

VAMDC

Virtual Atomic and Molecular Data Centre

D3.13

Final Dissemination/Training Report

Version 1.0

Grant agreement no: 239108

Combination of Collaborative Projects & Coordination and Support Actions







Project Information

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9	Queen's University Belfast	QUB	UK	Month 1	Month 42
10	Astronomska opservatorija	AOB	Serbia	Month 1	Month 42
11	Institute for Spectroscopy RAS	ISRAN	Russian Federation	Month 1	Month 42
12	Russian Federal Nuclear Centre All-Russian Institute of Technical Physics	RFNC-VNIITF	Russian Federation	Month 1	Month 42
13	Institute of Atmospheric Optics	ΙΑΟ	Russian Federation	Month 1	Month 42
14	Corporacion Parque Tecnologico de Merida	IVIC	Venezuela	Month 1	Month 42
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Abstract	The objective of D3.13 is to describe VAMDC Dissemination and Training Report for the whole project. This report corresponds to Activities in WP3: NA2 "Dissemination and Training".



Versioning and Contribution history

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WP3 ACTIVITIES DESCRIPTION

Work package number3			Star	t date	or sta	rting	event:	3			
Work package title	NA2: Diss		emination and Training								
Activity Type	COORD										
Participant id	1	2	3	4	5	6	7	10	13	14	15
Person-months per beneficiary:	6	9	3	18	14	8	1	12	6	11	3
(Total = EU + Node Contributions)											

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1. WP3 Objectives

Our objective is to attract new participants to the e-infrastructure, i.e. producers and users of data.

The key objective of the training and dissemination activity is to ensure that principle stakeholders are engaged in the development and implementation of the VAMDC E-infrastructure. This Work package will therefore provide for:

a) Dissemination of VAMDC services at national, EU and non-EU levels

b) Training of producers & users at master, PhD and professional levels (both academic and non-academic users)

Specifically this work package provides for:

1) An annual meeting, which showcases the work of the e-infrastructure, supports networking and scientific communication, and becomes the conference of choice for users and providers of atomic and molecular data

2) Organize topic based scientific workshops, twice a year, to bring together proposers, users and providers of A&M data to discuss data needs and how VAMDC can meet those needs.

3) Arrange teaching tutorials (on-line and face to face) on the VAMDC e-infrastructure

2. WP3 Milestones and Deliverables

Milestones

M3.1	CTT meetings	WP3	OU/UNIVIE	Months	Minutes of Meetings on
				10, 22, 34, 42	Internal Website
M3.2	Review of Conferences/Schools	WP3	OU/UNIVIE	Months 10, 22, 34	Agenda and Training material of workshops on Public Website



M3.3	Review of Regional	WP3	OU/UNIVIE	Months	Agenda and Training
	Tutorials			10, 22, 34	material of workshops on
					Public Website

Deliverables

D3.1 Dissemination and Training (D&T) Plan (PM 3) D3.2 Annual D&T Report to be included in report to EU – Year 1 (PM 10) Annual reports will provide publicly available summaries of the activity of the WP for each project year. Report will include a list of meetings/conferences attended to disseminate VAMDC to other communities. Annual reports will be for examined by the VAMDC Project Board. D3.3 VAMDC Level 1 Service Prototype (PM10) D3.4 VAMDC Annual Project Meeting 1 at OU (4) (PM12) An annual meeting will be organized at the end of each year of the project D3.5 Annual D&T Report to be included in report to EU – Year 2 (PM 22) D3.6 VAMDC Level 2 Service Prototype (PM22) D3.7 VAMDC Annual Project Meeting 2 at CMSUC (2) (PM24) D3.8 Annual D&T Report to be included in report to EU – Year 3 (PM 34) D3.9 VAMDC Level 3 Service prototype (PM34) D3.10 VAMDC Annual Project Meeting 3 at UNIVIE (5) (PM36) D3.11 VAMDC Service Release (PM40) D3.12 VAMDC Final Annual Project Meeting at CNRS (1) (PM42) D3.13 Final Report of Dissemination and Training to be included in final report to the EU *(PM42)* The final report will include a reflexive analysis of the effectiveness of the WP, and proposals for future activities beyond the lifetime of the project. This deliverable will be organized under Task 1.

