Materials Handbook

- Started for the APT project
- Continued in AAA
- Now accepted as the GenIV handbook

Stuart Maloy (LANL)
Phil Rittenhouse (ORNL, ret)

DECISION APPLICATIONS

Los Alamos

Rev. 4 of the Materials **Handbook** will be ready for distribution in October 2003

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15. Coolants/Fluids
16. 304L SS
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19. **NEW in Rev. 3** Design Properties of Mod 9Cr-1Mo (T91)
20. ***(New in Rev. 4)*** Design Properties of HT-9 and Russian Ferritic-Martensitic Steels
21. ***(New in Rev. 4)*** Design Properties of Tantalum
22. **NEW in Rev. 3** Design Properties of Lead-Bismuth Eutectic

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Recent Handbook Activities

Review and final revisions to Chapter 21 on Tantalum were Completed

- Original draft of the chapter was prepared by Hans Ullmaier of the ESS Project at Forschungszentrum Juelich

Handbook Chapter 18 on HT9 ferritic/martensitic stainless steel was drafted and reviewed

- First complete draft prepared by the Handbook Coordinator
- Based on a first partial draft prepared by Todd Allen on ANL
- Chapter includes selected information on Russian ferritic/martensitic steels of similar composition to HT9.
- Russian steels have higher Si content to provide increased resistance to attack in Pb-Bi eutectic.

Both chapters will be ready for inclusion in Revision 4 on the *Materials Handbook* in the Fall

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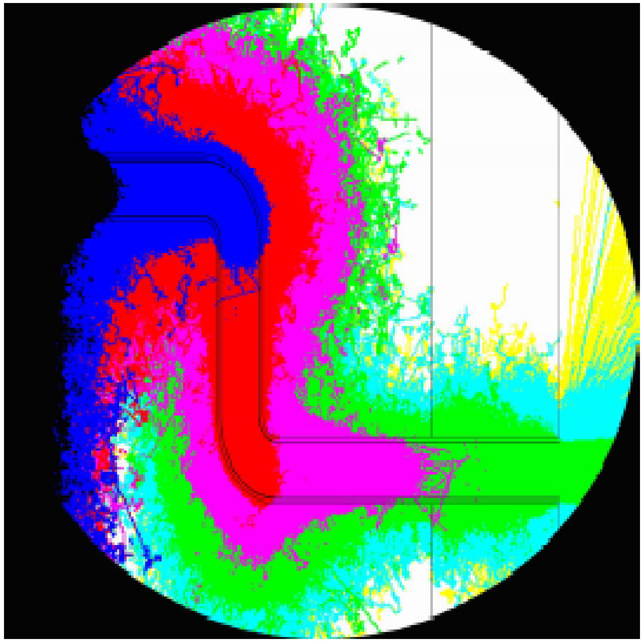
MCNPX Developments



Laurie Waters

High Power Targetry for Future Accelerators

September 11, 2003

MCNPX 2.5.d released August, 2003

John S. Hendricks, Gregg W. McKinney, Laurie S. Waters, Teresa L. Roberts, Harry W. Egdorf, Holly R. Trellue, Joshua P. Finch, Nate Carstens, LANL

