4FUN

"The FUture of FUlly integrated human exposure assessment of chemicals: Ensuring the long-term viability and technology transfer of the EU-FUNded 2-FUN tools as standardised solution"

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PP	Restricted to other programme participants (including the Commission Services)	
RE	Restricted to a group specified by the consortium (including the Commission Services)	
CO	Confidential, only for members of the consortium (including the Commission Services)	

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1 Introduction

1.1 Aims of the task

The project 2-FUN, funded under the EU 6th Framework Programme, produced a prototype software containing a library of models for the assessment of human exposure to chemicals, coupling environmental multimedia and pharmacokinetic models. The objective of the 4FUN project is now to convert this prototype into a widely used product integrating on the same platform multimedia, PBPK, and dose-response models. The final software, called MERLIN-Expo, will thus allow exposure assessments for different human populations (e.g. general population, children at different ages, pregnant women) including exposure through multiple pathways.

The main aim of task 2.7 (‘Analysis of previous success stories’) was to learn from the experience of other projects analysing success stories related to software initially developed in the frame of European/national research projects and now widely disseminated among the scientific/regulatory/consultancy world. Hence a number of research projects considered to be successful were found, selected and analysed in order to gain benefit from them.

The present deliverable aims to provide an overview of the analysis of these success stories. The information collected will help the development of new approaches and new possible strategies in order to improve the effectiveness and the dissemination of the 4FUN project, the evaluation of the potentialities of the project and the exploration of alternative or additional management plans.

In order to identify and analyse success stories, different steps were followed:

- Identification and selection of interesting projects
- Collection of information via a questionnaire
- Analysis of the answers

In the following paragraphs all these steps will be described.

2 Looking for interesting projects

2.1 Identification of interesting projects

As stated above and in the description of work, success stories should be related to European or National projects which developed software now widely disseminated.
Different strategies were adopted in order to identify potential interesting projects:

1. projects in which 4FUN partners were involved were considered
2. EU funded projects were found on the internet via:
   - http://cordis.europa.eu/fp7/projects_en.html where project details are published after the negotiation and the signature of the grant agreement between the European Commission and the beneficiaries
   - http://www.cefic.org/ which is the website of the European Chemical Industry Council
   - general search engines.

In this way, the following projects were identified:

1. **ACROPOLIS**: Aggregate and Cumulative Risk Of Pesticides: an On-Line Integrated Strategy (http://acropolis-eu.com/)
2. **AGRIXCHANGE**: A common data exchange system for agricultural systems (http://www.agrixchange.eu/)
3. **ANTARES**: Alternative Non-Testing methods Assessed for REACH Substances (http://www.antares-life.eu/)
4. **A-TEAM**: Advanced Tools For Exposure Assessment and Biomonitoring (http://www.birmingham.ac.uk/index.aspx)
5. **BIO_LCA_TOOL**: Simplified Life Cycle Assessment Tool.
6. **BROWSE**: Bystanders, Residents, Operators and WorkerS Exposure models for plant protection products (https://secure.fera.defra.gov.uk/browse/index.cfm)
7. **CAESAR**: Computer assisted evaluation of industrial chemical substances according to regulations (http://www.caesar-project.eu)
8. **CONTAMED**: Contaminant mixtures and human reproductive health - novel strategies for health impact and risk assessment of endocrine disrupters
9. **ConsExpo**: The software model ConsExpo is a set of coherent, general models that enables the estimation and assessment of exposure to substances from consumer products that are used indoor and their uptake by humans (http://www.rivm.nl/en/Topics/C/ConsExpo)
10. **CITINES**: Design of a decision support tool for sustainable, reliable and cost-effective energy strategies in cities and industrial complexes (http://www.citines.com/)

11. **ChimERA**: An integrated modelling tool for ecological risk assessment (http://www.cefic-lri.org/projects/38/21/LRI-ECO19-RUG-ChimERA---An-integrated-modelling-tool-for-ecological-risk-assessment/?cntnt01template=display_list_test)
12. **CREAM**: Mechanistic Effect Models for Ecological Risk Assessment of Chemicals (http://cream-itn.eu/)
13. **ERICA**: Environmental Risk from Ionising Contaminants: Assessment and Management (https://wiki.ceh.ac.uk/display/rpemain/ERICA+Tool)
14. **E-RISK**: Evidence-based risk management in global software development projects
15. **ESTOMAD**: Energy Software Tools for Sustainable Machine Design.
16. **EULER**: EUropean software defined radio for WireLEss in joint secuRity operations (http://www.euler-project.eu)
17. **FLOSSINCLUDE**: Free/Libre and open source software: International cooperation development roadmap.
18. **FOOTPRINT**: Functional tools for Pesticide Risk assessment and management (http://www.eu-footprint.org/it/index.html)
19. **G.EN.ESI**: Integrated software platform for Green ENgineering dESIgn and product sustainability.
20. **ICT 4 E2B FORUM**: European stakeholders forum crossing value and innovation chains to explore needs, challenges and opportunities in further research and integration of ICT systems for Energy Efficiency in Buildings (www.ict4e2b.eu)
21. **MAS DE NADA**: Modeling and Advanced Software Development for Electrical Networks in Aeronautical Domain Analysis.
22. **Modelkey DSS**: Models for Assessing and Forecasting the Impact of Environmental Key Pollutants on Marine and Freshwater Ecosystems and Biodiversity
23. **MOSAIC**: Open-Source API and Platform for Multiple Clouds
24. **OPENAIRE**: Open Access Infrastructure for Research in Europe.
25. **OPEN-SME**: Open Source Software Reuse Service for SMEs.
26. **ORCHESTRA**: Organising dissemination on results of projects on chemical evaluation, spreading techniques for risk assessment (http://www.eu-orchestra.org/)
27. **PROAST**: Software package developed by the Dutch RIVM for the statistical analysis of dose-response data http://www.rivm.nl/en/Documents_and_publications/Scientific/Models/PROAST)
28. **ROSETTA**: Rosetta s Way Back to the Source: Towards Reverse Engineering of Complex Software. In execution.
29. **TOX-TRAIN**: implementation of a TOXicity assessment Tool for pRActical evaluation of life-cycle Impacts of techNologies (http://toxtrain.eu/)
30. **SMARTLM**: Grid-friendly software licensing for location independent application execution.

2.2 Selection of interesting projects

The main aim of the analysis of previous success stories was to learn from other projects related to software developed in the frame of European/national research projects and which are now widely disseminated among the scientific/regulatory/consultancy world. Therefore, the projects identified and listed in the previous paragraph were scanned in order to verify their correspondence to the main aims of the task. Key persons were identified, their availability to collaborate was checked and finally the following projects were selected:

1. ANTARES (Nazanin Golbamaki)
2. CREAM (Ida Dolciotti)
3. ERICA (Boris Alonso)
4. FOOTPRINT (Igor Dubus)
5. Modelkey (Elena Semenzin)
6. ORCHESTRA (Rodolfo Gonella Diaza).

