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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Dissemination Level		
PU	Public	x
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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Abbreviations

CRA	Certification of environmental Risk Assessors
CEEP	Cremona Executive Education Programme
CIR	Chemicals Industry Regulations
CS	Case Study
EC	European Commission
EFSA	European Food Safety Authority
EU	European Union
EUSES	European Union System for the Evaluation of Substances
FP7	Seventh Framework Programme
GUI	Graphic User Interface
IHCP	Institute for Health and Consumer Protection
IPCHEM	Information Platform for Chemical Monitoring
JRC	Joint Research Centre
PBPK	Physiologically Based Pharmacokinetic
PCB	Polychlorinated biphenyl
PEC	Predicted Environmental Concentrations
PFOA	Perfluorooctanoic acid
QSAR	Quantitative Structure-Activity Relationship
QSPR	Quantitative Structure Property Relationships
SETAC	Society of Environmental Toxicology and Chemistry
SME	Small and medium-sized enterprise
TK	Toxicokinetic

1 Introduction

MERLIN-Expo, designed as a prototype tool by the 2FUN project, is here to answer the present conundrum of coupling environmental multimedia and pharmacokinetic models. It is seen as the future of chemical fate assessment and has been hailed as a highly promising tool by the European Commission for the assessment of human exposure to chemicals.

Current exposure assessment is recognised by many as a weak point in ecological and human health risk assessment due to a lack of integrated approaches for combined stressors, widespread use of over-conservative 'worst-case' scenarios, estimation of only external and not internal exposures and a lack of uncertainty and sensitivity analysis for the identification of key exposure drivers. However, contrived by the leading e-fate modelling minds of Europe, MERLIN-Expo arrives precisely when needed to liberate us from currently available tools that show major flaws and lack an integrated approach. Equipped with a flexible modular format, pharmacokinetic considerations, and uncertainty and sensitivity analysis functionality, MERLIN-Expo can enable robust, regulatory-relevant environmental and exposure assessments with ease and transparency. At a time when chemical risk assessment to human health is a major concern for policy and industry regulators alike, the need of such a tool has never been more evident.

Now under the 4FUN project, MERLIN-Expo will be taken to the market following thorough standardization processes and dissemination activities. With the help of the workshops and summer school outlined in this report a proper examination of MERLIN-Expo's strengths and weaknesses can be performed and end-user requirements can be identified. The Workshops and training events were organised in such a way as to reach out to as many people as possible in different locations across the EU and promote the tool. The aim was also to raise the skill level of regulators and enable a community of users to develop.

When this work package was first conceived (as specified in the Description of Work) we imagined that the best way to deliver training would be to have 4 training events, each of 1 week. During the 4-FUN project, the format of the training was debated intensely. The final decision on the format was based on the following factors:

- A sense that professional people would generally not be able to commit 1 week coming to an event (although students probably could).
- A sense that we needed a variety of options that could appeal to a variety of people
- The idea that it would be good to link to other events that were already planned (and this was more important than having a specifically Nordic workshop).
- The need to include people from other work packages as part of the training programme in order to harness their expertise
- The lack of legacy if we simply deliver face-to-face training

In the end, the original plan was modified by splitting the training programme into 7 portions. These were:

1) A training workshop for professionals working in regulatory agencies
2) A scientific training workshop delivered in Belgrade
3) A scientific training workshop delivered to the JRC in Ispra
4) A scientific training workshop delivered in Barcelona as part of the SETAC conference

5) A summer school delivered in Cremona (Italy) as part of the SETAC Summer Schools programme and the CEEP programme
6) A scientific training workshop delivered in Barcelona to coordinate with the Informa Chemicals Industry Regulations conference
7) An online training programme

Alongside this, the MERLIN-Expo tool was presented at various other conferences and seminars, but without a specific training element.

1.1 Purpose of this plan/ report

This report outlines the process of preparing and delivering the training programme, the experience of delivering the programme and the feedback received about the programme.

2 Regulatory Workshop (Paris, March 2015)

2.1 List of contributors.

4-FUN partners giving presentations

Emma Grange; James Garratt; Philippe Ciffroy; Boris Alfonso; Elisa Giubilato; Artur Radomyski; Zoran Banjac; Frederik Verdonck; Céline Brochot; Paul Quindroit.

Main authors of this section of the deliverable report

James Garratt; Rodyn Gilharry; Emma Grange

2.2 In advance of the workshop

This workshop in Paris was our first demonstration of MERLIN-Expo and therefore a lot of preparation was done beforehand to ensure all the materials were ready. Heavy promotion was done via email to encourage participants to register and all registration was kept track of by staff at Enviresearch Ltd. The agenda for the workshop was drafted by James Garratt and Emma Grange who then sent it out to the other partners for comments or modifications. The lecturers for the topics was chosen by who had the most experience and expertise in the relevant field. Each lecturer was in charge of creating his or her own PowerPoint slides for the workshop and the final versions were emailed to Enviresearch for the production of delegate packs. The logistics such as location and catering for the workshop were arranged by Philippe Ciffroy. As a 4FUN partner working in Paris he was the best person to take charge to this important task.

2.2.1 Intended Audience

As the name suggests the intended audience for this workshop were environmental regulators.

2.2.2 Number of Attendees

There were a total of 17 registered participants for this event with 18 actually showing up on the day of the workshop.

2.3 During the workshop

During the workshop, the main focus was on ensuring that all presentations were delivered according to the agenda, and that delegates felt supported throughout. We also wished to enable some discussion and peer-support within the workshop where possible. We wanted to take advantage of the opportunity to spot bugs and problems within the modelling tool, and to document them for fixing at a later date. These points were all delivered.

2.3.1 Peer-discussion

From the point of view of development of the MERLIN-Expo tool, the most important was the peer-discussion. There were 2 sessions dedicated to this: at the end of the first day and at the end of the second day. Good discussion was generated in the first, but the second was quite flat. The main themes from the discussion were as follows.

The advantages of MERLIN-Expo

People generally liked the tool. The reasons given were:

- You can easily construct a trophic web
- It is easy to use

- It has good functionality
- It is transparent (especially important for the uncertainty / sensitivity analysis)
- It is not anthropocentric (combines both human and environmental aspects)
- Easy to import and export to spreadsheets
- Data structure is robust
- Useful for risk assessment of contaminants, e.g. cadmium in food
- Potentially useful for analysis of emerging contaminants where there are few data
- It is in principle useful for biocides as a higher-tier approach
- It's most important applications may be in resolving difficult problems

The disadvantages of MERLIN-Expo

- It is complex and takes time if you are not initially familiar with it.
- As a regulatory tool, it is too complex for a first-tier assessment.
- Some elements may be questioned by the scientific community, e.g. half-lives in fish, QSAR models (so the user must pay attention to the applicability domain)
- Documentation is not currently available online
- Default values for substances depend on having an exact substance in mind. It would be useful to have a set of values for a 'generic' example for a class of contaminants, e.g. 'generic PCB'.
- Since EUSES is the 'standard' people would only turn to MERLIN-Expo if they needed a higher-tier approach.

Things to consider for future

- Case studies for specific risk assessment problems, to show the utility of the tool.
- Demonstrate how you can reproduce an existing model (e.g. EUSES) with a constrained MERLIN-Expo and then demonstrate the added value of additional options available within MERLIN-Expo.
- For future support, this should maybe continue to be an EC programme.
- Potential to link with the IPCHEM project in JRC
- Potential to link to the EFSA report on uncertainty and sensitivity to be published in June 2015.

2.4 After the workshop

2.4.1 Facilitator discussion

The group of trainers discussed together how things might be improved, and the feedback from the participants was reviewed. The key themes from the discussion were as follows.

Could have gone better

- It would have been good to get for all participants to get to the end of all the case studies.
- It would have been good for all facilitators to test the case studies before the workshop.
- There were quite a lot of bugs in the model.
- Some of the instructions for the case studies were not clear enough.

Things that went well

- We could answer most of the questions that were put to us.
- The model worked.

- The sensitivity analysis case study was impressively detailed.
- We started and finished punctually
- Delegates turned up.
- The level of support was strong (always somebody to help).

Notes for future courses

- Explain the 'connections' between the models better within the documentation.
- Maybe have simpler case studies, e. g. the PBPK case study might not need a river.
- For the SETAC workshop, we should omit the information on the 4-FUN project itself.
- We should add discussion on how to interpret the results.
- Sensitivity analysis could be performed on an existing case study.

2.4.2 Feedback forms.

The results from the feedback were generally very positive. The questions had a 5-point scale, and if we assume that points 4 or 5 represent success, then nearly every question was successful for 13 out of the 15 responses.

The cases where this was not true are as follows (number of responses rated 1-3):

- The content is relevant to my job (5)
- I will be able to use what I learned in this workshop (4)

Specific points for improvement from a tick-list were:

- Provide better information before the workshop (4)
- Improve the tests used in the workshop (2)
- Increase the content covered in workshop (2)
- Clarify the workshop objectives (1)
- Update the content covered in the workshop (1)
- Make the workshop more difficult (1)

In the free-text responses about possible improvements to the workshop, comments were received covering the organisation of the meeting, the training on the use of MERLIN-Expo and the training on the interpretation of the results from MERLIN-Expo.

Organisation

- Very clear logistics (the fact that the dinner was in Chatou, not in Paris, should have been clarified and a map from entrance to meeting room)
- Attendees were mostly from Anses, would be interesting to have the view and experience from other member states – maybe improve the communication / advertising of the project toward all EU?

Use of the tool

- Maybe to reduce the [number of] case studies and focus more on one case study; explore further the possibilities of the software
- Maybe provide more info on the sources used to input default parameter values.

- More explanations on sensitivity analysis. A bit difficult in interpretation, many diagrams with colours, but no so evident to understand every step. Maybe a more step-by-step method work on sensitivity analysis could help.

Interpretation of results

- Improve the interpretation of the results, graphics
- As a regulatory tool (and because other regulatory tools already validated exist), the output relevant for evaluation may be more clearly presented. As example, PEC calculations but for some compartment tools are missing for some uses (biocides ground water risk assessment etc.)
- To look at the results of the simulation and how they can be / are used.
- Comparison with classical tools to clearly show advantages / disadvantages should be stressed more

A few respondents gave feedback on the most and least useful elements of the training. These are shown in Table 1.

Table 1: Most useful and least useful elements of the Paris workshop as stated by the participants.

Most useful	**Least useful**
Very well prepared, organized, thought	Not all models still available in the tool
Many facilitators in the room during 'self-paced' workshops.	How to build models connecting external exposure to internal exposure
Time for discussions.	Also, comparison of MERLIN-Expo with other tools would be useful.
Nice tool!	Not so much things related to PPP assessment and residues in food
Practical cases	
Getting in a rather short time a good overview about the potential of this tool	
Everything was valuable. Thank you.	
Workshop intended for regulators	
Excellent format, good balance between lectures and practical work.	
After 2 days I think I will be able to use the software, the course was very efficient.	
To know what is in MERLIN-Expo	
Know how to use MERLIN-Expo and the different functionalities	
Practical sessions	
Uncertainty and sensitivity analysis	
PBPK model	

2.5 Conclusions from Regulatory Workshop in Paris

The workshop can be considered a great success. The notable points from all the data collected were that:

a) The MERLIN-Expo tool is a good tool and people are interested
b) The course was a good course, well organised, well presented and with a good balance
c) There are areas where we could improve. In particular
    i. The quality of the information provided before the workshop
    ii. The clarity of the instructions from the case studies
    iii. The interpretation of the results from the case studies
    iv. The comparison with other models

3 Scientific workshop, Belgrade (April 2015)

3.1 List of contributors.

4-FUN partners giving presentations

Aleksandar Vlajic; James Garratt; Johan Bierkens; Boris Alfonso; Zoran Banjac.

