MELCOR Code Development Status, Code Assessment, and QA

Larry L. Humphries, Randall Gauntt (SNL)
and
Hossein Esmaili (NRC)
MELCOR Code Development

• MELCOR is developed by:
  – US Nuclear Regulatory Commission
  – Division of Safety Analysis (DSA)
  – Office of Nuclear Regulatory Research

• MELCOR Development is also strongly influenced by the participation of many International Partners through the US NRC Cooperative Severe Accident Research Program (CSARP and MCAP)
  – Development Contributions – New models
  – Development Recommendations
  – Validation
**Current MELCOR Development**

**Code Readiness**
- code ready for applications
- code not ready for applications

**Code life-cycle**
- code conversion phase
- code development phase
- code maintenance phase

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**MELCOR 1.8.6**
- Molten pool models
- Core Package upgrade
- Released Fall 2005
- Code Maintenance
- Current Workhorse

**MELCOR 2.1**
- FORTRAN 95
- New input
- 2.0 beta version released Sept 2006
- 2.1 Release Sept 2008

**MELCOR 3**
- Current developmental version
MELCOR 3.0 Code Development Thrust Areas

Code reliability
- Validation
- QA
- Numerical stability

User Utilities
- Converter
- PTFREAD
- SNAP
- Uncertainty Engine

Code Enhancements
- New/improved modeling
- Code performance
MELCOR 2.1

- Source code ported to Fortran-95 by IBRAE
- Essentially equivalent to MELCOR 1.8.6 modeling
  - Many MELCOR1.8.6 execution issues resolved
  - Bit-for-bit parity between v1.8.6 & v2.0
  - New models added to M2.1
- Dynamically allocated memory
  - Arbitrary number of objects (CVs, FPs, Cells, etc.) limited by the available system memory
- Input deck converter
  - Can be used to ‘replace’ MELGEN to jumpstart use of code
  - Improvements to GUI
  - Double precision version
  - Debugged against assessments
Code Development: Code Reliability

MELCOR

User Utilities

Code Enhancements

Code Reliability
Software Quality Assurance

• Review of current SQA practices
  – Internal audit & review
• Code Configuration Management (CM)
  – Recently moved to ‘Subversion’ CM
• Assessment calculations of MELCOR 2.1
  – Currently underway
  – Regression testing and reporting
  – Automation of testing and reporting procedures
  – Nightly builds & testing
• Bug tracking and reporting
  – Bugzilla online
Software Quality Assurance

• Sandia Corporate Process Requirement 001.3.6 (CPR 001.3.6)

• The software management framework adapted from two internationally recognized standards
  – the Capability Maturity Model Integration (CMMI) ®
  – and ISO 9001
  – These standards provide elements of traceability, repeatability, visibility, accountability, roles and responsibilities, and objective evaluation

• Process areas
  – Project planning and oversight
  – Requirements Development and Management
  – Risk Management
  – Configuration Management
  – Technical Solution
  – Integrated Teaming
  – Integrated Product
  – Verification and Validation
  – Measurement and Analysis
  – Development and Lifecycle Support
Software Quality Assurance
Annual Re-evaluation

- Annually review of MELCOR SQA Practices.
  - Weighted average of team members
  - 0-None, 1-Little, 2-More, 3-Most
- Highlights areas of improvements.
  - Verification & Validation
  - Collected Improvement Data
  - Risk Management
  - Integrated Teaming
- Focuses attention on areas needing improvement
  - Requirements Development and Management
  - Integrated Product Development
- Sandia’s commitment to SQA
MELCOR Assessments

- **MELCOR 2.1 Assessment Matrix**
  - Over 70 calculations currently in the assessment matrix
  - Performed by Sandia National Labs and Russian Academy of Science
  - Results to be published with MELCOR 2.1 release

- **Example Experiments**
  - Phebus
  - Quench
  - OLHF/LHF
  - RASPLAV
  - LOFT
  - PANDA
  - FLECHT/SEASET
  - CORA13
  - LACE
  - NUPEC
  - Three-Mile Island

- **Test calculations cover a broad range of phenomenon**
  - Core uncovering (i.e., TMI-2 and LOFT-FP2),
  - Core damage/melt relocation (TMI-2, PHEBUS, LOFT-FP2)
  - Core to upper plenum natural circulation (TMI-2)
  - Natural circulation within SG tubes (i.e., IIST)
  - Core to lower plenum natural circulation (i.e., BACCHUS tests)
  - Lower head failure (i.e., LHF & OLHF)
  - FP release (i.e., ORNL HI & VI, VERCORS, PHEBUS)
  - Containment Thermal Hydraulics (i.e., CVTR, HDR, NUPEC, Marviken blowdown, CSTF ice condenser, PANDA etc.)
  - Aerosol Deposition (i.e., ABCOVE, SUPRA pool scrubbing, DEMONA, etc.)
Alternative TMI-2 Accident Benchmark Study

