## The Pacific Northwest National Laboratory Export Control Improvement Initiative

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# ABSTRACT

The Pacific Northwest National Laboratory has completed a two-year export control program improvement initiative that has significantly reduced its compliance risk with US laws and regulations that protect national economic interests and prevent the acquisition of critical technologies, technical data, and information. This paper highlights key processes and activities that underpin the improvement initiative. Improvements were broadly accomplished through upgraded research-focused training and laboratory awareness; process mapping of requirements to organizational procedures, development of information technology (IT) tools; and the management of high-risk export-controlled property, chemicals, and biological materials. IT tools put in place include: Improved Export Control Web Site, Export Control Service Request, Inbound Shipping Tool that allows staff to identify inbound shipments that are not related to procurement or the standard acquisition process, the Risk Engine that allows high-risk export controlled personal property to be managed from acquisition to final disposition, and the Technology Protection Integration Map that depicts spatial identification and control of high-risk personal property, projects, and people associated with export-controlled projects. To assure sustainability, the Technology Protection and Export Control organization staffing was increased, definitive administrative procedures were developed, and periodic self-assessment/assurance processes were established.

# INTRODUCTION

# The Challenge

The Department of Energy (DOE) national laboratories are exceptional organizations that deliver scientific and technological capabilities to address national priorities in fundamental science, energy, and security. This is done often by collaborating with academia, industry, and other governmental organizations. The complexity of research operations, collaborations, new technology breakthroughs, and security imperatives present an incredibly large, diverse, and multifaceted export control compliance challenge. The Pacific Northwest National Laboratory (PNNL) is no exception. Between 2019 through 2021, PNNL invested in significant improvements to its Export Control Program (ECP), recognizing that export controls are comprehensively linked to many of its business functions and research missions. Figure 1 illustrates the scope of export control involvement within PNNL.

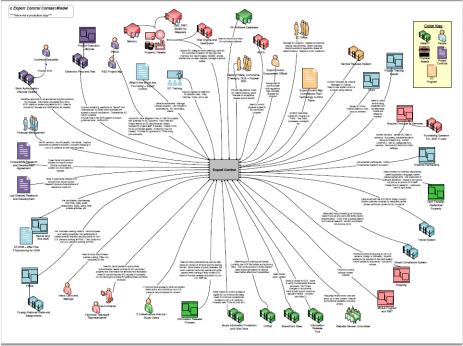


Figure 1. Export Control Context Model

This projectized effort had the overall objectives to:

- Determine key critical improvement areas and expectations for success
- Execute an integrated approach for implementation actions
- Verify improvement actions met success criteria.

The overall goal was to mitigate areas of greatest risk exposure to PNNL. Ten improvement areas were acknowledged with a total of over 1,000 individual project actions worked. The outcome was senior management commitment to export controls, beginning with the Laboratory Director, that flowed down through all organizations. New IT tools were developed, and processes were strengthened.

Our goals were achieved. The following sections of this paper discuss some of the key improvements.

# It's All about the People – Staffing for Success and Sustainability

Developing and sustaining any compliance program within the context of a multi-discipline national laboratory is a significant challenge. In past years, the export compliance organization (now referred to as the Technology Protection and Export Control [TPEC] Team) was under-resourced with limited visibility among the Management and Operations (M&O) program and research and development organizations. An immediate hurdle faced was quickly building a robust and sustainable export compliance program from a previously unstaffed organization that could meet the needs of a dynamic and diverse research portfolio.

Staffing was increased from three export control professionals to nine in a matter of just 18–24 months. While this was a welcome increase in resources, growing this quickly came with its own set of challenges. Constraints were immediately understood:

- Export control professionals cannot be grown overnight.
- Onboarding and training novice professionals quickly would be a considerable strain on the more experienced subject matter experts (SMEs).
- A large group of compliance professionals would need to represent a multi-disciplinary background that mirrored our research portfolio.

While the above by no means captures all the myriad challenges regarding managing sustainable growth, the key tactics employed to address these obstacles were:

- Hired new staff from early, mid, and late career candidate pools. Evaluated the scope of work; identified simple, moderate, and advanced tasks; and allowed these assessments to drive hiring decisions.
- Posted position descriptions had export/trade compliance as a preferred qualification, but not required which opened opportunities for lateral moves into Export Control (EC) from other disciplines.
- To prevent new-hires from becoming overly "stove-piped" into narrowly focused portfolios, leadership developed an organizational chart that attempted to find a balance between various factors such as mission requirements, experience levels, education/ backgrounds, and desires of individual staff.

Other elements that needed to be developed along the way to assist in managing the steep increase in workload as enhanced awareness about export risk began to permeate PNNL.