Franz X. Gallmeier, ORNL

Jean-Christophe David - CEA-Saclay

William B. Hamilton, HQC Professional Services

Julian Lebenhaft, Paul Scherrer Institute

Sponsors

Eric J. Pitcher, Doublas R. Mayo, Martyn T. Swinhoe,

Stephen J. Tobin, Thomas Prettyman- LANL

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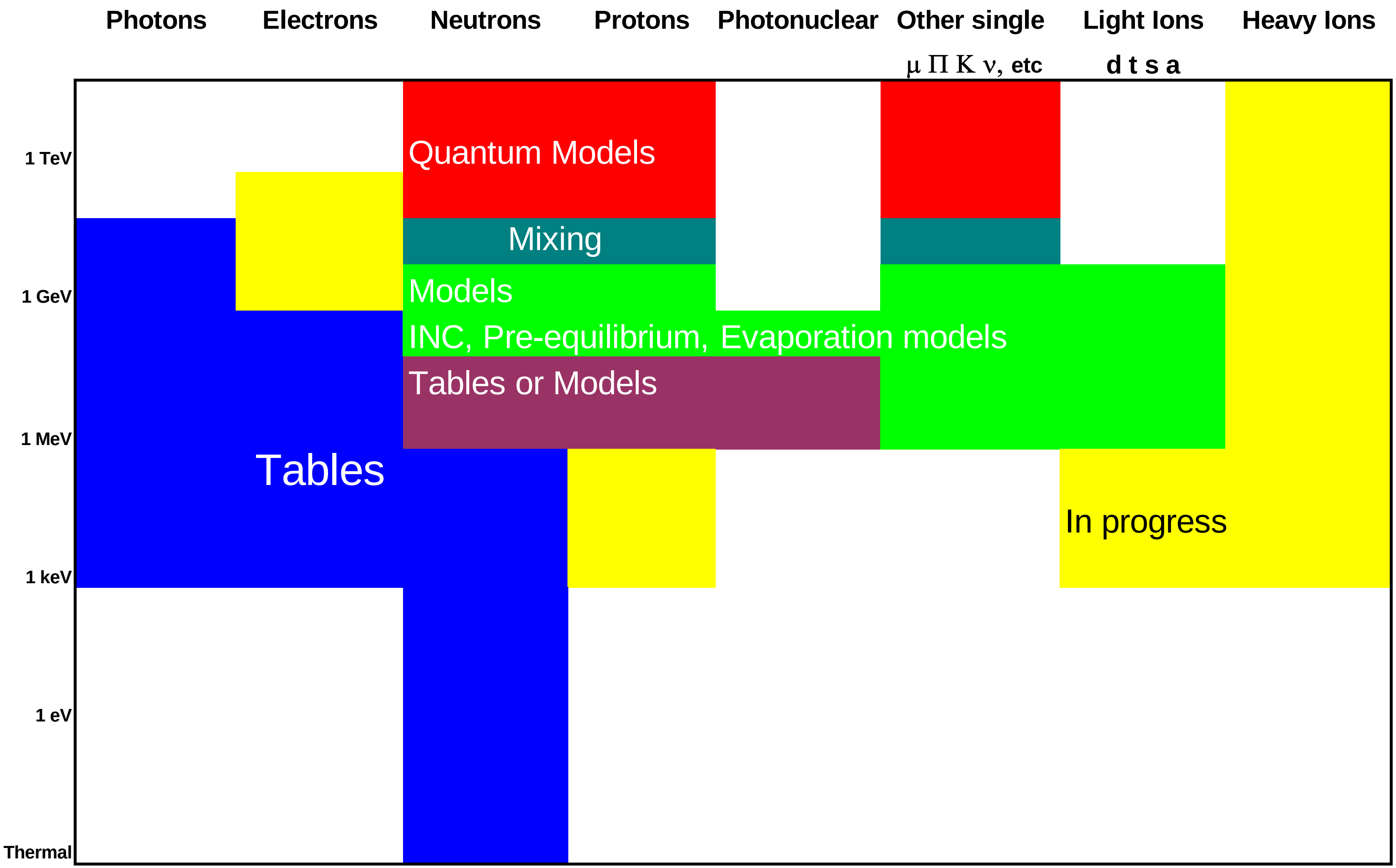
MCNPX Code Acceptance



MCNPX Events During Past Year

- Version 2.5.b released Nov 26, 2002
- Version 2.5.c released Apr 3, 2003
- Version 2.5.d released Aug, 2003
- 1113 beta testers, 250 institutions (28 users in progress)
- 5-day Classes
  - SCK-CEN, 20 students
  - Orlando, 15 students
  - Santa Fe Community College, 23 students
  - MD Anderson Cancer Center, 24 students
  - Santa Fe Community College, 16 students
- 2 summer students,
  - Nate Carstens- MIT (speedup of parallel KCODE Calcs.)
  - Josh Finch- Purdue (new test problems)

Funding

- AFCI
- Mars Odyssey
  - Water on Mars, July 2002 issue of Science, Distinguished Performance Award just announced
- Threat Reduction
  - Groundwork CINDER implementation work for delayed neutrons in active interrogation
  - Maritime cargo container project
  - Nonproliferation/Safeguards - various projects
- Heavy Ions
  - Rare Isotope Accelerator, NASA, AFCI fuels
- Isotope Production Facility

Code Applications as of 8/25/03

• Medical	70 groups	201 people
• Space reactors, cosmics	54 groups	115 people
• Fuel Cycles	50 groups	140 people
• Threat Reduction	47 groups	124 people
• ADS	45 groups	185 people
• Accelerator HP	33 groups	101 people
• Applied Physics*	31 groups	83 people
• Neutron scattering	16 groups	81 people
• Code development	18 groups	28 people
• Physics models, data eval.	9 groups	18 people
• Nuclear, HE, Astrophysics	8 groups	56 people

* Radiography, oil well logging, irradiation facilities, isotope production, detector development, environmental, high density energy storage