Annual D&T Plan revisions included in Revised Annual VAMDC Project Plans – Year 1,2,3

WP3 Leader	N. Mason (OU)	
Task Number	Leader	Other Partners
1 Coordination	N J Mason (OU)	F. Kupka (UNIVIE)
2 Annual meetings	N J Mason (OU)	All partners involved in WP3
3 Scientific	N J Mason (OU)	All partners involved in WP3
Workshops		
4 Training Tutorials	N Walton (CMSUC)	UCL; CPTM, INASAN, IAO
5 VAMDC Service	N Walton (CMSUC)	UU - CNRS

3. WP3 Tasks Description

Description of work

This activity provides the conduit for communicating both the aims and results of the VAMDC e-infrastructure. Dissemination activities are aimed at VAMDC's users, the wider European science community, European industrial stakeholders and policy makers. It is intended to provide an attractive platform to exchange and present results, develop new ideas



and to network with other data providers and e-infrastructures. This will be accomplished by organizing a high profile annual meeting, being represented at other appropriate conferences and hosting a series of targeted topical workshops and teaching tutorials.

- NA2 therefore consists of four tasks:
- 1) Coordination
- 2) Organizing an annual meeting and arranging representation at other relevant meetings
- 2) Organizing themed scientific workshops
- 3) Organizing training tutorials

Task 1: Coordination (Chair OU(4), Deputy Chair UW_A(5))

Dissemination activities will be a pre-requisite for all VAMDC's activities. Therefore each NA, SA and JRA will nominate a member to prepare the necessary material for disseminating the aims, objectives and results of these activities. Dissemination across the project will be coordinated by the **Communication and Training Committee (CTC).** The role of the communication and training committee is to propose a list of dissemination and training actions, to organize the general events linked to this project and to compile records of actions. It will be composed of NA2 partners and chaired by the WP3 leader (OU). The CTC will organise the communication and training section of the VAMDC web-site. This section will hold all records of dissemination and training actions and the CTC will be responsible for updating this section with announcements, news, proceedings, and presentations.

Task 2: Organisation of annual international conference and VAMDC's representation at other relevant meetings

<u>Annual meeting</u> The CTC will organise an annual international conference focused on the VAMDC e-infrastructure, its resources and services. The programme committee will be chaired by OU with UNIVIE as deputy. It will be aimed at users, producers and developers. It will include both academic and non-academic users. This major event will be held each year in a different part of the EU and proceedings will be published (both on line and subject to discussions with scientific publishers in hardcopy – note the UK Institute of Journal of Physics Conference Series have expressed interest in publishing such proceedings).

It is VAMDC's ambition that this meeting become a conference of choice for A&M database providers and for A&M data users (We wish at least one meeting to be combined with the international ICAMDATA conference).The conference will therefore aim to attract a wide audience including many of the key stakeholders we wish to engage with (industrialists, politicians, media). The Conference will also be the location of many of the VAMDC e-infrastructure's necessary management meetings.

Dissemination via EU national and international existing conferences

Yearly the CTC will establish a list of national and international conferences where oral presentations and demonstrations on VAMDC will be valuable. These national and international conferences will usually be conferences of producers and users. AOB will be responsible for collating the information and arranging with other partners VAMDC presence at such meetings. The CTC will accordingly prepare suitable display material (in electronic format and hard copy) for display at such meetings which can be *used by any of the VAMDC partners*.

Organisation of "regional" tutorials

Since the VAMDC e-infrastructure is planned as an international activity and includes international partners the CTC will also prepare a list of tutorials that will be held in non-EU countries in order to spread the knowledge and practice of the VAMDC infrastructure. These



tutorials will be organised by our non-EU partners (CPTM, INASAN, IAO, AOB) and will be aimed at people from those "regions".

Task 3: Scientific workshops

Central to the aims of the VAMDC is the formation of an infrastructure that responds to the needs of its user communities since the major impact of the e-infrastructure will be its adopting by scientific and technology communities. Therefore in order to ascertain the requirements of current and potential VAMDC communities and in order to inform the project we will host a series of themed workshops with such communities. These meetings may be stand alone or more usefully as part of the user community's own conference/meetings programme (through arranged VAMDC sessions). It is anticipated that two such meetings would be per year. Administration of these meetings will be arranged by the CTC.

Proposed topics follow those identified in Section 3 (Impact) and include; The astronomical and planetary science Community (with sessions held at the Euro planet RI meeting, SF2A, IAU meetings); The atmospheric science community (in collaboration with one of the HITRAN database meetings); The technology plasma community (at its European meeting ESCAMPIG); The fusion community (as part of the IAEA meetings for ITER itself part of the EURATOM programmed); The Lighting industry (hosted by Philips Itd) and the radiation sciences community (possibly in collaboration of GEANT meeting and the EU RADAM conference series). Each of the following partners will organize (and when necessary host) one or more such workshops; OU (plasma and radiation sciences); UCL and IAO (atmospheric science and Hitran); CMSUC, AOB, CNRS (astronomy and planetary science); UNIVIE and OU (fusion (with IAEA) and lighting).

