SAND2016-1749C

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MELCOR Computer Code Application Guidance for Leak Path Factor in Documented Safety Analysis

Final Report

U.S. Department of Energy
Office of Environment, Safety and Health
U.S. Department of Energy
1000 Independence Ave., S.W.
Washington, DC 20585-2040

~~May 2004~~ 2016

MELCOR 2.1 LPF Guidance Development (NSRD-10) Status

Presented by David Louie,Ph.D.

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2016 NFS Meeting – NSR&D sub-group,
March 1, 2016

U.S. DEPARTMENT OF ENERGY | NNSA National Nuclear Security Administration

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Acknowledgement

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- Collaborators for this project include: Dr. Larry Humphries, Mr. Kyle Ross and Dr. Salvador Rodriguez

Outline

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- History of MELCOR code development and its applications
- The use of MELCOR in DOE facilities
- MELCOR 2.1 LPF Guidance development tasks and progress
- Future expectation for MELCOR 2.1 LPF analysis

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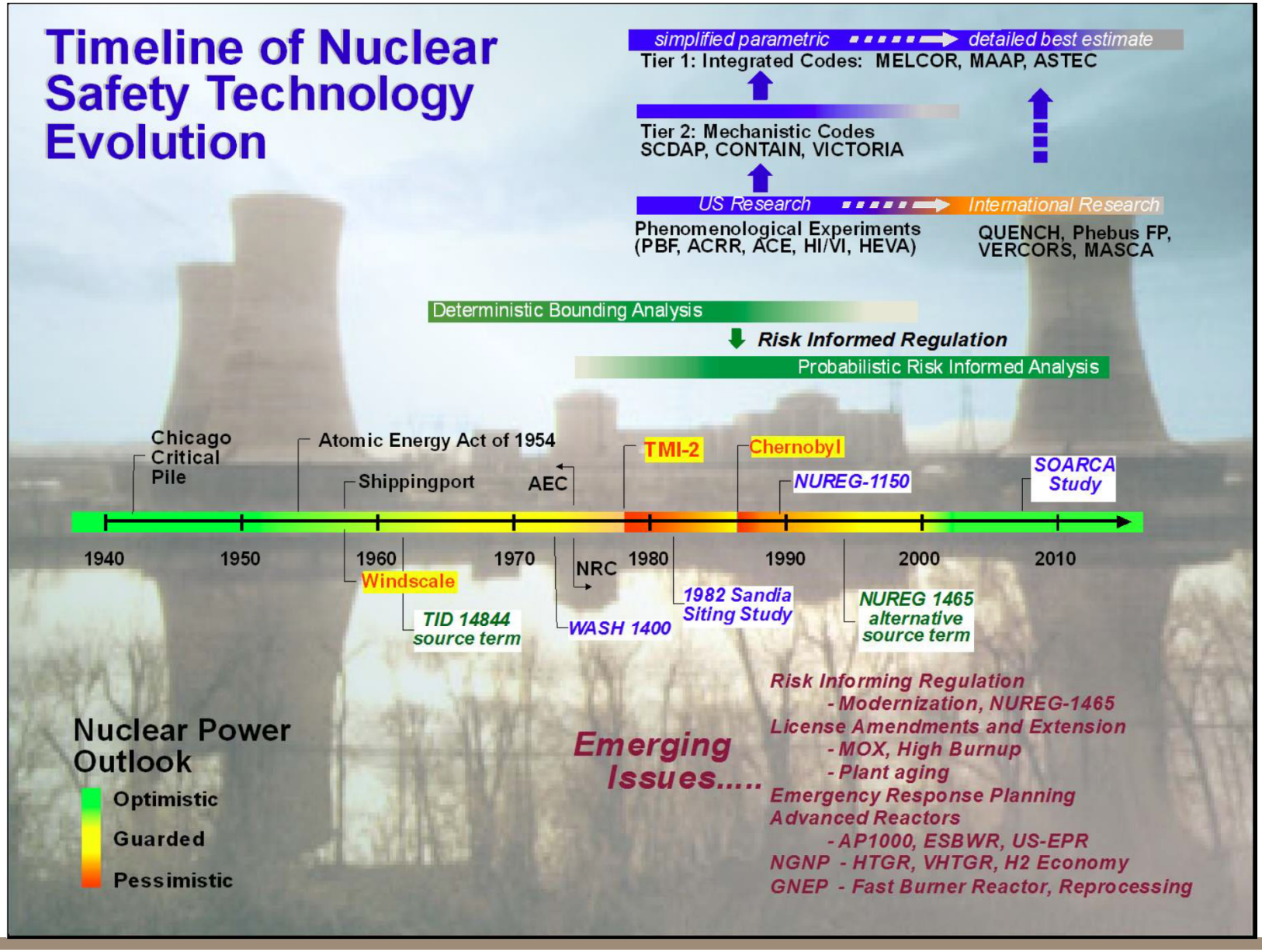
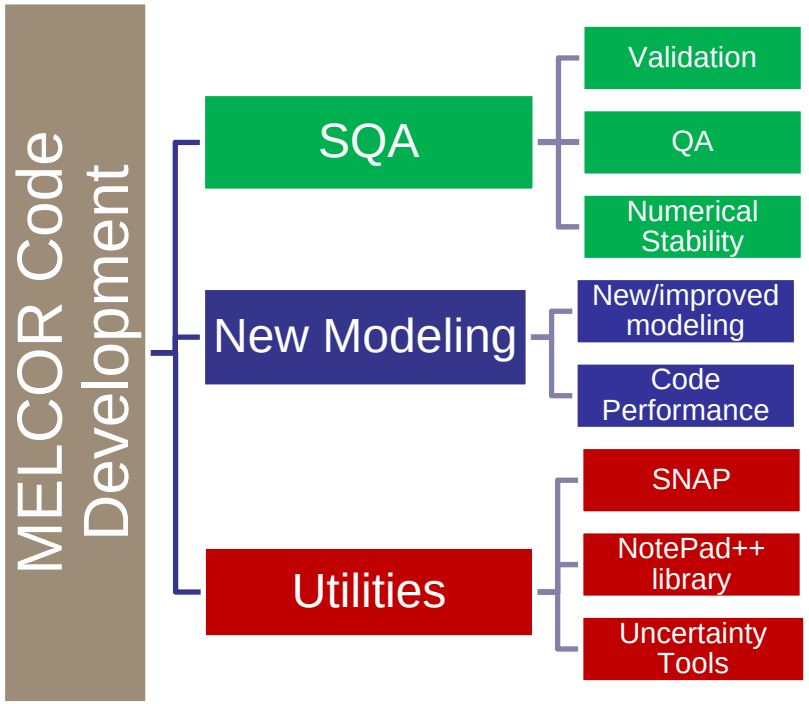
Timeline of Nuclear Safety Technology Evolution