- A service request system that could organize and manage the thousands of support requests.
- A website all staff could access that would provide key reference materials; web links to resources, videos, and training materials; and a web-based questionnaire that staff could provide answers in that would assist them in assessing their project's need to engage with TPEC.
- An aggressive communications campaign and holistic change management plan.

Export control regulations are large and spread across many agencies. Distilling these regulations into straight-forward requirement statements and then into policies and procedures was a considerable but critical lift. We now have a central repository that houses all our export compliance business rules and their corresponding requirements and implementing methods. This process is discussed later.

# It Starts at the Top – Laboratory-Level Participation

A common challenge facing export control professionals is communicating risk and securing buy in from organizational leadership. The regulatory requirements are complex and affect practically every facet of an organization. Communicating concepts and requirements that cut across M&O

programs can be confusing and problematic to senior leaders and managers overseeing specific operational programs without broad insight into overall organizational operations.

Compliance professionals are commonly challenged to develop systems that are easy, efficient, and effective. At the risk of oversimplifying the role of export control programs, they are attempting to do this while ascertaining specific risks associated with physical assets (high risk property), people and organizations (restricted party screening), paper (sensitive and proprietary information), purposes (what is the item or information ultimately used for?), and payments (finance).

With that backdrop, it is vital that compliance programs have staff with a broad set of skills that enable them to understand viewpoints of stakeholders and communicate effectively with them. Some of the skills needed include business and operational acumen, legal and regulatory training, technical and scientific understanding, communication skills, organizational understanding, and broad awareness of industry best practices. A single individual or narrow set of skills could not be broad enough to effectively manage this wide array of risks and domains. Through necessity, a team is required.

TPEC initially struggled to engage directly with programs without appearing to be managing risks owned by other organizations. This often resulted in defensive positions rather than collaboration. No program wants the optics of being "investigated" by compliance teams. Despite the challenges, we found common ground with organizations managing high risk personal property (HRPP), human resources, information releases, and other PNNL elements coping with similar challenges. As relationships developed, we recognized the need to reach out to our process improvement group. TPEC spent a significant amount of time working with process improvement professionals to help scope out the immensity of the regulatory requirements and distilling them down to business rules and began gathering data and identifying other areas of operations that could be affected by changes.

As the program began to develop, we identified a significant number of gaps that needed to be addressed and a considerable number of corrective actions were developed. It became clear that we needed a coordinated effort to accomplish all that was being asked. The lab provided the resources for a broad Program Improvement Plan (PIP), and a team of individuals representing a broad spectrum of programs and perspectives was identified to assist in the effort.

As the PIP progressed, the actions and team evolved over time, adding new members as new issues were uncovered and releasing others as their assigned tasks were completed. During this evolution, we soon realized that much of the scope and effort was focused on the operations and management side of the organization. However, as a research organization, the PIP team needed to assess the impacts on our research operations as well.

Project and line management within our research enterprise was willingly engaged, and with the support of Lab Leadership, TPEC pulled together, through PNNL's operations counsel, a Technology Protection Advisory Committee (TPAC). The TPAC was tasked with understanding the evolving regulatory landscape and assessing the research impacts with a focus on graded risk-based approaches. This committee was key to helping set the overall direction of the program. Through this committee we identified the various needs throughout the project lifecycle of research

programs. The TPAC identified improvement areas for various stages of this lifecycle, including pre-proposal, proposal, first funded reviews, project kick-offs, project reviews, and project closeout activities. During this process development, we looked at the various systems and stakeholders that would be engaged at each point and where overlapping requirements could be consolidated.

Throughout the program development, there was a need to design new systems. We worked closely with IT to develop requirements and user stories as well as identify and create data sources and fields necessary to obtain the needed information to make adequate decisions. This effort led to some truly novel approaches that brought together reports that revealed the scope of PNNL's risk in visual formats.

Throughout the process, we engaged with our local DOE site office leadership on a regular basis. The site office closely monitored our progress and asked tough questions to ensure that the PIP team was addressing those risk areas they perceived as most critical. Addressing the PIP in this manner fostered significant understanding, buy-in and trust.

## **Understanding the Flow Down of Requirements**

When establishing or improving an export control program, it is essential to understand what export

control requirements apply to scope of the business. The United States uses a complex set of overlapping regulatory regimes to control the export of weapon and dual-use technologies. As a DOE national laboratory, PNNL also must comply with complementary DOE requirements for protecting export-controlled technologies and information. See Figure 2 for a sense of the range of topic. Identifying requirements has several challenges: hundreds of pages of details, same terms for different things, different terms for the same things, different reporting requirements, and different controls for similar things.