Some of the projects identified were considered interesting in order to spread information about the 4FUN project to existing networks and to involve these networks in the dissemination activities. They were not included in the ‘success stories’ because they are still running, however were added to the list of interesting projects. The interesting projects are:

- ACROPOLIS
- A-TEAM
- BROWSE
- CONTAMED
- ConsExpo
- ChimERA
- PROAST
- TOX-TRAIN

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3 Collection of information

Measuring the success of projects and learning from failed projects can make a big impact on other projects. When evaluating a project, it is important to make the evaluation complete. Online surveys, email surveys, round-table discussions, questionnaires, interviews and one-on-one phone calls are excellent ways to evaluate a project. In order to reach the aims of the task 2.7, a questionnaire was developed and according to the availability of the different persons it was done in writing or via one-on-one phone calls.

The questionnaire was developed considering questions that need to be answered to demonstrate success and making sure that the questions could be answered unambiguously.

Twenty-two questions were developed considering different aspects:

- demonstrate whether the aims were achieved and the work was useful, know what was done, what went well, and what could have been improved. In this way it is possible to measure the success in relation to achieving the objectives and to gather information for improvements. If the project did not meet its objectives, it is usually a sign of insufficient resources or unclear objectives. Therefore, the following questions were developed:

  1. Brief description of the project: aims/ duration / consortium size/ type of project
  2. Were aims achieved?
  3. If not, what went wrong? What could have been improved?
  4. What would you do differently?
  5. What impact did the project have?

- Understand technical issues about the software development. This aspect can help to decide what changes might be made to the current project. The questions were:

  6. Was the software developed within a legislative framework?
  7. Which were the strengths and the weaknesses of the software?
  8. Was a standardization process included?

- Evaluate stakeholder satisfaction. If stakeholders are not satisfied, it is a sign there were inefficiencies in the project. It is important to verify whether the project provided benefits to its stakeholders. Successful projects create noticeable benefits. If the project has not realized benefits, it does not always mean the project was not executed successfully. The developed questions were:

  9. Were stakeholders involved?

10. If yes, how were stakeholders involved?
11. Did the software meet the needs of stakeholders?
12. How were the stakeholder needs identified?
13. What benefits were there for stakeholders?

- Evaluate end-user adoption. This aspect helps to determine if end-users are utilizing the software developed. If the project is successful, high-end user adoption and frequent use will be found. The addressed questions were:

14. Was the software delivered after the end of the project?
15. Are end-users still using the software? If not, why?
16. Who are the main users of the software?
17. What are the main reasons to use this tool?

- Financial issues. These issues are important to evaluate how the further maintenance of the software, and then its success, is funded. The questions were:

18. Is the software/tool currently sold? If yes, by whom?
19. What is the model price (or is it not free)?
20. How is the maintenance of the software managed? Are there any public or private funds to cover the maintenance costs?

- Dissemination activities. Some projects have excellent outcomes but they are not well disseminated among stakeholders. The success of a project is measured on how the delivery of the results went smoothly. The following questions were made:

21. What types of dissemination activities were done (eg: training courses, workshops, etc…)?
22. Were dissemination activities effective?

4 Summary of the information collected

For each selected project key persons were identified and contacted. The questionnaire was sent first by email, and then according to the availability of these persons, it was done by phone or by email.
The questionnaires fully compiled are shown in Annex I. Here a summary of the answers collected is reported.

All the selected projects were funded by the European Commission, however under different programs (e.g. LIFE, 6th Framework Programme, 7th Framework Programme, Marie Curie Initial Training Network, etc…). The consortia were usually quite big (between 7 to 26 partners) and made by different partners from all Europe. The duration was not less than 3 years.

As specified by the aims of the tasks, all projects developed software. However, the topics of the projects were different, and then the specific aims of the different software tools were diverse. The different aims do not interfere with the evaluation of success stories. The attention was mainly focused whether the projects met their objectives or not. Aims were always achieved, therefore software was developed (for ANTARES the main result was a characterization of the non-testing methods suitable for REACH; CREAM developed ecological models for the risk assessment on different organisms; ERICA provided an integrated approach to the assessment and management of environmental risks from ionising radiation; FOOTPRINT produced computer tools for risk assessment at the farm, catchment and national scales, and produced important advances in risk assessment; MODELKEY developed interlinked tools applicable to European freshwater and marine ecosystems; ORCHESTRA developed and promoted of the VEGA platform, a software containing predictive QSAR models, suitable for regulatory purpose).
Only two persons answered that something went wrong and could have been done differently. For FOOTPRINT, beta versions of the software tools were produced, but not released due to the lack of funding to finalise them and to support them in the long term. However, the two main scientists of the project created a start-up company (FOOTWAYS) and developed new improved tools partly based on the FOOTPRINT methodology. For Modelkey there was a problem of time lag between the starting of the project and the implementation of the related Directive by the local authorities. The final prototype was ready too late. Furthermore, stakeholders were involved late in the project and it was difficult to create collaboration with them.

The projects had different impacts. ANTARES made a survey of current methods for the compliance to the REACH legislation and identified criteria for the non-testing methods for the REACH legislation. CREAM represented a first step toward having general guidelines for the use of ecological models in the context of chemical risk assessments. Furthermore many scientific publications and presentations at conferences were made.The ERICA Integrated Approach and ERICA tool are widely used in the assessing of environmental risks from ionising radiation. FOOTPRINT demonstrated that the use of pesticides can be optimised to reduce impacts on water quality. Modelkey had many downloads, but in the context of research and not for the actual application within the Water Framework Directive. Within ORCHESTRA the organizations of events, courses and the production of videos containing interviews with regulators from ECHA and representatives from the chemical industry improved the understanding of the use of compute based models for regulatory purposes.

Except ERICA, the other software tools were developed within a legislative framework (e.g. CREAM with the legislation regarding the environmental risk assessment of pesticides, FOOTPRINT software was initially developed to support the Water Framework and the Sustainable Use directives, Modelkey was developed for implementing the Water Framework Directive, ORCHESTRA and ANTARES were developed in the framework of the REACH).
Strengths and weaknesses were different according to the different software tools, however user friendliness, simplify managing of large data sets, possibility of dealing with different situations were commonly seen as strengths.

The only project that took into consideration standardization was ORCHESTRA. Standardization was a key point in the ORCHESTRA project. Dealing with outcomes from multiple projects, interacting with possible users from different areas and with different backgrounds made it mandatory to create and to adopt standard methods. For example, while analysing the outcomes of the EC funded projects chosen as case studies, SWOT analysis were adopted. Furthermore, another example is the editing process of the online survey on “Benefits and barriers to the use of computer-based methods”. Also the VEGA platform, developed and promoted under ORCHESTRA, was, and currently is, developed paying attention to standardization. The possibility to reproduce and compare results is of key importance in every scientific field, therefore VEGA uses standard formats for inserting the molecules to predict and standardized parameters both for the prediction itself and the evaluation of the applicability domain.

Stakeholders’ involvement was an important issue in all the projects. Many efforts were done in order to keep stakeholders interested and informed on the projects, and to achieve their

needs. If stakeholders are not satisfied, it is a sign that there were inefficiencies in the project.