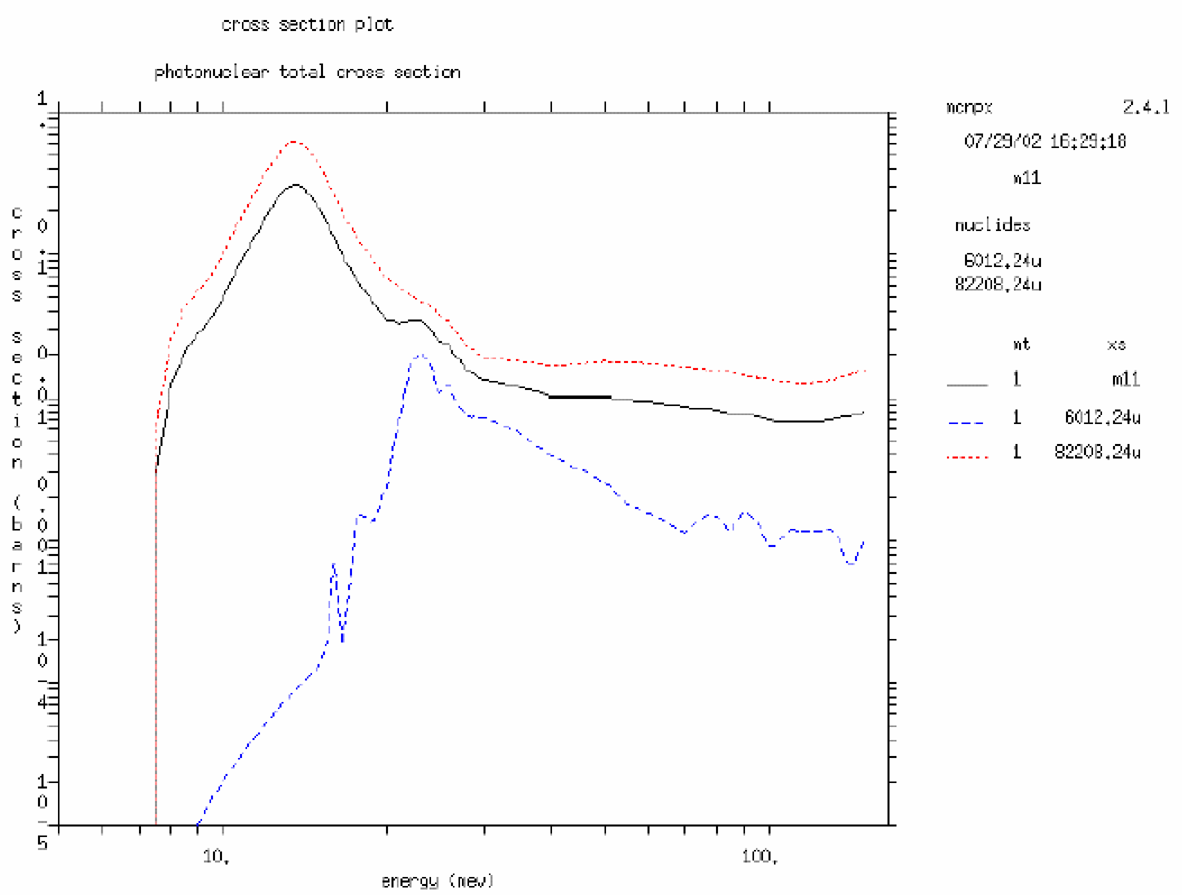
MCNP4C3 Features

- Macrobody geometry
- Superimposed mesh weight windows
- Interactive geometry plotting
- Perturbations
- Unresolved resonances
- Photonuclear reactions
- Delayed neutrons
- ENDF/B-VI physics
- PC enhancements
- ITS3.0 electrons
- Parallelization

MCNPX 2.4.0 RSICC Release - Sept 2002

- F90 modularity and dynamic memory allocation (GWM)
- Distributed memory mulitprocessing for all energies (GWM)
- Repeated structures source path improvement (LLC/JSH)
- Default dose functions (LSW/JSH)
- Light ion recoil (JSH)
- Enhanced color geometry plots (GWM/JSH)
- Photonuclear and proton cross section plots (JSH)
- Photonuclear and proton reaction multipliers with FM cards (JSH)
- Logarithmic interpolation on input cards (10log) (JSH)
- Specify cosine bins in degrees (JSH)
- Cosine bin specification for F2 flux tallies (JSH)
- Pause command for tally and cross-section plots (JSH)