• OECD/CSNI Alternative TMI-2 Scenario Benchmark
  – Participating codes: ASTEC v1.3, ATHLET-CD, ICARE/CATHARE V2, MAAP4, MELCOR 1.8.5, MELCOR 1.8.6
  – Objective to perform a benchmark on a well-defined plant (similar to TMI-2) and with prescribed boundary conditions

• Conclusions
  – Codes performed well in all phases with little or no tuning of parameters
  – Importance of adequate user training
  – Prediction of oxidation of molten mixtures
  – Prediction of UO₂ melting & interactions
  – Prediction of debris coolability
• The key quantities of interest obtained from Test M-8-2 include:
  – **Helium** (e.g., simulated hydrogen) mixing;
  – Containment **spray** performance
  – **Pressure** and temperature response and stratification.
Key phenomena in the LOFT LP-FP-2 tests were oxidation/hydrogen generation, relocation of core materials, forced convection, conduction, radiation, and fluid-structure heat transfer, pressure response.

Hydrogen Production from Oxidation of Zircaloy Cladding

CFM Cladding Temperature 0.25 m from Bottom of Module
• Key phenomena in the CORA-13 tests were oxidation/hydrogen generation, relocation of core materials, forced convection, conduction, radiation, and fluid-structure heat transfer.
MELCOR 2.1 Assessment
LACE-LA-4

- **Aerosol** Modeling
- Hygroscopic effects
  - Temperatures
  - Pressures
• **Key Phenomenon**
  - Core material relocation,
  - *temperature* histories,
    - Heat conduction/convection
    - fuel relocation
  - *hydrogen* production.
    - hydrogen production occurs during the initial steam phase before any relocation,
    - relatively insensitive to simulation parameters.
MELCOR Code Regression Testing

• Test Suite run on a distributed computer cluster
  – 10 Dell PowerEdge 2950s (40 runs)
    • 2 Dual Core, Hyperthreading 64-bit Xeon Processors, with 2MB cache, running at 3 GHz
    • 667MHz Front-side bus
    • 8GB RAM
  – DEF - tool for automatically launching jobs to distributed machines
  – Results archived in subversion

• Test Cases
  – Standard test cases chosen for physics coverage ~14 test cases
    • New cases will be added as validation calculations are run
    • Debug & optimized versions tested
    • Unix versions not tested as frequently (will test more frequently in future)
  – Special purpose cases to address particular bug issues
Regression Tests

• Regression testing performed with each interim code release

• Standard Test Suite
  – Qualifies the code for particular application
    • Analytical results
    • Using ISP or other recognized assessments
    • Baby problems
  – Formal regression testing report (made available to users)
  – Review test cases
    • Every major code release
    • Coverage testing

• Special Purpose Testing
  – Regression test for each resolved bug
  – Regression test for new feature or enhancement
  – Responsibilities of submitter (owner)
    • supply success criterion
    • review test results for success
  – Test case made inactive after three successes (still available for future testing)
MELCOR Code Regression Test Report

- **Auto-generated regression test report**
  - Readable and highly formatted report (PDF)
  - Auto-generation allows report for each interim code release
  - Reports to be made available to users

- **Side-by-side comparison of regression test results**
  - Comparison plots for two code versions
  - Event time tables

- **Test suite coverage tables**

- **Test case dimension table**

- **Pedigree information**

**Automated Nightly builds and regression testing (New!)**
Bugzilla site for bug reporting, tracking, and information
  - Available from SNL web page

Users submit bugs and details
  - OS, Hardware, affected packages, severity
  - Bug description
  - Attachments

Comments and attachments can be marked private and not visible to other users

Utilized more by MELCOR community
  - 90 bugs (M1.8.6) reported last 12 mos.
  - 68 bugs (M1.8.6) resolved
  - 22 bugs (M1.8.6) unresolved
Bugs Tracked in MELZILLA

- Automated applications for reporting issue management
  - Integrated with MSOffice, Bugzilla, and internal Wiki
  - Charts of open/assigned issues
    - Leveling bugs with developers availability
  - Timeline showing issues entered into bugzilla
    - Trying to reduce the length of time a bug is left open
    - Some issues are harder to resolve than others