Our approach addressed these challenges by first capturing the essential requirements as business rules. These are single topic, explicit statements

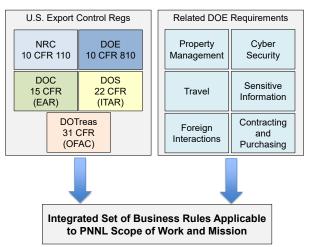


Figure 2. Integrating requirements.

using defined terms that tell workers whether they may or may not do something or give them the criteria and conditions they need for making decisions. We chose rules that applied to PNNL's work scope, and we maintained a close association between the business rules and the regulatory language, which contained important details needed for implementation. We reconciled terminology across the regulations and categorized the 250+ business rules to bring like requirements together. Figure 3 shows an excerpt from the business rule database.

BR Id# 🗊	Business Rule	BRCategory -	SubCat 🔽	SRD 🔽	Sect 👻
22	If the transferee, ultimate end-user, any intermediate consignee, or any other party to a transaction is a person denied export privileges, then it is prohibited to engage in any activity that violates the terms or conditions of a denial order.	EC License	Requirements	15 CFR Subchapter C (EAR)	732.3(g)
23	With some exceptions, all items <u>subject to the EAR</u> must not be exported to <u>embargoed</u> countries in any way (e.g., export, reexport, pass through during shipping, vessel ownership, etc.) without a license.	EC License	Requirements	15 CFR Subchapter C (EAR)	746
24	The EAR controls any item warranting control that is not exclusively controlled for export, reexport, or transfer by another agency of the U.S. government or is otherwise excluded from being <u>subject to</u> the EAR.		Identification	15 CFR Subchapter C (EAR)	730.3
25	Persons must not proceed with a transaction with the knowledge that a violation of the EAR, involving items on the CCL and within EAR99, has occurred or is about to occur. "Red flags" that might indicate a potential violation must be "checked out", inquiring about end-use, end-user, and ultimate country destination.	EC License	Requirements	15 CFR Subchapter C (EAR)	EAR Supple- ment 3
26	All activities conducted under ACT must be conducted in accordance with all implementations applicable to the 1830 contract, including export control.	Non-DOE Work	ACT	Clause H-29	TBD
27	ACT agreements must address export control relevant to the scope of the agreements.	Non-DOE Work	ACT	Clause H-29	TBD
28	All PNNL requests to the DOE Patent Counsel to assert copyright to technical data (other than in S&T articles and from CRADAs) must include a determination of whether the data is subject to export control.	Tech Transfer	Vetting	Clause I-135	(e)(1)(i)
29	PNNL must obtain permission to assert copyright to technical data, which is determined to be under export control restrictions, for the purpose of limiting commercialization in a manner that complies with export controls statutes and regulations.	Tech Transfer	Vetting	Clause I-135	(e)(1)(iii)(E)
30	<u>Software</u> must be subjected to export control review prior to designating it or any resulting derivative software as Open Source Software.	Software	Mark/Control	Clause I-135	(f)(9)
31	Technology transfer agreements with third parties must include notification that the export of goods and/or technical data from the United States may require an export control license or other authority and that failure to obtain such authority may result in criminal liability.		Mark/Control		(j)(2)
32	Internal export control reviews must be conducted when technology is transferred except for fundamental research as defined in National Security Decision Directive 189.	Technical Data	Release	Clause I-136	(j)(3)

Figure 3. Part of business rule database (defined terms are shown in blue)

Our next step was to identify the means to implement all the individual requirements, which can include processes, controls, training, IT systems, and SMEs. Since we were running an improvement effort, we identified existing implementations to update and define gaps needing new implementations. Export control requirements touch nearly every business function in PNNL, which

are owned by different functional teams. We worked with each functional team to update or create new implementations and to define what critical controls we would use to assure effectiveness and compliance. Figure 4 shows a small excerpt of the database of nearly 300 implementations mapped to business rules. The mappings of business rules to implementations were then codified in records of decision, which were approved by the requirement and implementation owners.

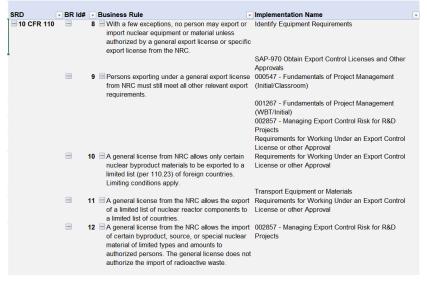


Figure 4. Excerpt of business rule to implementation map

We also used the database to show all the rules each implementation must address and to provide each functional manager a list of rules they are responsible for.