Within ANTARES stakeholders were involved in different meetings and seminars. Several meetings with industry and regulatory stakeholders helped in the identification of objectives and needs of stakeholders. Stakeholders were active partners of CREAM since the beginning of the project. Their needs were the starting point of the project. The ERICA project involved active participation of stakeholders. The work relied on an end-users group (EUG) established under the project, where a number of stakeholder dialogue methodologies were used to gather information based on end-users' experience, expertise and opinion. A one-day workshop dedicated to testing the ERICA integrated approach was organized. The ERICA e-newsletters were produced regularly to inform stakeholders of project progress. FOOTPRINT involved stakeholders mainly through the Advisory Committee of the project. Within ORCHESTRA stakeholders were involved during the whole lifetime of the project. Meetings and workshop were organized with regulators, as well as courses about the use of model and how to understand and evaluate its outcomes. Stakeholders' feedback was gained both during these events and with direct interviews. Furthermore several surveys, courses, exercises and interviews were organized.

The only project in which stakeholders' involvement was difficult was Modelkey. Basically they were not allowed to travel and to spend money for joining the training courses. The needs of stakeholders were identified taking into consideration the requirements of the water framework directive.

All the projects produced open source software, freely available, but users must be registered in order to make the download. The software tools are used mainly by industries and research, are not sold, and the maintenance is based on private funding. The platform VEGA-QSAR is maintained by the Mario Negri Institute, however other EC funded projects are continuing on the same area and contribute to the enhancement of the platform and the software. Modelkey is maintained via collaboration with other projects. The improvement done to the software lead to the publications of papers which is a good achievement from a scientific research perspective. Only the ERICA Tool is being maintained by a consortium (comprising the Norwegian Radiation Protection Authority, Environment Agency, Centre for Ecology & Hydrology, IRSN, the Swedish Radiation Safety Authority and CIEMAT). While FOOTWAYS sells its own tools (e.g.: Modul'O^{TM}, Tetris matrices, Footways Pro, etc…), the FOOTPRINT tool was not released (and is therefore not used nor sold). Annual subscriptions to use the web-based software tools, and consultancy services are used for maintaining the software and the company.

In general dissemination activities were related to the participation to international events and workshops (with small courses, oral presentations and posters) and the organization of meetings and courses with stakeholders (e.g. from chemical industries and regulatory bodies), the organization of seminars, events for industries. The CREAM project took advantage from the organizations of schools within the SETAC conference.

5 Overview of other successful stories

Despite the idea was that 'success stories' should be related to European or National projects which developed software widely disseminated, it was decided also to have a look at different kind of experiences. Therefore, the following 'successful stories' were investigated.

5.1 HYDRUS

HYDRUS is a model for simulating the movement of water, heat, and multiple solutes in variably saturated media. It is a wide used and well known model. One of the developers, Jirka Šimunek, was contacted in order to gather information.

HYDRUS-1D, which is a public domain Windows-based modeling environment for analysis of water flow and solute transport in variably saturated porous media, started as a governmental organization. However, the entire group fell apart, but people involved in the software development kept it going by themselves. Then, the GUI for HYDRUS (2D/3D) was developed in 3 years within the free time of the scientists involved at the beginning. Therefore, the model was kept alive by the constant support of the developers. The marketing for the model consists of a website (http://www.pc-progress.com/en/Default.aspx), conference presentations, and short courses (at least two per year, one in Europe and one in the USA). Furthermore, the model has a long list of scientific references.

5.2 FOCUS

Directive 91/414/EEC (the Plant Protection Products Directive) aimed to harmonise the overall arrangements for authorisation of plant protection products within EU by establishing agreed criteria for considering the safety of those products. The Directive and its six Annexes set out common rules and guidance on data requirements, data evaluation, risk assessment, the transition from a national to the EU authorisation system, the protection of commercial information, and public access to information on pesticides. A positive list of active substances (Annex I), that had been shown to be without unacceptable risk to people or the environment, was established. In the context of Annex VI of the Directive 91/414 it was stated: "… estimate, using a suitable calculation model validated at Community level, the concentration…". Therefore, it was necessary to provide guidance to the Member States, the European Commission, and industry on the role of modelling in the EU registration process and to provide tools for estimating environmental concentrations of active substances for the purpose of their assessment for inclusion in Annex I.

In 1993 FOCUS (the FOrum for Co-ordination of pesticide fate models and their Use) (http://focus.jrc.ec.europa.eu/) was established, as an initiative of the European Commission,

in order to harmonise the calculation of predicted environmental concentrations (PEC) of active substances of plant protection products in the framework of the EU Directive 91/414/EEC.

FOCUS was based on co-operation between scientists of regulatory agencies, academia and industry. The FOCUS Steering Committee consisted of the European Commission (DG SANCO), seven European Member States, and ECPA. The steering committee set different working groups dealing with different topics: ground water, surface water, landscape and mitigation, degradation kinetics and air.

Participants were scientists from governmental research institutes within EU, working for national registration authorities. Since 1993 the working groups developed scenarios and approved simulation models that are used to calculate the concentrations of plant protection products in groundwater and surface water in the EU review process according to Council Directive 91/414/EEC.

5.3 EUSES

The European Union System for the Evaluation of Substances (EUSES) is a decision-support instrument which enables government authorities, research institutes and chemical companies to carry out assessments of the risks posed by chemical substances to man and the environment (http://ihcp.jrc.ec.europa.eu/our_activities/public-health/risk_assessment_of_Biocides/euses/euses/?searchterm=None).

EUSES is a coordinated effort of: EU Member States, the European Commission, The European Chemicals Bureau, and the European Chemical Industry. The system is based on the EU Technical Guidance Documents (TGD) on Risk Assessment for New Notified Substances, Existing Substances and Biocides. The new EUSES 2.1.2 version (2012) is an update of EUSES 2.1, containing all Emission Scenario Documents for biocides.

The development of EUSES 2.1 was commissioned by the European Commission to the National Institute of Public Health and the Environment (RIVM, the Netherlands). The work was supervised by an EU working group consisting of representatives of the JRC-European Chemicals Bureau, EU Member States and the European chemical industry.

6 Conclusions

The answers collected to the main questions made are summarized in Table 1.

Table 1. Summary of the answers collected.

Main questions / Projects	Connection with legislative framework	Standardization process included	Stakeholders' involvement	Dissemination of results	Maintenance of the software
ANTARES	Yes	No	Yes	Yes	By the Institute leader of the software development
CREAM	Yes	No	Yes	Yes	By each software developer
ERICA	No	No	Yes	Yes	Via a Consortium
FOOTPRINT	Yes	No	Yes	Yes	Through annual subscription and consultancy service
Modelkey	Yes	No	Not very successful	Yes	Through different projects and internal funding
ORCHESTRA	Yes	Yes	Yes	Yes	By the Institute leader of the software development

The questionnaires and the study of the 'successful stories' helped to highlight some points that should be taken into account for making the MERLIN-Expo tool a success story as well.

