Chemical Security Analysis Center Projects

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Science and Technology Directorate

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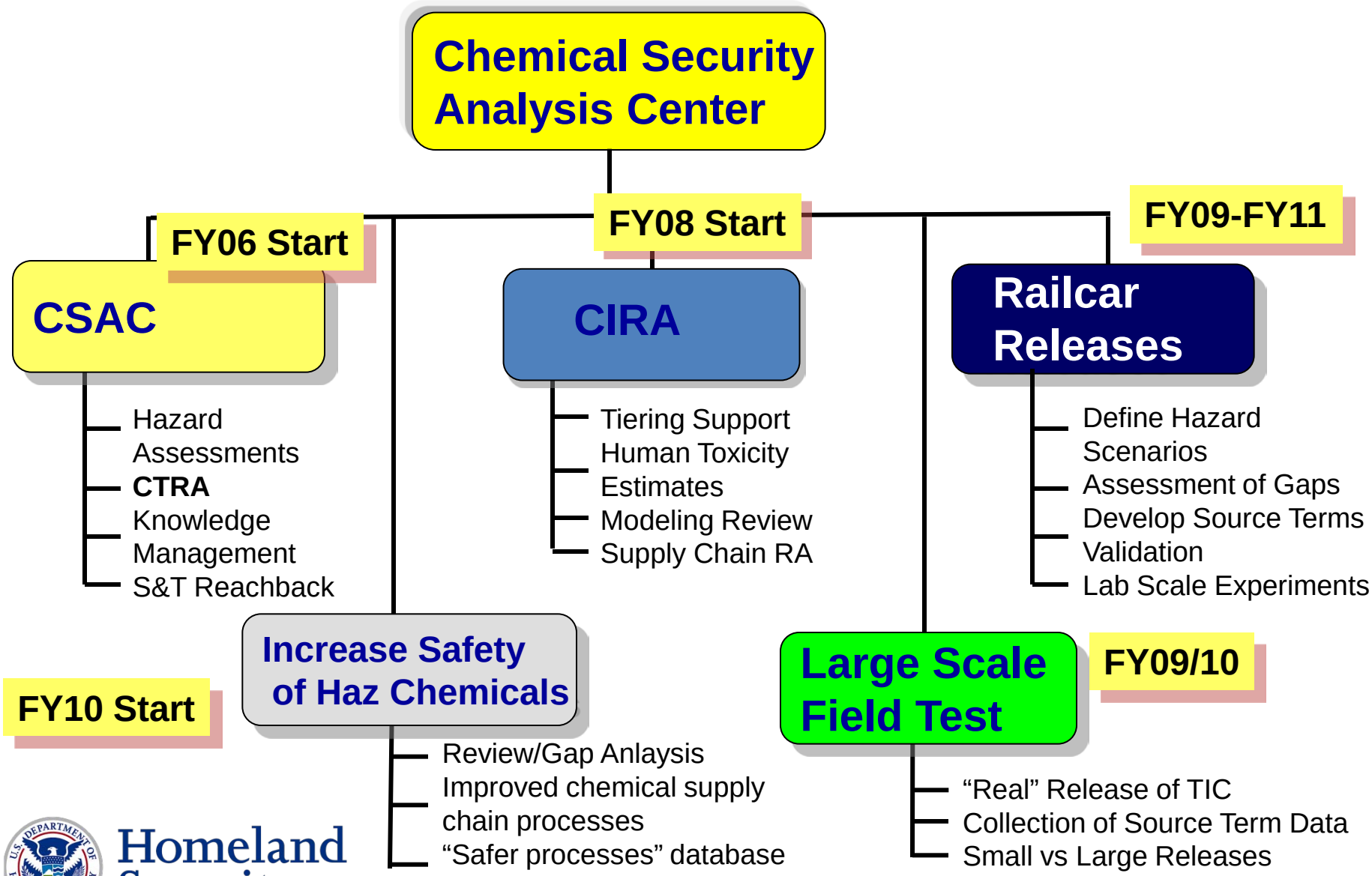
Chemical Security Analysis Center Structure



