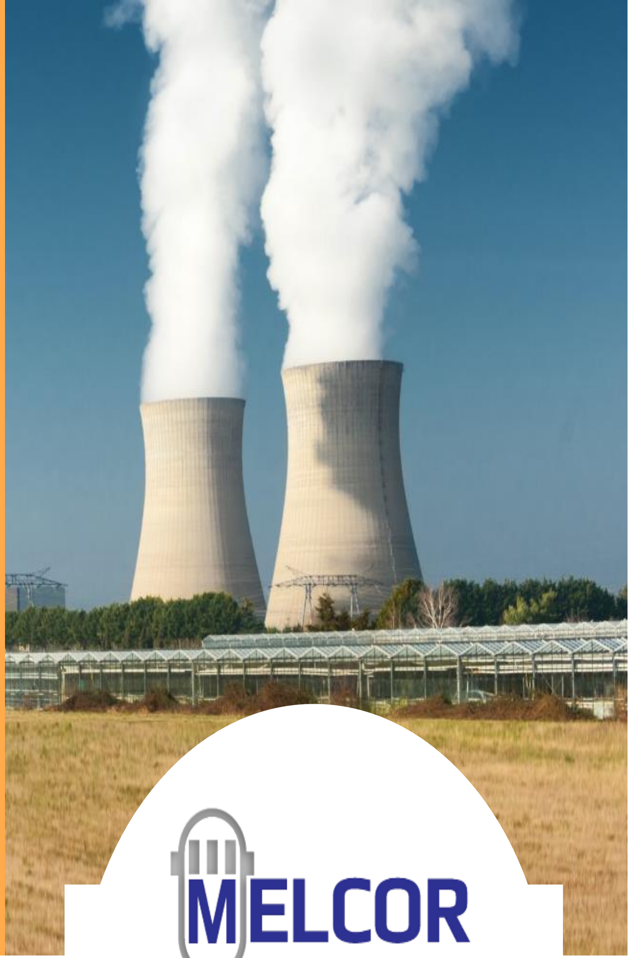
Sandia National Laboratories

Securing the future of Nuclear Energy



MELCOR

CAV and LHC Modernization Effort

2024 European MELCOR Users' Group Meeting

April 15th-18th, 2024

U.S.NRC

SAND2024-03574PE

U.S. DEPARTMENT OF ENERGY NNSA

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Overview

Effort underway to "modernize" the MELCOR CAV and LHC packages

- General strategy:
  - Convert to modernized input parsing
  - Convert CAV database to route through the field manager
  - Augment CAV data structures to "stride-one" as appropriate
  - Put CAV physics subroutines through the physics manager
- Consolidate LHC and CAV
  - Preserve capabilities of LHC,
  - Reconcile debris solution to CAV

Simultaneously, introduce CORQUENCH-style debris and concrete cavity solution algorithm as an alternative to CORCON-MOD3

- Implementation strategy
- Challenges

Progress Report

Summary

Modernized Input Parsing

Modernized C++ input parser is key to informing:

- Scalar and array data to support CAV and LHC solution,
- Parameters of a given code package,
- Field manager (database management),
- Physics manager

To translate an input record's information into field manager via the parser:

- Inform field manager about any parameters and data (scalar or array of some type)
  - Redesign elements of database as necessary
  - For example, flattening to stride-one arrays
- Develop the C++ function(s) to process input records
- Translate the relevant data into field manager
- Allocate/Get as necessary from field manager to use data in MELGEN/MELCOR

Progress:

- Supporting architecture of CAV-related parser largely in place
- Moving through the collection of input records slowly
- Using internal mechanisms to cross-check results from modernized parser

Field Manager & Database

MELCOR

Field manager is a new mechanism for database management

- Module/sub-module structure
- Leverage object-oriented FORTRAN practices and polymorphism
- Ensure automatic and good data allocations and initializations
- Eliminate memory issues
- Deftly handle time-level management and sub-cycling during run-time
- Simplify restart file read/write
- Interface with physics manager, plot manager, etc.
- Facilitate more efficient code development moving forward