MELCOR Code Development

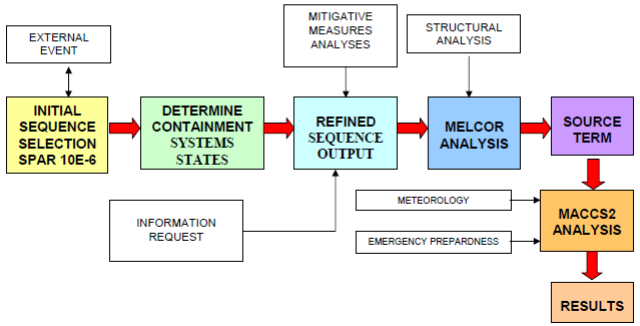
- MELCOR is developed by SNL for
  - US Nuclear Regulatory Commission
  - Division of Systems Analysis
- MELCOR Development is also strongly influenced by the participation of many International Partners through the US NRC Cooperative Severe Accident Research Program (CSARP)
  - Development Contributions – New models
  - Development Recommendations
  - Validation
- DOE-NE also may influence the development of MELCOR:
  - Sodium fast reactors – CONTAIN-LMR implementation
  - Small moderator reactors - NuScale



Code Applications

- Forensic analysis of accidents – Fukushima, TMI, PAKS
- Consequence Analysis SOARCA
- License Amendments
- Risk informed regulation
- Design Certification
- Preliminary Analysis of new designs
- Support of International Regulatory Bodies
- Non-reactor applications
  - DOE Leak Path Factor Analysis
  - Transport of radiological releases, toxins, and biohazards in buildings, building complexes
  - Chemical weapon demilitarization facilities
  - NRC Spent Fuel Reprocessing Source Term Tool development

SOARCA PROCESS



International Use of MELCOR

MELCOR Workshops & Meetings

- 2014 CSARP/MCAP/ MELCOR Workshop
  - September 8-12, 2014
  - Almost 100 registered
  - MELCOR full week Course
- 2014 Asian MELCOR User Group (AMUG)
  - October 13-17th 2014, Republic of Korea
  - Weeklong workshop
- 2015 European MELCOR User Group (EMUG)
  - Bel V & Tractebel, Belgium 2015
  - April 17-18, 2015
- 2015 CSARP/MCAP
  - September 14-18, 2015
  - Albuquerque, NM
  - No Workshop
- 2015 Asian MELCOR User Group (AMUG)
  - Hosted by CRIEPI
  - November 2015

MELCOR LPF Usage at DOE Facilities

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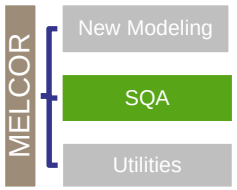
- MELCOR is the DOE designed Toolbox code
- MELCOR 1.8.5 LPF guidance and gap analysis reports (2004)
- MELCOR 1.8.5 and 1.8.6 have been used for LPF analyses
- LANL – Plutonium facility (TA-55), Waste Characterization Reduction and Repackaging Facility, Decontamination and Volume Reduction System Facility, Chemistry and Metallurgy Research Replacement Facility, Beryllium Technology Facility, Godiva Kiva
- LLNL – Plutonium facility (331)
- NNSS– Device Assembly Facility, Area G Tunnel
- Pantex
- SRNL – K Area Spent Fuel Storage Facility