Task 4: Training Tutorials

CMSUC and UCL will prepare material for the partners to use in training workshops both in their own countries and internationally. These tutorials will be focused in developing a user's competence to use the e-infrastructure and to interface it into their own operating systems; Short training sessions will be integrated into the Annual meeting. All partners will be required to nominate one member who will be able to 'train' and/or provide support for their national users. Our non EU partners (CPTM, INASAN, IAO) will also prepare a self-studying e-tutorial for VAMDC users who can not attend such tutorials. We (OU,UCL) will also prepare an e-tool for general public/more general stakeholders such that they can take a virtual guided tour of VAMDC including its current status: statistics, content, geography of clients and producers etc.

Task 5: VAMDC Service & Service Prototype Release

CMSUC, UU and CNRS will lead the coordinated release of the annual VAMDC prototype service. This will lead to the final release of the VAMDC service infrastructure. The annual prototypes will be reviewed at the yearly project meetings and available for assessment alongside the VAMDC annual reports.

The prototype services will contain the following functionality:

Level 1: Preliminary VAMDC service with simple data access to the core VAMDC data resources

Level 2: Enhanced interoperable data access to VAMDC data resources, all resources accessible

Level 3: Interoperable VAMDC data access with VAMDC tools available (client side or server side accessible via through workflow enactment engines)

VAMDC Service: Final full service, including access to resources from the wider community



(through the SA1 / Task 6 community call).



4. WP3 Final Report

Period: 01/07/2009 – 31/12/2012 WorkPackage: Working Group 3 WorkPackage Leader and co-Leader: OU (N J Mason) and UNIVIE (F Kupka) Participants in the WorkPackage: CNRS, CMSUC, UCL, OU, UNIVIE, UU, KOLN, AOB, IAO, IVIC, INASAN

Part 1

VAMDC Potential Impact and Dissemination Activities (not to exceed 10 pages)

Scientific research requires dissemination of findings and results. The aim of most scientists is that other people (be they other scientists, industry, government or the public) should learn of their work and use it. Today many of these exchanges are electronic with immense amounts of data being exchanged using all forms of modern information technology. This in turn requires scientists to adapt to conducting research with data that come in rapidly increasing quantities, varieties and modes of dissemination, often for purposes far more interdisciplinary than in the past. Accordingly, around the world 'data centres' and other more loosely defined organisations of data producers and users are participating in a revolutionary transformation in the manner in which data is exchanged. However it is widely recognised that there remain several major challenges to developing robust and integrated e-infrastructures that will allow data to be disseminated to user communities. In particular there is a strong need to:

 \cdot Develop close links between the user communities, the data producers and data centres based on modern technology.

 \cdot Establish better international coordination in order to promote data compilation and database activities, avoid duplication of efforts and ensure the use of the best available data.

The Virtual Atomic and Molecular Data Centre (VAMDC) was developed with the goal of building such a secure, documented, flexible, easily accessible and interoperable e-infrastructure for *Atomic and Molecular (A&M) data*. Atomic and molecular data underpins a wide range of diverse applications such as astrophysics, atmospheric science, the development of fusion energy, semiconductor manufacturing and other plasma based technologies, the lighting industry, detection and remediation of pollutants (and increasingly the detection of explosives and biological agents as may be used in terrorism) and is essential for understanding many biological processes including modelling radiation damage in cellular systems for therapy treatment. Indeed progress in many of these areas is limited by the availability of accurate quantitative information on the collisional properties and spectroscopic characteristics of interacting species.

However it is widely by the recognised by the A&M community that there remain several major challenges to developing a robust and integrated infrastructure that will allow A&M data to be disseminated to these user communities:

- (1) Data completeness and quality assessment and
- (2) Development of a data interface for data mining.



VAMDC has been built upon the expertise of existing AM databases, data producers and service providers with the specific aim of creating an infrastructure that on one hand can directly extract data from the existing data repositories while one the other hand is sufficiently flexible to be tuned to the needs of a wide variety of users from academic, governmental, industrial communities or from general public both within and outside the ERA. The main output of the VAMDC therefore has been the provision of the VAMDC e-science portal described in Section XXX however such a structure cannot be developed without a clear knowledge of the both the 'user' base and the 'suppliers' of the A&M data. Accordingly throughout the VAMDC project dissemination to and engagement with users and suppliers was core to the success of the programme.