"Array flattening" a major aspect of database modernization

- Simplifies coding
- Easier to add to a database
- Facilitates debugging
- Performance improvements
  - Restarts
  - Physics (finding/reducing cliff edge effects)

XMDC array in old format:

Cor%Cell(naxl, nrad)%Cellcomp(kcmp)%New%XMDC(ncrmat)

Flattened array

XMDC(ncrmat, kcmp, naxl, nrad, state)

Memory layout is contiguous in memory and "stride one"

CAV and LHC database translation into field manager is in progress

Physics Manager

Physics manager handles execution (implementation)

- Usually subroutines usually including all or part of a physics algorithm
- Can apply to other subroutines/procedures (not strictly related to physics)
  - Output processing and accounting operations
  - Inter-package communications
  - Database operations

Benefits:

- Facilitates development (new/alternate physics models)
- Separates data from implementation (a principle of modernized development)
- Facilitates external user development (new/alternate physics w/o source code access)
  - Opportunity for a flexible application programming interface (API)
  - Would eliminate sensitivities around source code distribution
  - Would facilitate incorporation of externally-developed models into MELCOR
  - Many possible applications:
    - Advanced users with ideas for modeling improvements or interest in specialized topics
    - Reactor simulator vendors,
    - Research/development

CAV and LHC have been completely routed through physics manager by now

CAV/LHC Consolidation

"Combine" CAV and LHC

- Take advantage of their many similarities
- Reconcile debris models
  - LHC debris was intended as simplified CAV debris originally
  - Database consolidation with field manager
  - Physics algorithms with physics manager
  - Open both CAV and LHC to alternatives (e.g. CORQUENCH)
- Retain the distinctives
  - CAV with its concrete cavity
  - LHC with its user-definable structures
- Preserve necessary capabilities despite the reorganization
- Reduce user burden in terms of MELGEN/MELCOR input
- Possibly reduce code maintenance burden
  - CF arguments and plot variables
  - MELGEN/MELCOR text output
  - Restart file read/write
  - Entire sequences of sensitivity coefficients
  - Other redundancies currently being tolerated

Effort not started in earnest, but facilitated by CAV/LHC FM/PM development

CORQUENCH in CAV

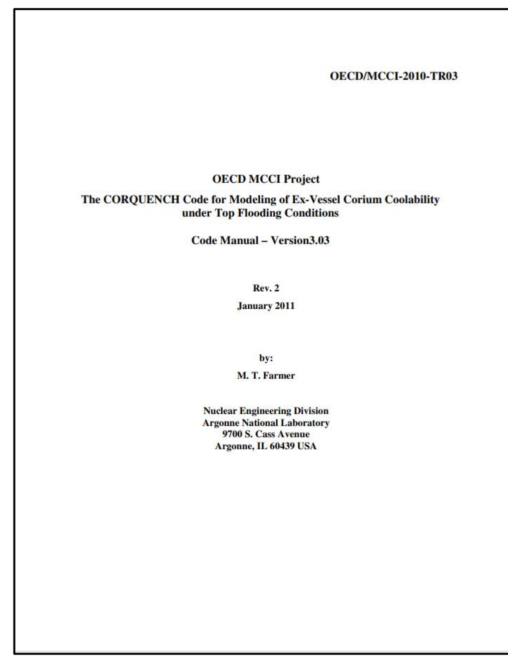
CORium QUENCHing (CORQUENCH)

- In support of Melt Attack and Coolability Experiment (MACE) and OECD/MCCI program
- Developed at Argonne National Laboratory since early 1990's (largely by Farmer)
- Targets integral analysis of heat/mass transfer processes of corium ex-vessel
- First-order analysis of plant accident scenarios
- Latest advancements include modeling related to debris spreading

Overlaps with CORCON-MOD3 for ex-vessel modeling, and uses some similar methods and models to accomplish modeling goals

Differences in important ways from CORCON-MOD3:

- Debris pool conceptualization (e.g. single layer)
- Solution methodology (simultaneous time integration)
- Concrete treatment (more detailed alternatives)
- Methods of predicting/computing the "trouble spots"
  - Incipient growth of crusts and crust dynamics
  - Transitions in heat/mass transfer processes
  - Treatment of certain phenomena (e.g. melt eruption)
- Excludes certain phenomena (RN release and VANESA)