Photonuclear Cross Section Plotting



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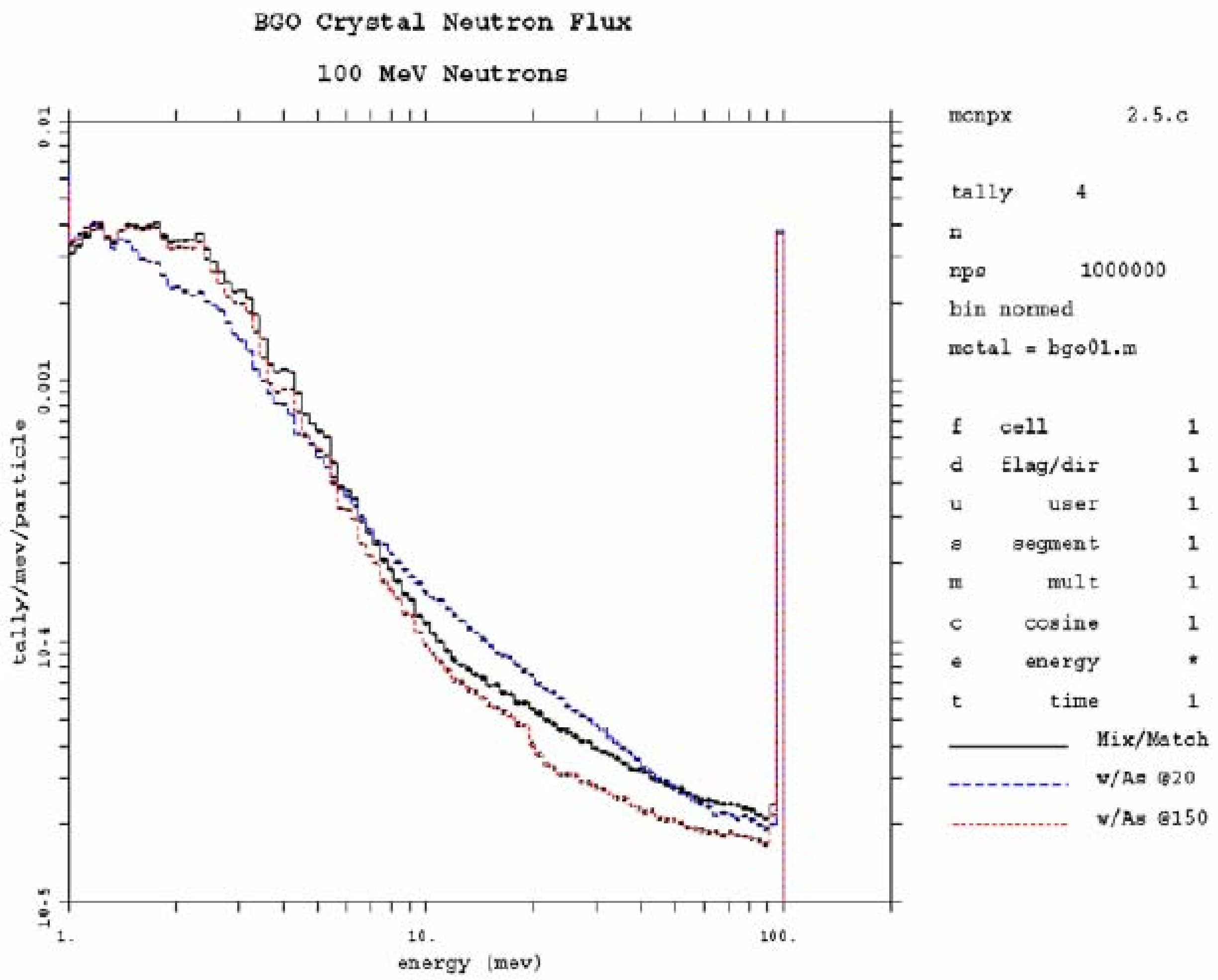
MCNPX 2.5.b Features

- CEM2k physics models (SGM, AJS, FXG,JSH)
- Mix and Match solution (JSH)
  - Isotope Mixing for different particles
  - Energy Matching between libraries and models
- Positrons enabled as source particle on SDEF card (HGH)
- Spontaneous fission (par=sf on SDEF card) (JSH)