Modern Software Quality Assurance Best Practices

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Emphasis is on Automation

Affordable solution

Consistent solution

- MELCOR Wiki
  - Archiving information
  - Sharing resources (policies, conventions, information, progress) among the development team.
  - Non-reactor application assessment
- Code Configuration Management (CM)
  - 'Subversion'
  - TortoiseSVN
  - VisualSVN integrates with Visual Studio (IDE)
- Code Review
  - Code Collaborator
- Nightly builds & testing
  - DEF application used to launch multiple jobs and collect results
  - HTML report
  - Regression test report
- Regression testing and reporting
  - More thorough testing for code release
  - Target bug fixes and new models for testing
- Bug tracking and reporting
  - Bugzilla online
- Validation and Assessment calculations
- Documentation
  - Available on Subversion repository with links from wiki
  - Latest PDF with bookmarks automatically generated from word documents under Subversion control
    - Links on MELCOR wiki
- Sharing of information with users
  - External web page
  - MELCOR workshops
  - LinkedIn User Group

Visualization and Graphical Interface

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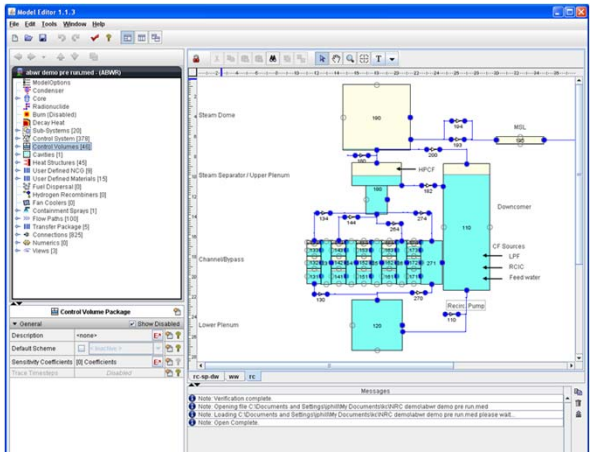
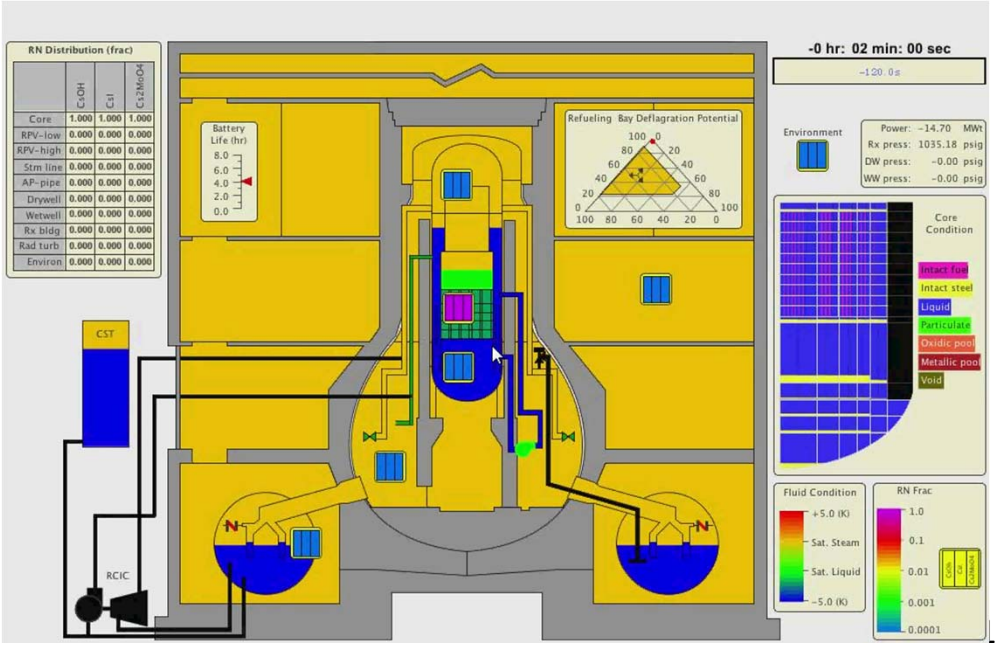
- Visualization is important for improving quality of calculations
  - Identification of modeling errors and issues
- Graphical user interface
  - Can reduce input errors
  - Simplifies input for new users
- SNAP MELCOR 2.1 Plugin
  - Version 1.0.0 - Released 7/17/09
  - Current version 2.1.1 – Released 2/24/12
  - Will convert a 1.8.6 input deck to 2.1 and back to 1.8.6
  - Sandia is working with SNAP developers to recommend enhancements for MELCOR plug-in
- 2011 workshop focused on the use of SNAP
- Model Editor -Components
  - Tree Structure organization
  - Arranged according to MELCOR package
  - ASCII view of object available
  - Organize components
  - DIFF capability for components
- Views
  - Trend plots
  - Custom animations
  - Others