External experts contributing to the training

Momir Paunovic

Main authors of this section of the deliverable report

James Garratt; Rodyn Gilharry; Aleksandar Vlajic

3.2 Preparing for the workshop

As the only workshop to be held in Eastern Europe the importance of this event in Belgrade could not be overstated. Equipped with the experience gained in the Paris workshop, lecturers and facilitators knew what to fix in the teaching material and how to modify the schedule to allow for smoother running of the workshop. Some changes where done to accommodate specific problems that were unique to the Belgrade workshop. For example, Aleksander Vlajic, the main coordinator of this workshop requested for the schedule of the second day be shifted by half an hour to an hour to accommodate students coming all the way from Novi Sad located about 90km out of Belgrade. Indeed if it was not for the help of Aleksandar, the workshop may not have ran as smoothly. As a Serbian working in Belgrade he was able to make a lot of the arrangements such as location, catering and preparation of course materials. After the Paris workshop each lecturer was in charge of modifying and editing their presentations and teaching materials accordingly and send their final versions to Aleksander. As most, if not all of the participants of this workshop were Serbians, Aleksander also took charge of keeping track of the registrations. The major steps in preparing for the workshop are discussed in the following sections.

3.2.1 Intended Audience

This workshop was planned for risk assessment scientists of Eastern Europe.

3.2.2 Number of Attendees

This workshop had an incredible turn out of around 20 participants.

3.3 During the workshop

During the workshop the priority was on delivering the presentations as clearly as possible and on sticking to the agenda. As most of the participants in this workshop were students, compared to Paris workshop, more effort was placed on making the presentations as easy to understand as possible. Speakers went out of their way to make attendees feel welcome, such as James learning some Serbian words to make the attendees feel comfortable. The MERLIN-Expo tool worked much better than in the Paris workshop while carrying out the simulations, facilitating our work. The tool had not been updated since Paris, so we believe that this was due to improved instructions, allowing fewer opportunities for the users to act independently. We also wished to enable some discussion and peer-support within the workshop where possible. Speakers did well in showing the applicability and potential of MERLIN-Expo.

3.3.1 Peer-discussion

Peer-Discussion was one of the most important activities in this workshop as it allowed us to assess the performance of the MERLIN-Expo tool and point out bugs and glitches not seen in the Paris workshop, but most importantly, it allowed us to get a feel of how the tool is being viewed by participants. Since the program worked exceptionally well in this workshop, there were not much comments regarding program glitches, but the participants did share their thoughts on the program. There were sessions dedicated to this at the end of both days. Some of the main points and questions that were discussed were as follows. Comments fell into the following categories.

MERLIN-Expo tool: what can it be used for?

- Where do we position our model in comparison to the other models?
- Can the model be used for higher tier in risk assessments?
- Can we specify what it can/can't be used for?
- Can it be used to estimate air pollution or exposure to air from oil companies and the population?
- Can we use it for inverse modelling, e.g. to estimate exposure from measured concentrations in blood?

MERLIN-Expo tool: comments on PBPK model

- It would be interesting to amend the metabolism part of the PBPK model. If you add an antidote, can it interact with the contaminant?
- Toxicokinetics (TK) could be different between sick /healthy individuals

MERLIN-Expo tool: comments on probabilistic analysis

- It would be good to have better conclusions for probabilistic analysis. What is 'important' or 'significant'? Most people should be able to interpret results in the same way.

MERLIN-Expo tool: comments on the substance database

- Which form are the metal contaminants, e.g. Lead, Mercury? It makes a big difference.
- PFOA (used in case study 2a) is very polar for an example organic
- It would be helpful to have information on how to add a new contaminant, including links to databases and Quantitative Structure Property Relationships (QSPR).

The workshop: areas for improvement

- More simple and clear instructions should be used in the case study examples.
- Terminology – The terms used in the instructions should be similar to that used in the software to avoid confusion when doing the case studies. Participants might get stuck finding a label in the software that is not named the same.
- All instructions should be included in the 'building a CS' outline, even the small simple steps.

- The GUI has many helpful or useful tricks and shortcuts, we should create a glossary that lists them to make participants and users of the model aware of them, such as 'double-clicking' does this, 'right-clicking' does that, etc.
- We should use easier case studies with fewer parameters in examples. Also re-think the order of how case-studies are presented.

Things to consider for future:

- Something that could make the tool more appealing or expand its versatility would be to create an online/open access library with some time series data and complete models/scenarios. This would allow researchers and regulators to simply download data directly instead of having to generate loads of time series data, which can be quite complicated, time consuming and tedious.
- Areas where the participants saw the possibility of future applications for the tool include:
  - Hotspots for concern and risk mitigation.
  - Environmental impact assessment for sites of new facilities.
  - New direction of research: contaminants, processes, sampling strategies etc.
- One of the attendees suggested to make the invertebrates' population model, this would make the model very useful in research and she would buy it together with her colleagues.
- Medical attendees expressed interest in the population model, but this was not available at the Belgrade workshop

3.4 After the workshop

3.4.1 Facilitator discussion

The group of facilitators and lecturers discussed together how things might be improved, and the feedback from the participants was reviewed. The key themes from the discussion were as follows.

Things that could have gone better

- Too much in one case study (CS 2b)
  - The copy/paste did not go well; too many little steps to successfully copy and paste data.
- First contact should be sooner and simpler, delegates want to be clicking and start using the tool from early on. Perhaps Case study 1 could be used better and allow for the delegates to get early exposure by using the 'open the file' option and allowing them to go through a solved case step by step.
- Case materials need to be better completed: you should be able to follow the case study even if you have not seen the introductory presentation.
- Functionalities could be better demonstrated especially import/export.
- Combine the two Uncertainty presentations.
- Late cancellations was a problem.
- There were no people from the business sector
- The facilitators were not the most experienced users. For some elements, there was very short notice to prepare.

Things that went well

- The facilitators did really well considering their experience.
- There was a good mix of people, a nice group.
- People were really interested in the tool, this may help with future support.

- Momir Paunovic's talk was excellent. He showed himself to be a true local expert.
- The recap and introduction went well.
- People felt at ease.
- The discussion at the end of day 2 went well.
- The Venue was good, both in location and catering.
- Finished on time.
- Fewer bugs than Paris.

Delivering consistent quality training

We had a discussion around how to deliver consistently good training on diverse topics, such as we find with MERLIN-Expo. It is complicated because not every specialist can be at every workshop. Some of the key questions were the following:

- How should a workshop be organised? As a standard package or as a specialist scientific course? If it is a standard package, then anybody could present the material, which would make it more widely accessible. However, it would mean that you would not necessarily get the in-depth analysis from a specialist in that particular area.
- Currently, success in the training workshops depends on the goodwill of presenters (to put the effort into preparation and then to turn up). Maybe attendance by the key presenters should be obligatory? It would certainly be easier if more 4 FUN partners could attend and cover their area of work. However, it makes the training package quite inflexible and vulnerable to the availability of key individuals.
- Each presenter needs to have a thorough understanding of the material. This was a problem for the first probabilistic presentation – how do you present someone else's message? So, even if it becomes a 'standard' package of materials, the trainer needs to be confident on the whole package.

3.4.2 Feedback forms.

Fifteen participants filled out the feedback form. The results from the feedback were very positive. The questions had a 5-point scale, and if we assume that points 4 or 5 represent success, then every question was successful for 12 out of the 15 responses.

Questions 1-13: the ratings on various elements of the workshop

Out of the 15 persons that filled out the form:

- 100% agreed that the workshop lived up to their expectations, gave them sufficient practice and was a good way for them to learn the content.
- 80% said the content was relevant to their jobs and 100% said they would be able to use what they learnt.
- 93% rated the workshop as either Excellent or Very Good.
- 87% are very likely to recommend MERLIN –Expo to a friend or colleague.

The cases where less positive responses were received are as follows (number of responses rated 1-3):

- The content is relevant to my job (3)
- The workshop objectives were clear to me (2)
- The pace of this workshop was appropriate (1)

Question 14: the tick list of options for improvement

Specific points for improvement from a tick-list were: (percentage of participants that choose the same option).

- Improve the instructional methods. (40%)
- Clarify the workshop objectives. (33%)
- Increase the content covered in the workshop. (27%)
- Add more video to the workshop. (27%)
- Provide better information before the workshop. (20%)
- Make workshop activities more stimulating. (20%)
- Make the workshop less difficult. (20%)
- Allot more time for the workshop. (20%)
- Improve the tests used in the workshop. (20%)

Questions 15-17: free-text responses to the workshop

In the free-text responses about possible improvements to the workshop, some participants commented

(1) "I would recommend more examples, case studies and practical work."
(2) "Change the order of demonstrations, start with simple and explain the basics of combining models."
(3) "Maybe the course lasts longer."
(4) "More work with real results."

When asked what was least valuable about the workshop most participants gave positive comments, such as:

> "Every information had value", "All is important."

However, there was one comment that said:

> "The most complicated demonstrations, they are too specific, difficult to follow and almost impossible to generalize."

When asked what was most valuable in the workshop, almost all participants agreed that it was the "case study examples and practical work in the tool".

3.5 Conclusions from Scientific Workshop in Belgrade

The workshop can be considered a great success. Some of the more notable points from the workshop and all the data collected were that:

a) The MERLIN-Expo tool is a good tool and people are genuinely interested in it.
b) The course was an excellent way of presenting the model and teaching how to use it, it had a good balance of lectures and practical examples.
c) Some participants felt that simpler and less specific case studies should be used, however this may be influenced by that fact that most of the participants were students and therefore they did not have as much exposure compared to other users, such as those in the Paris workshop for example.
d) Participants want to get their hands on the model from early on so maybe the structure and order of lectures and case studies could be changed in future workshops.
e) There are areas where we could improve. In particular

i. Clarify the workshop objectives
ii. Improve the clarity and simplicity of the instructions
iii. The interpretation of the results from the case studies

4 Short Course, SETAC – Barcelona (May 2015)

4.1 List of contributors.

4-FUN partners giving presentations or facilitating

James Garratt; Philippe Ciffroy; Boris Alfonso; Elisa Giubilato; Zoran Banjac.

Main authors of this section of the deliverable report

James Garratt; Rodyn Gilharry

4.2 Preparing for the Short Course

The opportunity to host a short course in the 2015 SETAC conference in Barcelona was a big opportunity for MERLIN-Expo to gain some exposure. SETAC is a large organization with risk analysis experts coming to their conference from all over Europe, and so if MERLIN-Expo is to catch the attention of regulatory experts it needs to take advantage of opportunities like this to gain notoriety and spark interest. The organizing of the short course was different from previous events because with SETAC being the main organizer we had to ensure we keep within their guidelines and schedule. Certain aspects of the short course such as venue and catering were handled by SETAC, which reduced the workload on us, however we were still responsible for the preparation of our own delegate packs. By this workshop, the teaching materials used were mostly all standardised and only slightly modified from event to event. Most errors had been detected and removed from past workshops and therefore editing was hardly ever required. Registration for the short course was monitored by SETAC and at the end of the registration deadline, they sent us a list of participants. The number of registered participants for this event was not as high as past workshops and this could have been as a result of a high registration fee charged by SETAC that many people were not willing to pay.

4.2.1 Intended Audience

The SETAC short course was aimed mostly towards academia and the education of students about MERLIN-Expo, however participants from the Industrial Sector were also encouraged to attend.

4.2.2 Number of Attendees

There was not a large turnout for this event, 10 people registered for the course but only 6 showed up on the day of the event

4.3 During the Short Course

During the short course, the priority was on delivering the presentations as clearly as possible and on sticking to the agenda. The only deviation from the agenda was a really helpful, special presentation done by Philippe Ciffroy where he tried to define new substances that could be used in the software. There was a total of six participants for the short course, of that two were from the industrial sector and four were students. Speakers did well in showing the applicability and potential of MERLIN-Expo.

4.3.1 Peer-discussion

There was no time for peer discussion.

4.3.2 Facilitator discussion

After the workshop, the facilitators met and discussed the events of the day. Their views fell into three categories: What could have gone better; things that went well; and notes for future courses.