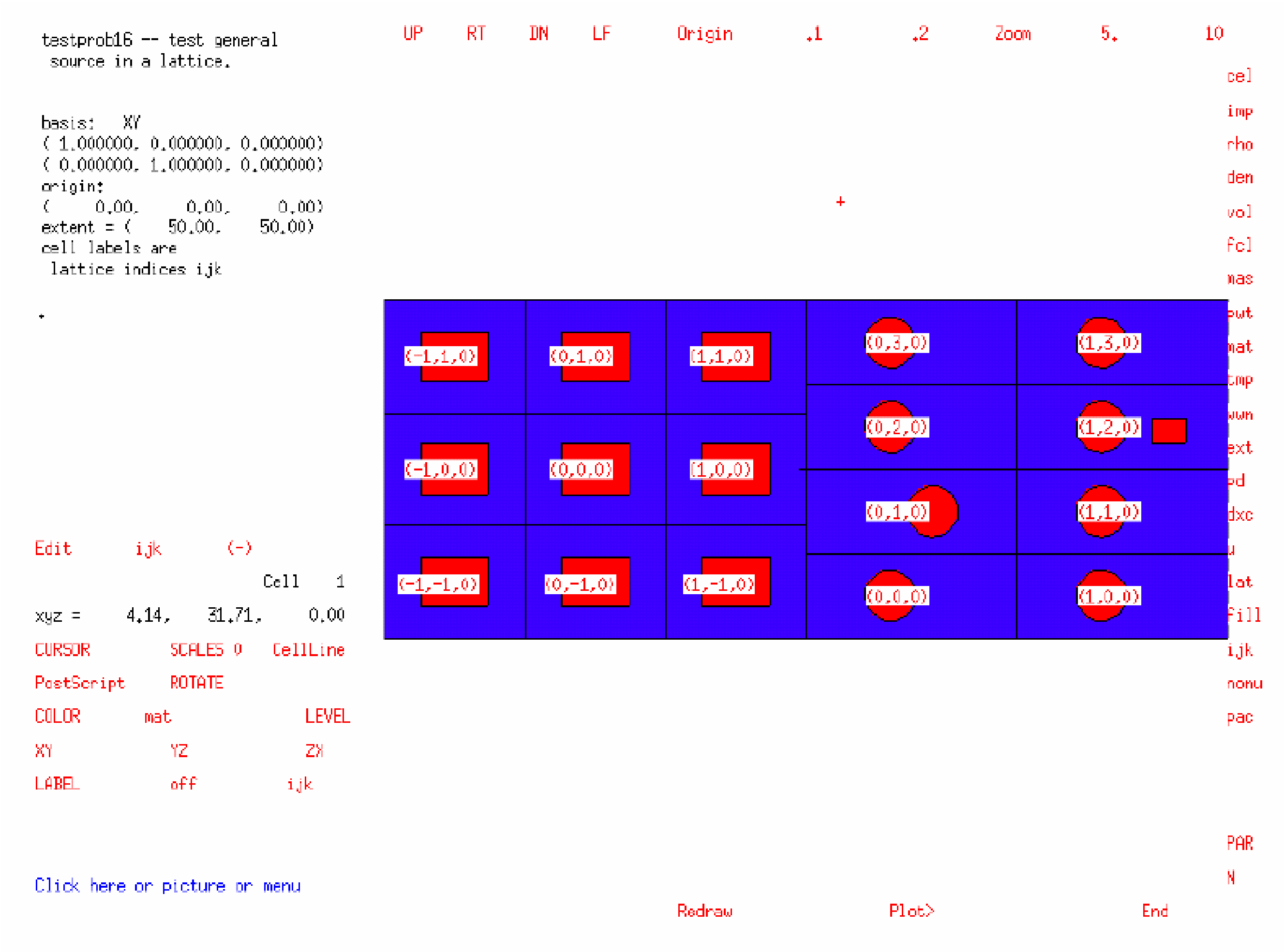
Mix and Match - Energy Matching



MCNPX 2.5.c Features

- MPI Multiprocessing (JL/GWM)
- i,j,k lattice indexing in geometry plots (JSH)
- Enable weight window generator in physics model region (FXG,JSH)
- Enable exponential transform in physics model region (FXG,JSH)
- Extend neutron model physics below 20 MeV (JSH)
- 3-He coincidence detector modeling (HGH/JSH)
- F90 Autoconfiguration (TLR)