Need to eliminate bugs that are unresolved for more than a month
Post-Workshop Bugs (M2.1)

- 218: Steady-State option leads to temperature on HS_ND record and warning in MELGEN
- 228: Logic error 4 in CVHMOM
- 229: Failure with converted input for VVER440
- 230: Error with unformatted EDF files
- 231: No error checks for time-dependent volume properties
- 234: File open warning in M_EXEC
- 236: PWR Shroud collapse temperature
- 238: Advanced B4C modeling
- 239: VVER calculation volume freezing – Film Tracking
- 240: CORA-13 COREU3 run-time error
- 241: Integer valued CF arguments
- 242: MELCOR 2.1 freezes
- 251: In CVH_INPUT CV_SOU the H2O_VAP for IDMAT isn’t functioning properly
- 252: COROXY call to COROXD can result in invalid memory writes
- 254: MACCS interface variables calculation bug
- 257: Component collapse parameters
- 259: Wrong listing of film tracking in MEGOUT_v2-0
- 260: Abnormal termination on EDF with Belikov error
- 261: LOGIC ERROR 4 in CVHMOM
- 262: Content of ERROR and WARNING Messages
- 265: NMPAIR on DCH_EL is supposed to be optional
- 266: Array bounds exceeded in elheat_NSI
- 267: Error flag not set in cvhbv1_NSI
- 271: IHX model incorrectly implemented
- 272: Input echo missing comments and global variables
MELCOR Developers Wiki Site – Internal Use

- MELCOR Developers Wiki
  - Archive records
    - Requirements
    - Testing reports
    - Quality Records
    - Assessment work
  - Information Sharing
    - Debugging Policies
    - Testing Policies
    - Code Development practices
    - Coding Conventions
    - Lessons Learned
    - Software Risk Management
    - Version Changes
MELCOR Web Page

- New Look
- Downloads
  - MELCOR executables
  - Converter executables
  - 2.1 GUI
  - Documentation
  - PTFREAD
  - Change Documents
- Workshop / CSARP information
- Bug reporting
- FAQs
- More? Regression reports,...
MELCOR Online: Downloading MELCOR

- Account login is your email address
- All authorized MELCOR users are given an account
  - First time users must receive authorization from USNRC
- Access from MELCOR website or go directly to https://melcor.sandia.gov/MelcorDownloads/MelcorDownloadStart.aspx
- You can follow its hierarchical links to access every file on the system

To quickly download the latest version of MELCOR, just click the “Latest News” link to see a page like this:

**Current News as of September 1, 2008**

MELCOR 2.1 has been released. View Change Document.

To download the latest version, click here.

Click on the appropriate link for the User’s Guide and Reference Manual.

**Other Options**

- Main Menu
- Old News
### MELCOR 1.86.YS Changes

<table>
<thead>
<tr>
<th>Subversion Branch Location</th>
<th>Start Revision # from SubVersion Repository</th>
<th>Finished Revision # from SubVersion Repository</th>
<th>Changed Files</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Trunk</td>
<td>920</td>
<td>NA</td>
<td>CoredT</td>
<td>Fixes problem with zero clad masses for the COR text editor for all the test problems. (Bug: 114)</td>
</tr>
<tr>
<td>Trunk</td>
<td>928</td>
<td>NA</td>
<td>CoredT, coruin</td>
<td>Fixes problem with steam starvation plot variable. Allows 7 parameters for COREVOL (coruin) and removes extra &quot;.&quot; in COR-STARV-OUT plot variable.</td>
</tr>
<tr>
<td>Trunk</td>
<td>915</td>
<td>NA</td>
<td>Cuthra</td>
<td>Disable the new &quot;not quite equilibrium&quot; modeling (Bug #60). This feature will be completed in the next code revision.</td>
</tr>
<tr>
<td>Trunk</td>
<td>914</td>
<td>NA</td>
<td>Enlrsn.f</td>
<td>Fixed problem with surface area calculated for H2 with multiplicity 0.0.</td>
</tr>
<tr>
<td>Trunk</td>
<td>654</td>
<td>NA</td>
<td>Curtge</td>
<td>Restored from rollback. Significant changes to curng by the to resolve some problems observed with the &quot;original YS&quot;, and also to resolve bug 147.</td>
</tr>
<tr>
<td>branches/1.86TS</td>
<td>730</td>
<td>841</td>
<td>coruin</td>
<td>Allow INDIVCT for pool scrubbing of all aerosol and vapor species</td>
</tr>
<tr>
<td>BCI/Developers/1joamu/trunk</td>
<td>598</td>
<td>564</td>
<td>CoredS, corps2, corsh1, corsh4, corshm.</td>
<td>Fixed end-dam-flag control function argument.</td>
</tr>
</tbody>
</table>
Code Development: Code Enhancements