OECD/MCCI-2010-TR03

OECD MCCI Project

The CORQUENCH Code for Modeling of Ex-Vessel Corium Coolability under Top Flooding Conditions

Code Manual – Version3.03

Rev. 2

January 2011

by:

M. T. Farmer

Nuclear Engineering Division
Argonne National Laboratory
9700 S. Cass Avenue
Argonne, IL 60439 USA

CORQUENCH in CAV

CORCON-MOD3 is the current calculational framework for ex-vessel debris in CAV

- Has served well in the past,
- Is difficult to debug and maintain, and very difficult to modify or improve
  - Physics and numerical methods of solution algorithm are intimately entangled
  - Several development efforts from recent years speak to the difficulty
    - Water ingression and melt eruption model development
    - Physics-based debris spreading
    - LHC "simplified CAV" debris modeling approach
- Is limited in its concrete/structural modeling capabilities (quasi-steady ablation only)

CORCON-MOD3 will remain an alternative in CAV moving forward

Incorporate CORQUENCH as a CAV/LHC alternative…why?

- Repository of knowledge gleaned from recent experimental program (Farmer, ANL)
- Different and theoretically more robust debris solution approach
  - Notionally easier debugging/maintenance and development
  - Better performance in severe accident calculations, particularly with wet cavities
- Improved (more detailed) concrete cavity modeling
- Well-documented models & methods consistent with experimental observations
- Translate F77-style CORQUENCH source & incorporate into actively developed code

CORQUENCH in CAV

Existing CAV database (including FM) at least partially applies to CORQUENCH

CORCON-MOD3 "switched off" and CORQUENCH "switched on" by PM

- The main CAV/CORCON-MOD3 run routine itself is subject to PM
- Introduce new physics via PM and select the new CAV/CORQUENCH run routine
- Simple CAV user input record indicates the switch

The CAV/CORQUENCH alternate run-step routine algorithmically (in brief):

- Enter routine during MELCOR time-step, check for cavity "awakening"
- If a cavity "wakes up", do a sequence of initialization calculations:
  - Concrete cavity initializations
  - Miscellaneous variable initializations
  - Debris/melt initializations
- If an awake cavity is continuing on, do normal CORQUENCH time-step integration:
  - Time integration loop - Integration of solution variables & computation of time derivatives
  - Given new "state" of debris, perform a series of checks and updates:
    - Conservation of mass, top crust and heat transfer, bottom and side crusts and heat transfer,
    - Debris/melt thermophysical properties, concrete properties, check bottom/side debris heat transfer
    - Ablation, debris/melt superficial gas velocity, check top debris heat transfer
    - Gas bubble diameter and terminal rise velocity, top crust growth
    - Debris source-in (COR), concrete off-gas and condensed material generation
    - Update overall energy balance and fluxes

Progress Report

CAV & LHC PM done except for new developments related to CORQUENCH

CAV FM in process

- CAV & LHC consolidation sort of simultaneous
- CAV/LHC C++ input parser development sort of simultaneous

CAV/CORQUENCH:

- Alternate CAV run step routine built
- Input structure to select alternate CAV run step routine built
- Studying CORQUENCH
- In process of conducting first-cut very simple MELCOR (CAV/CORQUENCH) to CORQUENCH comparison
  - Quasi-steady ablation, dry cavity, simple common L/CS concrete
  - One debris/melt constituent, same starting conditions
  - Excluding certain physics like debris pool chemistry, RN release, etc.
  - Bring along CAV FM and PM and input parser to extent CAV CORQUENCH requires
- Strategy moving forward is to iteratively build in complexity and benchmark

Summary

Described and reviewed CAV/LHC modernization:

- Modernized C++ input parser
- Field manager and physics manager in general terms
- Field manager and physics manager applied to CAV and LHC
- Ideas to consolidate CAV and LHC

Described ongoing CAV/CORQUENCH development effort

Aspiring to an update with actual MELCOR (CAV/CORQUENCH) vs. CORQUENCH benchmark results by CSARP/MCAP in June