It resulted important to have a **connection between the software and a legislative framework**. This point is also demonstrated by the story of the FOCUS, that in order to fulfil the requirements of the Directive 91/414/EEC developed standard scenarios and approved simulation models that are currently used in all Europe to calculate the concentrations of plant protection products in the environment. Furthermore, also the development of EUSES 2.1 was strictly related with risk assessment regulations. The MERLIN-Expo tool could be used within the framework of different legislations. The '4FUN European Observatory' (WP6) was planned to be created also in order to help connecting the tool with the relevant legislations. Furthermore, as demonstrated by the problems occurred within Modelkey, synchronised timing between new legislations and features of the tool is crucial. Therefore, 4FUN could take advantage of the '4FUN European Observatory' in order to keep the tool

updated according to requirements of the new legislations. However, a strategy to keep updated from a legislative perspective should be developed.

It is interesting to underline that an exception is represented by the success of HYDRUS. This software, in fact, was not developed for any regulatory purpose but it is a strong and reliable model for simulating the movement of water, heat, and multiple solutes in saturated media, and it is widely used. Therefore, another important point to consider in order to facilitate the use of the tool is to have a software which is **user friendly, flexible, fast and reliable**, all characteristics that appeared to be crucial in the projects investigated in the present deliverable.

Another important lesson learned from the success stories is that software should be **freely available**, but **registration for downloading** it should be **compulsory**. In this way it is possible to monitor the people interested in the tool that could be contacted in case of further developments or when organising training activities. The MERLIN-Expo tool follows the trend being freely available. The compulsory registration for downloading the tool will be taken into account.

Stakeholders' involvement is a critical issue. If stakeholders are not satisfied, it is a sign that there were inefficiencies in the project. Analysing the different projects it was shown that stakeholders were involved in different ways, such as: organizing **meetings**, **seminars** or **workshops**, **identify their needs**, promote their **active participation** (e.g. via end-users group), producing **e-newsletters** to inform on project progress, create an Advisory Committee of the project, organize **training courses** about the use of model and how to understand and evaluate outcomes. Furthermore, **surveys and interviews** could be useful as well. Training courses are crucial within the 4FUN project and will be carefully planned. Furthermore, the use of e-learning tools will be promoted within the project in order to reach stakeholders without asking them to travel and to spend money. Their active participation will be promoted using a forum where stakeholders can find easily the answers to their questions and interact with the software developers.

Dissemination of results is important to guarantee knowledge transfer: participation to **international conferences and workshops** (oral presentations and posters), and organization of **meetings and courses** with stakeholders, **events for industries**, **schools within the SETAC** conference. Furthermore, scientific publications in **peer reviewed journals** and in **books** can add an important scientific value. Some of these activities are already planned in the dissemination plan of the 4FUN project, but other should be considered. For example, schools could be organized within the SETAC conference, and a book could be written.

Standardization is an important aspect that not all the projects took into account. Within the 4FUN project standardization is highly considered with the aim to improve transparency and

accessibility of large exposure models by specifying the requirements for the information to be provided in the documentation along with guidelines on presentation. This will allow the user to better compare existing risk exposure models, and will also support the more rigorous formulation of risk exposure models.

Finally, it is important to monitor the **financial status** of the project in order to **avoid** the risk of the **lack of funding** during the course of the project. A detailed business plan was developed (WP7) in order to plan the long-term support of the tool (e.g. via private funding, creating a consortium, asking annual subscriptions and consultancy services, etc…). The maintenance of the software is a critical point that was addressed differently within the different projects. Asking for annual subscriptions, giving paid consultancy services, or creating a consortium could be the possible solutions for the future of the MERLIN-Expo tool.

In conclusion, the present deliverable gave the possibility of summarizing concrete suggestions to be taken into account for assuring the success of the 4FUN project. The key elements are:

- link between the software and legislation
- user friendly, flexible, fast and reliable software
- freely available software, but with compulsory registration for downloading
- keep stakeholders involved via e-learning, training schools, and forum
- organize schools within the SETAC conference, write a book
- standardize the tool
- monitor the financial status
- plan the long-term support of the tool.

7 References

Agarwal N., Rathod U. Defining success for software projects: an exploratory revelation. International Journal of Project Management. Vol 24, issue 4, May 2006, 358-370

Jianga J.J., Kleinb G., Discenzab R. Perception differences of software success: provider and user views of system metrics. Journal of systems and software. Vol 63, issue 1, 15 july 2002, 17-27

Annex 1

ANTARES (Alternative Non-Testing methods Assessed for REACH Substances) - Nazanin Golbamaki

1. Brief description of the project: aims/ duration / consortium size/ type of project

REACH legislation states that Non-Testing Methods (NTM) can be used within REACH. These methods include Quantitative Structure-Activity Relationship (QSAR) models and read-across. Before making an animal experiment the industry should verify if alternative methods exist. However, so far there is a deep gap of knowledge on which methods are available and can be used in practice. ANTARES aims to reduce this gap assessing NTM as an alternative approach for the REACH legislation. The NTM methods are examples of alternative methods which predict the effects of chemicals without the use of the real compound, but only on the basis of the compound structure. They include Quantitative Structure-Activity Relationship (QSAR) models and Read-Across.

The main objectives were: to verify the possible use and performance of the non-testing methods for REACH; to identify requirements and constraints originating from the REACH legislation which may affect the non-testing methods; to identify safety assessment factors for the non-testing methods; to identify the best applicability criteria for a safer use of the non-testing methods; to integrate different non-testing methods, achieving superior performance; to disseminate the results; to promote non-testing methods for legislative purposes.

LIFE (L'Instrument Financier pour l'Environnement) is the EU's funding instrument for the environment, launched by the European Commission and coordinated by the Environment Directorate-General. The general objective of LIFE is to contribute to the implementation, updating and development of EU environmental policy and legislation by co-financing pilot or demonstration projects with European added value.

The ANTARES project has been declared eligible under the programme component LIFE+ Environment Policy and Governance. LIFE08 ENV/IT/00435 (http://ec.europa.eu/environment/life/about/index.htm)

2. Were aims achieved?

Yes, the main result was a characterization of the non-testing methods suitable for REACH. We think the duration and size of the project were appropriate.

3. If not, what went wrong? What could have been improved?

4. What would you do differently?

5. What impact did the project have?

The following have been achieved during the project: survey of current methods for the compliance to the REACH legislation; identification of the criteria for the non-testing methods for the REACH legislation; identification of suitable experimental databases/data sets for the

ecotoxicological, toxicological and environmental endpoints for REACH; list of (Q)SAR models for the ecotoxicological, toxicological and environmental endpoints for REACH, and their review; validation of non-testing methods; identification of boundaries for best use of models (applicability domain) and of the assessment factors; architecture for integration of different non-testing methods for best performances and coverage of applicability.

6. Was the software developed within a legislative framework? Which were the strengths and the weaknesses of the software?

The software is user friendly and fast.