What could have gone better

- The room was claustrophobic, it would have been crowed if 10 participants had arrived.
- Only six out of the ten registered participants showed up. This is because some of the registered participants did not pay the fee and the price was thought to be off-putting.
- There was no time for group discussions. Due to the short amount of time available to cover such a large amount of information, we ran out of time and no discussions were held.
- Need to let people know where to go next. A shortcut to the website should have been placed on the memory stick.
- The Uncertainty and sensitivity case study was too rushed.

Things that went well

- Some people went through to the end with the instructions.
- The Venice case study went really well.
- We managed to fit a lot in such a short time.
- The short presentation by Boris was really helpful.

Notes for future courses

- Explore the effects of food intake rates for different ages of individuals.
- Perhaps extend the PBPK model to include 0-20 years.
- For the JRC agenda:
    - Morning: Theory and basic Introduction.
    - Afternoon: Present the PBPK model.
    - Day 2: Present the uncertainty and sensitivity case study.

4.3.3 Feedback forms.

The feedback forms used for this training event were standard issued SETAC evaluation forms. The results were collected and processed by SETAC. Figure 1 shows the responses to the thirteen questions. You can note that the majority of the responses were very positive showing the participants' contempt with the short course, with three out of the thirteen questions receiving all 'excellent' evaluations.

Some of the comments and recommendations included:

(1) "I am looking forward to further upgrades and application of MERLIN-Expo."
(2) "Very useful, thank you."
(3) "The manual is good. I would enlarge the slides on the pages so that they are readable. Also the case study text is hard to read."

4.4 Conclusions from the SETAC-Barcelona Short Course

The short course can be considered a success. Considering the limited amount of time available we were still able to cover a large amount of information and carry out a number of case studies. The participants seemed genuinely interested in the tool and impressed with its

capabilities. The only negative thing about the short course was the low number of attendees and because of this we couldn’t collect a lot of feedback.

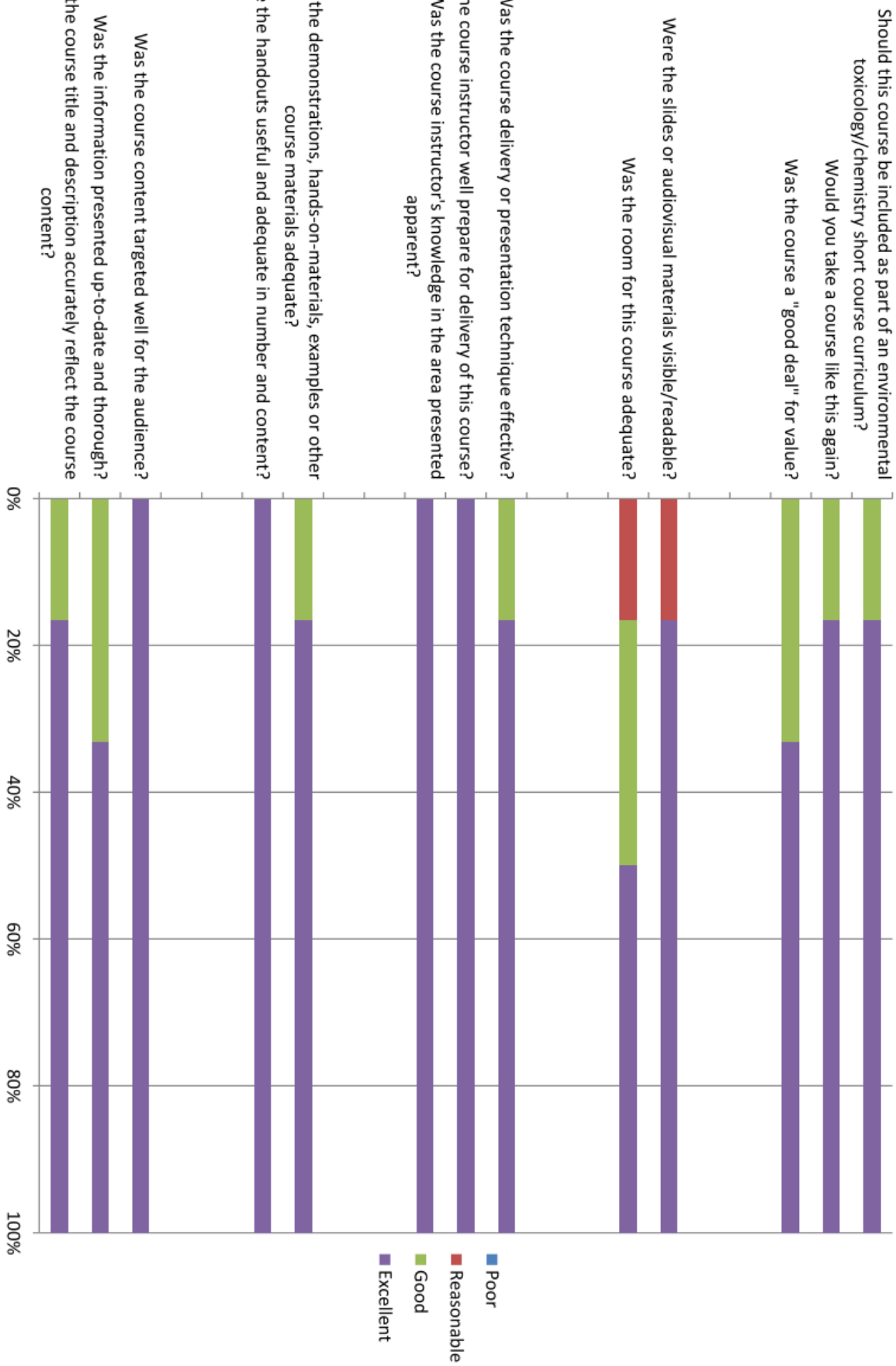

Figure 1. SETAC feedback forms review

5 JRC Workshop

5.1 List of contributors.

4-FUN partners giving presentations

Philippe Ciffroy; Boris Alfonso; Gabriella Fait; Elisa Giubilato; Artur Radomyski

(Some presentations were prepared by other 4-FUN partners: Zoran Banjac; Frederik Verdonck; Céline Brochot; Paul Quindroit)

Presenters from the JRC

Stylianos Kephalopoulos; Alexandre Zenié

Main authors of this section of the deliverable report

Gabriella Fait

5.2 Preparing for the Workshop

This workshop was held at the Joint Research Centre (JRC), located in Ispra (Italy), a Directorate General of the European Commission. It was organized thanks to the acquaintance between Alexandre Zenie and some members of the 4FUN consortium (Philippe Ciffroy, Elisa Giubilato and Andrea Critto). Alexandre Zenie works for the Institute for Health and Consumer Protection (IHCP), which is one of the seven institutes of JRC and provides scientific support to the development and implementation of European Union policies related to health and consumer protection. The institute carries out research to improve the understanding of potential health risks posed by chemicals, biocides, genetically modified organisms, etc..

The agenda was drafted by Philippe Ciffroy in collaboration with the partners involved in the training and Alexandre Zenie in order to adapt to the JRC requirements. An introductory presentation was added in order to highlight the main features of the MERLIN-Expo software and all the activities done (CEN standardization, trainings, 4FUN observatory).

The lecturers for this training were chosen considering the expertise in the relevant fields and the availability to travel to Italy. Each lecturer created his or her own PowerPoint slides for the workshop taking into account the previous experiences and the final versions were emailed to AEIFORIA for the production of delegate packs. The logistics such as location and catering for the workshop were arranged by JRC.

5.2.1 Intended Audience

Since this workshop was organized according to a specific request from Alexandre Zenie, the audience was made of JRC employees belonging to different institutes (mainly the Institute for Environment and Sustainability – IES, and the Institute for Health and Consumer Protection - IHCP).

5.2.2 Number of Attendees

The registrations to this event were collected directly by Alexandre Zenie. There were 16 participants; half of them followed the entire workshop, while the other half followed only specific parts.

5.3 During the Workshop

During the workshop, it was necessary to change and adapt the agenda several times in order to meet participants' needs. This occurred because the workshop was organized in the working environment of the participants.

5.3.1 Peer-discussion

The audience was made of people working at JRC, with deep knowledge in several areas related to the 4FUN project (exposure/risk assessment, epidemiology, toxicology, etc.). Therefore, participants were quite active, asked many questions, even quite specific on the features of the models, validation process, standardization, benchmarking, etc.. For instance, they asked how the natural bio-availability is included in the PBPK model, how the atmosphere model works, at which scale the model runs, whether it is possible to make repeated exposure and define continue exposure. Furthermore, they gave some suggestions, such as to include a dermal root model (at JRC there are people working on dermal model), to add an 'undo button' in order to have the chance to go back when changing a parameter, and to build standard scenarios.

5.4 After the Workshop

During and after the workshop, the trainers discussed together about positive and negative aspects of the training, the key topics were as follows.

5.4.1 Facilitator's Discussion

Things that could have gone better

- According to all trainers, a critical issue of the training at JRC was the fact that it was organized at the working place of participants. Thus, except for a group who attended the whole training from the beginning until the end, the other participants attended only some sessions, coming and leaving the training depending on their work commitments. This condition hampered the smoothly development of the training. Furthermore, also on request of the local contact point, it was necessary to change and adapt the agenda several times during the training in order to facilitate people who had to leave earlier
- In general, the audience was perceived not always entirely focused on presentations/exercises
- The discontinuous participation affected the understanding of the course contents and some participants were asking questions about the sessions they missed, thus slowing down presentations or exercises
- Some participants seemed not to have completely understood the applicability domain and the scope of the tool
- Some specific questions on the PBPK model (e.g., difference between modelling ingestion via the GI tract and modelling ingestion through direct input to the liver) could not be answered satisfactorily by the trainers due to limited knowledge on PBPK details.

Things that went well

- The location was fine and suitable to the number of participants, laptops were prepared in advance by JRC staff with the last version of MERLIN-Expo already installed
- Participants were all people working in research/policy-support at JRC, coming from different JRC units and with different backgrounds (exposure/risk assessment, epidemiology, toxicology, etc.)
- Participants were quite active, asked many questions

- The contents of the training course and the material were improved since the first training and were quite “robust” and well verified. Despite the difficulties related to the discontinuous participation, most of participants succeeded in running most of the practical sessions
- Despite the last-minute changes in the agenda, presentations and exercises went well and, from participants’ feedbacks, it seems that trainers managed to convey the main concepts
- A good overview of 4FUN activities was provided (presentations by Philippe Ciffroy and Gabriella Fait in particular), including not only MERLIN-Expo development but also benchmarking activities, demonstration through case studies with real monitoring data, CEN workshop/models’ documentation, training and educational activities. This was quite useful considering the purposes of the training, i.e. to explore possible interest in JRC staff to support in some way the further development and maintenance of the tool
- Uncertainty and sensitivity analysis features and the capability to perform long term dynamic simulations were appreciated as the most interesting and promising characteristics of the tool
- The presentation on the Venice case study and the associated practical session were integrated with the tutorial video on the fish model, which provided details on the processes included in the model and applicability domain. This seemed useful to support participants in better understanding what they do in the hands on session on food web modelling.

5.4.2 Feedback forms

General Notes:

(1) A total of 9 participants filled out the feedback forms and the overall response was very positive, the participants rated the training as either Excellent or Very Good.

(2) The participants seemed disposed to recommend the MERLIN-Expo tool to a friend or a colleague and showed interest in being informed on events, follow up activities, collaboration with the project, etc. Considering the high level of expertise of the audience this is a valuable feedback for the project.

(3) The participants agreed and strongly agreed (40% and 60% respectively) that the training was a good way to learn about the tool and almost all of them strongly agreed that the instructors were helpful.

(4) In general, participants gave good feedbacks to the training. The only points were some of them ‘neither agree nor disagree’ concerned: gathering sufficient practice and feedback, accomplishment of the objectives, ability to use what learned. It has to be underlined that the information previous to the training was not managed by the consortium, but directly by our contact person in JRC.

Figure 2 shows the rating of the questions from 1 to 12.