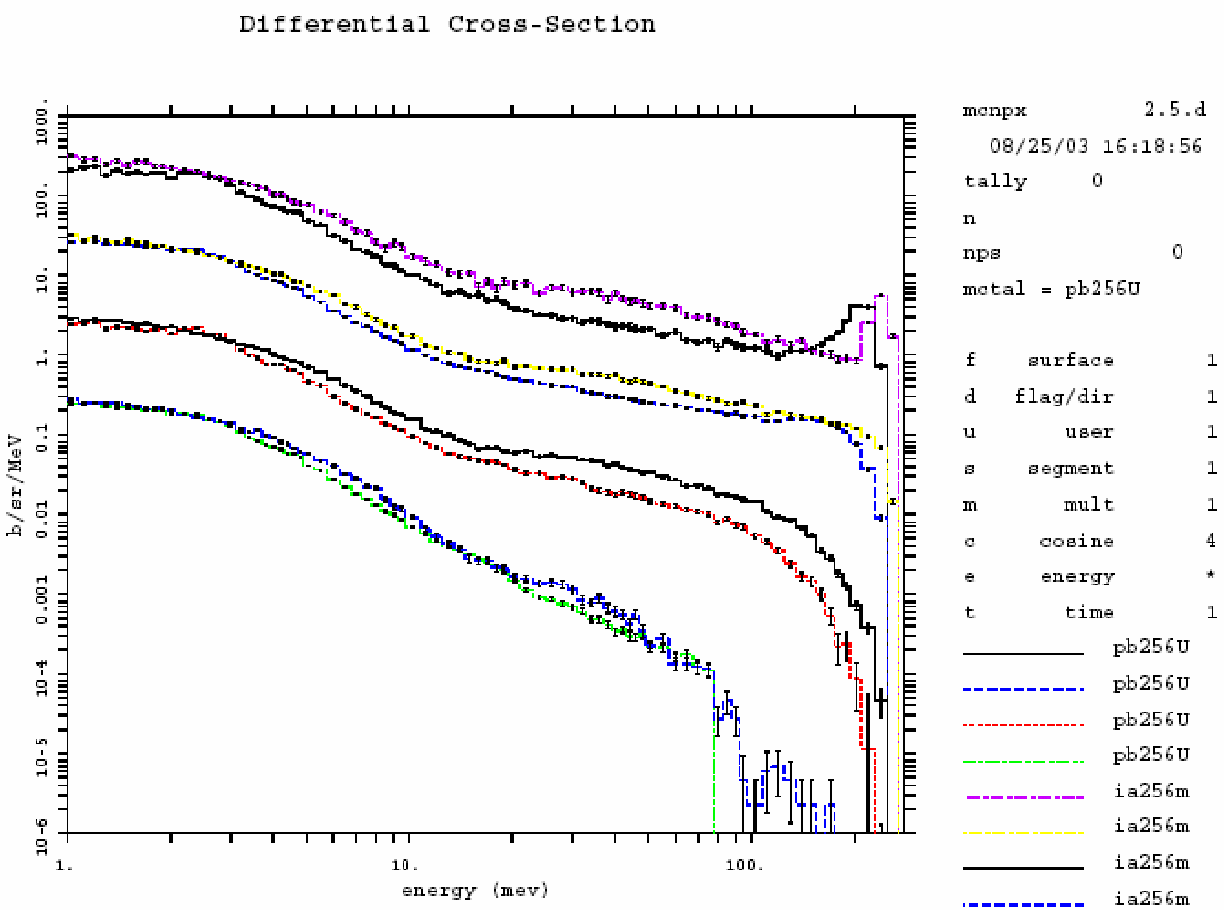
i,j,k Plotting on Lattice Cells



MCNPX 2.5.d Features

- INCL/ALBA physics models (JCD/JSH)
- Lattice tally speedup for rectangular meshes (GWM)
- Multiple particles on SDEF cards (JSH)
  - Can depend on other variables
  - Normalization
- Auxiliary input files, ‘READ’ card (JSH)
- Geometry plot of weight-window-generator superimposed mesh (JSH)
- Pulse-height light tally with anticoincidence, FT8 PHL (GWM)
- Coincidence capture tally and PTRAC file, FT8 CAP (MTS/SJT/DRM/JSH)
- Residual Nuclei Tally, FT8 RES (JSH)
- Inline generation of double differential cross sections and residuals (JSH)

Secondary Particle Plotting



Future Work

- User support and testing
- Error Analysis
  - Completion of perturbation techniques in model region
  - Data covariance analysis
- Criticality
  - Externally driven source
  - Improve stability of eigenfunctions
  - Improve parallel processing for KCODE calculations
- Transmutation
  - Inlining of CINDER’90 for transmutation work
  - Monteburns and Cinder are about to go up on the beta test page
- Variance Reduction
  - Variance reduction for pulse-height tallies
  - Detectors and DXTRAN for all neutral particles at all energy ranges
  - Secondary particle angle biasing for isotropic distributions
  - Next-event-estimators for charged particles

Future Work

- Physics improvements
  - Heavy ion and low energy transport improvements for fuels work
  - Upgrade physics models as they become available, e.g., LAQGSM/CEM, ISABEL
- Miscellaneous code features
  - Plotting of physics model total and absorption cross sections
  - Lattice tally contour plotting
  - Interactive tally and cross section plotting
  - CAD link
  - Integration of HTAPE tallies directly into MCNPX
  - Parabolic beam source
  - Addition of MCNP5 features
- Software Engineering
  - INTEL and 64 bit computer support
  - Improvements in autoconfiguration system
- RSICC Release in December 2003

TRACE Code Development and Applications

High Power Targetry for Future Accelerators

September 11, 2003

By

J. Elson and J. Lin

Nuclear Design and Risk Analysis Group (D-5)

Outline

- TRACE Overview
  - Roles
  - Sponsors
  - History
  - TRACE Modernization
  - Code Characteristics and Capabilities
  - Code Qualification and Software Validation
- TRACE Applications for Accelerator Systems
  - DELTA-Loop Performance Benchmarks
  - LANSCE-1L Test Facility Safety Studies

D-5 Roles

- Transient Reactor Analysis Computational Engine (TRACE) software development
- Software validation
- Software applications
- Consulting and training services

Sponsors

- US Nuclear Regulatory Commission (NRC)
  - Office of Nuclear Reactor Research (RES) - Primary Sponsor
    - Division of Systems Research; Reactor and Plant Systems Branch
  - Office of Nuclear Reactor Regulation (NRR) - Secondary Sponsor

- Knolls Atomic Power Laboratory (KAPL)