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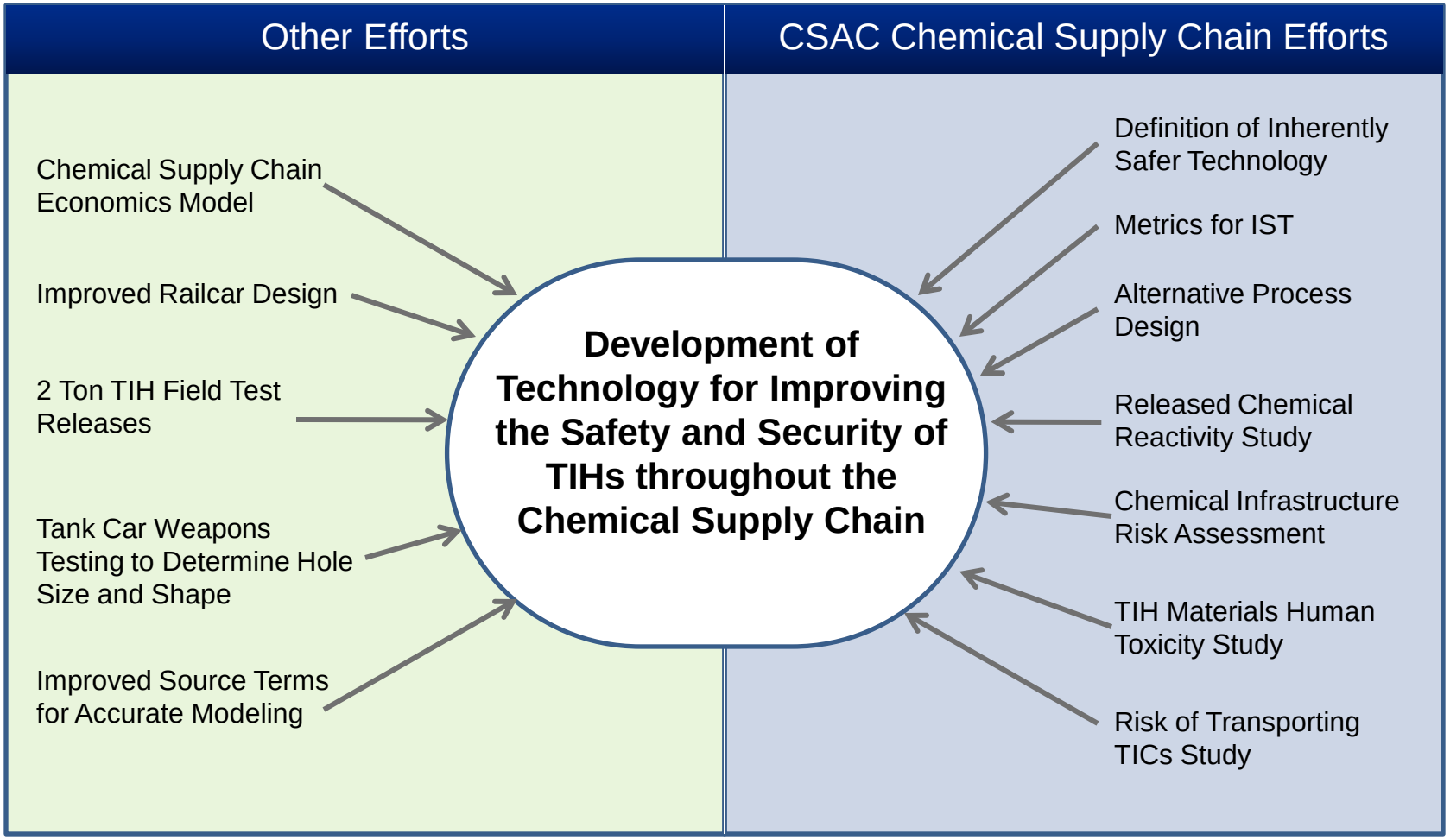
Chemical Supply Chain Efforts



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Increase Safety of Hazardous Chemicals

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Increasing Safety of Hazardous Chemicals

FY10 New Start

Increase Safety of Hazardous Chemicals

Define Inherently Safer Technology

- Review of Current Models
- Evaluate Models for Assessing Release within the Chemical Supply Chain

Metrics

- Develop Method of Tiering App A Chemicals
- Risk Based Approach to Assigning Tiers
- Reachback for CFATS

