Documentation for Department of Energy Toolbox

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Introduction

- Motivation
  - NRC guidance
    - OI PRM-012, "Software Quality Assurance for RES-Sponsored Codes," ML17047A448
    - MD 11.7, "NRC Procedures for Placement and Monitoring of Work with the U.S. Department of Energy (DOE)," ML112991579
    - NUREG/BR-0167, "Software Quality Assurance Program and Guidelines," ML012750471
  - Outdated version of MACCS approved for use in the DOE Safety Software Quality Assurance – Central Registry (Toolbox)
    - MACCS2 Version 1.13.1 vs. MACCS Version 3.10.0
  - 13 years since DOE MACCS2 Gap Analysis
    - Code modifications
    - Documentation and training updates

DOE Central Registry

- Safety Software Quality Assurance (SSQA) – Central Registry (DOE Toolbox)
  - Evaluated against DOE O 414.1D, "Quality Assurance" and DOE G 414.1-4, "Safety Software Guide for Use with 10 CFR 830 Subpart A"
  - Toolbox codes used by DOE contractors for safety analyses
- Benefits of toolbox codes:
  - the gap analysis evaluation performed provides valuable information on the code regarding application of SQA requirements,
  - the evaluation extends beyond the DOE SSQA criteria to the review of the code's capability to properly perform safety basis calculations,
  - the DOE specific guidance documents identify limitations and vulnerabilities not readily found in other code documentation, and
  - due to the established pedigree, assessments of the toolbox code by Field Offices and site contractors may be reduced in scope.

DOE Toolbox Codes

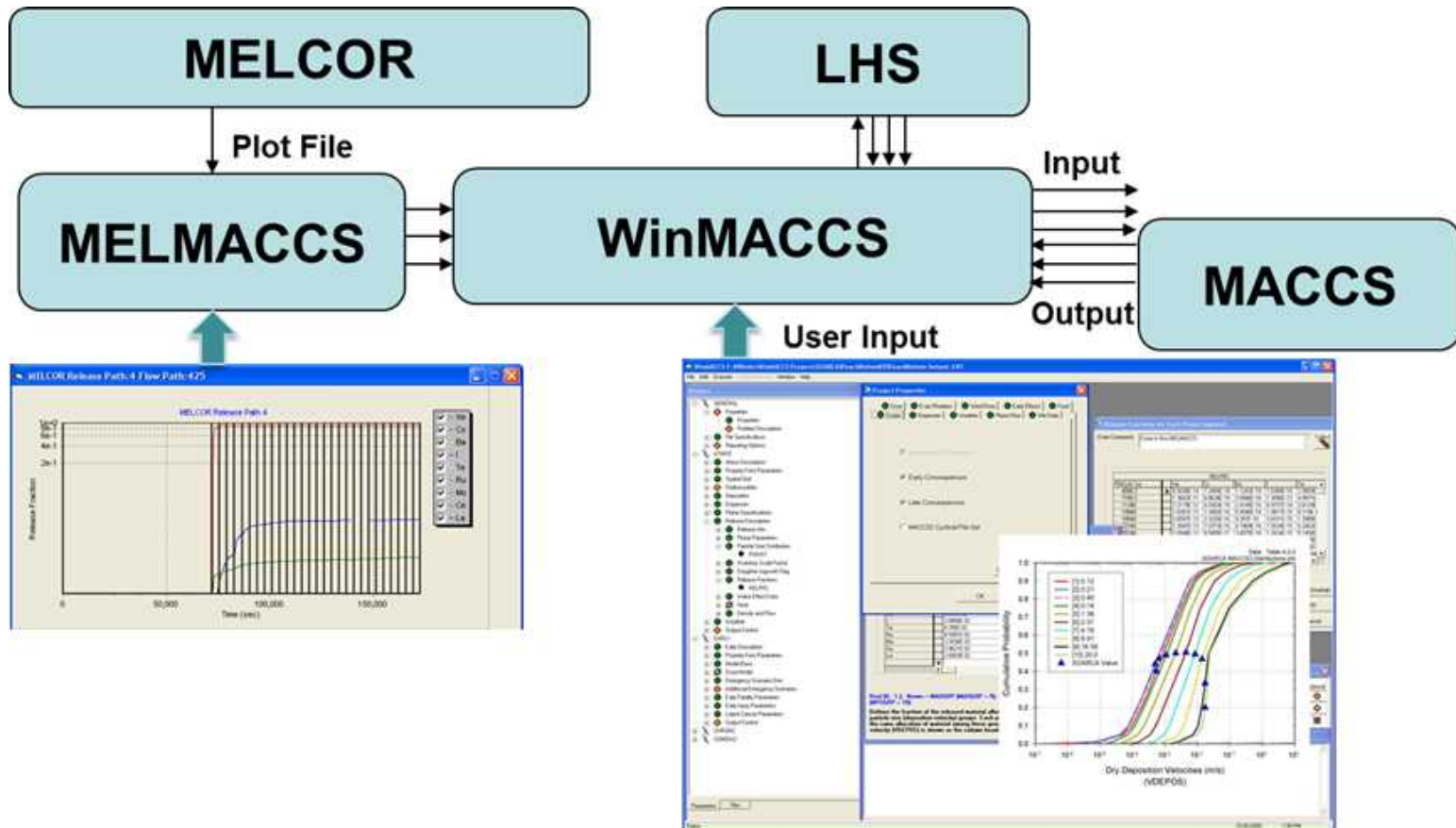| CODE	VERSION	YEAR APPROVED	OWNER
ALOHA	V5.4.4	2014	National Oceanic and Atmospheric Administration (NOAA)
CFAST	V3.1.7 and V5.1.1	2004	National Institute of Standards and Technology (NIST).
EPIcode	V7.0	2004	Homann Associates, Inc.
GENII	V2.10.1	2013	Pacific Northwest National Laboratory (PNNL)
HotSpot	V2.07.01	2010	Lawrence Livermore National Laboratory (LLNL)
IMBA	IMBA Expert ™ USDOE Edition V4.0.28	2006	UK Health Protection Agency (HPA)
MACCS2	*V1.13.1*	*2004*	*Sandia National Laboratories (SNL)*
MELCOR	*V1.8.5*	*2004*	*Sandia National Laboratories (SNL)*