- All new code development will be performed in MELCOR 2.1
- MELCOR 1.8.6 – Code Maintenance only
Code Development
HTGR - COR Package Updates

- New reactor models (like present PWR, BWR)
- PBR (pebble bed)
  - New components
    - Pebble fuel
    - New heat transfer coefficients
  - Effective thermal conductivity
    - radiation/convection/conduction
  - Coolant friction loss
- PBR (prismatic)
  - New components
    - Reflectors
    - Hexagonal graphite blocks
  - cell-cell conductive/radiative heat transfer
- Graphite oxidation models
- On-going work
  - Fission product release and transport from HTGR fuel
  - Plant demonstration calculations
• Fueled part of pebble is fuel component
  – $\text{UO}_2$ with extra COR material as graphite
• Unfueled shell is clad component
  – Clad material becomes graphite
• Center reflector component
• Outer reflector component
• Fuel radial temperature profile for sphere
  – Provides peak and surface pebble temperature
    • Better reactor simulation
Radial cell-cell conductive/radiative heat transfer added
  • Uses effective bed conductivity (Zehner-Schlunder with modifications for thermal radiation)
Axial cell-cell conduction modified to use effective bed conductivity
Coolant friction factor is for pebble bed (Ergun equation) when PBR model is invoked
  • Achenbach correlation being investigated
Coolant heat transfer uses pebble bed heat transfer coefficients
PMR COR Model

- More “rod-like”, requires fewer changes to COR
- Fuel compacts represented as fuel component
- Part of hex block associated with a fuel channel is “thick” clad component
  - Temperature gradient in clad as well as fuel
- Reflector components
- Radial cell-cell conductive/radiative heat transfer added
  - Single effective thermal conductivity
Graphite Oxidation Models

- Oxidation of graphite by steam and air
  - The air oxidation rate is implemented as (Richards, 1987)
  \[ R_{OX} = 122.19 \exp \left( - \frac{20129}{T} \right) P^{0.5} \]
  - The steam oxidation model is implemented as (Richards, 1988)
  \[ R_{OX,steam} = \frac{k_4 P_{H_2O}}{1 + k_5 P_{H_2}^{0.5} + k_6 P_{H_2O}} \quad k_i = K_i \exp \left( - \frac{E_i}{RT} \right) \]

- Maximum rates limited by gaseous diffusion to surface

- Reaction Products
  - Currently, the air reaction produces CO
  - Steam reaction produces CO and H₂
  - The CO/CO₂ mole ratio is given by (Kim and NO, 2006)
  \[ f_{CO/CO_2} = 7396e^{-69604/RT} \]
• **Point kinetics for operating reactor applications**
  – Model developed by UNM
    • Stable over wide range of timesteps
  – Temperature-dependent reactivity feedback from COR components
    • Fuel/Moderator/Reflector generalized weighting for spatially averaged feedback
  – External reactivity insertion via control functions
    • Generalized and flexible

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**Sample Test**

- Initial power level is 268 MW
- $0.50$ reactivity oscillation (CF)
  - Period is $2\pi / 0.05 = 125$ s
- Doppler feedback from fuel and moderator
- PK Model turned on
- Oscillation started at 400 s
HTGR COR Model Testing

• PBR Testing of new COR model
• Deck adapted from Texas A&M PBR deck
  – Pebbles represented as fuel/clad components instead of debris
  – Steady state problem
    • 268 MW reactor power
    • Run to 1500 s
  – Reactor is older Pty Ltd design as in Reitsma (2006)
HTGR Ongoing Work

- Fission product release and transport from HTGR fuel
  - Release
    - Review PARFUME models
    - Devise simplified MELCOR model (Booth?)
  - Transport
    - Plate out
    - Surface sorption
    - Dust liftoff
- Plant demonstration calculations
  - Use of point kinetics for accidents w/o SCRAM
  - Consider coupling of 2D neutronics (ie PARCS) with COR
- HTGR RCCS model
  - Removal of heat from vessel
- Plant components
  - Gas turbine
  - Heat exchangers
  - Helium circulator
HTGR Ongoing Work contd

- **Stratified flow for air ingress**
  - Original scenario was that air entered by diffusion
    - 10hr timescale
  - CFD simulation shows that air enters via stratified flow and circulation (Kim, 2008)
    - 260s timescale