MELCOR

New Modeling

SQA

Utilities

MELCOR Documentation

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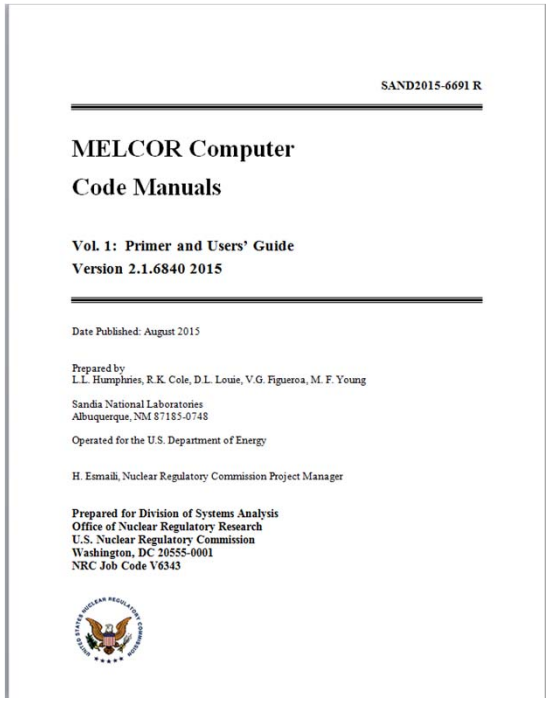

SAND2015-6691 R

MELCOR Computer
Code Manuals

Vol. 1: Primer and Users' Guide
Version 2.1.6840 2015

Date Published: August 2015

Prepared by
L.L. Humphries, R.K. Cole, D.L. Louie, V.G. Figueroa, M. F. Young

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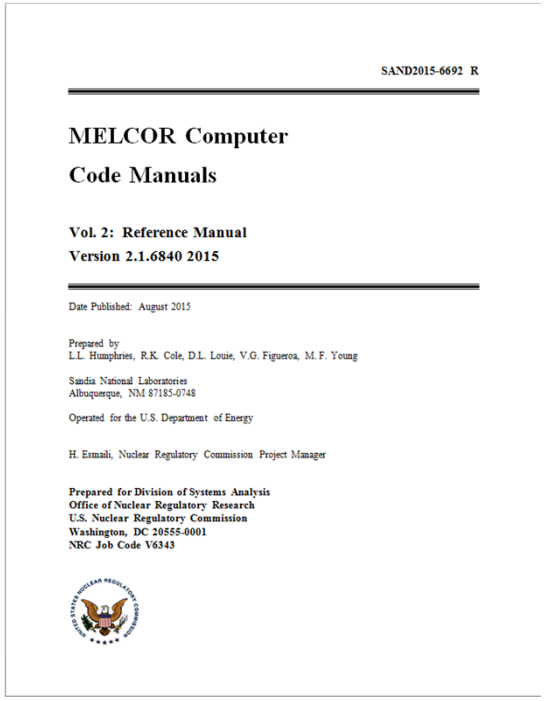
Prepared for Division of Systems Analysis
Office of Nuclear Regulatory Research
U.S. Nuclear Regulatory Commission
Washington, DC 20555-0001
NRC Job Code V6343



SAND2015-6692 R

MELCOR Computer
Code Manuals

Vol. 2: Reference Manual
Version 2.1.6840 2015

Date Published: August 2015

Prepared by
L.L. Humphries, R.K. Cole, D.L. Louie, V.G. Figueroa, M. F. Young

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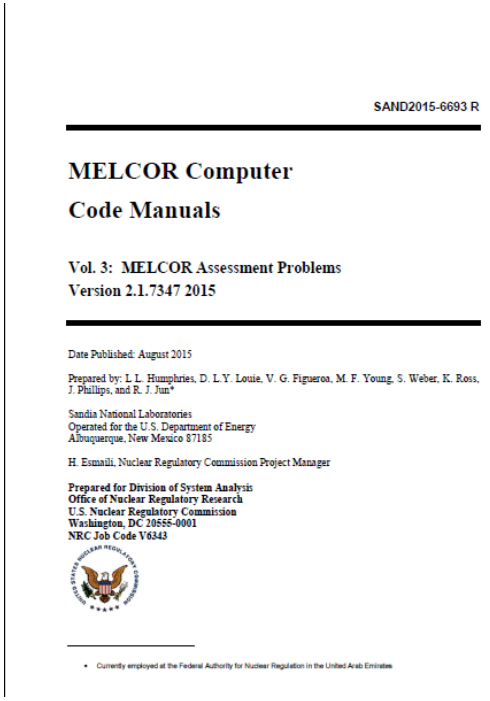

SAND2015-6693 R

MELCOR Computer
Code Manuals

Vol. 3: MELCOR Assessment Problems
Version 2.1.7347 2015

Date Published: August 2015

Prepared by: L.L. Humphries, D. L.Y. Louie, V. G. Figueroa, M. F. Young, S. Weber, K. Ross, J. Phillips, and R. J. Jun*