7. Was a standardization process included?

We checked the different software programs according to a standardized check list

8. Were stakeholders involved?

Yes, in different meetings and seminars (see the next question)

9. If yes, how were stakeholders involved?

The following is the list of events towards industry performed during the ANTARES project:

F.I.S. (Fabbrica Italiana Sintetici), Montecchio Maggiore, Italy - Seminar on the use of QSAR models for toxicity evaluation

APR 20 2012: S.I.S.T.E., Milan, Italy - Seminar on alternative methods for cosmetics (Regolamento 1223/09: Nuove metodologie e piattaforme informatiche)

MAR 8 2012: 8ª Conferenza Sicurezza Prodotti - A che punto siamo con il REACH, Milan, Italy

FEB 16 2012: Gent, Belgium - QSAR Workshop at ARCHE Consulting

DEC 15 2011: Milan, Italy - 2nd National Conference: Rethinking the equation REACH = Regulation

OCT 5-7 2011: Milan, Italy - Chem-Med 2011 - The International chemical event

JUN 20 2011: Lisbon, Portugal - Training Workshop on QSAR as a Tool in Chemical Risk Assessment

MAR-APR 30-1 2011: Barcelona, Spain - OSIRIS Fourth Annual Meeting

MAR 22 2011: Istituto Mario Negri, Milan, Italy - Course on "Il metodo QSAR e sue applicazioni pratiche nel Regolamento REACH"

MAR 8-9 2011: Leipzig, Germany - OSIRIS ITS Stakeholder Workshop

FEB 3 2011: Milan, Italy - 6° Conferenza Sicurezza Prodotti: REACH

DEC 15 2010: Milan, Italy - Workshop Centro Reach "Prepararsi al 2011: come realizzare attività dif R&S e servizi professionali, insieme al Centro Reach"

NOV 17-18 2010: Brussels, Belgium - Cefic-LRI 12th Annual Workshop on "Reduction of uncertainty Enabling Decision Making"

JUN 16-17 2010: Stresa, Italy - Workshop of ICCA/CEFIC/JRC "Integrating New Advances in Exposure Science and Toxicity Testing: Next Steps"

MAY 11 2010: Istituto Mario Negri, Milan, Italy, Centro Reach - Course on QSAR methods

FEB 24 2010: Milan, Italy - Workshop of Federchimica "The LRI Long Range Research Initiative"

FEB 9 2010: Istituto Mario Negri, Milan, Italy, Centro Reach - Course on QSAR methods

10. Did the software meet the needs of stakeholders?

Yes

11. How were the stakeholder needs identified?

Several meetings with industry and regulatory stakeholders guided us through the identification of objectives and needs of both groups.

12. What benefits were there for stakeholders?

ANTARES had covered a vast range of activities in building models for industry use, comparison of the existing models for prediction of toxicity for a large number of toxicity endpoints (38 endpoints covered), identifications of needs of regulatory and industry stakeholders for characterization of toxicity and ecotoxicity of chemicals.

13. Was the software put on the market after the end of the project?

The software is freely available through VEGA QSAR platform: http://www.vega-qsar.eu/

14. Are end-users still using the software? If not, why?

Yes

15. Who are the main users of the software?

Industry and research

16. What are the main reasons to use this tool?

Early identification of chemical structures that may lead to toxic effect of the chemical, the software is user friendly, free and the performance of different predictive models is documented in related manuscripts and compared to other models available (commercial and free models).

17. Is the software/tool currently sold? If yes, by who?

No

18. Which is the model price (free access, etc…)?

Free access

19. How is the maintenance of the software managed? Are there any public or private funds to cover the maintenance costs?

The platform VEGA-QSAR is maintained by the Mario Negri Institute, however other EC funded projects are continuing on the same area and contribute to the enhancement of the platform and included software.

20. What types of dissemination activities were done (eg: training courses, workshops, etc…)?

Seminars for the European regulatory bodies, international events participation, courses and initiatives, events for industries, workshops and seminars, meetings with national regulatory

bodies. The complete list of dissemination activities is available at: http://www.antares-life.eu/index.php?sec=events

21. Were dissemination activities effective?

Yes

CREAM (Mechanistic Effect Models for Ecological Risk Assessment of Chemicals) - Ida Dolciotti

1. Brief description of the project: aims/ duration / consortium size/ type of project

CREAM was a Marie Curie Initial Training Network, funded by the European Commission within the 7th Framework Programme and started in September 2009. The duration was 4 years, but for bureaucratic reasons it was prolonged for another year (http://cream-itn.eu). The consortium consisted of 13 partner institutions and 10 associated partners from industry, regulatory authorities, and research organizations.

Current risk assessments focus on risk at the level of individual organisms, but according to EU directives the protection goal for most species aims at achieving sustainable populations. Population-level effects depend not only on exposure and toxicity, but also on important ecological factors that are difficult to fully address empirically. Mechanistic effect models (MEMs) enable the integration of these factors, increasing the ecological relevance of risk assessments and providing understanding on how chemicals interact with ecosystems. CREAM developed and experimentally validated a suite of MEMs for organisms relevant for chemical risk assessments of chemicals, primarily pesticides. CREAM included 20 PhD and three postdoc projects.

2. Were aims achieved?

Yes, all projects were related to the developing of ecological models for the risk assessment on different organisms of interest for the environmental risk assessment of pesticides

3. If not, what went wrong? What could have been improved?

4. What would you do differently?

5. What impact did the project have?

The project represented a first step toward having general guidelines for the use of ecological models in the context of chemical risk assessments. The project had a positive impact; many scientific publications and presentation at conferences were made.

6. Was the software developed within a legislative framework? Which were the strengths and the weaknesses of the software?

Toxicological models are not yet included in the legislation regarding the risk assessment to evaluate the risk of pesticides in the environment. Ecological models are becoming important in the context of chemical risk assessments. However, no general guidelines exist for their development and use. The project was a first step to provide a tool for regulatory agencies to assess the environmental risks of pesticides.

CREAM developed a suite of MEMs, all models have both strengths and weaknesses.

7. Was a standardization process included?

The CREAM represented the first step towards the implementation of a good modelling practice: a standard framework for the transparent and comprehensive documentation of ecological models and the underlying modelling process – the TRACE documentation. Documentation encompasses the whole modelling process: development, testing and analysis. The TRACE documentation framework can only become established as a standard if it is applied and refined by numerous projects. The CREAM project encompassed several ecological modelling projects with the objective of application in chemical risk assessment. All modelling projects applied the TRACE framework for documentation. Accordingly, CREAM functioned as a test bed, and is producing a collection of examples for TRACE.

8. Were stakeholders involved?

Yes, within the consortium there were representatives from industries, academia, and national environmental protection agencies

9. If yes, how were stakeholders involved?

Stakeholders were active partners since the beginning of the project.

10. Did the software meet the needs of stakeholders?

Stakeholders' need were the starting point of the project because they needed to make more effective the process for the assessment of toxicity

11. How were the stakeholder needs identified?

Needs were identified by the stakeholders taking part in the project

12. What benefits were there for stakeholders?

The benefit was making a first step toward a platform for ecological models for chemical risk assessments (as the FOCUS for fate models).

13. Was the software put on the market after the end of the project?

No

14. Are end-users still using the software? If not, why?

15. Who are the main users of the software?

Industries, agencies and mainly academia

16. What are the main reasons to use this tool?

Having mechanistic effect models for different population-level effects to carry out risk assessments

17. Is the software/tool currently sold? If yes, by who?

No

18. Which is the model price (free access, etc…)?

Most of the models are open source and free available online

19. How is the maintenance of the software managed? Are there any public or private funds to cover the maintenance costs?