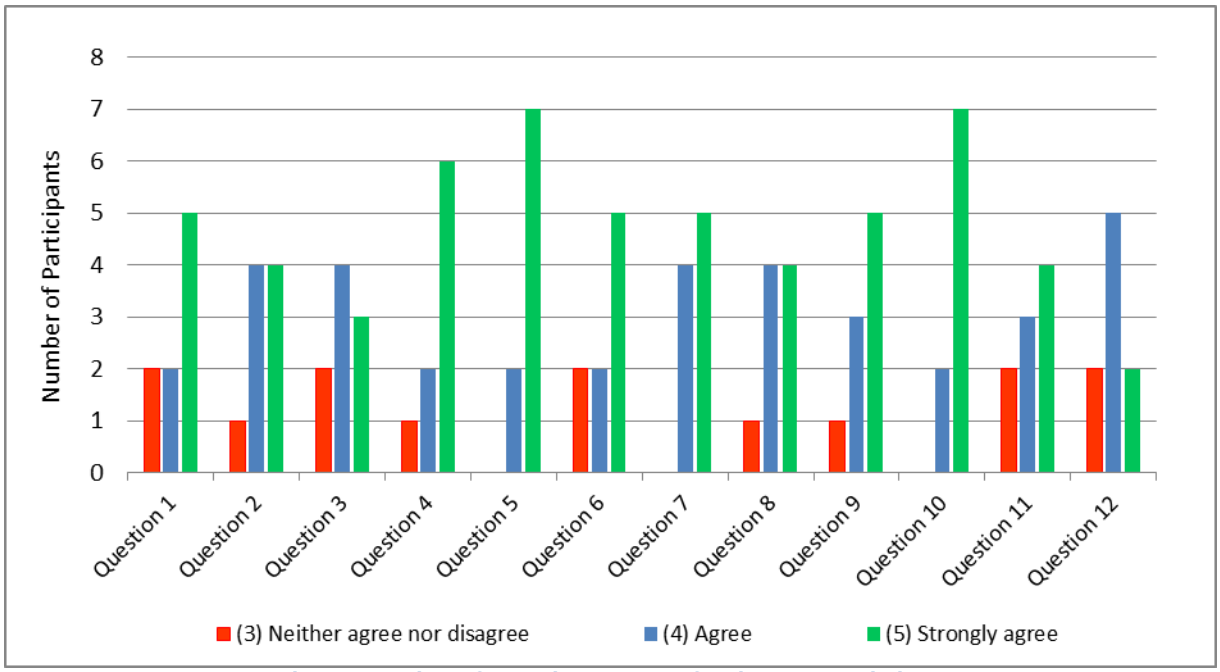

Figure 2 Rating of questions 1 to 12 for the JRC workshop

Q1. I was well informed about the objectives of this training.

Q2. This training lived up to my expectations.

Q3. The content is relevant to my job.

Q4. The training objectives were clear to me.

Q5. The training activities stimulated my learning.

Q6. The activities in this training gave me sufficient practice and feedback.

Q7. The difficulty level of this training was appropriate.

Q8. The pace of this training was appropriate.

Q9. The instructors were well prepared.

Q10. The instructors were helpful.

Q11. I accomplished the objectives of this training.

Q12. I will be able to use what I learned in this training

Improvement Recommendations:

- Question 14 in the feedback form allows the participant to choose certain ways in which they would improve the training. Most participants chose not to fill out this section. However, some of them ticked a few options: improve the training organization; improve the tests used in the training; provide better information before the training; update the content covered in the training. Two of the participants ticked the option related to use more video tutorials in the training.

Free Comment Section:

- In the feedback form there was a question that allowed the participant to write down his or her personal suggestions in order to improve the training. Only few participants gave us his/her opinions. One of them suggested improving some case study data and the explanations of the data. Another participant proposed to do the sensitivity analysis in the 1st day or at the beginning of day 2 and to give more insight on this

topic, for example adding a reference list of papers published in the framework of the project

- No participant filled question 16 related to what was least valuable about the training
- Question 17 asked what was most valuable about the training. Only few participants answered this question indicating the hand on sessions and the support by trainers as the most valuable about the training.

5.5 Conclusions from the JRC training

The training at JRC can be considered a success. Considering the difficulties given by the changes done to the agenda, we were able to cover all the planned topics and carry out all the practical case studies. The participants showed interest in the tool and were able to carry out the case studies, meaning that MERLIN-Expo is a straightforward and easy-to-use tool. The negative thing about the training was the interruptions due to the discontinuous participation of the participants.

6 Cremona Summer School 2015 (29th June – 3rd July)

6.1 List of contributors.

4-FUN partners giving presentations or chairing sessions regarding MERLIN-Expo

Gabriella Fait; Nicoleta Suciu; James Garratt; Ettore Capri; Philippe Ciffroy, Boris Alfonso; Elisa Giubilato; Céline Brochot; Johan Bierkens; Zoran Banjac

4-FUN partners giving presentations on topics outside the 4-FUN project

Philippe Ciffroy (on behalf of Nicholas Roth); Damia Barcelò; Antoni Ginebreda

External expert contributors

Roberto Gilioli; Emilio Benfenati; Frederic Bois; Andrea Saltelli.

Main authors of this section of the deliverable report

Gabriella Fait; Nicoleta Suciu; James Garratt; Rodyn Gilharry

6.2 Preparing for the summer school.

The Cremona Summer School sponsored by SETAC was a good opportunity for MERLIN-Expo to gain exposure to a younger demographic that will become the future of regulatory science and chemical fate modelling. The summer school was aimed at junior modellers, research students, post-docs and anyone in the early stages of their career. The main organiser of this event were Gabriella Fait and Nicoleta Suciu who took charge of keeping track of the registrations, producing the delegate packs and arranging the logistics. Thanks to their hard work and excellent organisation, the summer school turned out to be a big success. A large number of participants registered for the event and over the course of five days a variety of lectures and case studies were presented following an agenda designed by Gabriella and Nicoleta. Each lecture and case study presented in the summer school was revised an edited by the lecturer responsible of delivering it, to match the new requirements of this event.

This school was supported by SETAC, who included it as part of their professional training programme ‘Certification of Environmental Risk Assessors’ (CRA). To allow this to happen, we needed support from a University. We negotiated with the Università Cattolica del Sacro Cuore (sede di Piacenza) to award credits for successful completion of the summer school. For all this to happen, we devised an evaluation scheme to monitor how well the students had learned the concepts that we aimed to teach. Our evaluation scheme consisted of a combination of short written responses and interpreting results obtained using MERLIN-Expo.

The course was held within a 2-hour drive of Milan, and we took the opportunity to take the participants to the Milan EXPO, which had the theme of ‘Feeding the Planet; Energy for Life’. There we had special discussion sessions on themes of food security and safety. We had a guided visit at Future Food District where Ms. Boccaletti, the person responsible for communication, explained to the students about the Future Food project. We visited the EU pavilion where Julia Beile, Deputy Director of the EU Pavilion, presented the EU scientific programme for Expo to the students and answered their questions. Furthermore, at the Piacenza pavilion Alba Brancato, EFSA scientific officer, gave a presentation on ‘Pesticide risk assessment and characterization in food. The European approach’, which was followed by an interesting discussion.

as well as time to explore the booths. This provided a very relevant extension to the learning in the classroom.

6.2.1 Intended Audience

Because the event in Cremona is a summer school, the event was mostly targeted towards research students and early career scientists in risk assessment.

6.2.2 Number of Attendees

The Summer school was considered to be a great success with 16 participants attending the event.

6.2.3 Evaluation of the students

All the students achieved the required level to be awarded the credits and the two highest performers (who both scored an impressive 29 out of 30) were given a prize: the book 'Global Sensitivity Analysis', kindly donated by Andrea Saltelli.

6.3 After the summer school

The goal at the end of the summer school was to go over the events that had transpired over the past week and to reflect on the performance of both the lecturers and students in the summer school. This could identify possible strengths and weaknesses in the content of the summer school that could then be addressed to improve the quality of the MERLIN-Expo workshops.

6.3.1 Facilitator discussion

After the summer school a few of the facilitators met and had a quick discussion about the summer school and the events that took place. Their views fell into three categories, things that could have gone better, things that went well and notes for future courses.

<u>Could have gone better</u>

- Took time to get going; using the tool took a while.
- Get concrete earlier, too much theory in the first days.
- Availability of experts was a constraint.
- General lectures on regulation, is IRA necessary?
- Benfenati gave a great lecture; we should have put him earlier in the day on Tuesday.
- River practical missed a bit of detail, Celine's practical was too long. The one she used in Paris was faster.
- The copy and pasting of excel values; we should focus more on using the import function.
- When selecting chemicals, it is annoying that the setting is always on 'default'.

<u>Things that went well</u>

- Level of Organisation
- Quality of speakers
- High level course
- Visit day was good, it was on this day that socialising started.
- Participants were enthusiastic about repeating the course next year.
- Perfect location

<u>Notes for future courses</u>

- Reduce the amount of theory covered and start the practical exercises earlier.

- Get the regulatory a bit more scientific by finding a balance between regulatory and scientific discussions in the lectures, i.e. explain the regulatory standards without losing the scientific debate.
- For Celine's practical, as it is a long practical, establish an appropriate stopping point. This would work as a goal for the slow learners and faster learners could continue beyond this point if they wanted to.
- For practicals involving copy and pasting values from excel, the data list should not be too long. For long data lists the use of the import function should be encouraged.

6.3.2 Feedback forms.

General Notes:

(1) A total of 15 participants filled out the feedback forms and the overall response was very positive, over 90% of the participants rated the summer school course as either Excellent or Very Good.

(2) The participants seemed especially impressed with the level of instructors and lecturers present at the summer school and almost all of them strongly agreed that the instructors/lecturers were helpful and well prepared.

(3) All of the participants either agreed or strongly agreed that the summer school was a good way for them to learn the content, over 85% strongly agreed that they were well informed about the objectives of the summer school and over 90% strongly agreed that the summer school plenary lectures and practical sessions stimulated their learning.

(4) In our pursuit of continually improving our workshops and always providing an excellent learning experience, we should strive to only obtain 4 or 5 ratings in the feedback forms, so even though no question received a negative rating, if we consider a rating of 3 (neither agree nor disagree) as a negative response, then there quite a few areas where improvements can be made. Figure 3 shows the questions that received at least one rating of 3.

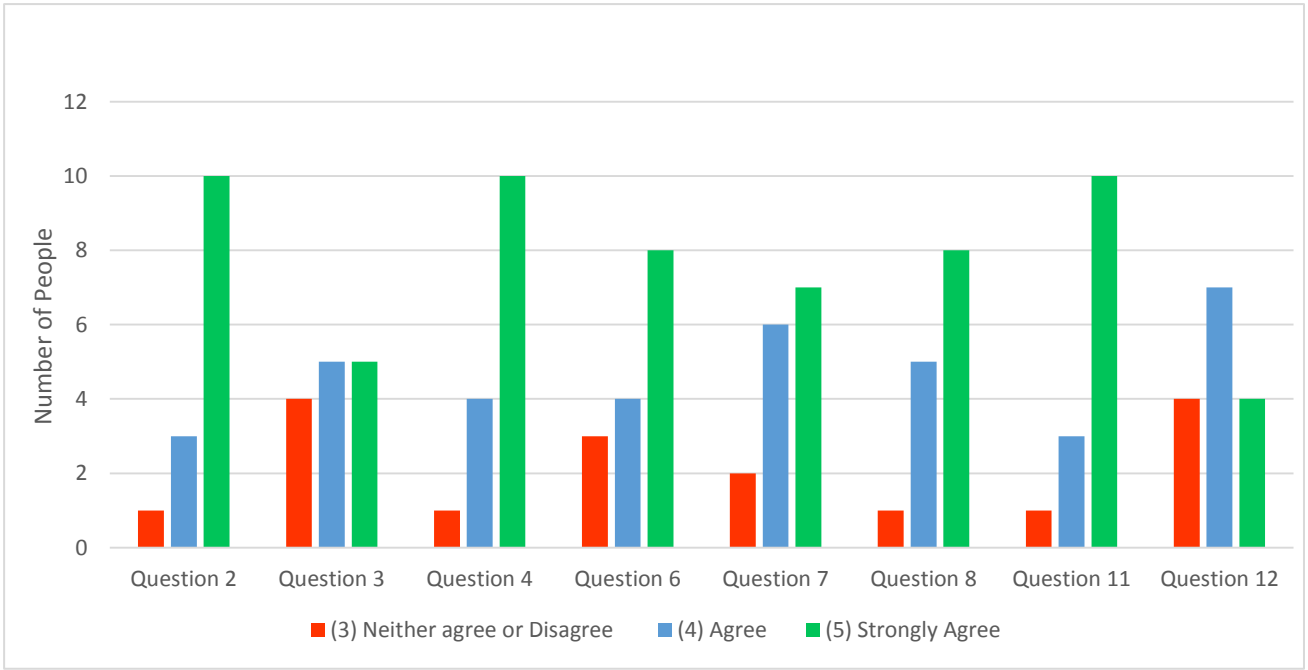

Figure 3. Questions that received the worst ratings in the Summer School

Q2. The summer school plenary lectures and practical sessions lived up to my expectations.