MACCS DOE Applications

- U.S. DOE, "MACCS2 Computer Code Application Guidance for Document Safety Analysis," DOE-EH-4.2.1.4-MACCS2-Code Guidance, 2004

- DOE Regulatory Applications
  - Calculating the centerline Total Effective Dose Equivalent (TEDE) incurred by the Maximally Exposed Offsite Individual (MOI) evaluated at the 95th quantile dose level
  - Sensitivity studies to show relative benefits of evacuation, sheltering, interdiction and shielding
    - Not usually used in Documented Safety Analyses (DSAs)

- DOE DSAs utilize ATMOS and EARLY modules with specific recommended parameter inputs

Recommended DSA Parameters

Modeling Characteristic	Recommendation
Receptor Distances and Meteorology	Maximally Exposed Individual (site-boundary)
Meteorology Conditions	Stability Class F and low windspeed (1-1.5 m/s)
Dispersion Parameters	• > 100 meters: P-G, Tadmor-Gur, Briggs • < 100 meters: Eimutis-Konicek
Mixing Layer Height	Local site-specific seasonal and time-of-day mixing layer height
Surface Roughness	Site-specific AMS (1977) model
Release Duration	Site-specific
Exposure	2-hours
Deposition	• Dry deposition, no wet deposition • 1 cm/s for unfiltered, non-tritium, non-noble gas; 0.1 cm/s filtered; 0.04 cm/s – 0.8 cm/s tritium gas or HTO
Dose Conversion Factor	ICRP-60 (biokinetic), ICRP-68/72 (dose coefficients), ICRP-26 (metabolic), ICRP-30/48, FGR 11 or 12
Pathways	Inhalation, cloudshine, groundshine
Breathing Rate	3.33E-04 m^3/s
Dose Commitment	50-year
Heat	Conservative ground-level release
Protective Actions	None
Meteorological Sampling	Stratified Random Sampling
Meteorological Data	1-year of hourly weather data

MACCS and associated tools

- MACCS2 transitioned to simply MACCS in version 3.8.0.2 (June 2014) and the graphical user interface WinMACCS

Current Status

- DOE toolbox approved code
  - MACCS2
  - Version 1.13.1 (no longer supported)
  - 2004
  - Sandia National Laboratories