Gap Analysis

- Review Current Estimates for Appendix A Chemicals
- Revise Based on New Methods
- Identify Data Gaps

Safer Processes

- Identify Processes
- Example Process

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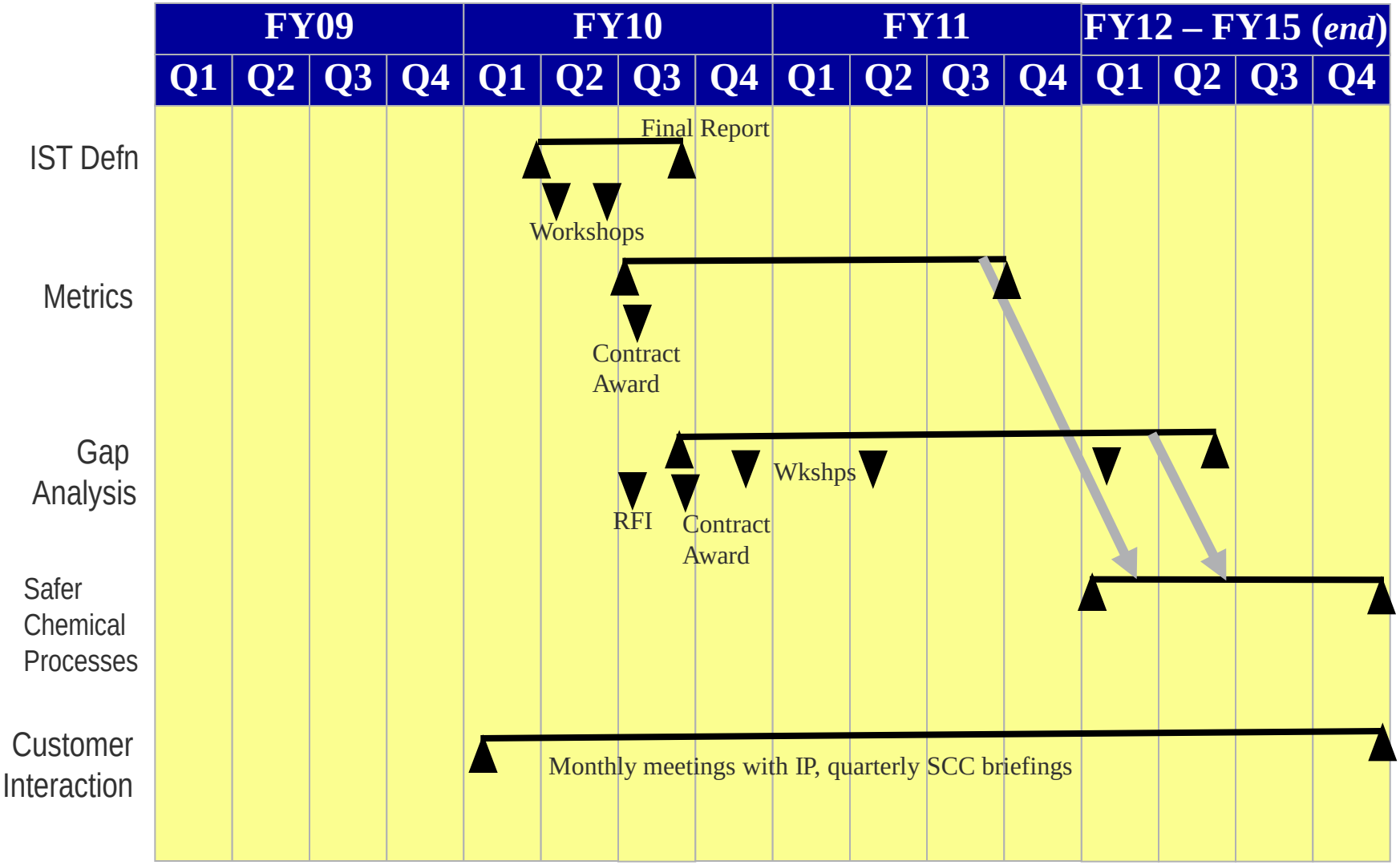
Increase Safety of Hazardous Chemicals Gantt Chart



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Summary

- Increasing safety and security of hazardous materials is not a simple problem
- There is currently no way to measure ISHC across the supply chain
- Developing a common definitive definition of IST is key
- Understanding how new processing increases safety and security is essential (Metrics)
- IST is one component of ISHC
- Be aware of unintended consequences

ISHC can be considered as recommended means to reduce risk and increase safety across the chemical supply chain only though consideration of the entire CSC process.