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Volume I: User Guide

SAND2015-6691 R

Volume II: Reference Manual

SAND2015-6692 R

Volume III: Assessments

SAND2015-6693 R

MELCOR Code Validation

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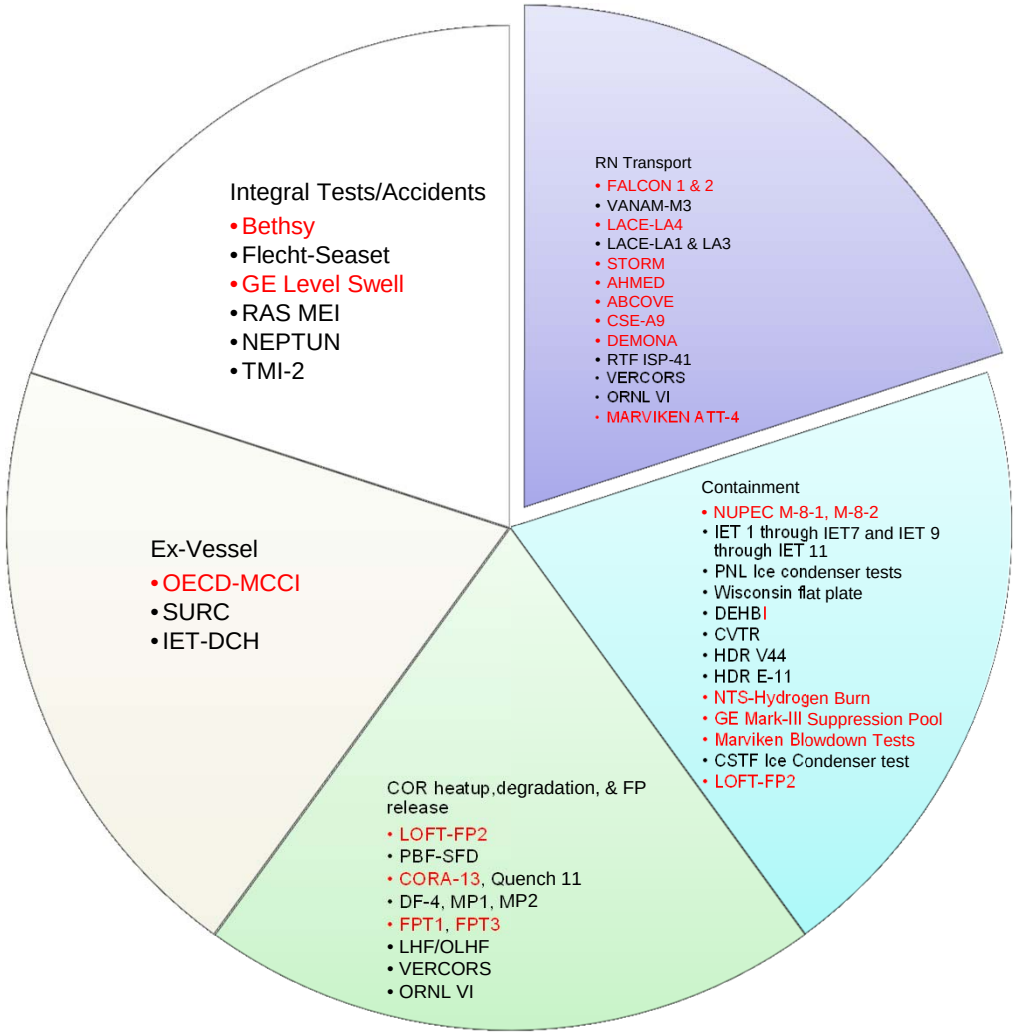
- Separate effects tests
  - More tightly controlled conditions
  - Limited or specific range of phenomena
- Integral tests
  - Combine many simultaneous physics aspects
  - Often less precisely characterized test conditions
  - Broader range of phenomena investigated
- Actual Accident Studies: TMI-2, Fukushima
  - Combines all relevant physics at full scale
  - Least well instrumented and characterized "experiment"
  - An ultimate basis for code validation
    - Bearing in mind, not every accident should be expected to be the same as TMI-2
- Participation in multiple International Standard Problems



NSRD-10 Major Objectives

- Replace the obsolete MELCOR 1.8.5 LPF Guidance Report in the DOE Repository
  - MELCOR 1.8.5 or 1.8.6 is not supported by Sandia
  - Only verification tests included
- MELCOR 2.1 LPF Guidance Report development include:
  - Validation tests
    - reactor and non-reactor experiments, particularly for aerosol physics
    - Analytical tests
  - Verification tests
    - Version to version comparison - MELCOR 1.8.5, 1.8.6 and 2.1
    - Additional verifications other than those in MELCOR 1.8.5 guidance report
  - Best practices for common accident scenarios encountered at DOE facilities
  - Replace 1.8.5 with 2.1 version of MELCOR in DOE Toolbox