We used a risk assessment method to identify priorities for which implementations to work on first and to help identify critical controls for the highest risk areas. We adapted an approach called factor

analysis of information risk (FAIR<sup>TM</sup>), which is primarily used to assess information risk. To do this we defined scenarios of threats against all types of export-controlled technologies, estimated frequencies and magnitudes of loss using industry data, and used a Monte Carlo method to estimate risk impacts before and after applying controls. We prioritized the impact of cost and time to implement, the impact on productivity, and breadth of benefit. Figure 5 illustrates the type of output that was generated. This analysis provided a basis for selecting implementation approaches, prioritizing work, and selecting critical controls. Other sections in this paper illustrate a few of the implementations that were developed and how adoption of the new or changed implementations was promoted across the laboratory.

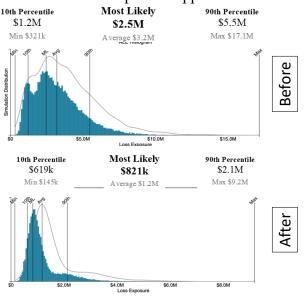


Figure 5. Impact Analysis

The integrated set of requirements will be continually managed over time. The export-control regulations themselves change and evolve over time to accommodate new technologies and new risks, and the changes must be incorporated into the program. Implementations need to be monitored to assure effectiveness and to make sure they remain compliant when they are changed to accommodate process improvements or changes in other external requirements.

## Management of HRPP and Assets

The management of HRPP is executed throughout the asset lifecycle. From procurement to excess, PNNL has placed people, processes, and tools to identify and safeguard HRPP. At the point of acquisition, descriptive data is collected on equipment that can be reviewed by the Risk Engine tool, Figure 6, and classified by an export control professional matrixed to Property Management.

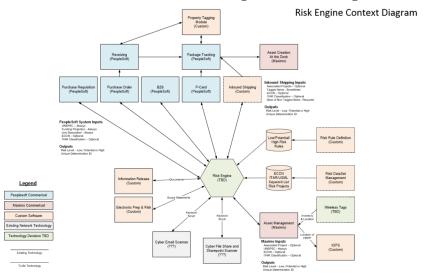


Figure 6. Risk Engine

Additionally, assets obtained from outside of the acquisition process are reviewed by ECP through the new Inbound Shipping tool. These tools and processes allow for HRPP to be identified as early in the asset lifecycle as possible, as illustrated in Figure 7.



Figure 7. HRPP asset lifecycle

PNNL's Property System, Maximo, along with the Property Management Specialists, is the tagging and tracking mechanism that holds the details for each tagged piece of equipment. Maximo also allows for PNNL to uniquely identify HRPP and display the export control classification number (ECCN) or International Traffic in Arms Regulations (ITAR) number (DDTC). Maximo holds over 39,000 tracked pieces of equipment, of which 6% are considered HRPP. Property custodians can see their equipment details and act on their equipment in Assets, a front-facing IT interface

integrated with Maximo for custodian use. Staff can also generate an Outbound Shipping Request through Assets, which automatically routes the request to the appropriate SMEs, including ECPs, to ensure all actions are completed before property is shipped off campus.

The ECP is an integral part of PNNL's excess process. As part of the ECP Program's improvement initiative, the excess request form was updated to allow the addition of shop-made or fabricated equipment to be reviewed by our export control professionals. HRPP and non-tracked equipment are also reviewed by ECPs prior to final approval. HRPP that can be sent to the scrapyard is isolated from non-HRPP, and its destruction is witnessed by a member of the Property Management team. ITAR equipment is safeguarded for future demilitarization.

Through a mixture of people, processes, and tools, PNNL is managing its HRPP from cradle to grave in a cost-effective manner. A strong relationship between the Export Control Office and Asset Management along with integrated tools is key to managing the risk.

# Addressing Export Controlled Technical Data, Information and Software

At PNNL, we are in the business of generating new and novel approaches and technology-based solutions. At any giving time, there are roughly 2000 active projects at the organization that cover the spectrum of potential export control risks. Assessing EC risk is a challenge because the nature of the work we conduct may not necessarily align with technologies currently identified on control lists. Current regulatory guidance has shifted, and US regulators have begun looking more closely at "Emerging" and "Foundational" technologies with an eye towards a continually evolving control list focusing on new technologies in key industries. Where in the past we may have been able to rely on certain fundamental research exclusions within the regulations to permit non-US-Person access to research areas, the risk of potential "deemed exports" significantly increased. A deemed export is the release of controlled technology to non-US-persons while they are physically present in the US This release is deemed to be an export to that non-US-person's home country. With a significant number of foreign researchers working in research areas under more scrutiny, PNNL needed to address how we identified and controlled proprietary information, technical data, software, and other types of sensitive information.