The project does not deal with the maintenance of the software. Each developer takes care of the maintenance.

20. What types of dissemination activities were done (eg: training courses, workshops, etc…)?

As a Marie Curie Initial Training Network, CREAM was designed to provide training for ecological modellers. Workshops involving persons from industries and agencies were organized to use the models via key studies.

SETAC winter schools and one-day courses at SETAC were organized in order to teach people how to use the models. Participants paid a fee. Announcements were done at the SETAC website. Two main conferences were organized, at the middle and at the end of the project, all participants were invited and also students from different universities and other agencies (as EPA, etc…) attended the conferences

Furthermore, many works were presented during sessions at of different conference (e.g. SETAC EU and US).

The conference was opened to external contributions that referred to the research topics of CREAM. The workshop was open for up to 100 participants including representatives from European regulatory agencies, chemical companies and consultants. Keynote presentations by project members and invited scientists were given on different aspects of the CREAM background.

21. Were dissemination activities effective?

Yes

ERICA (environmental risks from ionising contaminants: assessment and management) - Boris Alonso

1. Brief description of the project: aims/ duration / consortium size/ type of project

The ERICA project (EC contract no. FI6R-CT-2004-508847).

The objectives of ERICA was to provide an integrated approach to the assessment and management of environmental risks from ionising radiation with emphasis on biota and ecosystems, and to develop the ERICA Tool, which is a software programme with supporting databases that together with its associated help will guide users through the assessment process. Duration: 36 months

Project coordinator: Swedish Radiation Protection Authority (SE)

Project partners: Swedish Nuclear Fuel and Waste Management Company (SE); Facilia AB (SE); Södertörn University College (SE); Norwegian Radiation Protection Authority (NO); Agricultural University of Norway (NO); Spanish Research Centre in Energy, Environment and Technology (ES); UK Environment Agency (UK); University of Liverpool (UK); Natural Environment Research Council (UK); Westlakes Scientific Consulting (UK); Finnish Radiation and Nuclear Safety Authority (FI); French Institute for Radiological Protection and Nuclear

Safety (FR); Électricité de France (FR); German National Research Centre for Environment and Health (DE)

More than 60 European scientists contributed to the ERICA Integrated Approach. Facilia AB played a vital role not only with the scientific contribution but also with technical support for the development of ERICA Tool.

The ERICA project was partly funded by the EU under the Sixth Euratom Framework Programme (FP6 Euratom). It brought together over 50 scientists from 15 organisations and 7 countries.

2. Were aims achieved?

The final deliverable of the project, D-ERICA, describes the integrated approach. https://wiki.ceh.ac.uk/download/attachments/115017395/D-Erica.pdf?version=1. The ERICA tool can be downloaded from http://www.erica-tool.com/

3. If not, what went wrong? What could have been improved?

4. What would you do differently?

5. What impact did the project have?

The ERICA Integrated Approach and ERICA tool are widely used in the assessing of environmental risks from ionising radiation.

6. Was the software developed within a legislative framework?

No.

7. Which were the strengths and the weaknesses of the software?

Strengths: the ERICA tool guides the user through the assessment process, recording information and decisions as the assessment progresses. The ERICA tool simplifies the managing of large data sets underpinning the assessment approach and prevents the potential to introduce errors when performing numerous calculations manually.

Weaknesses: It does not address situations where an organism may inhabit more than one ecosystem, or where a radioactive release may impact upon more than one ecosystem. The ERICA Tool does not allow for multiple input sources into an area.

8. Was a standardization process included?

No

9. Were stakeholders involved?

The ERICA project involved active participation of stakeholders. The work relied to a great extent on an end-users group (EUG) established under the project, where a number of stakeholder dialogue methodologies were used to gather information based on end-users' experience, expertise and opinion. The end-users group (EUG) was created with 52 international and national organisations from Europe, Australia, Canada, Japan, and the USA. The EUG was composed of regulators, academia, industry, NGOs, and inter-governmental organisations. This forum enabled the project to host eight events to discuss issues based on specific themes, including assessment frameworks and scientific knowledge

gaps; ionising radiation and other contaminants; decision-making and stakeholder involvement; scientific uncertainties; a consensus seminar; management, compliance and demonstration; an ERICA tool testing day; and a local stakeholder event. WP3 in conjunction with WP1 organised a one-day workshop with the EUG to test the ERICA tool and developed a training pack for the ERICA Open Event, organised in Paris, February 2007. WP3 also developed the deliverable D8 relating to decision-making and options to be considered at the formulation stage, which will impact on the scope of the assessment.

10. If yes, how were stakeholders involved?

The EUG events focused on exploring individual 'experiences in order to draw out useful information for the project. The EUG participants were asked to provide a short summary of their experience and a comprehensive evaluation of the work plans for the four ERICA Work Packages (WPs). The comments and suggestions from the EUG were included and reproduced accurately in form of deliverables.

https://wiki.ceh.ac.uk/display/rpemain/ERICA+reports

A one-day workshop dedicated to testing the ERICA integrated approach, i.e. the ERICA assessment tool prototype and the draft deliverable D-ERICA, was held. Seven EUG members attended and six ERICA Consortium participants. EUG members were asked to provide feedback on use of the tool and its guidance. As a result, a list was collated containing comments, improvements and software bugs.

The ERICA e-newsletters were produced regularly to inform stakeholders of project progress and seek views on WP issues.

11. Did the software meet the needs of stakeholders?

Yes

12. How were the stakeholder needs identified?

See answers to question 9 and 10.

13. What benefits were there for stakeholders?

As a result of the cooperation with the EUG members, a number of important changes and additions have been made to the Integrated Approach and to the tool.

14. Was the software put on the market after the end of the project?

No, the tool is freely available at http://www.erica-tool.com/. All new users have to register before receiving a download.

15. Are end-users still using the software? If not, why?

Yes.

16. Who are the main users of the software?

Those interested in assessing the radiological risk to biota.

17. What are the main reasons to use this tool?

The tool simplifies the use of the ERICA Integrated Approach. It incorporated databases. The ERICA Tool and the Integrated Approach are well documented.

18. Is the software/tool currently sold? If yes, by who?

No, the tool is free.

19. Which is the model price (free access, etc…)?

No, the tool is free.

20. How is the maintenance of the software managed? Are there any public or private funds to cover the maintenance costs?

The ERICA Tool is being maintained by a consortium comprising the Norwegian Radiation Protection Authority, Environment Agency (England and Wales), Centre for Ecology & Hydrology (UK), IRSN (France) the Swedish Radiation Safety Authority and CIEMAT (Spain).

21. What types of dissemination activities were done (eg: training courses, workshops, etc…)?

The ERICA e-newsletters were produced regularly to inform stakeholders of project progress and seek views on WP issues. The ERICA project produced a number of deliverables during the lifetime of the three-year project.