Atomic molecular data user and provider communities

At the outset of the project VAMDC targeted those scientific communities that had a track record of being large users of A&M data. These included;

- (i) Astrochemistry (and planetary science)
- (ii) Atmospheric Sciences
- (iii) Fusion Energy Research
- (iv) Lighting Industry
- (v) Plasma technologies
- (vi) Radiation Sciences

These communities are also strongly linked to A&M providers, indeed it is important to recognise that within the EU research community most A&M data is developed for specific applications and is not produced in isolation as a purely scholarship activity (as it was in the mid to late 20th century). For example most spectroscopic and collisional studies today are funded as part of applied research programmes rather than for their own sake with the rapid expansion of molecular spectroscopy arising from the need to study atmospheric chemistry whilst the spectroscopy of atomic ions has been driven by the need to interpret astronomical observations or provide benchmarks for fusion devices. VAMDC's interactions each of these fields will be discussed in turn.

Astronomy and Planetary Science

The VAMDC project was largely led and initiated by the astronomy research community in recognition of the role A&M data plays in the interpretation and modelling of astronomical and planetary science data. VAMDC was therefore built upon a the wide range of users coming from the astrophysical community and many of the initial databases within the VAMDC portal are those developed by, and for, the astronomy and planetary science communities. Accordingly the VAMDC partners were strongly integrated with major astronomy and planetary science projects including The ALMA and Herschel telescopes which will produce a data 'deluge' that will dwarf any previous datasets. Similarly during the course of the VAMDC project the Cassini-Huygens mission to Saturn and Titan has highlighted the need for large datasets of A&M data on complex hydrocarbons, whilst the discovery of exoplanets and subsequent exploration of their atmospheres has led to an urgent need for access to spectroscopic data (at elevated temperatures). VAMDC partners have been integral to the development of several other EU projects in which the VAMDC ethos and structure have been demonstrated. These include the International Virtual Observatory Alliance (IVOA); The European Virtual Observatory (EURO-VO) and the UK's Virtual Observatory, AstroGrid. VAMDC has also been engaged with both the GREAT and LASSIE ITNs (allowing a new generation of Early Stage Researchers to engage with the VAMDC



portal and its databases); The COST Action CM0805 'The Chemical Cosmos' which hosted a series of workshop in which data needs were reviewed and the ESF EUROGENESIS Eurocore. VAMDC members are also strongly connected with the forthcoming GAIA and Rosetta missions whilst providing input into the current Martian missions (Mars Express and the MSL Curiosity Rover mission - in which the new GhoSST database developed under auspices of VAMDC is particularly important).

The VAMDC project has been particularly engaged with the EUROPLANET Research Infrastructure (http://www.europlanet-ri.eu) which has operated concomitantly with the VAMDC project. The Europlanet project has developed the Integrated and Distributed Information Service (IDIS). The task of IDIS is to provide an easy-to-use web-based platform to give access to available planetary science data needed to interpret observations or to solve open questions and exploit synergies between space-based missions and capabilities of ground-based observatories. A set of tools for describing, accessing and combining information and data from different sources has been developed, with the objective to offer a Virtual Observatory access to many data essential for planetary research from European and non-European sources. Thus the goals of IDIS and VAMDC overlap and several of VAMDC's partners are also members of Europlanet RI, indeed two of the VAMDC databases (GhoSST and KIDA) have been developed under the auspices of both projects. VAMDC has featured at the Europlanet Annual conferences (the European Planetary Science Congress EPSC) in EPSC7: IFEMA-Feria de Madrid, Spain, 23-28 September 2012; EPSC6 held jointly with the US Division of Planetary Sciences at La Cité Internationale des Congrès Nantes Métropole, France, 02-07 October, 2011; EPSC5: Angelicum Centre -Pontifical University of Saint Thomas Aquinas, Rome, Italy, 19-25 September, 2010 and EPSC4: Kongresshotel, Postdam, Germany, 13-18 September, 2009. Thus VAMDC reached in excess of 3,000 Planetary Scientists.

Atmospheric science : Understanding the physics and chemistry of the terrestrial atmosphere and thence climate change with all its social and economic consequences has required the construction of the some of the largest, most complex computational models in the world today. The development of such models is performed as an iterative process that is often driven by experimental observations. Such field observations are predominantly based on spectroscopic techniques and hence require a rich and diverse database of atomic and molecular photoabsorption cross sections to both determine the absolute concentrations in the terrestrial atmosphere and to quantify their role in the atmospheric radiative transport problem. Such data is then used construct the models which predict the influence of natural/anthropogenic phenomena in our atmosphere. The models presently include more than a 100 atomic and molecular species with data drawn from both experiments and theory which must be sourced, validated, tabulated and cross referenced. The international database for this community is HITRAN the high-resolution transmission molecular absorption database. HITRAN is a compilation of spectroscopic parameters that a variety of computer codes use to predict and simulate the transmission and emission in the atmosphere. The database is a longrunning project started by the Air Force Cambridge Research Laboratories (AFCRL) in the late 1960's in response to the need for detailed knowledge of the infrared properties of the atmosphere but today HITRAN its analogous database HITEMP (high-temperature spectroscopic absorption parameters), are now being developed at the Atomic and Molecular Physics Division, Harvard-Smithsonian Center for Astrophysics. HITRAN is one of the core databases in the VAMDC suite and the VAMDC Consortia (in particular UCL node) have been integral to the development of the most recent Hitran updates. VAMDC has been