NSRD-10 Work Breakdown Structure

- Task 1- Summarize existing LPF materials and the important aerosol physics to be validated
  - Completed – a summary letter report submitted
- Task 2 – Summarize existing reactor experiments for DOE facility applications
  - In progress
- Task 3 – Validation calculations using experiment data in DOE-HDBK-3010
  - In progress
- Task 4 – Develop best practices for MELCOR LPF
- Task 5 – Final report (SAND) – MELCOR 2.1 LPF Guidance Report

Task 1 Reviews and Findings

- Review of existing MELCOR 1.8.5 LPF guidance report (2004)
  - Findings
- Review of LA-UR-03-7945*
  - Findings
- Important aerosol physics to be validated for LPF
  - Findings
- Review of MELCOR 2.1 Manuals for LPF applications
  - Findings

*Jordan, H., and Leonard, M., Attenuation of Airborne Source Terms in Leak Paths, LA-UR-03-7945, Los Alamos National Laboratory, Los Alamos, NM, October 2003

Task 1 Summary and Conclusion

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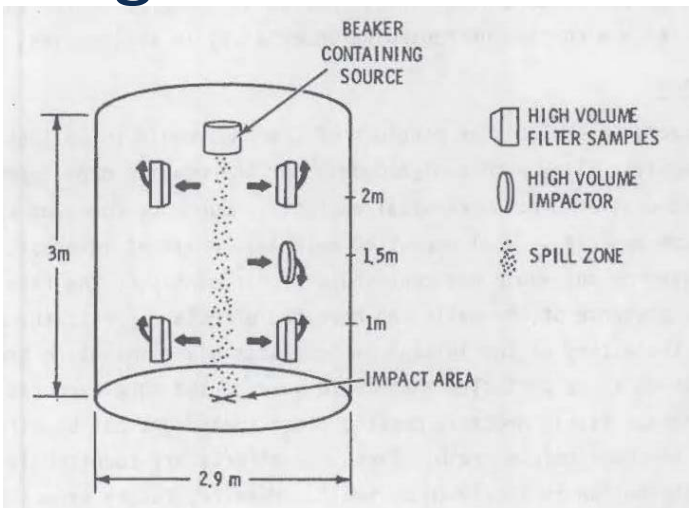
- Possible best practice recommendations
  - Use exact MAR with agglomeration and/or deposition disabled, instead of using “1” g mass
  - For modeling the environment volume, use time-independent volume instead of very large volume of in order of 10^{10} m^3
  - Use the CCF model in the FL package to better represent counter-current situation in fire scenario
  - Use new filter models in MELCOR 2.1 for modeling the HEPA filter conditions for accident conditions
  - Use SPR package to model the water fire sprinkler system
  - Use control function to model solid combustible burn for fire scenarios
- Important aerosol physics models to be validated
  - Agglomerations
  - Deposition
  - Resuspension
- Improvement needs (not a part of this research) for MELCOR 2.1
  - Dynamic hot gas layer for fire scenarios
  - Solid/liquid combustion models in Burn package for fire scenarios

