models are programmed by using @Risk (Palisade ©, NY) or R (R: A language and environment for statistical computing; URL: http://www.R-project.org). While R is free software, @Risk is not, which limits the reuse of these models. Recently, the FDA released version 4.0 of its web-based risk assessment tool FDA-iRISK® (FDA-iRISK® version 4.0.; URL: https://irisk.foodrisk.org/), that offers users a well-structured template to develop their own QMRA model. The new features include first, separation and quantification of variability and uncertainty through 2D Monte Carlo analysis, second, incorporation of predictive models, third, data importing from FDA databases, fourth, database with shared FDA-iRISK® models, and finally, models accounting for multiple hazards and foods among others. A different approach is applied by a new software called FSK-Lab (Food Safety Knowledge Lab; URL: https://foodrisklabs.bfr.bund.de/fsk-lab/) from BfR. FSK-Lab allows users to create, import, modify, run and export QMRA models in different languages, like R, MATLAB (MATLAB and Statistics Toolbox, The MathWorks, Inc., Natick, Massachusetts, United States) or KNIME (KNIME; URL: https://www.knime.com/). Besides that, this software allows to combine existing QMRA models facilitating the construction of new or adapted QMRA. Some other resources, like FoodRisk.org (FoodRisk.org; URL: http://foodrisk.org) are also of high relevance. The latter is an open information portal to assist professionals involved in microbial risk analysis and food safety. It contains unique datasets, tutorials, and links to numerous tools and information sources.

Current challenges
One of the current challenges in microbiological food safety is the difficulty to exploit and apply the knowledge generated/present in predictive microbiology and QMRA studies and software tools. This represents a severe obstacle for the establishment of timely risk assessment using the most up to date knowledge. Thus, the microbiological food safety community would benefit by having knowledge efficiently shared in a transparent and consistent way in order to facilitate its exploitation and application in microbiological risk assessment and management.

This transparent and consistent way can be achieved, for instance, by the development of a user-friendly model repository that stores the knowledge in a standardized format. Thereby users can download models and information about models facilitating their reusability, and also they can easily contribute to develop the model library by uploading models in different programming languages according to the tool they used to build it. This step is made through a standard format allowing to have the same level of information about model regardless of software or tools used. But before this is possible, some previous steps on harmonization, such as transparency and consistency, are necessary.

Transparency and consistency
Transparency in modelling consists in documenting all the different steps followed within the model generation process, including references for all data used, as well as the assumptions, ranges of applicability, limitations and uncertainties. Consistency principle is a crucial element for allowing model comparison. It means that methods or terminology, once adopted must be applied consistently in future. Also same definitions must be used for similar situations. With the development of new experimental technologies, food microbiologists and risk assessors are now confronted with large datasets that are computationally analyzed for extracting the biological information of interest. Facing the statistical complexity of data analysis and the heterogeneity of available software tools, Cohen-Boulakia *et al.* [39•] argue that some scientific results will not stand the test of time. Indeed, no one will be able to reproduce results that are dependent of programmes that may not be maintained in the future. Thus, tackling the transparency and consistency of how the results were produced is one of the main scientific challenges. This is essential to enable other researchers to check previous conclusions and build upon them. There are different strategies promoting the adoption of these best practices recommended, for example publishing data into repositories like FigShare or Zenodo [40], or as supplement to a publication or publishing data itself in so called 'Data journals' [41].

Whatever the approach, metadata are key to provide a transparent and consistent description of research results. Harmonized and detailed metadata are the foundation to search for and find datasets, and to be able to reuse

knowledge in another context. Data warehouses typically offer a list of metadata to describe the datasets they host. They may also require a minimum of metadata when submitting datasets. In this sense, a guideline called 'Minimal Information Required in the Annotation of Models' (MIRIAM) has been created to define the minimal information required in the annotation of models within the Systems Biology community [42]. It is now possible to assign a unique reference (DOI) to a dataset, providing a long-term reference to a digital object. DOI is a service offered by a DOI Registration Agency. Agencies collect metadata, assign DOI names, and offer other services such as reference linking. For example, DataCite [43] a non-profit organization not geared to a particular thematic area, can deliver DOIs for datasets as long as a metadata list defined by DataCite is provided. It supports different standards for metadata, such as Dublin Core (Dublin Core; URL: http://dublincore.org), IDF (International DOI Foundation) metadata kernel, and OECD dataset Metadata.