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Accurate Modeling of Large Scale Toxic Inhalation Hazard Releases (Railcar)

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Impetus for Project

- Current dispersion models overestimate the downwind chlorine hazard from railcars
- TSA-led effort identified a number of S&T "gaps"
  - Dispersion models use source terms which are not valid for rapid, large release of liquid chlorine
  - Large releases, due to slow kinetics of heat absorption, form stable source blankets with persist for minutes to hours
  - Lethal effects are in the near field (~500 meters)
  - Chlorine vapor and aerosols are dense and initially flow with gravity
- Subject matter expert consensus is problems are due to
  - Incorrect source term definition
  - Incorrect toxicity values
  - Degradation of toxic cloud not accounted for
- Most "conclusions" to date have been anecdotal

Large Scale Toxic Inhalation Hazard Releases

FY09 New Start

Modeling Large-Scale Toxic Chemical Transport Releases

Gap Analysis

- Literature review of previous work
- SME Workshop
- Documentation and prioritization of knowledge/capability gaps

TIH Cloud Degradation

- Systems Assessment
- SME Workshop for definition of key modeling parameters
- Experimentation to determine rate/capacity of TIH removal from reactions

Effect of Terrain and Obstacles on TIH Transport

- Investigation of physical behavior of TIH transport
- Modeling SME workshop to determine best implementation of findings

Source Term Analysis & Development

- Analysis of existing data
- Experimentation to fill identified knowledge gaps
- Development of recommendations for improving modeling methodologies

Project JackRabbit Support

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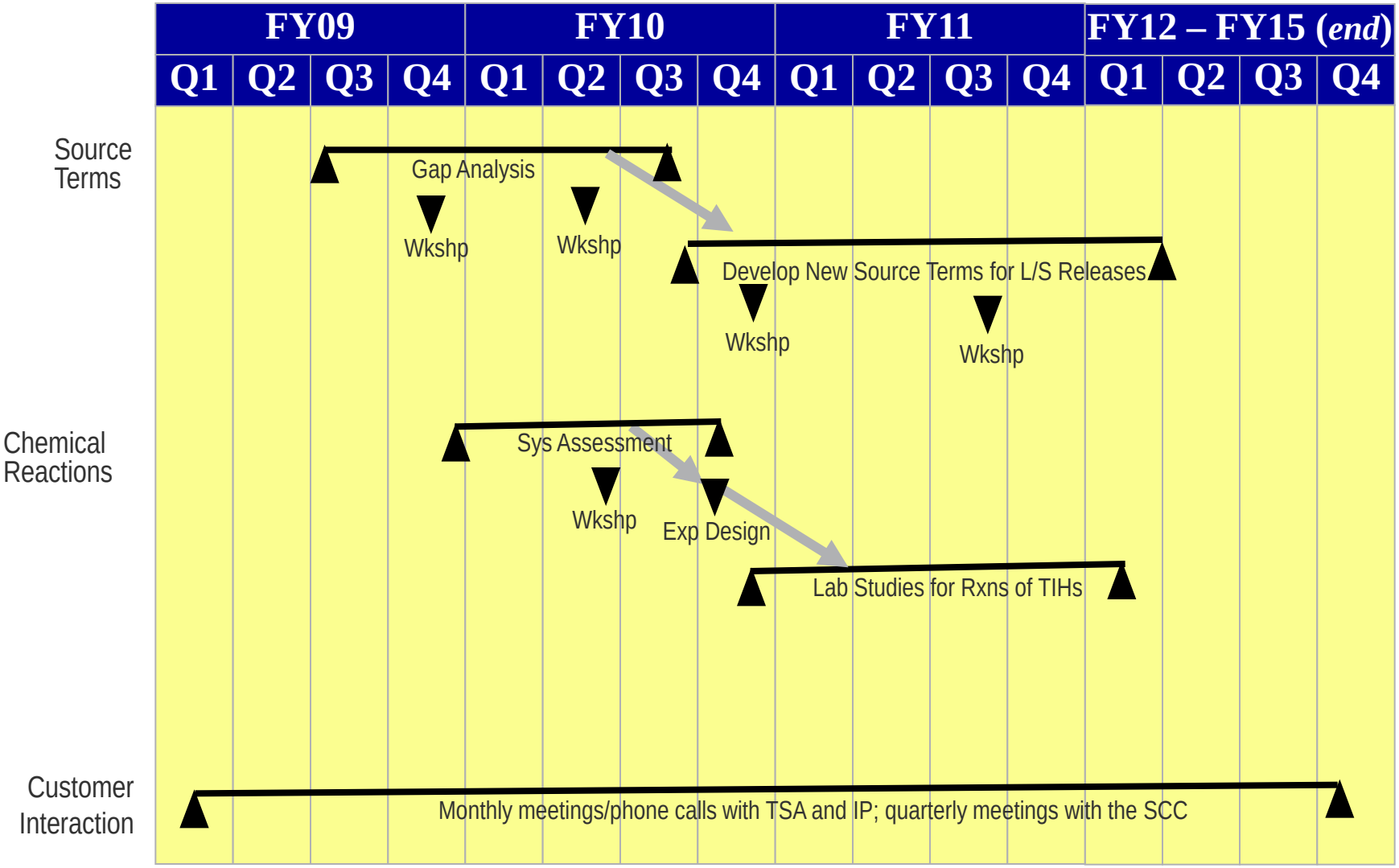
Model Large Scale Releases