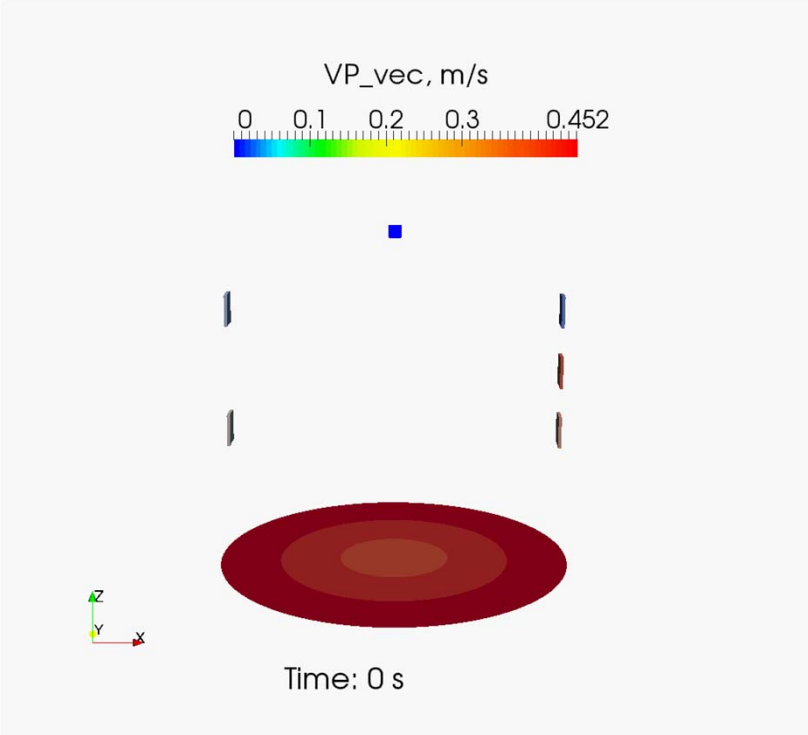
Task 2/3 – In progress

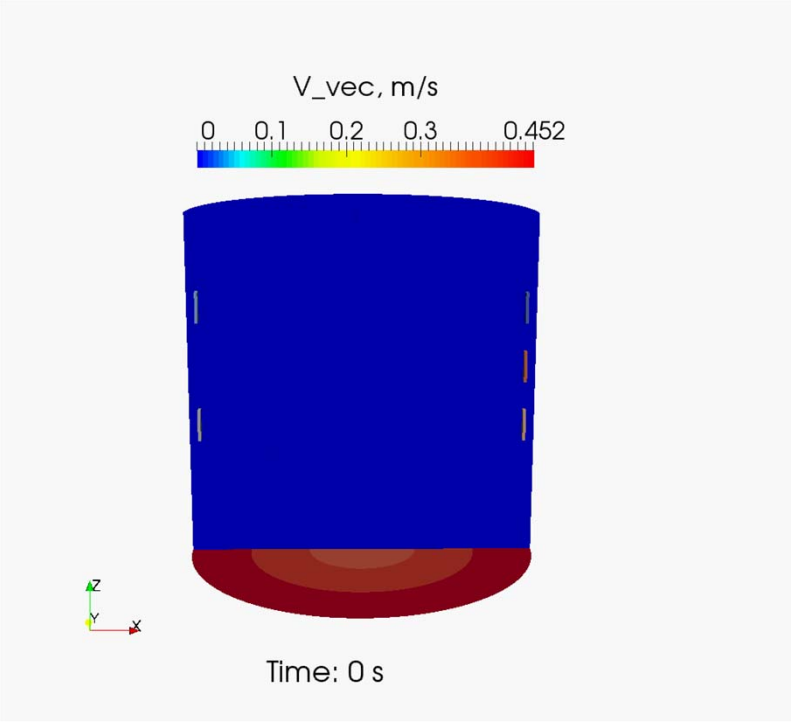
- Review of MELCOR 2.1 Assessment Report (SAND2016-6693R)
  - Chapter 2 –analytical validation useful
    - No aerosol validation
  - Chapter 3 – experiment validations
    - Applicable for Aerosol physics validations, water spray validations
- Other recent international experiments on aerosols
  - DIANA experiment (0.7 m cube with 1 HS @330K, 1 HS @ 291 K)
- LA-UR-03-7945
  - Analytical aerosol transport two-volume problem
- DOE-HDBK-3010 experiment data, PNL aerosol experiments
  - Pressurized powder release experiment
  - Spill experiment - CFD code provides initial fluid velocity since aerosols in MELCOR does not affect hydrodynamics

Spill Tests (PNL-3786) using FUEGO Simulation

- 100 g of TiO_2 falls from a beaker at the ceiling of PART volume.
- Particle size – 1.7 µm
- FUEGO simulation
  - 100,000 particles
  - Filters @ 1.4 m^3/min
  - Impactor @ 0.56 m^3/min







Future Expectation

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- MELCOR 2.1 LPF Guidance Report is completed by September 2016
- Upon DOE approval, replace to the obsolete MELCOR 1.8.5 guidance report
- DOE may conduct QA and Gap Analysis for the Sandia MELCOR Program
- MELCOR 2.1 is ready to be used in DOE LPF analysis, replacing the old LPF analysis using obsolete versions of MELCOR
- Create DMUG (DOE LPF MELCOR user group) meeting?
- Conduct training across DOE complex

Back up slides or hyperlink

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Aerosol Physics Validations

Physics	Comments and Suggestions
Agglomeration	It is important to validate this model because it identifies the degree of the aerosol interaction during the initial release from an accident. This research will identify experiment data to be used to validate this model in MELCOR
Deposition	A number of deposition models have been included in MELCOR (gravitational, diffusive, and thermophoresis). Although MELCOR 2.1 allows the user to turn off one to all three of these deposition mechanisms, we will assess if one or more of these deposition models can validate using experimental data. In addition, MELCOR 2.1 contains turbulent deposition models that are only available for heat structure surfaces (non-pool surfaces). Turbulent deposition models can be validated through experimental data for high Reynolds number regime, straight pipes, including bend geometry.
Plugging	Currently MELCOR 2.1 does not contain plugging models. Although models are available for plugging, we may examine the available models. Consideration of plugging in LPF analyses may not be conservative in terms of the release.
Resuspension	MELCOR 2.1 contains a resuspension model from SAND2015-6119[1] using the force balance between aerodynamic forces and adhesive forces to the surfaces. This simple model is a function of wall shear stress, friction factor, gas velocity and surface roughness. The validation of this model is important, particularly if sufficient flow exists to entrain the deposited aerosol to the air stream. Thus this research will include the resuspension validation.

[1] Young, M.F., Liftoff Model for MELCOR, SAND2015-6119, Sandia National Laboratories, Albuquerque, NM July 2015.