represented at the biennial HITRAN Database Conferences held during the project -11th conference at Harvard 16-18 June, 2010 and the 12th conference held in Reims August 29-31, 2012. VAMDC members were already present at the 10th meeting also held in Harvard June 22-24, 2008). VAMDC was also represented and a participant in a myriad of workshops and conferences, at which HITRAN was reviewed, developed and exploited including the Atmospheric Spectroscopy Applications (ASA) series. The success of the integration of HITRAN and VAMDC is perhaps summarised by the inclusion of Dr Larry Rothman of the Atomic and Molecular Physics Division, Harvard-Smithsonian Centre for Astrophysics and chair of HITRAN in the VAMDC follow-on project SUP@VAMDC.

Fusion Energy Research

Atomic and molecular collisional and spectroscopic processes play an important role in magnetic fusion devices as they influence the energy balance of the confined plasma, the plasma transport and radiation properties and are used as the basis for many plasma diagnostic methods. The design and operation of several fusion device systems, such as neutral beam heating, impurity control and thermal power and particle exhaust systems, require large amounts of A&M collisional and spectroscopic data. The need for coordination of A&M data acquisition efforts on an international scale therefore became evident at the beginning of the 1970's and has been part of the central programme of the International Atomic Energy Agency (IAEA) which has therefore (in collaboration with several National programmes) assembled recommended international A&M data for fusion. Indeed since such work has been led by the IAEA Atomic and Molecular Data Unit (www-amdis.iaea.org). Accordingly developing a partnership between VAMDC and the ITER A&M data unit was a central goal of the VAMDC. This has been extremely successful with the head of the ITER A&M data unit Dr Bas Braams becoming a key member of the VAMDC community. VAMDC members have extensively participated in ITER A&M data unit meetings and several VAMDC protocols and have been adopted by IAEA databases e.g. the VAMDC XSAMS has now been adopted. VAMDC members are also playing a lead role in the data evaluation and recommendations of A&M datasets prepared under the auspices of IAEA and will play an integral role in preparing the ITER A&M data unit's guidelines for evaluating theoretical data in 2013. Through these strong ties VAMDC has been widely engaged with the EU fusion community and is poised to play a key role in the IAEA's A&M data recommendations/standards for the ITER programme.

Lighting Industry

General purpose lighting consumes about ¹/₄ of all electricity produced, hence there is a great interest in improving lighting technologies and a field of research in which ERA has International expertise (e.g. with Philips Ltd). However despite the long and distinguished history of the lighting research community in establishing the required databases the present status is still unsatisfactory particularly for the new technology developments exploiting new gas species (e.g. mercury free fluorescent lamps using pure Xe, phosphorous and metal alloys such as InSb). As an exemplar of combining fundamental research with commercial applications the VAMDC project engaged with members of the lighting research communities to establish the necessity for databases for the development of future light sources. A special topical workshop (Atomic and Molecular Data Needs for Lighting) was held as part of the XX ESCAMPIG in Novi Sad, Serbia July 13-17, 2010. This meetings highlighted that many of the databases used by industry were 'closed' and that, while the industry would welcome access to the VAMDC portal it was essential that such access was confidential to the specific user (and not open to examination by commercial competitors) whilst industrial databases



could not be made open access due to commercial sensitivities. This and subsequent meetings thus highlighted the difficulties in both fulfilling the 'open access' requirement of EU (Framework) supported research with commercial needs and the challenge of VAMDC tendering for and supplying data on a commercial basis as part of its sustainability plan.

Plasma technologies.