Q3. The plenary lectures and practical sessions content is relevant to my job.

Q4. The summer school objectives where clear to me.

Q6. The activities in this summer school gave me sufficient practice and feedback.

Q7. The difficulty level of this summer school was appropriate.

Q8. The pace of this summer school was appropriate.

Q11. I accomplished the objectives of this summer school.

Q12. I will be able to use what I learned in this summer school.

Improvement Recommendations:

- Question 16 in the feedback form allows the participant to choose certain ways in which they would improve the Summer School. Most participants chose not to full out this section because they felt that there was no need to improve the summer school, which is a very positive response for us. However, there were a few people that ticked a few options of how to improve the summer school and these are summarized in Figure 4.

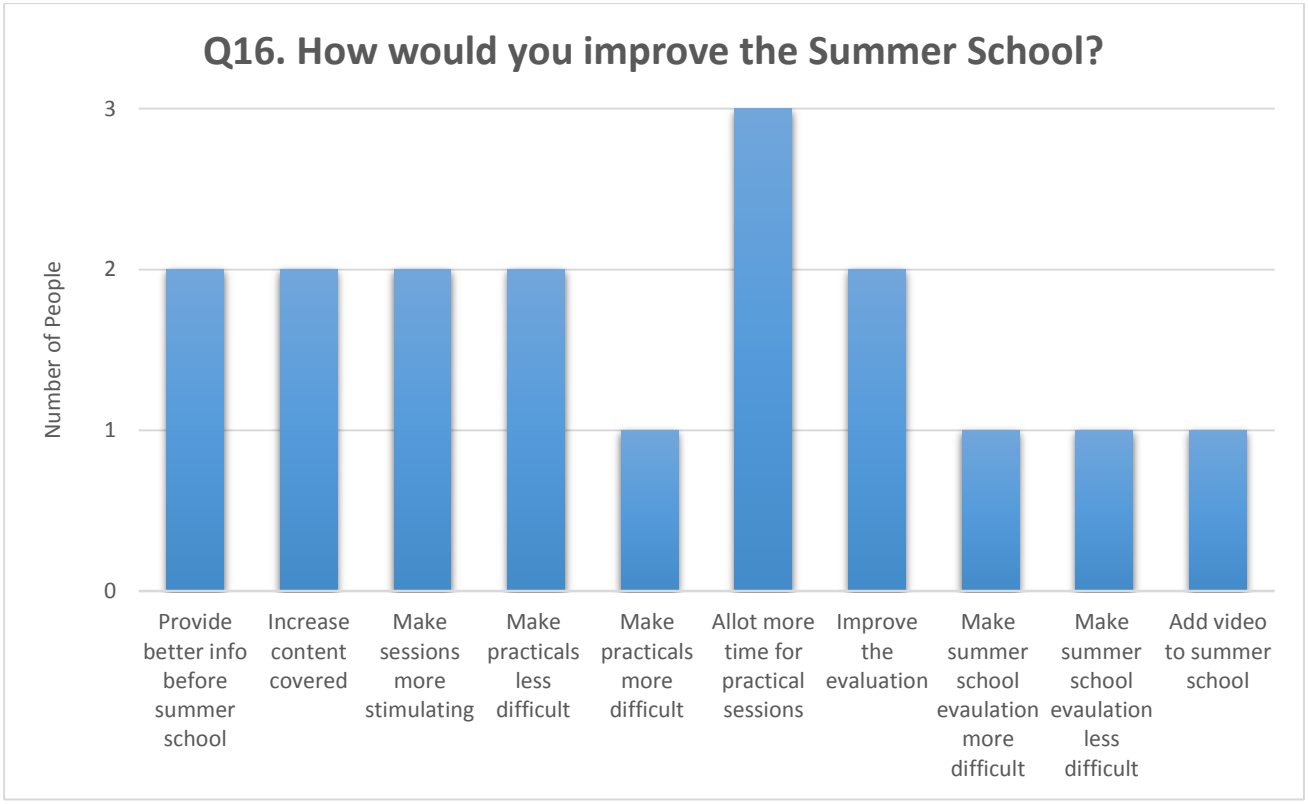

Figure 4. Responses to Question 16 for the Summer School

- In question 17, participants could also write personal remarks of how they thought the summer school could be improved. Most did not write anything but the few remarks obtained are listed below.
  i. 'Expo was really interesting, but should be done in a room not in an open space, due to the noise'.
  ii. 'Should be held twice a year and also contain other topics'.
  iii. 'Pre-Course exercises? Quality in the level of detail required for the evaluation questions'.
  iv. 'More case study presentations and group discussions'.

Free Comment Section:

- In the feedback form there were a few questions that allowed the participant to write down his or her personal comments about the summer school such as question 17 discussed above.
- Question 18 asked what was least valuable about the summer school and again few comments where written in this section as most participants indicated that they felt everything was valuable. However there were two comments that indicated they felt the least valuable part of the summer school was the 'visit to the expo' and the 'introduction on regulations'.
- The section that received the most comments was question 19 that asked the participants what they felt to be most valuable about the summer school. Many positive comments were given in this section and are listed below.
    a. 'Lecturers were very well prepared'.
    b. 'Excellent speakers, good organization and social events, beautiful location'.
    c. 'I appreciate the variety of subjects covered, with clever interconnections and great speakers who were able to adapt to different levels of knowledge in the audience'.
    d. 'This summer school can be very beneficial to my current and future research work and give me the opportunity to meet other researchers'.
    e. 'Combination of theory and practical sessions'.
    f. 'Sensitivity and uncertainty analysis'.
    g. 'Lessons held by Experts; high quality lessons'.
    h. 'High level of lecturers' profiles, good organization of contents and timing'.
    i. 'Learning a new tool for IRA, very qualified experts'.
    j. 'Use of MERLIN-Expo'.
    k. 'Practical sessions, sensitivity analysis'.
    l. 'Great speakers; top experts in field. Interaction with modelling software'.
    m. 'Learning the modelling tool and lectures from experts'.

6.4 Conclusions from Summer School in Cremona

The summer school can be considered a great success. Participants were especially impressed with the high level of lectures and experts in the field available for discussions. Some notable points and comments that summarizes the whole summer school were:

a) The MERLIN-Expo tool is a good tool and people are genuinely interested in it.
b) The course was an excellent way of presenting the model and teaching how to use it.
c) Some participants felt that some pre-course exercises could be given beforehand to better prepare the participants for the course.
d) Participants want to get their hands on the model from early on so maybe the amount of theory covered at the beginning could be reduced and the course could be more concrete from earlier.
e) The comment that ranked the highest in how to improve the summer school was, 'Allot more time for practical sessions'.

7 MERLIN-Expo Barcelona Workshop (22 September 2015)

7.1 List of contributors.

4-FUN partners giving presentations

James Garratt; Philippe Ciffroy; Boris Alfonso; Zoran Banjac; Gabriella Fait.

Main authors of this section of the deliverable report

James Garratt; Rodyn Gilharry

7.2 Preparing for the workshop

This workshop was intended to coordinate with a major international conference in the Chemicals Industry that is held annually in Barcelona: the Informa Chemicals Industry Regulations (CIR) conference. The reason for trying to coordinate with this conference was to link with people from consultancies or industry who might be in Barcelona anyway. Thus we chose to hold the workshop on the day before the CIR conference (22 September 2015). We attempted to make a formal link with Informa to help to promote the event, but we were not able to establish a meaningful working relationship with them. Therefore we made all the publicity ourselves by email.

It was a short course, designed to give participants a feel for the capabilities of the tool but not an in-depth understanding. This workshop was similar to the previous one in Barcelona: the SETAC short course from May 2015. The agenda for this workshop was based on the agenda for the SETAC course. Additionally there was a presentation on the regulatory acceptability and the benchmarking, which was first used at the JRC workshop.

The final list of participants included regulators, consultants and academics.

7.2.1 Intended Audience

This workshop was planned for commercial and industrial regulatory professionals.

7.2.2 Number of Attendees

This workshop had 9 participants.

7.3 During the workshop

This workshop had as its priority the showcasing of the capabilities of the tool. Therefore, the presentations left plenty of room for discussion, to allow questions from the participants on how the tool might be applied in practice. Some of the practical sessions were reduced to demonstrations in order to give time to work through the whole agenda. The practical sessions that were performed interactively were simplified to give everyone a good chance to get to the end of the practical. Additional practical work was supplied for those who worked extremely fast or wanted to do more after the end of the workshop.

7.3.1 Peer-discussion

There was a lively discussion at the end of the workshop about the advantages and potential problems with the MERLIN-Expo tool. The key themes from this discussion are indicated below.

Advantages of MERLIN-Expo

Global sensitivity analysis is not found in most tools that are available. The uncertainty and sensitivity analysis was a particular strong point.

Could in principle be used to evaluate multiple sources of a substance, e.g. a substance that is found naturally as well as being a metabolite of an anthropogenic substance.

Could establish whether critical tissue concentrations are exceeded when there are multiple routes of exposure.

There has been some regulatory interest (e.g. JRC, ECHA, EFSA, ANSES, AGES)

Potential problems of MERLIN-Expo

Not clear whether time-series data can be included in the sensitivity analysis

Does not fit neatly with regulations on plant protection products

It would be helpful to build a dermal exposure module

It is not clear the extent to which model error has been considered (i.e. the equations and relationships correct?).

Still needs more developments to become acceptable to regulators (although ECETOC does allow consideration of 'robust arguments' and MERLIN-Expo could provide this).

You need quite advanced knowledge to be able to use it.

7.4 After the workshop

7.4.1 Facilitator discussion

The group of facilitators and lecturers discussed together the best bits of the day and the bits that we could do better if we go on to repeat courses like this in future.

Things that we could do better

- We could make sure that each case study relates to a specific skill in how to manipulate MERLIN-Expo
- We concentrate on ensuring people know how to do particular operations and generate the results (for example, greater use of existing simulations and .eco or .eas files)
- We could talk more about parameters: where to get them, why are these defaults chosen?
- We could make better use of the registration forms to get to know the audience before the workshop.
- We constantly need to be aware of getting our timing right.

Things that went well

- We had a great audience: really well qualified and experienced
- We put a lot in a short time
- We were able to make presentations that were not in our specific fields of expertise.

7.4.2 Feedback forms.

Eight participants filled out the feedback form. The results from the feedback were very positive. The questions had a 5-point scale, and if we assume that points 4 or 5 represent success, then every question was successful for 5 out of the 8 responses.

Questions 1-13: the ratings on various elements of the workshop

Out of the 8 persons that filled out the form, all agreed that:

- The workshop objectives were clear
- The workshop stimulated their learning
- The difficulty level was appropriate
- The instructors were well prepared
- The instructors were helpful
- The workshop was a good way to learn the content.