To assist in that effort, we reevaluated the fundamental research exclusions within the regulations to verify our processes identified early projects that could pose a risk. In our project proposal and risk capture tool, known as Electronic Prep and Risk (EPR), we reworked screening questions to ascertain if projects would engage in sensitive topics, have publication restrictions, foreign national restrictions, or would be developing proprietary technologies meant to be commercialized.

Efforts were coordinated with our Foreign Visits and Assignments (FVA) office to assure we addressed gaps associated with site access approvals. The FVA office and TPEC worked together to address training and process gaps to make certain foreign nationals working at the lab had appropriate approved scope within their security plans that included detailed descriptions of individual project work rather than overly broad explanations with limited value. Project scope continually evolves, and people transition between projects and programs. This required significant outreach to hosts and managers to ensure they were aware of the risks and requirements to update the foreign national's security plans.

The updates to EPR and the FVA system enabled TPEC to address access control risks more fully, but we still needed validation tools.

Working closely with IT a tool was developed allowing the team to bring together numerous data streams reflecting export control risks associated with projects, information, time billing, and property. This tool, known as the Technology Protection Integration Map (TPIM), is depicted in Figure 8(a) and (b).



Figure 8. Technology Protection Integration Map

We worked again with project leadership to identify the stage within the project life cycle that technology control plans (TCPs) would be needed. A TCP is meant to capture the high-risk areas of project research and identify any physical or electronic access controls, FN access restriction, and licensing requirements.

# **Export-Controlled Biological Materials**

To maintain a rigorous adherence of the export control laws of the United States, it was essential to reorganize the management of high-risk biological materials based on the regulations of the Chemical Weapons Convention (CWC). A catalog of the export-controlled biologicals was created by compiling an index from the relevant regulation lists of the CWC to cross reference with the inventory of PNNL. These regulations included:

- 1) Chemical Weapons Convention Regulations (CWCR)
  - a. Schedule 1 Chemicals (Ricin and Saxitoxin) (15 CFR 712)
- 2) United States Munitions List (USML) of the ITAR controlled by the State Department (22 CFR 121)
  - a. Category XIV-Toxicological Agents, including Chemical Agents, Biological Agents and Associated Equipment
- 3) Commerce Control List (CCL) of Export Administration Regulations (EAR) controlled by the US Department of Commerce (DOC)/Bureau of Industry and Security (BIS 2020)
  - a. Category 1-Materials, Chemicals, Microorganisms, and Toxins

- i. ECCN1C351 (Export Control Classification Numbers)
- ii. ECCN1C353
- iii. ECCN1C354
- iv. ECCN1C991

Biological Agent Name	Reg ID	Туре	Form	Category	Regulation List	<b>Regulation Category</b>	Regulation	Footnotes
	<b>↓</b> †	v v		~ ~	✓	<b>~</b>	SubCategory	💌 (see Tab)
Abrin	1393-62-0	Toxin	Toxin	EC Bio	CCL-EAR (DOC)	ECCN1C351	d.1.	10, 14
Abrin	1393-62-0	Toxin	GMO Toxins or toxin	EC Bio	CCL-EAR (DOC)	ECCN1C353	a.3.	10, 14, 16
			subunits					
Abrin	1393-62-0	Toxin	Vaccine(s)	EC Bio	CCL-EAR (DOC)	ECCN1C991	a.	10, 14
Abrin	1393-62-0	Toxin	Immunotoxin(s)	EC Bio	CCL-EAR (DOC)	ECCN1C991	b.	10, 14
Abrin	1393-62-0	Toxin	Medical Products	EC Bio	CCL-EAR (DOC)	ECCN1C991	d.	10, 14
Abrin	1393-62-0	Toxin	Diagnostic and food	EC Bio	CCL-EAR (DOC)	ECCN1C991	e.	10, 14
			testing kits					
Aff. Goat anti-Ricin	AB-AG-RIC	CRP Antibody	Antibody	EC Bio	USML-ITAR (State Dept)	USML Cat14	(g)(4)(i)	5
Aff. Rabbit anti-SEB	AB-AR-SEB	CRP Antibody	Antibody	EC Bio	USML-ITAR (State Dept)	USML Cat14	(g)(4)(iii)	5
Aflatoxins	1162-65-8	Toxin	Toxin	EC Bio	CCL-EAR (DOC)	ECCN1C351	d.2.	10, 14
Aflatoxins	1162-65-8	Toxin	GMO Toxins or toxin	EC Bio	CCL-EAR (DOC)	ECCN1C353	a.3.	10, 14, 16
			subunits					
Aflatoxins	1162-65-8	Toxin	Vaccine(s)	EC Bio	CCL-EAR (DOC)	ECCN1C991	a.	10, 14
Aflatoxins	1162-65-8	Toxin	Immunotoxin(s)	EC Bio	CCL-EAR (DOC)	ECCN1C991	b.	10, 14
Aflatoxins	1162-65-8	Toxin	Medical Products	EC Bio	CCL-EAR (DOC)	ECCN1C991	d.	10, 14
Aflatoxins	1162-65-8	Toxin	Diagnostic and food	EC Bio	CCL-EAR (DOC)	ECCN1C991	e.	10, 14
			testing kits					
African horse sickness virus		Virus	Organism	EC Bio	CCL-EAR (DOC)	ECCN1C351	a.1.	7, 14
African horse sickness virus		Virus	Gene(s) or GMOs	EC Bio	CCL-EAR (DOC)	ECCN1C353	a.1.	7, 14, 16
African horse sickness virus		Virus	Vaccine(s)	EC Bio	CCL-EAR (DOC)	ECCN1C991	a.	7, 14
African swine fever virus		Virus	Organism	EC Bio	CCL-EAR (DOC)	ECCN1C351	a.2.	7, 14
African swine fever virus		Virus	Gene(s) or GMOs	EC Bio	CCL-EAR (DOC)	ECCN1C353	a.1.	7, 14, 16
African swine fever virus		Virus	Vaccine(s)	EC Bio	CCL-EAR (DOC)	ECCN1C991	a.	7, 14