Plasma based technologies are one of the largest commercial industries in the world today. The selective and highly anistropic etching of materials and the controlled deposition of thin films in the fabrication of microelectronic structures are among the most important methods of plasma-assisted materials processing, plasma polymerisation and plasma-assisted surface modification. Plasma-based processes are used in some 40% of the steps in the manufacture of semi-conductor chips. For modelling the behaviour and properties of such chemically active plasma, detailed quantitative information is required for the most important collisional and radiative processes taking place both in the gas phase and on the surfaces in turn requiring an enormously detailed database. The plasma industry has recognised this need for more than a decade and most of the major plasma focused companies have supported or developed commercial databases but they are often incomplete and crucially many lack rigorous academic review. The A&M databases for most technological plasma applications therefore remain inadequate for a full understanding of the corresponding plasma chemistry dynamics and full exploitation of the optimization of these reactive plasmas. A coordinated international effort to improve the current status of the A&M database relevant to such plasma technologies has therefore been highlighted by both academic and industrial communities for the future advancement of technological development. Accordingly the VAMDC initiative has been welcomed by the plasma research community, both in the EU and internationally. Strong links have been established with the PLASIMO project (http://www.plasimo.phys.tue.nl) which has adopted VAMDC schema and protocols and exploited the Quantemol packages developed by the UCL node of VAMDC. VAMDC has also been integral to the EU-Japan Plasma Series (e.g. at the 8th EU-Japan Joint Symposium on plasma processing which included a workshop on Atomic and molecular database for plasma and surfaces 16-18 January 2012 and 7th EU-Japan Joint Symposium on plasma processing Liblice, Czech Republic 23rd to 26th April 2009) allowing the VAMDC ethos and 'product' to be disseminated amongst the Japanese and Korean research communities (including leading Plasma industries such as Toshiba, NEC, Hitachi and Samsung). Talks are on-going about incorporating plasma databases into the VAMDC portal for example LXcat an open-access website coordinated by Dr L.C. Pitchford University of Toulouse, France for collecting, displaying, and downloading ELECtron SCATtering cross sections and swarm parameters (mobility, diffusion coefficient, reaction rates, etc.) required for modeling low temperature plasmas.

Radiation Sciences. The effect of increased exposure to low doses of radiation in our daily lives has led to concerns that this may have long term health effects e.g. through damage of cellular DNA. Similarly the use of ionizing radiation in medical therapy relies of a better understanding of how to control/induce damage of DNA within cancerous tissue. Both problems are explored by the development of complex radiotherapy models on the nanoscale (e.g. using GEANT formalism), incorporating fundamental A&M data for example low energy electron collisions with the DNA components (e.g. nucleobases) and other biomolecules such as nucleosides, amino acids and in study of cellular walls, lipids. However the database both for the spectroscopy and collisional cross sections for such compounds is both scarce and too date data has not been assembled in a single database. VAMDC



interactions with the Radiation Damage community through its workshops (and in particular the 'RADAM' conference series) led to a collaboration between VAMDC and the RADAM communities via the COST supported Action MP1002 IBCT-NANO (<u>http://fias.uni-frankfurt.de/nano-ibct/overview/</u>) to develop the RADAM database in accord with the structures, protocols and schema of VAMDC. This will be the first purpose built database to follow the VAMDC structure and the compilers of this database were trained by VAMDC members.

Thus the VAMDC project has a strong dissemination programme with those communities that both use and provide A&M data. Links established during the course of the project are not only set to endure but will be integral to the development of both VAMDC and these partners (e.g. HITRAN, IAEA Atomic and Molecular data unit and RADAM).

Engaging with other stakeholders

Whilst much of VAMDC's dissemination programme was necessarily aimed at A&M data users and providers as described above the VAMDC consortia engaged a wider range of stakeholder groups including;

- Industrial and commercial partners
- Government and policy makers
- The general public and
- The international community.

Industrial and commercial partners: Efforts were made to target potential industrial and commercial partners, particularly SMEs who are an obvious user of the VAMDC e-infrastructure but traditionally have had the greatest problems in utilising databases in part because of the lack of metadata on such sites, problems in ease of access and the high cost of commercial databases which are beyond the affordability of most SME research budgets. The VAMDC with its stated aim of accessibility, interoperability and open access provides a new (and long required service) for such SMEs. As mentioned above workshops were held with two targeted industries the lighting and plasma industries. Such links were further fostered through one node's (UCL) own SME 'Quantemol'.however such discussions also highlighted the difficulties in both fulfilling the 'open access' requirement of EU (Framework) supported research with commercial needs and the challenge of VAMDC tendering for and supplying data on a commercial basis as part of its sustainability plan.