The cases where less positive responses were received are as follows (number of responses rated 1-3):

- I was well informed about the objectives of this workshop (2)
- This workshop lived up to my expectations (1)
- The content is relevant to my job (1)
- The activities in this workshop gave me sufficient practice and feedback (3)
- The pace of this workshop was appropriate (1)
- I will be able to use what I learned in this workshop (2)

Question 14: the tick list of options for improvement

Specific points for improvement from a tick-list were: (number of responses that choose the same option).

- add more video to the workshop (1)
- allot more time for the workshop (3)
- improve the instructional methods (1)
- increase the content covered in the workshop (1)
- make the workshop less difficult (1)
- provide better information before the workshop (2)
- slow down the pace of the workshop (3)

Questions 15 and 16 asked what improvements could be made and what was least valuable. These questions elicited some useful indicators for the future:

- “provide more time for study”
- “the practical sessions were a bit too ambitious. Perhaps better with pure demonstrations and/or less fiddling with parameter import”
- “perhaps participants may be asked to bring their personal examples”
- “cut and paste / filling in single parameter values” (is not a valuable use of time in a workshop)

Question 17 asked what was most valuable. There were several encouraging responses to this.

- “introduction to the general philosophy of the tool and a hands-on experience in using the tool.”
- “practical experience”
- “practical sessions”
- “the PBPK module session, due to my personal professional interest”

Question 18 asked for an overall evaluation. All responses were either ‘very good’ or ‘excellent.’

Question 19 asked whether participants received all the information that they needed before the event. All responses were either ‘all of the information’ or ‘most of the information.’

Question 20 asked how likely participants were to recommend MERLIN-Expo. All responses were ‘very likely.’

7.5 Conclusions from the Barcelona Workshop

As the final workshop, we would have hoped to have progressed a lot in our delivery since May 2015. In many ways this was true and the delivery was a lot smoother and clearer. However, we still received comments that we tried to cram too much information into too short a time. If training is to be part of the future of the open market offering of the MERLIN-Expo tool, then we need to play to the evident needs of participants. That is:

a) Practical skills in using the tool
b) Concepts and applications taught using scenarios and examples that have been built in advance
c) A limited scope of what is covered in a day (maybe a focussed day on one particular aspect).

Overall, we can see that we have greatly improved our workshops throughout this 6-month programme but they are still not perfect. If workshops like this are to be delivered on a commercial basis in future, there is still some effort required to ensure that they provide the right information in the right way.

8 Online Courses

8.1 List of contributors.

4-FUN partners preparing and organising materials

James Garratt; Charles Hazlerigg; Emma Grange; Philippe Ciffroy; Taku Tanaka; Erik Johansson; Annika Johannson; Boris Alfonso; Céline Brochot

OpenTea coordinator

Gabriele Sacchetini

Main authors of this section of the deliverable report

Gabriele Sacchetini; James Garratt; Rodyn Gilharry

8.2 Online course platform

The desired legacy of the 4-FUN project is that people around Europe (and indeed the world) will use the MERLIN-Expo tool to help them to improve their assessments of chemical fate and exposure. To achieve such a legacy, our 6-month programme of face-to-face training courses is not enough. We need to leave some kind of virtual training programme available so that people can access training into the future. For this reason, an online course was developed.

After various negotiations, OpenTEA was the platform contracted to host the MERLIN-Expo online courses. The course aims to familiarise the user with the new MERLIN-Expo tool by completing a number of tutorials, with the possibility to obtain a certification of attendance.

Gabriele Sacchettini was the person in charge of designing the web page and kept in constant communication with Enviresearch Ltd to ensure we were updated with his progress.

8.3 Structure of the Online Course

The course is composed of 9 modules, covering the background to MERLIN-Expo, some of the key models within the MERLIN-Expo library and an example of building a scenario. Users have the possibility to join the course anytime from anywhere and do not need to follow a specific order to take each modules.

Each module is composed of 5 easy steps which web-User can go through using an arrow control included on the top of the web page:

1. Introduction: Short description of the module + rule to complete the module;
2. Content: Video tutorial of approximately 20 min supported by a PowerPoint presentation + contact details together with a small bibliography of an expert that User could contact for clarifications;
3. Examination test (3 Multiple choice questions which users can try unlimited times with detailed feedback comments in case of wrong answers);
4. Feedback questionnaire (4 multiple choice questions and one open answer question requesting rating and personal opinion on the Content of the module);
5. Forum where participants could share opinions and experiences (divided into rooms, for each Module and an additional one for the overall course).

The modules are supported by Webinars: currently 6 are envisaged. The first, of these, has been delivered by Philippe Ciffroy at the opening of the course. Members of the 4-FUN

consortium have agreed to deliver other webinars throughout the end of 2015 and early 2016 to cover their specialism.

8.4 Certification

To obtain the certification, users will need to register into the course completing all modules included (Webinars are considered optional). To complete each module, a user will need to watch completely the video tutorial answering correctly to each question (a track system is in place to verify user performance).

8.5 Administration of the course

The registration is free as well as the release of the certification. Potential users simply go to the OpenTea website to register (http://www.opentea.eu/en/member/new/&platform=1), after which they will be able to log in on the course website (http://www.opentea.eu/en/e-learning/courses-The-Future-of-Environmental-and-Human-Health-Exposure-Modelling-of-Chemicals.10/).

The course is constantly moderated by the OpenTea coordinator, who is in charge of control, the correct operating of each feature, assisting Users in case of problems as well as interacting with them to enhance interest and increase motivation.

8.6 Preparation of the Materials.

Preparing the materials for the online course was a long and tedious process but resulted in the production of high quality materials. It was decided that the courses should be delivered via audio-visual means, therefore PowerPoint presentations, scripts and a voice recordings were needed for each course module. The PowerPoints and scripts were made by the lecturer in charge of the course and sent to Enviresearch, where it is was proof read and edited. We made sure that each PowerPoint was done using the same template and those that were not in the same format were edited to match. After the scripts were proof read and checked for grammatical mistakes, they had to be read and recorded to produce the Voice for the audio-visual presentation.

The Voice recordings were done by Charles Hazlerigg, an employee at Enviresearch Ltd., using the Camtasia Studio 8 software. He recorded all the scripts written for the eight modules produced so far and even re-recorded some scripts previously recorded by Emma Grange, another Enviresearch employee and 4FUN partner, to ensure consistency. This was a very time consuming task as sometimes the script had to be recorded more than once to get the proper tone, however Charles got all of them done in a timely manner and is a big part of why the materials produced are of such good quality. After the recordings were done the files, along with the PowerPoint presentations and script were sent to Boris Alfonso, a senior software developer at Facilia in Sweden and 4FUN partner. Boris then had the job of combining the presentation with the voice recording to form one audio-visual presentation, using the script to ensure the recording and PowerPoint slides were timed precisely, he produced excellent lecture presentations.

After the video tutorial presentations were finished by Boris they would be sent back to Enviresearch where they would be combined with other pieces of information about the module and sent to Gabriele to upload onto the Online course Platform. There was a specific outline in regards to what pieces of information was needed for each module as shown below. Appendix A shows an example of how this information would be complied and sent to Gabriele.

Out of the 9 modules, 6 were complete before the launch date of 10 September, 2 more became available during September and the final one was published in October.

8.7 Launch of the Online Courses and the opening Webinar

8.7.1 Before the webinar

The Online courses were scheduled to be launched in the summer of 2015. The first launch date was set for the beginning of July, however due to delays in the production of some of the online course materials the launch date had to be postponed. Due to the long chain of people the course materials have to go through before they are finalised, a hold up in one section significantly affects the progress of the rest. The final launch date was held on 10th of September by means of a Webinar (with Philippe Ciffroy) on OpenTEA.

In the beginning of September, potential participants received an invitation mail requiring a registration. Registered participants received an additional mail by the OpenTEA responsible the day before the Webinar including direct link as well as technical IT requirements to join the meeting. Moreover an additional reminder mail was sent to all registered participants 2 hours before the meeting. Prior to the webinar, Philippe and Gabriele conducted a technical test of the video / sound and resolved some problems due to firewalls and connectivity.

8.7.2 During the webinar

During the webinar, the web-classroom was hosted by Gabriele Sacchetini, who moderated the activity including coordination between speakers and interactions with the users (through web-chat).

The webinar started at 11.00 CET with an actual duration of 66 minutes (effective duration of 54 minutes) and proceeded as shown in Table 2.

Table 2: Timings of the elements of the first Webinar

Session	Leading	Time spent (min)
Introduction	Moderator	2
Oral presentation	Invited expert (Philippe Ciffroy)	36
Q&A	Moderator + Invited expert	16

In summary:

- 26 Users registered to the webinar
- 23 Participants (21 Attendees + 2 Speakers)
- 14 sentences coming from the chat including 8 explicit questions (All of them discussed by speakers).
- The attendance rate was similar along all the duration of the webinar meaning that most of the part of the attendances (19) followed the webinar since the beginning until the end.

8.8 Preliminary feedback

8.8.1 The online course

As at 25 September 2015, there were 21 registered Users. 4 Users registered without entering into the course, 8 connected for less than 5 minutes while the rest (12) have been actively participating into the course with an average time spent of 40.8 minutes. No interactions have been detected into the forum. However these numbers are not surprising

as the course still needed to be completed and it was very recently officially launched through the first Webinar.

8.8.2 The opening webinar

A Feedback questionnaire was received by all Attendees at the end of the Webinar. It was composed by the 4 multiple choice questions and one open answer question. Results are shown in Table 3.

Table 3: Summary of responses to questionnaire on the first Webinar

Q1-4	How would you rate this Webinar based on…?			
	clarity of messages	scientific consistency	exhaustiveness of the contents	overall quality
Very good	6	6	3	5
Good	6	6	10	5
Ok	1	1	0	3
Bad	0	0	0	0
Very Bad	0	0	0	0
Total answers	**13**	**13**	**13**	**13**

Q5	Do you have any comment? What would you like to be discussed during next webinar?
	• Thank you. It was very interesting and nice overview of Merlin Expo tool. I am looking forward to next session. • This is an interesting tool. However, with so many different processes going on in the models, and with only a handful of case studies tested, I wonder how confident we can be that the conclusions drawn from the model are meaningful? As someone whose work is focused on the regulatory side of exposure modelling, it seems to me that this tool is likely to be some way away from regulatory acceptability, even at higher tiers. • Practical case studies • I thought that Philippe did a great job!
Total answers	**4**

8.9 Conclusions and final considerations

- The fact that the attendance rate was constant during the webinar confirms that the general structure of the webinar and the overall length could be replicated also for the next ones.
- Feedbacks received (either from the questionnaire either from the overall participants' interactions) are encouraging in terms of participants' interest in joining next events.
- Number of participants at the event can be considered good taking into consideration the kind of high specialised scientific topic webinar wants to address and the fact that the e-learning course still needs to be completed.
- Video of the webinar will be edited in a suitable format and included in the e-learning course
- The online course can act as a focus for future interest in the MERLIN-Expo tool and will provide a definite and concrete way of allowing potential users to get training in the tool.

9 Overall Conclusion from the Training Programme

The goal of the training programme was to reach out to potential users of MERLIN-Expo to inspire them to find applications for the tool. The training programme has been very successful in reaching a broad range of potential users from industry, consulting, regulation and research.

Face-to-face courses were delivered to 85 individual participants. Added to this there are approximately 12 participants already active on the online training programme, and 21 attended the opening Webinar. Overall we have reached around 100 people.

Moving into the future, we are planning additional training events. The online course will be supported for a period of time and it should be possible to deliver face-to-face training on a more commercial basis. We have ample feedback from the training that we have delivered already that can help to define how future training should be conducted. Themes that have come out of the training up to now include:

i) People love practical sessions. This is much more important than long presentations about theory. But people don't like repetitive tasks as part of a practical and this would need to be avoided.
ii) Practical sessions need to be carefully optimised to ensure the maximum learning for the minimum time. There are various skills, which people will need to use MERLIN-Expo successfully and our practical sessions need to focus on teaching those skills and then moving on. We should make our practical sessions focussed on tasks (e.g. 'build a food web'; 'link two rivers').
iii) There was enthusiasm for video within the courses.
iv) Timing is key. If you try and cram too much into a short course, everything is rushed and people don't like that. There are 2 solutions: longer courses or less content. This dichotomy will need to be addressed.
v) Before the course, the quality of the information that is communicated to the participants needs to be of the highest standard.