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Gap Analysis Task

- Modeling Large-Scale Toxic Chemical Transport Releases
- Gap analysis for source emissions, dispersion, deposition and consequence assessment for toxic inhalation hazard (TIH) chemicals
- SAIC performer conducted 2 SME and stakeholder workshops, identified and prioritized gaps
- Key Findings and Recommendations:
  - Seven chemicals identified as highest risk: Cl_2, NH_3, HCl, SO_2, HF, C_2H_4O, HCN
  - There were 32 prioritized recommendations that were consolidated into priority gap areas
  - Overwhelming agreement that large-scale experimentation with TIH chemicals should be top priority (with particular emphasis on chlorine)
  - Several source term considerations dominate the remainder of the top priority gap areas

Prioritized Gap Areas	
1.	Large scale tests of TIH chemicals
2.	Determination of range of mass fluxes
3.	Rainout from flashing flow
4.	Roughness, slope, and obstacles
5.	Chemical reactions
6.	Specification of local conditions
7.	Understanding variability
8.	Improved consequence modeling
9.	Deposition in urban areas

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Chemical Reactions Task

- The Effect of Chemical Reactions on Toxic Inhalation Hazard (TIH) Material Concentration in Vapor and Aerosol Clouds
- Applied Research Associates (ARA) completed comprehensive literature review and analysis for priority chemicals identified in Gap Analysis Task
- Key Findings and Recommendations:
  - Reactions with water *strongly relevant* for *all* TIHs investigated
  - Photolytic reactions *strongly relevant* for **chlorine**, but not for any other TIHs
  - Reactions with soil *marginally relevant* for **chlorine**, but not for any other this
  - Reactions with building materials *not a relevant* removal mechanism for any TIHs
  - Reactions with atmospheric gases *not a relevant* removal mechanism for any TIHs
  - Recommendation is to focus experimental work on **chlorine**, due to its highest toxicity and highest reactivity vs. other TIHs
  - Experiments are recommended to fill data gaps for the reaction rate and capacity of chlorine with soil, vegetation, via photolytic decomposition/reaction

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2010 TIC Release Field Test (Jack Rabbit)

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Test Objectives

1. Characterize the vapor/aerosol cloud movement, behavior, and physiochemical characteristics to determine its comparison with known observations and testing of large-scale releases of the testing materials.

2. Determine if ammonia can potentially act as less expensive and less dangerous dense gas for studying the component phenomena of large scale releases of dense gas TIH materials.

3. Evaluate instrumentation that can be used for the study of the large-scale release of the testing materials, and develop and evaluate testing methodology for future additional and potentially larger-scale tests.