Another important set of commercial enterprises with which VAMDC engaged were *academic publishers*. Publishers are the main resource from which databases draw their material and therefore integral to the functionality of any database is its ability to access, quote and review published data. Indeed most databases require that the data they incorporate is already published and thus its authenticity and reliability has been subject to 'Peer review'. In turn data providers need their data to be referenced in order to justify their own funding, however, once within any database individual datasets are seldom specifically referenced. With the advent of open access publishing a whole variety of issues on data procurement, validation and referencing are being raised. VAMDC therefore sought to engage with two of the main European publishers of A&M data (IOPP in the UK and Springer) to explore how data in the VAMDC e-infrastructure may both be accumulated and referenced by users. A pilot project with IOPP is currently under development.



Government and policy makers: Being the first data infrastructure that is dedicated to providing a common platform for the application of A&M knowledge across science and technology VAMDC believes it can act as an exemplar for e-infrastructures dedicated to data production, curation and dissemination. In collaboration with IAEA and partners in USA, Korea and Japan VAMDC is establishing the 'agenda' for such data projects and in its successor project (SUP@VAMDC) it will produce a roadmap that will ultimately lead to a global e-infrastructure for the assembly, curation and access of the immense amounts of A&M data that will underpin the scientific knowledge base that will be required to meet (and overcome) the greatest scientific challenges of the early 21st century (e.g. climate change, space exploration , human health and crucially, the continued technological advances that will drive the global economy). VAMDC has sought to explain this vision to government and policy makers at both national and international level and the success of these activities might be demonstrated by support funding to partners from their national agencies as well as award of the SUP@VAMDC project.

Public outreach: The preparation and operation of databases and e-infrastructures at first sight does not appear conducive to public engagement but this is not true. The collection, storage and utilization of data has major social and economic consequences and whilst A&M Data Storage is not controversial compared with data on the human genome, genetic disease etc. many of the legal requirements are the same. For example discussion of who owns the data, the role of open access and how it influences publishing and the whole social context of scientific data is a topic of wide interest. Accordingly VAMDC aimed to disseminate it role and activities to the widest possible audience. Individual partners disseminated information on their role and that of VAMDC in general to their own local media while the VAMDC e-infrastructure was part of the larger Astrochemistry exhibition in Brussels in June 2011 (The Year of Chemistry) to which MEPs, Framework VII managers, COST and ESF staff was invited and the general public had access over a weekend. In the follow on project Sup@VAMDC such links are to be developed further to include teachers and amateur science communities (citizen scientists) who may use VAMDC as both a teaching and research resource.

Dissemination Methodology

<u>Coordination</u> Dissemination across the project was coordinated by the Communication and Training Committee (CTC) whose role was to propose a list of dissemination and training actions, to organize the general events linked to the VAMDC project and to compile records of actions. The CTC with member roles was as follows:

Nigel J Mason (Chair, organiser of workshops for data users and date providers and host first annual meeting at OU 2010)

Friedrich Kupka (Vice-Chair) (also host of the 3rd annual meeting Vienna 2012)

Claudio Mendoza (Organiser of Regional workshops in Latin America)

Nicholas Walton and Guy Rixon (VAMDC service and prototype release, Host 2nd annual meeting 2011)

N. Piskunov (user tutorials and Prototype release)

M.S. Dimitrijevic (Organiser of Regional workshop in Balkan region June 2012)

T.A.Ryabchikova (Organiser of Regional workshops in Russia)

K Benson (tutorials)



The Project co-ordinator (Marie-Lise Dubernet was also responsible for much of the VAMDC project's dissemination and outreach.

The central VAMDC website <u>www.vamdc.eu</u> holds records of dissemination and training actions and the CTC was responsible for updating this section with announcements, news, proceedings, and presentations. A more public focussed website dedicated to dissemination of the final VAMDC portal was designed by F. Kupka and T. Rank-Lueftinger of Vienna node for post project guidelines to the wider user community (website XXX).

The CTC also produced a newsletter ((editors F. Kupka, T. Rank-Lueftinger of Vienna node) which was circulated to the infrastructure members and other interested parties.

Organisation of VAMDC annual meetings;

An annual meeting was organised to coordinate the activities of the VAMDC project and provide an opportunity to engage with user and producer communities. The first meeting held at the Open University in 2010 was severely disrupted by the volcanic eruption in Iceland which closed European airspace. The second held in March 2011 included representatives from user communities and publishers, as did the Third meeting held in Vienna February 21-24, 2012. The final VAMDC meeting including meeting of WP3 was held in Observatoire de Meudon November 13-16. Some of the presentations at the Board meeting were filmed by F. Kupka. Two sessions of the meeting included presentation by potential users and data providers of the VAMDC database in particular the developing RADAM database, NIST and members of the Plasma community. The second session featured members of the data provider community and reviewed methodologies for data evaluation, this included review of data evaluation techniques currently used by VAMDC databases (KIDA and HITRAN, CDMS) and the emerging project by IAEA to coordinate worldwide atomic and molecular data evaluation. A Special session was arranged with publishers during which ideas of further dissemination of the VAMDC project were discussed (special issue & review articles) and the open access model of VAMDC reviewed. At outreach session was also organised including presentation form the Hands on Universe project. Full programmes including websites may be found on www.vamdc.eu.