Within the context of the 4-FUN project, we have delivered an excellent training programme with innovation and imagination all the way through. The 4-FUN partners have been committed to the process and have made it work and have had fun delivering the training. Overall, this has been one of the most rewarding elements of the 4-FUN project, both for the participants and the presenters.

10 Appendices

10.1 Appendix A: Online Course Materials needed per Module

Details for Completed modules:

(6) PBPK / human model

- Name of Module: The Human Model – A physiologically based toxicokinetic model
- Video Tutorial:
  http://media.facilia.se/4fun/training/camtasia/HumanIntakeModel_Tutorial/HumanIntakeModel_Tutorial_player.html
- Multiple Choice Test:

  (1) What are two functions of the human intake model in MERLIN-Expo that can be used in certain decision frameworks?

  (i) Indicating what concentration of the compound or chemical substance is lethal to people.
  (ii) Predicting the internal dosimetry of the compound in target tissues
  (iii) Identify the different ways in which the compound has entered the body.
  (iv) Predict the concentrations of biomarkers measured in biomonitoring studies.

  (a) (i) only
  (b) (i) and (ii) only
  (c) (ii) and (iv) only
  (d) (i) (ii) and (iv) only

  Answer: (c)
  Rationale: The PBPK model used in MERLIN-Expo does not indicate what concentration of the compound is lethal to people. That is not the purpose of a modelling tool, the tool simply calculates the concentration found in different areas by considering the diffusion and transport of the chemical throughout the body. Once this concentration is known it can be compared to standard levels of concentration found in medical or scientific journals to determine whether the concentration of the compound is considered to be lethal. The model also does not identify ways in which the compound enters the body, this should be known by the user and is an input parameter for the simulation. The model can predict the internal dosimetry of the compound in target tissues that is related to the outset of the toxic effects and can also predict the concentration of biomarkers measured in biomonitoring studies, such as the concentration of blood in urine.

  (2) Toxicokinetics can be described as the fate of a compound in a living organism and is usually determined by the ADME processes. Which of the letters shown below is not correctly matched to its meaning in the ADME acronym?

  A – Absorption of the compound in the organism
  D – Distribution of the substances in the organs via the circulatory system
  M – Mechanisms by which the substances are broken down
  E – Excretion of the substances from the body via urine or bile, etc.

(a) A
(b) B
(c) M
(d) E
(e) None of the above
Answer: (c)
Rationale: All of the letters and their meanings are correct except for M. M stands for metabolism, which is the irreversible transformation of the parent compound into metabolites. Although metabolism is a mechanism by which the substance is broken down, an acronym has an established meaning and should be not open to interpretation, regardless of how close the meaning is.

(3) The human intake (PBPK) model in MERLIN-Expo is sub-divided into 25 compartments and incorporates two routes of exposure: the inhalation in the alveolar space and the ingestion in the stomach lumen or liver. True or False?

(a) True
(b) False
(c) Cannot say from the presentation
Answer: (b)
Rationale: The PBPK model is actually subdivided into 23 compartments not 25, however the two routes of exposure are inhalation and ingestion.

(4) What are some of the assumptions made for modelling the gas exchanges in the MERLIN-Expo PBPK model?

(i) The gas exchanges are located in the alveolar space and not in other parts of the respiratory tract.
(ii) one-directional airflow was assumed in the region of gas exchange
(iii) Air moves through the lungs with a constant flow rate equal to the alveolar ventilation rate.
(iv) Because gas exchanges are assumed to be very rapid, equilibrium is rapidly reached between air in the lungs and the blood in the alveoli.

(a) (i) and (ii) only
(b) (i) and (iv) only
(c) (i) (ii) and (iv) only
(d) (i) (ii) (iii) and (iv)
Answer: (d)
Rationale: All of the statements give above (i) – (iv) are true assumptions made for modelling gas exchanges in the human intake model.

- Additional materials: None
- Contact email address of an expert: Celine Brochot <Celine.BROCHOT@ineris.fr>
- Short Description:

  The human model implemented in MERLIN-Expo is a physiologically based pharmacokinetic (PBPK) model that describes the relationship between an external dose and the internal dosimetry using parameters related to the anatomy and the physiology of the individual and

physico-chemical properties of the contaminants. The goal of the PBPK model is to simulate the toxicokinetics of contaminants in humans, i.e. the amounts or concentrations in different organs/tissues, under various exposure conditions.

10.2 Appendix B: Workshop Agendas

10.2.1 Paris Workshop Agenda

Day 1 26th March, 2015

Time	Presenter and topic
10:30 – 11:00	Welcome and coffee
11:00 – 11:15	*Lecture* Speaker: **Emma Grange / James Garratt** • Roundtable • Introduction to the course and the course objectives • Current approaches in human health and exposure assessment and their deficiencies • Advanced methods and the future for environmental and human health exposure modelling.
11:15 – 12:00	*Lecture* Speaker: **Philippe Ciffroy** • The 4FUN project: objectives • Innovative issues of the MERLIN-Expo tool • Documentation available for end-users • Overview of the library of models in the tool
12:00-12:30	*Lecture* Speaker: **Boris Alfonso** • Overview of the general structure and format of the MERLIN-Expo tool • Simple demonstration of the software
12:30 – 13:30	Lunch
13:30 – 15:00	*Practical session - Case study 1(Transport of a contaminant in a river)* Facilitated by: **Philippe Ciffroy** • First contact with MERLIN-Expo • Running a simulation with one model only • Connecting two models together
15:00 -16:30	*Practical session – Case study 2(Food web modelling in the Venice lagoon)* Facilitated by: **Elisa Giubilato and Artur Radomyski**
16:30 – 17:00	Coffee break
15:00 – 15:30	*Lecture* Speaker: **Zoran Banjac** • The Erbo Valley case study.
17:00 – 17:30	*Lecture* Speaker: **Frederik Verdonck** • Applications of the tool, usefulness of the tool in aiding regulatory decision making. • Benchmarking against other modelling tools
17:30 – 18:00	• Discussion, opportunity for questions • End of session
Evening	Social event

Day 2 27th March, 2015

08:30 – 08:50	Welcome and coffee
08:50 – 09:00	Speaker: **Emma Grange / James Garratt** • Recap of yesterday's sesssion • Overview of today's topics and activities
09:00 – 09:30	*Lecture* Speaker: **Céline Brochot** • The PBPK model
09:30 – 11:00	*Practical session – Case Study 3 (Human food chain)* Facilitated by: **Céline Brochot and Paul Quindroit** • Predicting contaminant concentrations in human tissue using the MERLIN-Expo tool
11:00 – 11:30	Coffee break
11:15 – 12:00	*Lecture* Speaker: **Philippe Ciffroy** o Uncertainty and sensitivity analysis
12:00-12:30	*Practical session – Case study 4(Uncertainty/Sensitivity on simple case study)* Facilitated by: **Philippe Ciffroy** • Using the MERLIN-Expo tool to perform o probabilistic and deterministic simulations o uncertainty and sensitivity analysis
12:30 – 13:30	Lunch
13:30 – 14:30	*Practical session – Case study 4(Uncertainty/Sensitivity on simple case study)* Facilitated by: **Philippe Ciffroy**
14:30 – 15:00	*General discussion* Led by: **Emma Grange / James Garratt** • Summary of the day and close of session.

10.2.2 Belgrade Workshop Agenda

Day 1 Monday 20 April 2015

Time	Presenter and topic
10:30 – 11:00	Welcome and coffee
11:00 – 11:10	*Introduction* Speaker: **Aleksander Vlajic / James Garratt** • The objectives of the course • Introduction to the speakers
11:10 – 12:00	*Lecture* Speaker: **Dr. Momir Paunovic** • Management challenges in water sector in developing countries - Serbian and regional experience
12:00 – 12:45	*Lecture* Speaker: **Zoran Banjac** • The 4FUN project: objectives • Innovative issues of the MERLIN-Expo tool • Documentation available for end-users • Overview of the library of models in the tool
12:45 – 13:30	Lunch
13:30 – 14:00	*Lecture* Speaker: **Boris Alfonso** • Overview of the general structure and format of the MERLIN-Expo tool • Simple demonstration of the software
14:00 – 15:00	*Practical session - Case study 1 (Transport of a contaminant in a river)* Facilitated by: **Zoran Banjac** • First contact with MERLIN-Expo • Running a simulation with one model only • Connecting two models together
15:00 – 15:30	*Lecture* Speaker: **Zoran Banjac / Johan Bierkens** • General overview of case study work • Modelling emerging and priority contaminants in the Ebro river • Modelling historical heavy metal contamination • Ecological and human exposure to POPs in the Venice lagoon
15:30 – 16:00	Coffee break
16:00 - 18:00	*Practical session – Case study 2a (Food web modelling in the Venice lagoon)* Facilitated by: **Zoran Banjac** *Practical session – Case study 2b (Modelling historical heavy metal contamination)* Facilitated by: **Johan Bierkens** *Extension Work : for further personal practice* *Case study 2c (Food web modelling in the Venice lagoon)*
18:00 – 18:30	*General discussion* Facilitated by: **James Garratt**
Evening	Social event

Day 2 Tuesday 21 April 2015

09:30 – 09:50	Welcome and coffee
09:50 – 10:00	Speaker: **Aleksander Vlajic / James Garratt** • Recap of yesterday's sesssion • Overview of today's topics and activities
10:00 – 10:30	*Lecture* Speaker: **James Garratt** • The PBPK model
10:30 – 11:00	*Practical session* Facilitated by: **James Garratt** • Predicting contaminant concentrations in human tissue using the MERLIN-Expo tool
11:00 – 11:30	Coffee
11:30 – 11:45	*Demonstration* Led by: **James Garratt** • Demonstration of predicting contaminant concentrations in human tissue
11:45 – 12:00	*Lecture* Speaker: **Boris Alfonso** • The documentation for the tool.
12:00 – 13:00	Lunch
13:00 – 13:30	*Lecture* Speaker: **James Garratt** Uncertainty and sensitivity analysis

13:30 – 14:30	*Practical session – Case study 4 (Uncertainty/Sensitivity on simple case study)*
	Facilitated by: **Johan Bierkens**
	• Using the MERLIN-Expo tool to perform
	  ○ probabilistic and deterministic simulations
	  ○ uncertainty and sensitivity analysis

14:30 – 14:45	*Demonstration and discussion on Case study 4* Led by: **James Garratt**
14:45- 15:20	*General discussion* Led by: **James Garratt**
15:20 – 15:30	*Wrap up* Speaker: **Aleksander Vladic** • Review of supporting information available: online training tutorials, user guides etc, where to find the model documentation. • Summary of the day and close of session.