Nowadays the research field of genomics is probably the most advanced area of transparent and consistent knowledge exchange in food microbiology. The large genomic datasets obtained by NGS are usually made publicly available on genome repositories, mainly promoted by the fact that journals in this field usually demand it. Some journals are specifically dedicated to the announcement of new genomic sequences, for example, Genome Announcement. In the same way open software tools used for the exploitation of these datasets are made publicly available in repositories like for example, GitHub or bitbucket [44].

Researchers involved in the field of predictive microbiology and QMRA modelling are certainly less advanced in transparent and consistent knowledge exchange than, for instance, in the field of genomics or Systems Biology [42]. However, some examples can be pointed out. Recent studies on the creation of food safety model repositories for predictive microbial models [45••] are likely to provide tailor-made solutions also for this research domain. In November 2016, EFSA launched Knowledge Junction, a curated, open repository that makes use of Zenodo. This repository aims at exchanging evidence and supporting material used in risk assessments, such as QMRA models, datasets, guidance documents, etc. An example of a shared model is a *Listeria monocytogenes* QMRA for three ready-to-eat foods developed in @Risk software [46]. In addition, the Interactive online Catalogue on Risk Assessment (ICRA) is also an example of an open repository of QMRA models that allows users to compare and contrast models from the same pathogen and/or commodity (ICRA; URL: http://icra.foodrisk.org/).

Although a few repositories for data and models related to microbial responses are available [47], in general there is no practice within food microbiology to systematically make all raw data accessible when a study is published. However, dealing with modelling practices associated with these data, the parameters obtained after fitting models to dataset are now generally included in scientific publications. To apply and reuse these data, the related environmental conditions are needed and this is an area where more detailed reporting in scientific publications would be beneficial, as pointed out by predictive microbiology validation studies [7]. To improve transparency some predictive microbiology application software explicitly share the equations and their parameter values and others include references to the scientific studies where models were developed (M Filter *et al.*, 8th International Conference on Predictive Modelling in Food, Paris, France, September 2013). In addition, results from product validation studies have been used to improve the reliable application of models for assessment and management of microbiological food safety. These product validation results included values for indices for model performance and the range of applicability for specific models with respect to the food products and environmental conditions for which the models were successfully validated [7]. To ensure the complete exploitation of knowledge it would be essential to share, for example, firstly, raw data collection, secondly, criteria of inclusion in the analysis, thirdly, script/tool/algorithms used in the modelling generation process, and finally, complete description of food product or laboratory media characteristics. Defining transparent criteria for inclusion of data is important, including the data quality measurement of an obtained kinetic parameter, the number of points of the kinetics and the minimal difference between the inoculated level and maximum level [48]. The documentation of the fitting procedure is also important. Recent examples for fitting procedures with different tools and fitting approaches can be found in Plaza-Rodriguez *et al.* [45••]. The option to provide Supplementary materials in almost every journal in the field should encourage the exchange of knowledge. Some recent studies indicate that more and more data and software scripts will be made publicly available (e.g. [49,50]).

Transparency and consistency are also a challenge for QMRA. During the last decade, verification and validation have gained a large interest within the scientific community because of the requirement to assess the possible errors affecting the results obtained by software code. Over the years, many attempts have been made to standardize the terminology of verification and validation, but several distinct definitions are still associated to this concept [51,52]. Code and calculation verification are a crucial issue, particularly in the field of risk assessment where computer codes are used to assess the probability of failure of real systems. However, the concept and the practice of code verification are not well developed in the community of QMRA. Among the possible reasons for

that are the large variety in scientific background of QMRA modellers, the difficulty to fully understand all details of a QMRA model in the programming language used and the time pressure that is typical associated with performing QMRA in risk assessment agencies, where risk managers need timely assessments to make timely decisions, for example when an outbreak arises. Validation of QMRA models is challenging. Currently, risk assessors can verify intermediate results of their models [52] and try to validate the risk estimate by comparing it with epidemiological data. However, this is difficult as both epidemiological data and QMRA results are associated with large uncertainty [53].