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Jack Rabbit Participating Organizations

Jack Rabbit

TSA
Sponsor

DHS-CSAC
Manager

Dugway
Performer

Naval Surface Warfare Center - Dahlgren

- *Corrosive effects on military electronics*
- *On-site source modeling*

Center for Toxicology and Environmental Health

- *Instrumentation deployment – AreaRAE and MiniRAE detectors*
- *Fielding DHS S&T detectors*
- *Live plume mapping*

Air Force Research Lab Wright Patterson AFB

- *Compatibility testing with aircraft materials*
- *Long-term stress testing*

Signature Science, Inc.

- *Cloud Concentration*
- *Source Analysis*

Air Force Research Lab

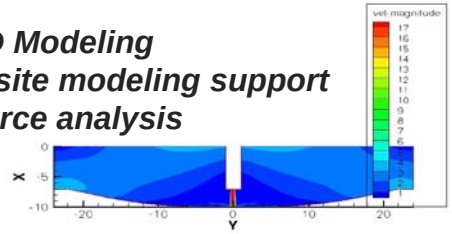
- *Soil Core Sampling*
- *Reaction Analysis*

Other Government Organization

- *Unmanned Aerial Vehicles*
- *8mm HD video*
- *Other data*

Forsvarets Forskningsinstitutt (FFI)
The Norwegian Defense Research Establishment

- *CFD Modeling*
- *On-site modeling support*
- *Source analysis*



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Pilot Test Releases (1 Ton)

Cl_2 5 min

NH_3 1 min

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Chemical Infrastructure Risk Assessment

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Chemical Infrastructure Risk Assessment

Chemical Infrastructure Risk Assessment

Dispersion Modeling Review

- Review of Current Models
- Evaluate Models for Assessing Release within the Chemical Supply Chain

Chemical Supply Chain Risk

- Develop Scenarios
- Expand CTRA Scenarios
- Develop New Modules

Toxicity Estimates

- Review and Revise Current Estimates for Appendix A Chemicals
- Identify Data Gaps
- Develop Non-Lethal Estimates

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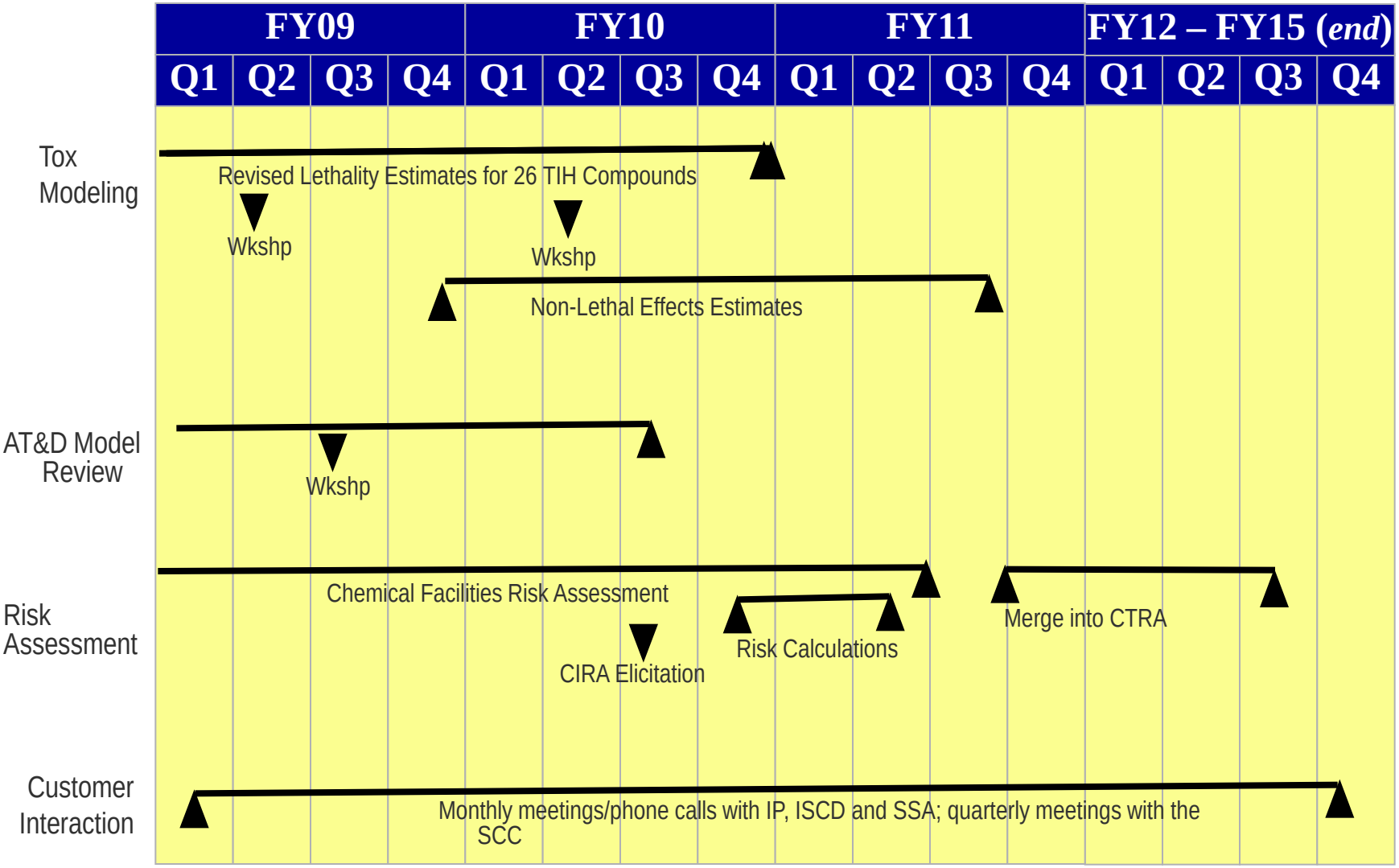
Chemical Infrastructure Risk Assessment Gantt Chart