Review of MELCOR 1.8.5 LPF Guidance Report

Area	Comments and Suggestions
MELCOR description	It describes MELCOR 1.8.5, which became obsolete
Suggests to include cracks of the structures in seismic events	This phenomenon is discussed further in the aerosol physics section.
Models door gaps	It is important phenomenon to be modeled in LPF analyses, particularly for a nuclear facility as shown in Figure 1 since exterior doors contain gaps to allow inflows to maintain the intent of the ventilation system. We will review the door gap data provided in this report.
Evacuation	MELCOR 2.1 contains control functions that can be used to model the open and close of the doors for evacuation purposes.
MELCOR 1.8.5 specific input requirements	Many of specific input requirements no longer apply for MELCOR 2.1. For example, a recommended 10^{10} m^3 for the environment is no longer needed because MELCOR 2.1 contains time-independent volume that could be used to model the environment. This reference recommended the use of 1 g/cc for modeling aerosol density; however, this density is for water. Therefore, when a dried condition is modeled, it may not truly represent the density of the aerosol. In this case, the actual density should be used.
Sample problems for MELCOR	The data for pressure drop for range of wind speed will be verified. We have conducted verification tests (in terms of version-to-version comparison) using the sample problems provided in this report for MELCOR 1.8.5, 1.8.6 and 2.1. We also added additional verification problems to the sample problem sets.
MELCOR limitation	This report pointed out a number of improvement needs for MELCOR 1.8.5, including those specified for LPF applications. Since then, the MELCOR Quality Assurance (QA) program was strengthened by a QA plan to track code changes, user bug reporting, code-review, code documentation (see Table 3 for details) and code configuration management. This research will provide a number of validation tests with known experiments and analytical calculations specifically for LPF applications. This research will provide a list of best practices to use MELCOR for LPF applications.

Review of LA-UR-03-7945

Area	Comments and Suggestions
Aerosol physics related to LPF	This report includes a summary of aerosol attenuation phenomena, including fire sprinkler system and filters as attenuation methods. This will address in the aerosol physics section below.
Gas and vapor	This topic will not be discussed further in this research
Analytical LPF approach	We may include these analytical analyses
LPF analysis using MELCOR	Although MELCOR 2.1 does not have solid combustibles as a part of the Burn package, the powerful feature of the control function models (CF package) in MELCOR allows the user to model the solid combustible efficiently. A demonstration of this model will be included in this research.
Lack of hot gas layer	This report includes the inadequacy of MELCOR 1.8.5 for modeling stratified hot gas layer in the fire scenarios. This is still true for MELCOR 2.1. A user still has to model this hot layer using the technique described in this report.
Lack of counter-current flow (CCF) model	This is not true for MELCOR 2.1. A CCF model has been implemented in the FL package. Similarly, this report states the requirement of fire code analysis for the input of the MELCOR calculations.
Small MAR models in MELCOR	The MELCOR 1.8.5 models described in this report tended to use “1” g aerosol mass as the initial source term for calculating LPF. Once LPF is obtained, the result is scaled back to the actual MAR involved in the accident. The use of such small mass by the authors and most safety analysts in the DOE complex is to yield conservative LPF values to minimize agglomeration and deposition [1]. However, this approach may undermine the aerosol physics, particularly for agglomeration, which may not be scaled linearly. In addition, because of the ability to disable the desired aerosol physics, we suggest modelling actual MAR from the source terms when using MELCOR 2.1 for LPF analyses (see the aerosol physics section more details).

[1] Siebe, D.A., et.al, Ensuring Conservatism/Lessons Learned in Leak Path Factor Calculations with MELCOR, LA-UR-07-2386, Los Alamos National Laboratories, Los Alamos, NM 2007.

Selected Review of MELCOR 2.1 Manuals

Area	Comments and Suggestions
CVH package	Significant improvements went into MELCOR 2.1 over MELCOR 1.8.5 for this package, such as atmosphere sound speed model (comparison to CONTAIN), time-independent volume (use for modeling environment), and properties (or time-) specified volume
FL Package	Some improvements include CCF model, flow blockage, and MACCS interfaces.
RN Package	Significant improvement went into MELCOR 2.1 over MELCOR 1.8.5: essentially no restriction on number of classes to be modeled, normalization of RN inventories, and treatment of MAEROS aerosol coefficients in terms of temperature and pressure. The aerosol filter model has been extended to allow specification of decontamination factor (DF) by particle size as well as by class. Each DF can be represented by a constant or control function. Beginning in MELCOR 2.1, many of the aerosol physics models can be turned off for individual mechanisms to allow specific aerosol testing. This turn-off feature includes for aerosol deposition and agglomeration. Turbulent deposition model has also been implemented. Recently, a resuspension model from SAND2015-6119
CF Package	One of the powerful models in MELCOR is the control function (CF) package. This package allows the users to model any models that use parameters in MELCOR for many applications. For example, opening and closing of the doors for evacuation can be modeled using CF. In MELCOR 2.1, CF_Formula is the powerful CF, allowing it to program a formula, such as a reaction, a pump curve, and an algebraic equation. For example, a reaction of solid combustible and oxygen can be modeled using CF.