22. Were dissemination activities effective?

Yes

FOOTPRINT (Functional Tools for Pesticide Risk Assessment and Management in Europe) - Igor Dubus

1. Brief description of the project: aims/ duration / consortium size/ type of project

FOOTPRINT (Functional TOOls for Pesticide RIsk assessmenNt and managemenT) was a research project funded by the European Commission as part of its 6th sixth Framework Programme for Research and Technological Development (FP6).

The project aims at developing methodologies and first versions of computer tools to evaluate - and reduce - the risk of pesticides impacting on water resources in the EU (surface water and groundwater). The project started in January 2006 and benefits from DG Research support for 3.5 years, i.e. until June 2009. The project involved 15 partner organisations from 9 European countries.

2. Were aims achieved?

The aims of the FOOTPRINT project were achieved. First versions of the 3 computer tools (risk assessment at the farm, catchment and national scales) were produced. The project also produced important advances in risk assessment science and a database of pesticide environmental properties (FOOTPRINT PPDB).

3. If not, what went wrong? What could have been improved?

4. What would you do differently?

Beta versions of the software tools were produced, but these could not be released due to the lack of the funding to finalise them and to support them in the long term.

The two main scientists on the project resigned from their research position at the end of the EU project to create a start-up company (FOOTWAYS) and to develop new improved tools partly based on the FOOTPRINT methodology. FOOTWAYS now developed 5 software tools which are operational across all EU countries: Proziris (pesticide registration), Footways Pro (reporting to the Commission), Modul'O (catchment and river basin action plans), Tetris matrices (improved agricultural advice) and Bluetiful (farm scale optimisation of crop protection practices).

5. What impact did the project have?

The project demonstrated that use of pesticides can be optimised to reduce impacts on water quality.

6. Was the software developed within a legislative framework?

The FOOTPRINT software was initially developed to support the Water Framework and the Sustainable Use directives. The FOOTWAYS tools have been designed to support these 2 directives and also the registration regulation (1107/2009/EC)

7. Which were the strengths and the weaknesses of the software?

Strengths: the software was conceived to be used in any EU country and at any scale (from fields to countries).

Weaknesses: the methodology relied on a pre-modelling approach which proved unfeasible. FOOTWAYS adapted the methodology to address the shortcomings and the FOOTWAYS tools, now rely on on-demand modelling.

8. Was a standardization process included?

No

9. Were stakeholders involved?

Yes

10. If yes, how were stakeholders involved?

Through the Advisory Committee of the project.

11. Did the software meet the needs of stakeholders?

Yes, but the software tools could not be finalised (see above). New tools were developed by the project coordinator and a colleague.

12. How were the stakeholder needs identified?

We carried out specific workshops based on the first beta versions of the tools.

13. What benefits were there for stakeholders?

New tools for pesticide risk assessment and management which did not exist before.

14. Was the software put on the market after the end of the project?

The FOOTPRINT tools were never released, but new tools partly based on the FOOTPRINT methodology were put on the market.

15. Are end-users still using the software? If not, why?

End-users are using the FOOTWAYS tools.

16. Who are the main users of the software?

We have a wide range of users of the FOOTWAYS tools: Ministries, water agencies, risk agencies, local authorities, agricultural advisory services, farmers cooperatives, farmers, food industry.

17. What are the main reasons to use this tool?

Limitation of the impact of pesticides on water resources.

18. Is the software/tool currently sold? If yes, by who?

FOOTWAYS sells its own tools. The FOOTPRINT tool was not released (and is therefore not used nor sold).

19. Which is the model price (free access, etc…)?

Annual subscriptions to use the web-based software tools, and consultancy services.

20. How is the maintenance of the software managed? Are there any public or private funds to cover the maintenance costs?

Private funds only.

21. What types of dissemination activities were done (eg: training courses, workshops, etc…)?

FOOTPRINT tools: initial trainings with beta versions of the software tools.

FOOTWAYS tools: commercialisation, training, support and maintenance.

22. Were dissemination activities effective?

FOOTPRINT: no.

FOOTWAYS: yes.

Modelkey (Models for Assessing and Forecasting the Impact of Environmental Key Pollutants on Marine and Freshwater Ecosystems and Biodiversity) - Elena Semenzin

1. Brief description of the project: aims/ duration / consortium size/ type of project

The project was funded by the EC 6th Framework programme in "Sustainable Development, Global Change and Ecosystems" (Contract-No. 511237 (GOCE)) (http://www.modelkey.org/). It started in 2005 and ended in 2010. The consortium was made by 26 partners from 14 different EU countries.

The main aim was to support the implementation of the water framework directive, trough different tools focusing of toxic substances in water, looking for emerging substances other than the 33 priority substances. MODELKEY had a multidisciplinary approach aiming at developing interlinked tools as well as state-of-the-art effect-assessment and analytical methods applicable to European freshwater and marine ecosystems: to assess, forecast, and mitigate the risks of pollutants on fresh water and marine ecosystems and their biodiversity at a river basin scale; to provide early warning strategies on the basis of sub-lethal effects in vitro and in vivo; to provide a better understanding of cause-effect-relationships between changes in biodiversity and the ecological status; to provide methods

for risk assessment and decision support systems for the selection of the most efficient management options to prevent effects on biodiversity and to prioritise contamination sources and contaminated sites; to strengthen the scientific knowledge at European level in the field of impact assessment of environmental pollution on aquatic ecosystems.

2. Were aims achieved?

The main aims were achieved; in particular models were developed, a database was created and the system for supporting decision-making was settled.

3. If not, what went wrong? What could have been improved?

There was a problem of time lag between the starting of the project and the implementation of the Directive by the local authorities. The final prototype was ready when the local authorities had already found tools for implementing the directive. Furthermore, end users were contacted late in the project. It was difficult to have the participation of stakeholders to trainings, workshops and to the project itself. Therefore not all the workshops planned were carried out, the solution was to make one-to-one person meeting, but it was not feasible. The improvement could have been to contact the stakeholders at the very beginning of the project, in order to get info on their needs and to create collaboration with them, or to involve more stakeholders within the consortium.

4. What would you do differently?

Involve stakeholders from the beginning to gather their needs, and take care of their participation

5. What impact did the project have?

There was a good scientific feedback, the software was tested by end users and some scientific publications were done. However, local authorities preferred easier approaches There were many downloads, but in context of research and not for the actual application within the directive.

6. Was the software developed within a legislative framework? Which were the strengths and the weaknesses of the software?

The software was developed considering the water framework directive and its guidelines. However, it was difficult to cover all the phases of implementation of the directive. The software allowed to evaluate the ecological and socio economic status of water bodies, but did not consider the last phase of the directive regarding the measures for intervention plans. The software was useful for managing a big amount of data

7. Was a standardization process included?

No

8. Were stakeholders involved?

Yes, but stakeholders involvement was difficult because they were not allowed to travel and to spend money in doing courses in EU.

9. If yes, how were stakeholders involved?

The stakeholders' involvement was due to the networking activities carried out by partners

10. Did the software meet the needs of stakeholders?

In general yes, but having stakeholders in the projects since the beginning would have contributed to improve more the software

11. How were the stakeholder needs identified?

The needs of stakeholders were identified taking into consideration the requirements of the directive.