Software development for knowledge exchange

A considerable number of software tools aiming to reuse the generated knowledge in the areas of predictive microbiology and QMRA are available, like ComBase (ComBase; URL: https://www.combase.cc), PMM-Lab (PMM-Lab; URL: https://foodrisklabs.bfr.bund.de/pmm-lab/), MicroHibro (MicroHibro; URL: http://www.microhibro.com/) and GroPIN (GroPIN; URL: http://www.aua.gr/psomas/gropin/). Users of specific predictive microbiology software tools have been able to exchange information such as product characteristics, storage condition, kinetic parameters and the related predicted responses. As one example the FSSP-software has used a XML-file format for this purpose since 2004 (Food Spoilage and Safety Predictor (FSSP); URL: http://fssp.food.dtu.dk/). However, communication mechanisms allowing the exchange of knowledge between different tools have not been established yet. This absence of communication increases the difficulty of users to reach the output of interest and might be a brake of the development of this research field. In the last years, the application of existing XML-based information exchange formats for the microbiological food safety modelling domain has been proposed. Specifications were provided by Plaza-Rodriguez et al. [45••], which promoted the consistent adoption of existing standards (NuML/SBML/SED-ML/OMEX) in order to create a common description language for predictive microbial models (Predictive Modelling in Food Markup Language-PMF-ML). PMF-ML has already been used to provide parameterized predictive microbial models to journals [50] and has facilitated the direct information exchange between different software tools from the domain of predictive microbiology (ComBase, GroPIN to PMM-Lab; PMM-Lab to R).

Recently, a Food Safety Knowledge Markup Language (FSK-ML; URL: https://foodrisklabs.bfr.bund.de/rakip/) has been suggested (Filter et al., Workshop 2, 10th ICPMF. Córdoba, Spain, September 2016) in order to create a common description language for QMRA models. The FSK-ML format adapts certain specifications of the PMF-ML format, while maintaining the highest possible synergies between both formats (M Alba Aparicio et al.,

COMBINE 2016. Newcastle upon Tyne, UK, September 2016). This will help microbiological food safety models encoded in a software-independent manner (using PMF-ML) to be easily interpreted by FSK-ML import and export functions in the future.

Future perspectives

The knowledge continuously generated by the microbiological food safety community should be efficiently shared in order to be able to reuse it for risk assessment and management. The creation of standard-based publicly available knowledge repositories could promote this knowledge sharing. Specifically, the development of harmonized data formats, controlled vocabularies and open source software code libraries, as suggested by Plaza-Rodriguez et al. [45••], will facilitate knowledge first, transparency and consistency and second, exchange between software tools in predictive microbial modelling and QMRA.

On this basis, we propose to put additional efforts into harmonization of knowledge as the first step to achieve these objectives (Figure 1). The markup language FSK-ML has been created to address many of the specific needs of the predictive microbial modelling and QMRA area described in this paper. This open exchange format can serve as the basis for harmonization of the large amount of available data and models. It is important to note that this harmonized markup language does not require to 're-implement' legacy models, but allows to create harmonized description around the original model (code).

Once placed into a harmonized description, models and data should be annotated. For this, it is necessary to define which metadata are relevant for describing models in the predictive microbial modelling and risk assessment domain, for example, by establishing lists of controlled vocabularies for relevant metadata concepts, and elaborate consistent rules for information annotation. We suggest to use or to extend existing metadata concepts and controlled vocabularies. For example the Dublin Core schema could be used to describe the general metadata associated to a model (title, creator, rights, etc.). Other more specific formats, such as the Standard Sample Description-SSD2 proposed by EFSA could be used to describe metadata associated to the description of the food product and microbial hazard considered in a model [54]. It is necessary to create a 'Minimal Information Required in the Annotation of Risk Assessment Models' (MIRARAM) guideline. This guideline would be similar to the MIRIAM guideline [42]. Even though some metadata would not be defined as mandatory, this would be highly important information, for example, when it comes to the interpretation of model-based predictions.