DECISION APPLICATIONS

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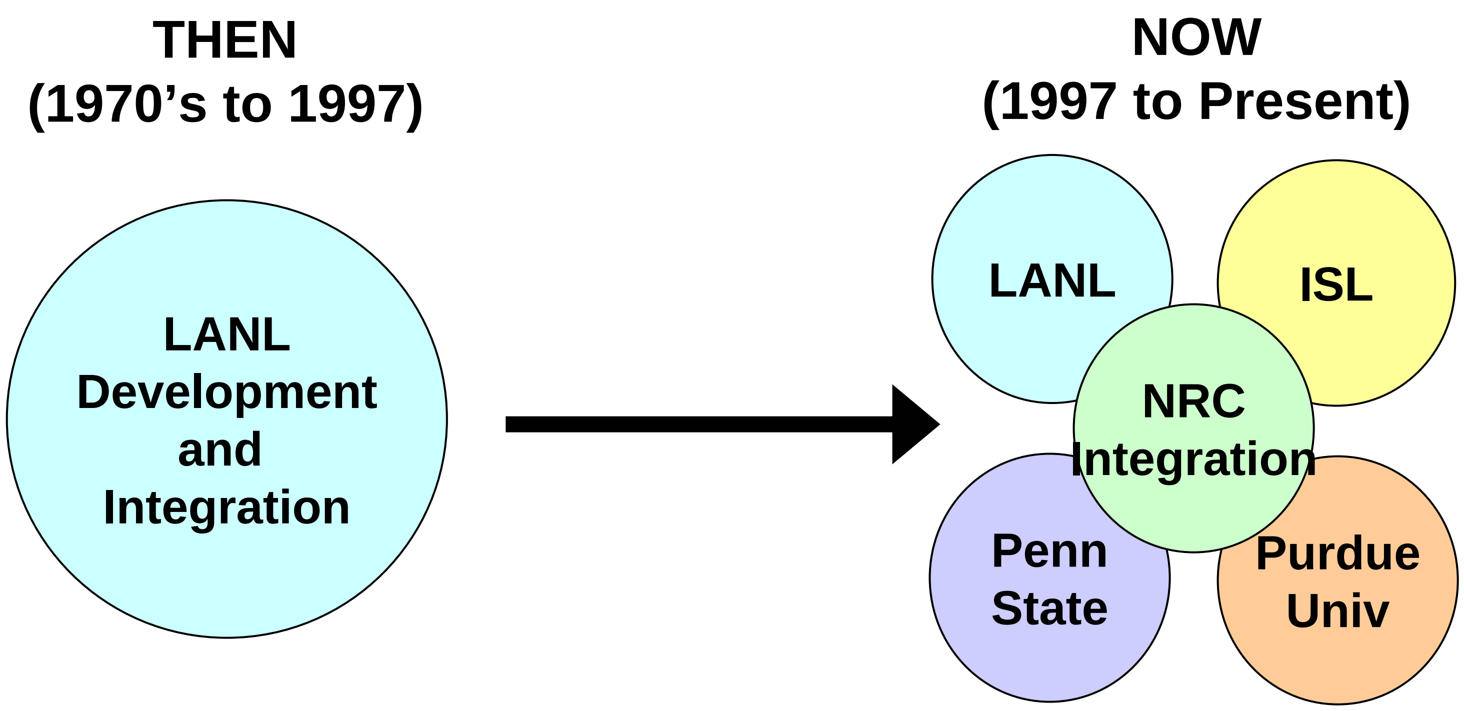
History

- TRACE under continuous development for the U. S. Nuclear Regulatory Commission (NRC) since early 1970
- TRACE continues to evolve with increasing understanding of complex two-phase, multi-component fluid phenomenology
- NRC sponsored multiple codes for 20 years
- NRC has now selected TRACE as the sole platform for future development
- Ambitious multi-institution development program underway

TRACE Development Environment



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TRACE Modernization Effort

- Modernized a legacy code...
  - Updated non-ANSI-standard code to Fortran 95
  - Added new component models
    - Added BWR component models to what was previously a PWR code
    - Added RELAP5 components (e.g., single-junction component)
  - Enhanced numerical solution algorithms
  - Added multi-dimensional kinetics (PARCS code)
  - Added new material properties (Na, He, Pb-Bi, other)
  - Updated the Validation Test Matrix

TRACE Modernization Effort

- Modernized code is highly modular and object-oriented
  - Order of magnitude easier to maintain and modify
    - Liquid metal fluid properties added to TRAC-M and tested within 2 staff-weeks
    - Prior versions of code may have required several staff-months for the same task
  - Enhanced parallelization

TRACE Characteristics and Capabilities

- Modular, object-oriented F95 standard coding
- Generalized two-phase thermal-hydraulic modeling capability (plants & test facilities)
  - Two-fluid model - 6 equation model
  - Multi-dimensional VESSEL component
  - All other components modeled in one dimension
    - Pumps, pipes, valves, etc.
  - Primary, secondary, and containment may be simulated

TRACE Characteristics and Capabilities

- Multiple fluid modeling capability
  - Primary and secondary loops can be modeled with different working fluids
  - Available fluid models include H_2O, D_2O, He, Pb-Bi, Na, N_2, air, oil, and RELAP5 H_2O
- Non-condensable gas model (H_2, air, etc.)
- Trace species tracking capability
  - Track trace gas and/or liquid species
  - Includes solubility models for trace species
- Fluid volumetric heating and fluid decay heat models