Scientific workshops and regional meetings

VAMDC presented and discussed its activities, objectives and tools in a series of international meetings with different user and provider communities as discussed above. In addition VAMDC was represented at the major International Conference of Atomic and Molecular DATA (ICAMDATA) held biennially in Vilnius, Lithuania in 2010 and, most recently, in NIST September 30 - October 4, 2012. An ICAMDATA Satellite Meeting entitled VAMDC-USA chaired by Yuri Ralchenko and Marie-Lise Dubernet was held on October 5, 2012. The purpose of this meeting was to expose VAMDC to the US community and vice versa as well as to initiate collaborations between database providers and users with VAMDC. Regional meetings were held in Caracas to disseminate VAMDC to the Latin South American community. AOB Organized a Regional Workshop on Atomic and Molecular Data in Belgrade, Serbia, 14-16 June 2012, see: Erreur ! Référence de lien hypertexte non valide. the meeting included participants from Slovenia, Croatia, Bulgaria, and Serbia. Similarly INASAN and IVIC and IAO hosted a Regional meeting in Russia Chair T.A.Ryabchikova for Moscow region users http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/MoscowTut http://www.astro.uu.se/valdwiki/Nik in Moscow 04-2012 Tutorials



CMSUC and UCL were tasked with preparing material for the partners to use in training workshops both in their own countries and internationally. Considerable material is available on the VAMDC website for users and this was used in the two regional meetings in Belgrade and Moscow in 2012. Kevin Benson (UCL) developed training tutorials and support material for a VAMDC-plugin used in the Taverna Workflow Management System. The material includes video material as well as screenshots. Ready to use workflows have been uploaded to the social workflow sharing website 'myExperiment' to allow end-users to instantly run workflows on the VAMDC infrastructure. http://www.myexperiment.org/search?query=vamdc&type=all. The public website will also provide a direct link to such material for future users.

Deliverables

D3.1 Dissemination and Training (D&T) Plan - DONE http://www.vamdc.eu/public-deliverables/14-deliverables-wp3/

D3.2 Annual D&T Report to be included in report to EU – Year 1 - DONE Annual reports will provide publicly available summaries of the activity of the WP for each project year. Report will include a list of meetings/conferences attended to disseminate VAMDC to other communities. Annual reports will be for examined by the VAMDC Project Board. <u>http://www.vamdc.eu/public-deliverables/14-deliverables-wp3/</u>

D3.3 VAMDC Level 1 Service Prototype - DONE – Demonstrated at Review Meeting 1 (Talk-4.pdf and Talk-5.pdf) http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/RmCycleOne

D3.4 VAMDC Annual Project Meeting 1 at OU – DONE – An annual meeting will be organized at the end of each year of the project http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/PmCycleOne/

D3.5 Annual D&T Report to be included in report to EU – Year 2 – DONE – http://www.vamdc.eu/public-deliverables/14-deliverables-wp3/ (*this report*)

D3.6 VAMDC Level 2 Service Prototype - DONE - – Demonstrated at Review Meeting 1

http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/RmCycleTwo/

D3.7 VAMDC Annual Project Meeting 2 at CMSUC - DONE – An annual meeting will be organized at the end of each year of the project <u>http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/PmCycleTwo/</u>

D3.8 Annual D&T Report to be included in report to EU – Year 3 – DONE – http://www.vamdc.eu/public-deliverables/14-deliverables-wp3/ (this report)

D3.13 Final Dissemination/Training Report



D3.9 VAMDC Level 3 Service Prototype - DONE - – Demonstrated at Review Meeting 111

http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/RmCycleThree/

D3.10 VAMDC Annual Project Meeting 3 at UNIVIE - DONE – http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/PmCycleThree/

D3.11 VAMDC Service Release - DONE - – http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/RmCycleFour/

D3.12 VAMDC Final Project Meeting at Paris Observatory - DONE – http://voparis-twiki.obspm.fr/twiki/bin/view/VAMDC/PmCycleFour/

D3.13 Final D&T Report– DONE – http://www.vamdc.eu/public-deliverables/14-deliverables-wp3/

Deviations from the contract (Annex I) and reasons for them (if applicable) none

Failures to achieve critical objectives and/or not being on schedule and reasons for them (if applicable)

N/A

Proposed corrective actions (if applicable) N/A