Heat and Mass Transfer Correlations
- MELCOR code should be able to model the CONTAIN correlations by default
- Modify the MELCOR film tracking model and default model parameters based on the CONTAIN parity

Engineered Safety Features (ESF) Enhancements
- heat exchanger models
- fan cooler models

Improvement of SPARC Models
- Review the SPARC98 model for possible improvements over the earlier SPARC90 model

Improvement of VANESA Models
- improvements for ex-vessel fission product release. Specifically, the modeling of Ru and Mo releases

Others…
Code Development: User Utilities

- Code reliability
- User Utilities
- Code Enhancements

MELCOR
• **SNAP**
  - Symbolic Nuclear Analysis Package developed by API – MELCOR Plug-in

• **PTFREAD**
  - EXCEL add-in for generating plots, analyzing data, creating AVI’s, generation of regression reports

• **MELCOR 2.1 GUI & Converter**
  - Utility for generating MELCOR 2.1 input decks and converting existing MELCOR 1.8.6 decks to new format

• **Uncertainty Software**
  - Suite of tools for running MELCOR in batch, Monte Carlo sampling of variables and analyzing statistics

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**Supporting Applications**

• **Best Estimate with Uncertainty Quantification**

• **Powerful tool for risk-informing regulations**
New AVI format indicates temperature of component by color

Flow velocities
- If horizontal flow paths exist
  - Vertical component
    - linear interpolation of the vertical flow velocity at the flow path junction height horizontal velocity
  - Horizontal component
    - taken from the horizontal flow path.
  - Vector is positioned at the radial center of the CV & the horizontal flow path junction height.
- If a horizontal flow path does not exist
  - The vertical velocity component in a control volume is calculated as the average of all inlet and outlet vertical flow velocities and a vector is drawn at the center of the control volume.
This is a new PTFread calculated variable and is accessed by selecting CALCULATED when asked to specify the MELCOR package for the variable:

- Mass is summed over a user-specified range of materials
- Mass is summed over a user-specified range of components
- Mass is summed over a user-specified range of rings
- Intact and/or conglomerate masses can be indicated
- Wildcards can be used to sum over an entire range

PTFREAD variable Format (as appears in the header row on the data sheet):

- SumMass(intact or conglomerate, material, component, elevations, rings)
- Example: SumMass(*,SS:SSOX,*,1:2:3:4:5,*)

Option for elemental mass in oxide (SSel)

- Only the elemental mass of Fe is included in the sum (does not include Oxygen mass)
New MELCOR Output Format
HTML

- **HTML Time Edits**
  - Specified with global input
    - MEL_HTMLFILE ‘DEMON_Out.htm’
  - File for each time edit
  - Links to other time edits
  - Links to package edits/tables
- **Other Links**
  - SNL/Bugzilla
  - I/O files
  - Code Manuals
  - Graphical Diagrams
    - Node Diagram
    - Temperature contours
Other MELCOR Changes

Code reliability

MELCOR

User Utilities

Code Enhancements
Intel Visual FORTRAN Compiler

- Compaq Visual FORTRAN v 6.6C is current developmental compiler
  - Did not want to make any changes until after 2.1 was released
- Intel Visual FORTRAN will become the new development platform
  - No technical support for CVF
  - Problems with CVF rebuilding entire project
  - Problems with error checking
- Advantages to Intel Compiler
  - Able to build true 64-bit code for 64-bit operating systems
    - Performance improvements
  - Better support for F95 code
    - Error checking
  - Currently the only compiler we are supporting on Linux
  - Improvements to the programmer interface (Visual Studio.NET)
    - Automatic keyword completion
    - Integration with subversion
  - Capability to automatically convert CVF projects
• This and future MELCOR releases will be node-locked
  – Each installation will require a separate license to run
  – A license will only work on the computer for which it was issued
• All licenses will expire
  – Normally within one year
  – Period may be shorter for special releases
  – The version of MELCOR released at this workshop will expire on 1 February 2009
• Check the MELCOR website for upcoming release dates
MELCOR Licensing - Requirements

• Two files now required besides the MELCOR and MELGEN executables:
  – calu_nl.dll
    • Contains the CALU (Cross-plAtform Licensing Utility) software that is called by both MELCOR and MELGEN
    • Any media we provide MELCOR on will also include this DLL
  – Product.key
    • Contains your license
    • This file is requested via email
• Both files must be in the same folder as your MELCOR executable or it will not run
Summary

Code reliability
- Validation
- QA
- Numerical stability

User Utilities
- Converter (Discussed in following presentation)
- HTML Output
- Etc.

MELCOR Code Development

Code Enhancements
- New/improved modeling
- Code performance