- Currently distributed versions
  - U.S. Nuclear Regulatory Commission is the primary code sponsor
  - MACCS version 3.10.1.2
  - WinMACCS version 3.10.0
  - Various other preprocessors (MelMACCS, SECPOP)

2004 MACCS2 Gap Analysis

- Gap analysis evaluated MACCS2 Version 1.12

- Conclusions by order of priority
  - correcting know defects
  - upgrading user technical support activities
  - providing training on a regular basis
  - revising software documentation
    - Software Quality Assurance Plan
    - Software Model Description including software requirements and software design
    - User's Manual including user instruction, test case description, and software configuration and control
    - Error notification and corrective action process

SQA Review Activities

DOE O 414.1D SQA Work Activity	Potential SQA Documents
1. Software Project Management and Quality Planning	− Software Project Management Plan (SMPMP) and/or − Software Quality Assurance Plan (SQAP) − Software Safety Plan
2. Software Risk Management	− Various document types can be used to cover risk management
3. Software Configuration Management	− Software Configuration Management Plan (SCMP) or related documents
4. Procurement and Supplier Management	− Contractual documents or other software procurement and use agreement documentation
5. Software Requirements Identification and Management	− Software Requirements Specifications (SRS) or related document
6. Software Design and Implementation	− Software Design Document (SDD), Model Description, Programmer's Reference Manual, or other related documents
7. Software Safety	− SDD − Software Safety Analysis documentation
8. Verification and Validation	− Verification and Validation Report − Test Case Description and Outcome Report; Other testing documents
9. Problem Reporting and Corrective Action	− Software Error Notification and Corrective Action Report
10. Training of Personnel in the Design, Development, Use and Evaluation of Safety Software	− User Instructions or User Manuals − Training Packages and User Qualification
11. Model Validation and Evaluation	− Test results and evidence that code output was compared to experimental results or against equivalent output from an independent code and differences resolved

MACCS SQA

- The MACCS SQA plan begins with MACCS2 Version 1.12
  - No plan to back-validate or back-QA
- Configuration Management System
  - QA Training
  - Software Requirements Document
  - Implementation Document
  - Test Plans
  - Source Code
  - Sample Files
  - Data Files
  - User's and Models Manuals
  - Test Results
  - Bug Tracking Database (Bugzilla)
  - Client Data
  - Distribution Package

MACCS SQA Configuration Management

- Subversion (SVN)
    - Apache Tortoise SVN
    - MACCS Server
    - Version Numbering, for example Version 1.15.00.02 where:
        - 1 - major revision number, incremented by PI approval
        - 15 - incremented when released to the NRC or to the public
        - 00 - incremented if a special (branch) version was released a particular person or group
        - 02 - minor modification number, incremented by the developer and used to track incremental development
- SQA Forms
    - Requirements
    - Software Implementation
    - Software Testing
    - Software Regression Checkout
    - Training Completion
    - Data Verification

Supporting Documentation

SQA Review Activity	Document Title	ADAMS Accession Number
Software Project Management and Quality Planning	MELCOR Accident Consequence Code System (MACCS) Software Quality Assurance Plan, Version 1.6	ML17174A930
Software Configuration Management	History of MACCS and WinMACCS	ML17047A451, ML17047A452
Procurement and Supplier Management	MACCS User NDA and Terms of Use Clause	ML17038A477
Software Design and Implementation	MELCOR Accident Consequence Code System (MACCS): Model Description	ML063560409
Training of Personnel in the Design, Development, Use and Evaluation of Software	MACCS Analyst Training and Qualification Plan, Ver. 2.0	ML17047A453
Training of Personnel in the Design, Development, Use and Evaluation of Software	P-301 Consequence Analysis Course	ML17047A455
Model Validation/Performance	Comparison of Average Transport and Dispersion Among a Gaussian, a Two-Dimensional, and a Three-Dimensional Model	ML043240034

Conclusion

- Lack of support for MACCS2 1.13 necessitates inclusion of MACCS 3.10+ in the toolbox

- Improvements since 2004

  - Code enhancements

  - Documentation

  - Training

  - Error notification and bug reporting (https://melzilla.sandia.gov/)

  - Configuration management

- Request to DOE for inclusion of MACCS 3.10 in the Safety Software Central Registry (2017)

Questions