After the models and data have been harmonized and annotated, they should be compiled in a publicly available food safety knowledge repository. This repository

Figure 1
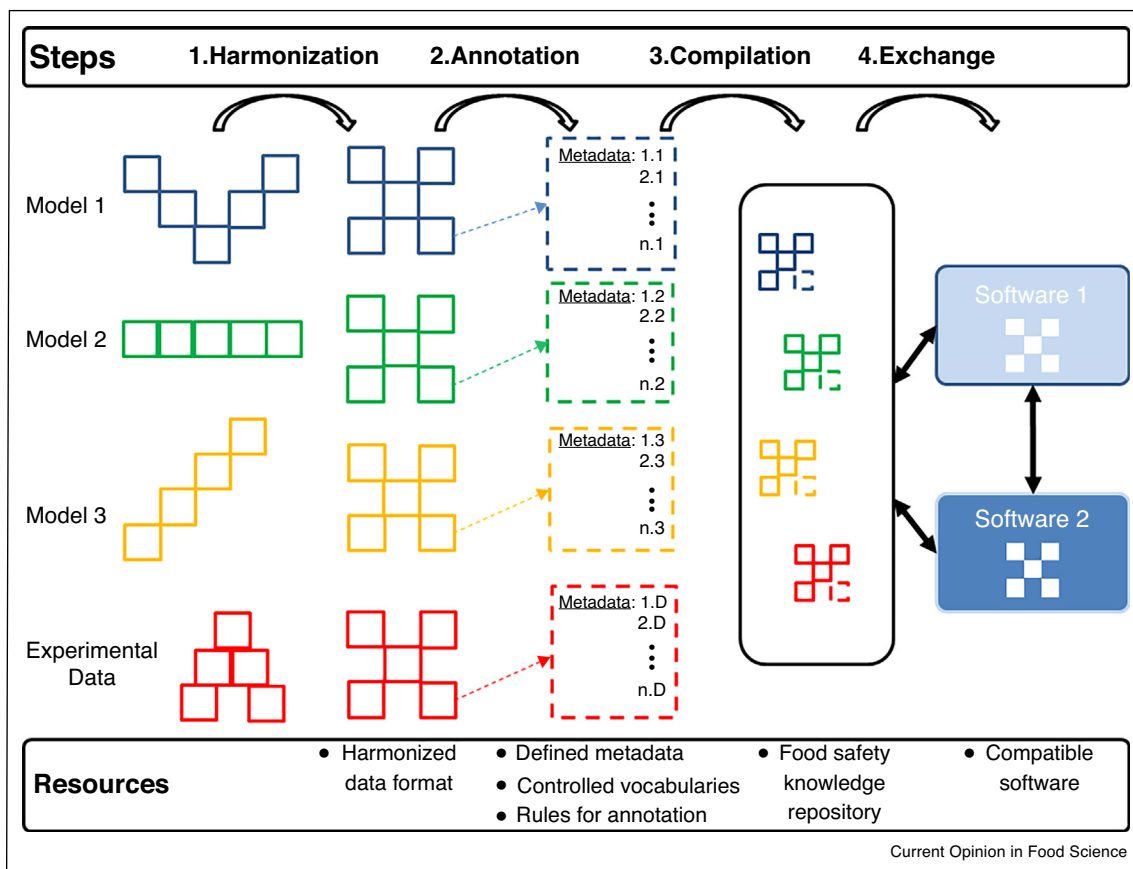
Steps and resources needed to reach transparent and consistent integration and exchange of knowledge in the microbiological food safety community.

would provide free, immediate and permanent access to data and models described in the harmonized data format. All software tools supporting the harmonized data format would be able to exploit the knowledge shared in this repository. Therefore, the use of the harmonized format would be a bridge between different software tools, data or model repositories and research groups in the future (Figure 1). It would be necessary to extend and validate the exchange of models and data to demonstrate that external tools can import and/or export them. This would be facilitated through the development of new open source software libraries and converter tools that should be made freely available to the scientific community.

Figure 2 shows important aspects of a food safety knowledge repository such as firstly, the end users and their main objectives, secondly, the principles involving the sharing and reusing of knowledge, and finally, important benefits for the microbiological food safety community.

Table 1 further illustrates the potential interests of using a food safety model repository. Such repository should be accessible for both 'non-expert users', that is, persons who intend to use the available models mainly for making predictions without too much interest in the modelling process, and 'expert' users.