12. What benefits were there for stakeholders?

The benefits were related to the possibility of assessing the ecological and socio economic status in order to prioritize water bodies and individuate hot spots areas

13. Was the software put on the market after the end of the project?

No, because there was no interest at national level

14. Are end-users still using the software? If not, why?

No, because stakeholders already had their tools

15. Who are the main users of the software?

The users are researches. Furthermore collaboration with China for the evaluation of water quality will allow to apply it to other conditions and to improve it a bit

16. What are the main reasons to use this tool?

17. Is the software/tool currently sold? If yes, by who?

No

18. Which is the model price (free access, etc…)?

Free download online, after registration

19. How is the maintenance of the software managed? Are there any public or private funds to cover the maintenance costs?

The maintenance was done without funding or via collaboration with other projects. The improvement done to the software lead to the publications of papers which is a good achievement from a scientific research perspective

20. What types of dissemination activities were done (eg: training courses, workshops, etc…)?

A workshop and a final conference were organized. The work was presented at several scientific conferences and published in scientific journals. The testing was carried out only online

21. Were dissemination activities effective?

Yes, but it was not possible to perform all the activities planned; the plan was changed during the course of the project taking in consideration the difficulties for involving stakeholders. For example the testing was done only online, and then it was completely rearranged.

ORCHESTRA (Organising dissemination on Results of projects on Chemical Evaluation, Spreading Techniques for Risk Assessment) - Rodolfo Gonella Diaza

1. Brief description of the project: aims/ duration / consortium size/ type of project

ORCHESTRA was an EU project, funded to disseminate recent research on computer-based in silico methods for evaluating the toxicity of chemicals. The main aim of the project was therefore to promote wider understanding, awareness and appropriate use of in silico methods.

The project consortium was composed by 7 beneficiaries and included scientists involved in toxicology and the development of in silico methods, and social scientists specializing in the analysis and responsible communication of science research. During its 36 months of duration ORCHESTRA directly interacted with a range of stakeholder organizations and individuals, including for examples chemical industries, consultants, policy makers, model developers, etc.

2. Were aims achieved?

Yes, ORCHESTRA successfully organized events, interviews, open questionnaires and produced a series of informative documents and videos. Moreover, the project actively contributed in the development and promotion of the VEGA (www.vega-qsar.eu) platform, a software containing predictive QSAR models, suitable for regulatory purpose, developed by several projects and institutions (e.g. CAESAR project, US EPA, etc.).

3. If not, what went wrong? What could have been improved?

4. What would you do differently?

5. What impact did the project have?

Thanks to the involvement of experts in communications, ORCHESTRA contributed in the improvements of the dissemination of results obtained by projects involved in alternative methods. The organizations of events, courses and the production of videos containing interviews with regulators from ECHA and representatives from the chemical industry also improved the understanding of the use of compute based model for regulatory purposes.

6. Was the software developed within a legislative framework?

ORCHESTRA contributed in the development of VEGA, which contains several models developed for example within the REACH regulation framework. Moreover, VEGA has been provided with several tools which help the user to better understand and support the predictions obtained by the models.

7. Which were the strengths and the weaknesses of the software?

VEGA provides users with additional information about the reliability of the prediction, evaluating if the submitted molecules are within the Applicability Domain (AD) of the model. In some cases the software also provides reasoning of the prediction, such as the presence of known structural alerts. An important feature, which is also the most important basis for the AD evaluation, it is that VEGA provides users with similar compounds present in the

models' dataset, showing both the structure and the experimental values, thus giving the possibility to make decisions of the prediction obtained. Considering the use of VEGA within the regulatory perspective, a possible limitation is that the software doesn't automatically provide the QSAR model reporting format (QMRF).

8. Was a standardization process included?

Standardization was a keyword of the ORCHESTRA project. Dealing with outcomes from multiple projects, interacting with stakeholders possible users from different areas and with different backgrounds made it mandatory to create and or adopt standard methods. For example, while analysing the outcomes of the EC funded projects chosen as case studies, the so-called SWOT analysis (Strength – Weakness – Opportunities – Threats) were adopted. Another important example was the editing process of the on line survey on "Benefits and barriers to the use of computer-based methods". Also VEGA was, and currently is, developed paying attention to standardization. Keeping in mind that the possibility to reproduce and compare results is of key importance in every scientific fields, VEGA uses standard formats for inserting the molecules to predict and standardized parameters both for the prediction itself and the evaluation of the applicability domain.

9. Were stakeholders involved?

Yes, from different areas (e.g. chemical industry, regulatory bodies, etc)

10. If yes, how were stakeholders involved?

Stakeholders were involved during the whole lifetime of the project. Meetings and workshop were organized with regulators, as well as courses about the use of model and how to understand and evaluate their outcomes. Stakeholders' feedback was gained both during these events and with direct interviews. These feedbacks were then used for example to improve the usability and the features included in VEGA.

11. Did the software meet the needs of stakeholders?

Yes, VEGA received positive feed backs from stakeholders

12. How were the stakeholder needs identified?

Several surveys, courses, exercises and interviews were organized.

13. What benefits were there for stakeholders?

The supporting information provided by VEGA for the predictions were judged very useful by stakeholders, for the interpretation and the evaluation of the prediction itself.

14. Was the software put on the market after the end of the project?

The software is open source and is therefore available for free download and usage at www.vega-qsar.eu

15. Are end-users still using the software? If not, why?

In order to download VEGA, the users must be registered to the website and downloads (as well as the accesses to the website) are monitored. From these information people are still

downloading and using the software. Moreover, VEGA is still promoted and disseminated mainly by ORCHESTRA's main beneficiary, the Mario Negri Institute.

16. Who are the main users of the software?

VEGA currently counts almost 1500 registered users from chemical industry, regulatory bodies and academia.

17. What are the main reasons to use this tool?

VEGA contains predictive QSAR models for several (eco)toxicology endpoint as well as for environmental and physico-chemical properties. The number of models present is expected to grow. All the models included have been developed within regulatory frameworks and are provided with the dataset used and with documentation and information. Moreover, as already explained, a series of tools have been integrated in VEGA, to help users in understanding the results and their reliability.

18. Is the software/tool currently sold? If yes, by who?

The software is currently maintained and updated and is available at the official website: www.vega-qsar.eu

19. Which is the model price (free access, etc…)?

Open source / free use and download.

20. How is the maintenance of the software managed? Are there any public or private funds to cover the maintenance costs?

VEGA is maintained mainly by Istituto Mario Negri with contributions and supports from several other institutions (see www.vega-qsar.eu/contributors.html for more information).

21. What types of dissemination activities were done (eg: training courses, workshops, etc…)?

The main dissemination activities were, and still are, the participation to international events and workshops (with small courses, oral presentations and posters) and the organization of small meetings and courses with stakeholders (e.g. from chemical industries and regulatory bodies).

22. Were dissemination activities effective?

Being mostly face-to-face activities, feedbacks and comments have been continuously collected. VEGA has been appreciated and the number of registered users is still growing.