Figure 9. A snapshot of the EC biologicals list

This compilation generated 594 entries of EC biologicals with 8 types (bacterium, CPR [C-reactive protein], antibody, fungus, Joint Biological Agent Identification and Diagnostic System [JBAIDS], polymerase chain reaction [PCR] kit, toxin, vaccine and virus) and 13 forms (antibody, diagnostic and food testing kits, fungus, gene[s] or GMOs, GMO toxins or toxin subunits, immunotoxin[s], medical products, micro-organism/toxin, non-natural genetic agents or elements, organism, product, toxin, and vaccine[s]). This list can be searched by type, and the search further narrowed by choosing the form of the type of biological.

With a complete catalog of EC biologicals, the PNNL inventory can be cross-referenced then updated with further warnings and actions based on the regulation or when new orders of biological materials are made.

# **Export-Controlled Chemicals**

It was also prudent to reorganize the management of high-risk chemicals in the PNNL inventory. This endeavor began by creating a catalog of EC chemicals based on Chemical Abstract Service (CAS) registry numbers the following regulation lists of the CWC:

- 1) CWCR
  - a. Schedule 1 Chemicals (Most are regulated under ITAR [State Dept.] except Ricin and Saxitoxin, which are regulated under EAR [DOC]) (15 CFR 712)
  - b. Schedule 2 Chemicals (Some Schedule 2 chemicals are controlled under ITAR and others under EAR) (15 CFR 713)
  - c. Schedule 3 Chemicals (All regulated under EAR) (15 CFR 714)
  - d. Amendment to Schedule 1 Chemicals (Costanzi Research 2020)
- 2) USML of ITAR (DDTC)

- a. Category V–Explosives and Energetic Materials, Propellants, Incendiary Agents, and Their Constituents
- b. Category XIV–Toxicological Agents, including Chemical Agents, Biological Agents and Associated Equipment
- 3) CCL of EAR (BIS 2020)
  - a. Category 1-Materials, Chemicals, Microorganisms, and Toxins
    - i. ECCNs include 1C011, 1C111, 1C350, 1C351, 1C355, 1C607, 1C608, 1C992, 1C997, and EAR99
    - ii. ECCNs 1A984, 1C395, 1C995 define concentration (mixture %) of the chemicals regulated in 3a.i.

The chemical names with corresponding CAS registry numbers were categorized by chemical type, regulation list, regulation category, regulation subcategory and concentration (% mixture) of the chemical. Many of the EC chemicals are found on more than one regulation list; the concentration of the chemical defines which regulation controls them. For example, hydrogen cyanide is a Schedule 3 (15 CFR 714) chemical regulated by the CWCR (CWC) when found in a mixture of 80% or above. If the concentration is between 30–79%, it falls under ECCN1C335 of the CCL and ECCN1C995 if under 30%.