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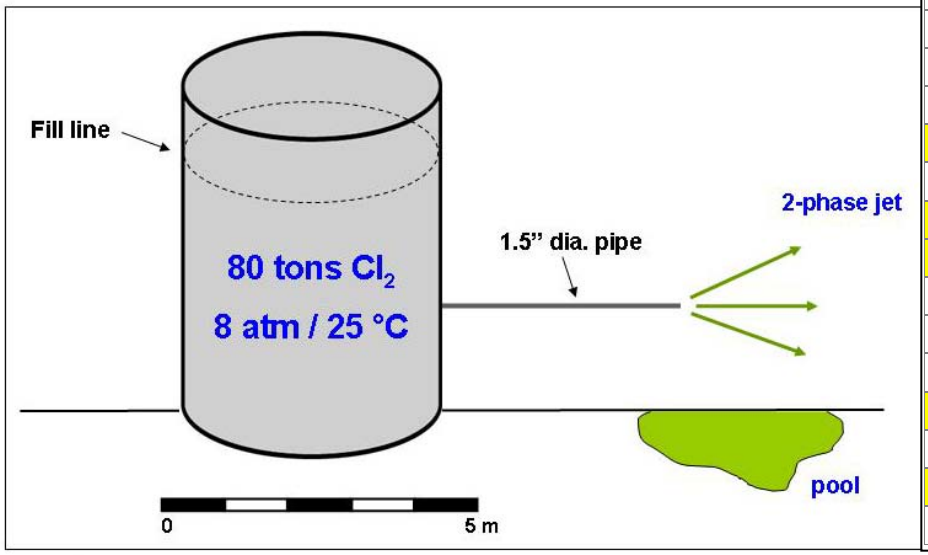
Dispersion Model Review

- Initial test scenario to characterize models
  - Initial screen reduced 172 models to 14; secondary screen reduced to 5
  - Identify strengths and limitations relevant to the risk assessment application
  - Identify methods to compare models on a common basis
  - Review of field trial data sets relevant to large-scale toxic industrial chemical (TIC) releases (Prairie Grass)
  - Review of past evaluations of models suitable for simulating large-scale TIC releases



Model	Developer
ADORA	BlazeTech Corp. (Cambridge, MA)
BREEZE HAZ[1]	Trinity Consultants (Dallas, TX)
CAMEO / ALOHA	NOAA/EPA
CHARM	BEE-Line Software (Austin, TX)
D2-Puff	IEM Inc. (Baton Rouge, LA)
HGSYSTEM	Shell Research Ltd. (Chester, UK)
HPAC	DTRA
MIDAS-AT	ABS Consulting (Rockville, MD)
NARAC (ADAPT / LODI)	Lawrence Livermore National Laboratory
OMEGA / ADM	SAIC (McLean, VA)
PHAST / PHAST Risk	DNV Corporation (Oslo, Norway)
QUIC-URB / QUIC-PLUME	Los Alamos National Laboratory
TRACE	SAFER Systems LLC (Camarillo, CA)
VLSTRACK	NSWC Dahlgren Division