10.2.3 SETAC Short Course Agenda

3rd May, 2015

Time	Presenter and topic
08:00 – 08:15	Coffee
08:15 – 08:30	*Welcome* Speaker: **James Garratt** • Introduction to the course and the course objectives • Current approaches in human health and exposure assessment and their deficiencies • Advanced methods and the future for environmental and human health exposure modelling • The MERLIN-Expo tool and its key features • The 4FUN project, introduction to the other speakers.
08:30 – 09:15	*Lecture 1* Speaker: **Philippe Ciffroy** • The 4FUN project: objectives • Innovative issues of the MERLIN-Expo tool • Documentation available for end-users • Overview of the library of models in the tool
09:15 – 09:45	*Lecture 2* Speaker: **Boris Alfonso** • Overview of the general structure and format of the MERLIN-Expo tool • Simple demonstration of the software
09:45 – 10:00	Coffee Break
10:00 – 10:20	*Lecture 3* Speaker: **Elisa Giubilato** • General overview of case study work • Ecological and human exposure to POPs in the Venice lagoon
10:20 – 12:00	*Practical session – Case study 1 (Venice lagoon)* Facilitated by: **Elisa Giubilato** • Food web bioaccumulation modelling in the Venice lagoon *Extension Work : for further personal practice* *Case study 1(b) (Modelling historical heavy metal contamination)*
12:00 – 13:00	Lunch
13:00 – 13:10	Speaker: **James Garratt** • Recap of the morning sesssion, overview of the afternoon's topics and activities
13:10 – 13:45	*Lecture 4* Speaker: **James Garratt** • The PBPK model
13:45 – 14:30	*Practical session – Case study 2 (Human food chain)* Facilitated by: **James Garratt** • Predicting contaminant concentrations in human tissue using the MERLIN-Expo tool
14:30 – 14:45	*Lecture 5* Speaker: **Philippe Ciffroy** • Uncertainty and sensitivity analysis (Theory)
14:45 – 15:00	Coffee break
15:00 – 15:15	*Lecture 6* Speaker: **Philippe Ciffroy** • Practical Introduction to uncertainty and sensitivity analysis in MERLIN-Expo.

15:15 – 16:15	*Practical session - Case study 3 (Uncertainty/Sensitivity)* Facilitated by: **Philippe Ciffroy** • Using the MERLIN-Expo tool to perform o probabilistic and deterministic simulations o uncertainty and sensitivity analysis
16:15 – 16:45	Review & Questions
16:45 – 17:00	Couse Evaluation / Feedback

10.2.4 JRC- IHCP Training Agenda

21st May, 2015

Time	Presenter and topic
10:00-10:15	Welcome address and Training course expectations **Stylianos Kephalopoulos (EC JRC/L1)** Training course agenda and modalities **Alexandre Zenié (EC JRC/L1)**
10:15 – 11:00	*Lecture* Speaker: **Philippe Ciffroy (EDF)** • The 4FUN project objectives and its relation to MERLIN-Expo tool • Innovative issues of the MERLIN-Expo tool • MERLIN-Expo documentation for end-users • Overview of the models library in the MERLIN-Expo tool
11:00 – 11:15	*Coffee break*
11:15-12:00	*Lecture* Speaker: **Boris Alfonso (FACILIA)** • Overview of the general structure and format of the MERLIN-Expo tool • Quick tour on MERLIN-Expo capabilities
12:00 – 13:30	*Lunch*
13:30 – 14:00	*Hands on session – Preliminary Case study (Lead poisoning : a very simple example just to learn how to use MERLIN-Expo)* Facilitated by: **Boris Alfonso (FACILIA)** • First contact with MERLIN-Expo • Learn the design of MERLIN-Expo • Running a simple simulation with one model only
14:00 – 14:30	*Lecture* Speaker: **Gabriella Fait (AIEFORIA)** • Applications of the tool, usefulness of the tool in aiding regulatory decision making. • Benchmarking against other modelling tools
14:30 – 15:00	*Lecture* Speakers: **Philippe Ciffroy (EDF) & Elisa Giubilato (Università Ca'Foscari)** • General overview of case study work • Modelling historical heavy metal contamination • Modelling emerging and priority contaminants in the Ebro river • Ecological and human exposure to POPs in the Venice lagoon
15:00 – 15:15	*Coffee Break*
15:15 – 17:15	*Hands on session – Case study 2 (Food web modelling in the Venice lagoon)* Facilitated by: **Elisa Giubilato & Artur Radomyski (Università Ca'Foscari)**
	Hands on session – Case study 2b (Optional for 'fast students': Metal contamination in Flanders) Facilitated by: **Gabriella Fait (AIEFORIA)**
17:15 - 18:00	*General discussion* Facilitated by: **Philippe Ciffroy (EDF)**

22nd May, 2015

Time	Presenter and topic
09:00 – 09:30	*Lecture* Speaker: **Philippe Ciffroy (EDF)** (prepared by **Céline Brochot (INERIS)**) • The PBPK model
09:30 – 10:00	*Hands on session – Case Study 3, Part 1 (Human food chain)* Facilitated by: **Philippe Ciffroy (EDF)** • Predicting contaminant concentrations in human tissue using the MERLIN-Expo tool
10:00 – 10:15	*Coffee break*
10:15 – 11:00	*Hands on session – Case Study 3, Part 2 (Human food chain)* Facilitated by: **Philippe Ciffroy (EDF)** • Predicting contaminant concentrations in human tissue using the MERLIN-Expo tool
11:00 – 11:30	*Lecture* Speaker: **Philippe Ciffroy (EDF)** • Uncertainty and sensitivity analysis and MERLIN-Expo tool

11:30- 12:00	*Practical session – Case study 4, Part 1 (Introduction to Uncertainty/Sensitivity analysis)*
	Facilitated by: **Philippe Ciffroy**
	• Using the MERLIN-Expo tool to perform
	  ○ probabilistic and deterministic simulations
	  ○ uncertainty analysis

12:00 – 13:30	Lunch
13:30- 15:00	*Practical session – Case study 4, Part 2 (Introduction to Uncertainty/Sensitivity analysis)* Facilitated by: **Philippe Ciffroy (EDF)** • Using the MERLIN-Expo tool to perform ○ sensitivity analysis
15:00 – 15:15	*Coffee break*
15:15 – 15:45	*General discussion* Facilitated by: **Philippe Ciffroy (EDF)**
15:45 – 16:00	*Trainees Satisfaction Survey (compilation and delivery)*
16:00 16:30	*Closing of the training course*

10.2.5 Cremona Summer School Agenda

Monday, 29 June 2015		**Chairman**
Morning Session		
10:00 – 11:00	Registration	
11:00 – 12:00	Speakers: James Garratt (ENVIRESEARCH) and Ettore Capri (UCSC) Roundtable Introduction to the course and course objectives Overview of the programme	James Garratt & Ettore Capri
12:00 – 13:00	Speaker: Nicolas Roth (SCAHT) Lecture: Integrated risk assessment	
13:00-14:00	*Lunch*	
Afternoon Session		
14:00-15:30	Speaker: Roberto Gilioli (ECHA) Lecture: Overview of legislation for risk assessment	James Garratt & Ettore Capri
15:30-16:00	*Coffee*	
16:00-16:45	Speaker: Philippe Ciffroy (EDF) Human exposure modelling: innovative issues and standard documentations	
16:45-17:30	Speaker: Boris Alfonso (FACILIA) Practical Session: MERLIN-Expo tool: general overview and simple demonstration of the software	
17:30-17:45	Recap of Day 1 and general discussion	
	Free dinner	

Tuesday, 30 June 2015		**Chairman**
Morning Session		
9:00 – 9:10	Brief introduction to Day 2	James Garratt & Nicoleta Suciu
9:10-10:40	Speaker: Damia Barcelo and Antoni Ginebreda (CSIC) Lecture: Occurrence of pharmaceuticals in Iberian rivers: prioritization and modeling	
10:40-11:00	*Coffee*	
11:00– 12:30	Speaker: Zoran Banjac (CSIC), Johan Bierkens (VITO), Elisa Giubilato (Ca' Foscari) Lecture: General overview of three case studies: emerging and priority contaminants in the Ebro river (Spain); historical heavy metal contamination (Belgium); ecological and human exposure to POPs in the Venice lagoon (Italy)	
12:30-13:30	*Lunch*	
Afternoon Session		
13:30-15:00	Speaker: Emilio Benfenati (Istituto Mario Negri) Lecture: QSAR Models	James Garratt & Nicoleta Suciu
15:00-15:30	*Coffee*	
15:30-17:00	Speaker: Elisa Giubilato (Ca' Foscari) Practical Session: food web modelling in the Venice Lagoon	
17:00-17:30	Recap of Day 2 and partial evaluation	
18:00	*Visit to Museo del Violino (MdV) and Gala dinner*	

Wednesday, 01 July 2015		**Companions**
9:00 – 20:30	Visit to EXPO Milan 2015	Ettore Capri, Philippe Ciffroy, Gabriella Fait, Nicoleta Suciu

Thursday, 02 July 2015		**Chairman**
Morning Session		
9:00 – 9:10	Brief introduction to Day 3	James Garratt & Gabriella Fait
9:10-10:40	Speaker: Philippe Ciffroy (EDF) Lecture: Transfer and fate of contaminants on the environment	
10:40-11:00	*Coffee*	
11:00– 12:30	Speaker: Philippe Ciffroy (EDF) Practical Session: Transfer of a contaminant in a river	
12:30-13:30	*Lunch*	
Afternoon Session		
13:30-15:00	Speaker: Frederic Bois (INERIS) Lecture: Theory of PBPK modelling	James Garratt & Gabriella Fait
15:00-15:30	*Coffee*	
15:30-17:00	Speaker: Celine Brochot (INERIS) Practical Session: Predicting contaminant concentrations in human tissue using the MERLIN-Expo tool	
17:00-17:30	Recap of Day 3 and partial evaluation	
20:00	*Social Dinner*	

Friday, 03 July 2015		**Chairman**
Morning Session		
9:00 – 9:10	Brief introduction to Day 4	James Garratt & Nicoleta Suciu
9:10-10:40	Speaker: Andrea Saltelli (SVT) Lecture: Uncertainty analysis/ sensitivity analysis	
10:40-11:00	*Coffee*	
11:00– 12:30	Speaker: Philippe Ciffroy (EDF) Practical session: Uncertainty/sensitivity analysis of a simple case study	
12:30-13:30	*Lunch*	
Afternoon Session		
13:30-15:30	Final Evaluation Feedback and closure of the course	
15:30	*Departures*	

10.2.6 Barcelona September Workshop Agenda

22nd September

Time	Presenter and topic
11:00 – 11:15	Welcome and coffee
11:15 – 11:30	*Welcome* Speaker: **James Garratt** • Introduction to the course and the course objectives • Current approaches in human health and exposure assessment and their deficiencies • Advanced methods and the future for environmental and human health exposure modelling • The MERLIN-Expo tool and its key features • The 4FUN project, introduction to the other speakers.
11:30 – 12:00	*Lecture 1* Speaker: **Philippe Ciffroy** • The 4FUN project: objectives • Innovative issues of the MERLIN-Expo tool • Documentation available for end-users • Overview of the library of models in the tool
12:00 – 13:00	*Lecture 2* Speaker: **Boris Alfonso** • Overview of the general structure and format of the MERLIN-Expo tool • Simple demonstration of the software o *Case study 1 (Lead poisoning in a child)* *If there is time, show a training video on one of the modules within MERLIN-Expo*
13:00 – 13.45	Lunch Break
13:45 – 14:15	*Lecture 3* Speaker: **Gabriella Fait** • Regulatory context of MERLIN-Expo • Evaluation and benchmarking • General overview of case study work
14:30 – 15:30	*Practical session – Case study 2a (Modelling emerging and priority contaminants in the Ebro river)* Facilitated by: **Zoran Banjac** *Extension Work : for further personal practice* *Case study 2b (Food web modelling in the Venice lagoon)*
15:00 – 15:30	*Lecture* 4 Speaker: **James Garratt** • The PBPK model
15:30 – 16:15	*Practical session – Case study 3 (Human food chain)* Facilitated by: **James Garratt** • Predicting contaminant concentrations in human tissue using the MERLIN-Expo tool *Extension Work : for further personal practice* *Continue with case study 2b (Food web modelling in the Venice lagoon)*
16:15 – 16:30	Coffee break
16:30 – 16:45	*Lecture 6* Speaker: **Philippe Ciffroy**

	• Practical Introduction to uncertainty and sensitivity analysis in MERLIN-Expo.
16:45 – 17:45	*Practical session - Case study 3 (Uncertainty/Sensitivity)* Facilitated by: **Philippe Ciffroy** • Using the MERLIN-Expo tool to perform o probabilistic and deterministic simulations o uncertainty and sensitivity analysis
17:45 – 18:15	Review & Questions
18:15 – 18:30	Couse Evaluation / Feedback