				Exp	oort Contro	Chemio	cals							
				Regulation		Regulation	Amount regulated	ECCN1A984-Amt	<b>Regulation List</b>	ECCN1C395-Amt				ist
CAS	*	Chemical Name	Type of Chemical	List 👻	Regulation Category	SubCategory *	(%) 👻	Regulated (%)	Section *	Regulated (%) 🎽	Section *	Regulated (%) 🎽	Section	Ŧ
				CWCR Scheduled Chemicals										
74-90-8	3	Hydrogen cyanide	Blood agent	(CCL-EAR [DOC])	Schedule 3 Chemicals	Part A3	≥ 80%							
			CWC Schedule 3 chemical or mixture											
74-90-8	3	Hydrocyanic acid; Hydrogen Cyanide	containing Schedule 3 chemical	CCL-EAR (DOC)	ECCN1C355	b.1.c.	30-79%					<30% by wt	b.2.	

Figure 10. Two entries for hydrogen cyanide in the EC chemicals list

The CWCR lists of scheduled chemicals (CWC) and the USML (22 CFR 121) include several entries of "families" of chemicals (Ex. "Schedule 1 Chemical Part A1: [1] 0-Alkyl [ $\leq$ C<sub>10</sub>, incl. cycloalkyl] alkyl [Me, Et, n-Pr or i-Pr]-phosphorofluoridates, e.g., Sarin: 0-Isopropyl methylphosphonofluoridate and Soman: 0-Pinacolyl methylphosphonofluoridate"). Comprehensive lists of the chemical families were assembled by conducting substructure searches using the SciFinder database (CAS 2021) and consist of all stereo isomers (R and S derivatives), isotopes, and mixtures. The PubChem database (NIH) was used to cross check chemical names and structures, with CAS registry numbers.

For some chemical families, the lists generated by SciFinder (CAS 2021) contained hundreds of entries. In the future, it will be prudent and comprehensive to use a cheminformatics approach using the Simplified Molecular Input Line Entry System (SMILES) (DAYLIGHT 2019) identifier of the chemical structure of interest against the family substructure. The current list of EC chemicals includes 1685 entries. It should also be noted that this database only includes commercially available chemicals.

From the list generated above, a unique chemical group for each sub-category was developed and established in the relational database managing our chemical assets and regulatory requirements. Each group was described with the source regulation section and was associated with a meta-group and a meta-meta-group. The group was coded to screen inventory from general staff view, identified to the appropriate control band, identified as a chemical requiring a notification upon

purchase as specified, and identified as pertaining to the regulatory subject matter owner that has jurisdiction over the group.

After the groups were developed, they were applied to existing constituent and product records, or new product and constituent records were developed, as needed. Each newly added product and constituent were characterized, associating the environmental reporting requirements; chemical data such as physical state, density, and molecular weight, properties; and hazards with each, as well as applying the Export Control code(s) associated with the chemical. Group assignments on specified concentration ranges were made where applicable. As many of these chemicals are not commercially available, Safety Data Sheets were not available for most. Based on information from SciFinder (CAS 2021), PubChem (NIH), and *Handbook of Chemical and Biological Warfare Agents*, Second Edition (Ellison 2007) , the data and properties of the chemical families were assigned to the chemicals based on their family groups when Safety Data Sheets were unobtainable.

The product definition was automatically associated with container records for chemicals in inventory or on order with the same chemical name.

The group triggers a warning message to the chemical management staff member entering an order for a chemical when ECP approval of the order is required, i.e., for ITAR CAT5 and CAT14 chemicals. Inclusion of the source regulation in the group description allows the export control SME to quickly identify the regulatory source of requirements pertaining to a chemical using a Names, Properties, and Hazards report for the chemical. An inventory report on the group or meta-group will produce all the inventory identified to that group or meta-group. Automated reports of new or existing inventory of export-controlled chemicals can be created to periodically notify SMEs.

Example:

Chemical C Group Code	Chemical Groups Chemical Group De	Display Hazard No on Purchase escription	ntification e? Hazard Notification Message Tex		Restric- y ted?	Combo Group?		Operational Significance		Group Domain	Catego	ry/Owner )		
	ITAR USML CA	<u> </u>	Add Export Control SME Aard		V		$\overline{\mathbf{v}}$	H	ŧ	PRODUCT	± EC		± -	-
1	E				Γ				Ŧ		±		±	
1	2					Γ			±		±		± .	•
					-1									
Chemical Grou	up XA11 👱 is	included as summary	I in the Chemical Meta Group	AR	ŧ									
Chemical I	Meta Group	± is included i	n the Chemical Meta Meta Group EC	ŧ										
Chem Meta Met			al Meta Meta Groups											
Group Code	Chemical Meta M	eta Group Description	1											11
EC ±	EXPORT CONT	ROL GROUPS												-

Figure 11. Chemical Group XA11 is described as "ITAR USML CAT14:A1I."