AIChE/CCPS Guidelines for Use of Vapor Cloud Dispersion Models (2nd ed.) by S. R. Hanna, P. J. Drivas, and J. J. Chang (1996)

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Models Under Evaluation

- CHARM 11 (BREEZE Software; Dallas, TX) – commercial/proprietary
  - Eulerian grid model that incorporates dense gas effects; uses 1970s-era West Wind Model for wind field modeling and Myrup-Ranzieri diffusivity model for dispersion. Contains integrated industrial source emissions models and can model complex terrain and obstacles.

- HPAC 5.0 (U.S. Defense Threat Reduction Agency) – U.S. Gov't. & contractors
  - Second-order closure Gaussian puff techniques (SCIPUFF model) for passive dispersion; incorporates dense gas effects. Contains IFAC model for weapon-on-target industrial facilities releases and ITRANS model for industrial transportation releases. Can model complex terrain, obstacles, and meteorology.

- PHAST 6.53.1 (DNV Software; London, UK) – commercial/proprietary
  - Gaussian plume passive dispersion model coupled to dense gas dispersion model. Contains integrated industrial source emissions models. Flat terrain with no obstacles only. Related product "PHAST Risk" is customized to output event-tree-parameterized casualty estimates.

- TRACE 9.1 (SAFER Systems; Camarillo, CA) – commercial/proprietary
  - Gaussian plume passive dispersion model coupled to dense gas dispersion model. Contains integrated industrial source emissions models. Flat terrain with no obstacles only.

Project Prairie Grass Conclusions

- For the most part, HPAC, PHAST, and TRACE perform similarly across the selected releases
  - These models generally underpredict the observed arc-maximum 30-minute dosages, particularly under less stable atmospheric conditions and at farther arcs
    - Predicted arc-maximum dosages fall off more rapidly with distance than do observations
  - Cloud footprints bit too wide under stable atmospheric conditions

- CHARM appears to behave differently from the other models
  - Cloud widths at dosage levels of interest and arc-maximum dosages do not vary much with atmospheric stability class
    - Problem with how the model treats atmospheric stability effects?
  - Clouds tend to be narrow
    - This behavior also observed in chlorine tank test scenario
    - Narrow clouds fit the observations better for releases under stable conditions
  - The underpredictions of the arc-maximum dosages are orders of magnitude more severe than for other models for the more stable releases at shorter distances
    - Model is severely underpredicting the worst-case scenarios
  - Arc maximum dosages fall off relatively slowly with distance (as do the observations)
  - These results need to be vetted through the CHARM developer

Chemical Supply Chain Risk Assessment

- Apply Probabilistic Risk Analysis (PRA) methodology to assess the acute risk to human health and the national economy due to a terrorist event in the chemical supply chain for Appendix A Chemicals
- Progress
  - Scenario Backbone for Event Tree complete
  - Data collection for scenarios nearly complete
  - 7 different attack scenarios
  - Scenario/Event Tree workshop to be held in August
  - Economic model developed, data collection almost complete; being integrated into PRA Risk Engine
  - Elicitation and Module development to start in September
  - 1st CIRA RA to be provided in FY11
  - Economic Requirement document complete

Realistic assessment of the risk of each Appendix A chemical with respect to intentional events within the chemical supply chain

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Summary

- Highly attended workshops
  - Toxicity estimates January 2009, March 2010
  - Dispersion modeling (IDA) September 2008
  - IST (TAMU) January 2009
  - Economic Model April 2009
  - Scenario and Event tree August 2009
- CIRA represents a focused effort concentrating on development of a more robust CSC module for future integration into the CTRA
- Although there are significant challenges, the benefit DHS and chemical industry will be significant
  - Improved toxicity estimates for better consequence estimates
  - Model comparisons between government and industrial models
  - Relative risk and major contributors to risk by chemical

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