Conclusions

Resources and knowledge generated within the microbiological food safety community are increasingly important and numerous. In the last years, advances have been made in new methods for obtaining and processing experimental data, in new model structures and algorithms, together with the creation of databases and software tools to generate and apply mathematical models in the field of predictive microbial modelling and QMRA. New resources facilitating transparent and consistent knowledge exchange would be beneficial to improve microbiological food safety. Synergies between existing resources, like databases and software tools, could be exploited. Therefore, the establishment of harmonized data formats and the development of consistent rules for knowledge annotation would be essential. In addition, the creation of an open access food safety knowledge

Figure 2
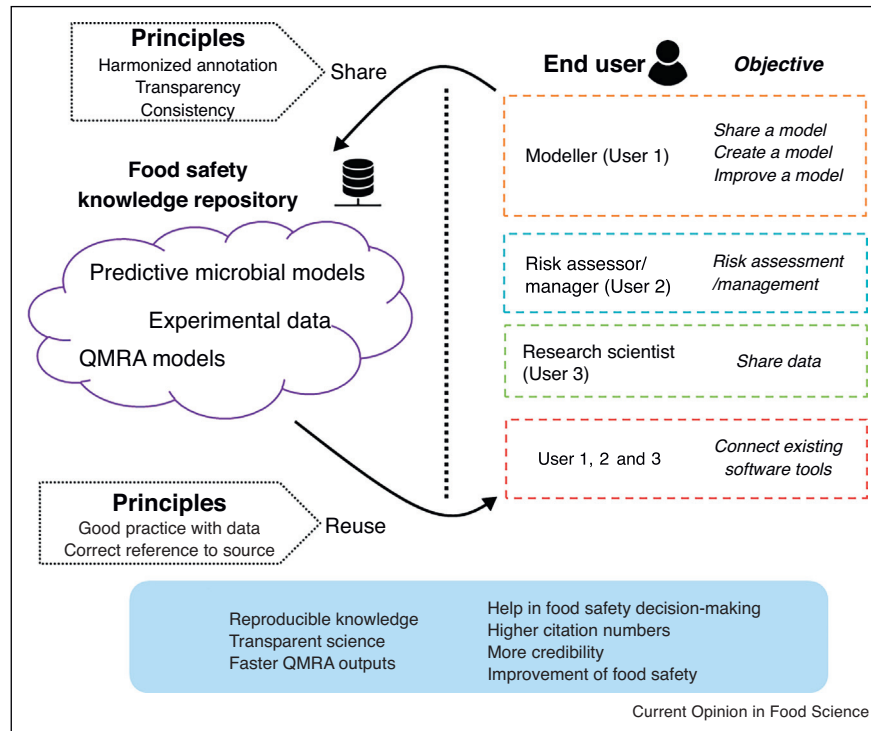
General overview of principles, end users and benefits for the microbiological food safety community when using a food safety model repository.

Table 1

Some user stories of a food safety model repository.

End user	Objective	Description of the user case
Modeller	Share a model	A modeller wants to share his model with the scientific community by making it publicly available and re-usable. In order to accomplish this, he can upload the model into the food safety knowledge repository. The model should be described in a harmonized language.
	Create a model	A modeller can easily search for available knowledge that is stored in the food safety knowledge repository, and then be able to re-use it in a software tool of his preference that is compatible with the harmonized language.
	Improve a model	A modeller wants to improve his own model or another model stored in the food safety knowledge repository. The model can be uploaded from the food safety knowledge repository, improved and uploaded again in the repository using the harmonized language.
Risk assessor	Risk assessment	A risk assessor wants to perform a new risk assessment. The description is the same as for the Modeller/Create a model.
Risk manager	Risk management	A risk manager can easily search for available knowledge on a new risk question using the food safety knowledge repository.
Research scientist	Share data	A microbiologist/food microbiologist wants to share experimental results with the scientific community. The data can be easily uploaded in the food safety knowledge repository. This example has a similar principle as ComBase database (URL: https://www.combase.cc).
All above users	Connect existing tools	A user wants to re-use a PM model describing growth that is available in a software tool or database in a QMRA model constructed in another software tool. If these software tools have an export function to download/upload the knowledge in a harmonized format, the build-up of a QMRA would be faster and use the most up to date knowledge.

repository would facilitate the exchange of information within the microbiological food safety community. These would be beneficial for the whole food safety community in many aspects such as the easier application and reuse of exiting knowledge, and consequently faster responses for industries and authorities in the case of food safety emergencies and the harmonization in decisions made during risk management.

Conflict of interest

The authors declare no conflict of interest.

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