- 1. A notification to "Add Export Control SME <name of SME> to acquisition as approver in PES order" is displayed when chemicals with this group are purchased.
- 2. Chemical inventory in this group is restricted from general view in inventory reports.
- 3. HCL3 is an Industrial Hygiene field, indicating that chemical use documentation is required for use of chemical products assigned to this group.

- 4. Operational significance is our control banding designating the amount of risk—physical, economic, or political—associated with a chemical. XA11 chemicals pose a high risk, so XA11 chemicals must be tracked to the room they are stored in, rather than just to the fire code control zone. If one is missing, a high degree of diligence must be exercised to find it or determine its fate.
- 5. Group domain indicates that the group is active based on the product assignment rather than the constituent assignment. When the group domain is product, the group is also recorded in the constituent record so that if any future products list it as a constituent, a determination of the applicability of the group will be considered.
- 6. Category/owner ID is EC. The owner has the responsibility to supply information regarding any new, modified, or retired regulatory requirements.
- 7. XA11 is a member of meta-group ITAR (EXPORT CONTROL BASED ON INTERNATIONAL TRAFFIC IN ARMS REGULATIONS), and ITAR is a member of meta-meta-group EC.

Product Name PHOSPHONOFLUORIDIC ACID, METHYL-, CYCLOOCTYL CYCLOOCTANOL, METHYLPHOSPHONOFLUORIDATE 2	Preferred Name or Synonym Product #  P  106891  S  106891 
Product #  106891  Physical L  Concentration Read.    Comment	
Manufacturer # Manufacturer Name	MSDS #
Pure Chemical Name / Constituent PHOSPHONOFLUORIDIC ACID, ME + 9024384 9024384 14719 9024384 14719 9024384 14719 9024384 14719 9024384 14719 9024384 14719 9024384 14719 9024384 14719 9024384 14719 90240 14719 1	Number PCT of Product Primary Constituent?
Chemical Group Code  Chemical Group Description    UNL1  UNSTABLE(REACTIVE) LIQUIDS - CLASS 1    WRL1  WATER-REACTIVE LIQUIDS - CLASS 1    XA11  ITAR USML CAT14:A11	Concentration Greater Than % Up To %

Figure 12. Product with this constituent associated with XA11 group

VXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX							ical Names, Properties, a	
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Bitcome  Construction  P  2000								
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Buildenood Locality Local								
Buildenood Locality Local					Inclusion of / Francis		Manage & Programme	
Creation  Construction  1    15893  Partial Barrier Line  Construction  1573-38-3  1000 cm    15993  Partial Line  Densety (gr/l, line)  1573-38-3  1000 cm    1000  Construction  15900  15900  1000 cm    1000  Through Ministry  15900  Construction  1000 cm    1000  Through Ministry  Review Ministry  Construction				,				PHOSPHON
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35893  14735-38-3  200    L  15990  1599				CAS No.			Chem No.	
Physical Las  Density (sp. 1)  LSS 00 LSS 00 al, LSS 00	208.21		14710-78-1					106881
Sale  (gm/c)  Loss  Rat (mp/k)    N  HSGB No.  Loss  Kat (mp/k)    N  TPQ (b)  HSGB No.  Kat (mp/k)    TPQ (b)  Thraddal  Kat (mp/k)    Periodicity (Hauth)  Thraddal  Connect    Periodicity (Hauth)  Reviewed  Review Status    Catableant Nume  Periodicity (Hauth)  Reviewed    Medicity (Hauth)  Reviewed  Review Status    Medicity (Hauth)  Status  Status    Medicity (Hauth)			147127-2012		Describe		Thursteel	1000001
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WRL1 WATER-REACTIVE LIQUIDS - CLASS 1 0.0 100.0 M No								

Figure 13. Chemical Names, Properties, and Hazards report for this chemical, showing regulatory source of requirements

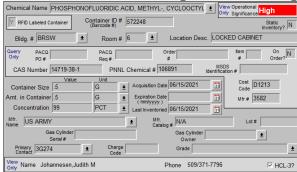


Figure 14. Container of this product (example)

## CONCLUSIONS

This paper gave insight into several improvements made by the Pacific Northwest National Laboratory to its export control program, organizational staffing, flow down of regulatory requirements, and several IT tools put in place for protection of high-risk export-controlled assets and biological and chemical materials. The Department of Energy's National Laboratories advance scientific and technological discoveries and innovations addressing the most complex problems facing our nation. Having a strong export control program underpinned by professional staff, strong processes, and leading-edge technical tools strengthens our national security, cybersecurity, and economic security.

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