TRACE Characteristics and Capabilities

- Single-phase and multi-phase heat transfer models
  - Includes liquid metal heat transfer models
- Multi-dimensional heat structure models
  - Cylindrical, rectangular, and spherical heat structures
  - Multiple materials
- Generalized radiation heat transfer modeling

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TRACE Characteristics and Capabilities

- PWR and BWR capability within the same code version
- Enhanced BWR fuel assembly models
  - Partial length fuel rods
  - Water rods and channels with diameters and geometry different from fuel rods
- Point and multi-dimensional kinetics
  - PARCS code allows for multi-dimensional, transient coupling
  - Point kinetics model also available

TRACE Characteristics and Capabilities

- **Multiple processor capability**
- **External component model**
  - **Allows different parts of a model to run on different processors**
  - **Can be used to couple TRACE to other computer codes or models (e.g. CFD, etc.)**
    - **TRACE coupled to HMS CFD code with one staff-week effort (high-level waste tanks)**

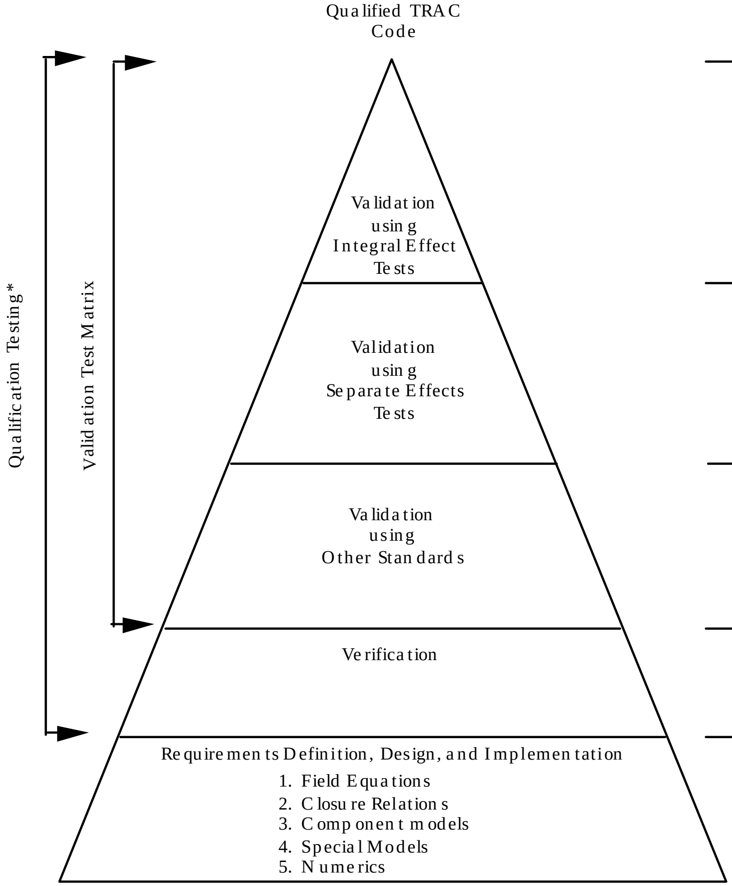
TRACE Characteristics and Capabilities

- Runs on a variety of platforms
- Platform-independent graphics and restart files
- Input can be generated by GUI front-end (SNAP)
  - SNAP takes basic plant geometric and materials data and generates input files for TRACE
  - SNAP can read RELAP5 input decks and generate TRACE input models

Code Qualification and Software Validation

- TRACE code has been validated to ensure that all code features, models, and integrated calculation capabilities are tested
- Large data base of assessments against LWR actual plant data and experiments
  - Separate effects tests, component effects tests, integral effects tests, and other standard tests
- TRACE Validation Test Matrix includes ~1000 test problems
- TRACE adheres to NRC Software Quality Assurance requirements

Code Qualification Overview



Description	Documentation
Integrated Code Behavior • Field Equations • Closure Relations • Component Models • Numerics • Special Models Scenario Applicability Scaling to Plant Conditions	Qualification Test Plan Qualification Test Procedures Qualification Test Report Acceptance Test Plan Acceptance Test Procedures Acceptance Report User Documentation
Focus on Closure Relationships (e.g., Correct Equations Used) Few Phenomena/ Processes Simple Geometry Controlled Boundary Conditions	
Specified Design Features/ Functions Equilibrium Problems Concept Problems Analytical Problems Numerical Method Tests	
Reviews Audits Peer Inspections Informal Tests	Verification and Validation Plan Review and Audit Packages Peer Inspection Packages Informal Test Plans, Procedures, Results
Analyze Requirements Develop Preliminary Design Develop Detailed Design Develop Code Units Inspections Reviews	Requirements Documents Verification and Validation Plan Software Project Plan Software Design Documentation Qualification Test Plan and Procedures Acceptance Test Plan and Procedures

* For additional information see NUREG/ BR-0167, "Software Quality Assurance Program and Guidelines," US NRC (February 1993)

Fig. 2-1. Code Qualification Overview*

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Software Validation

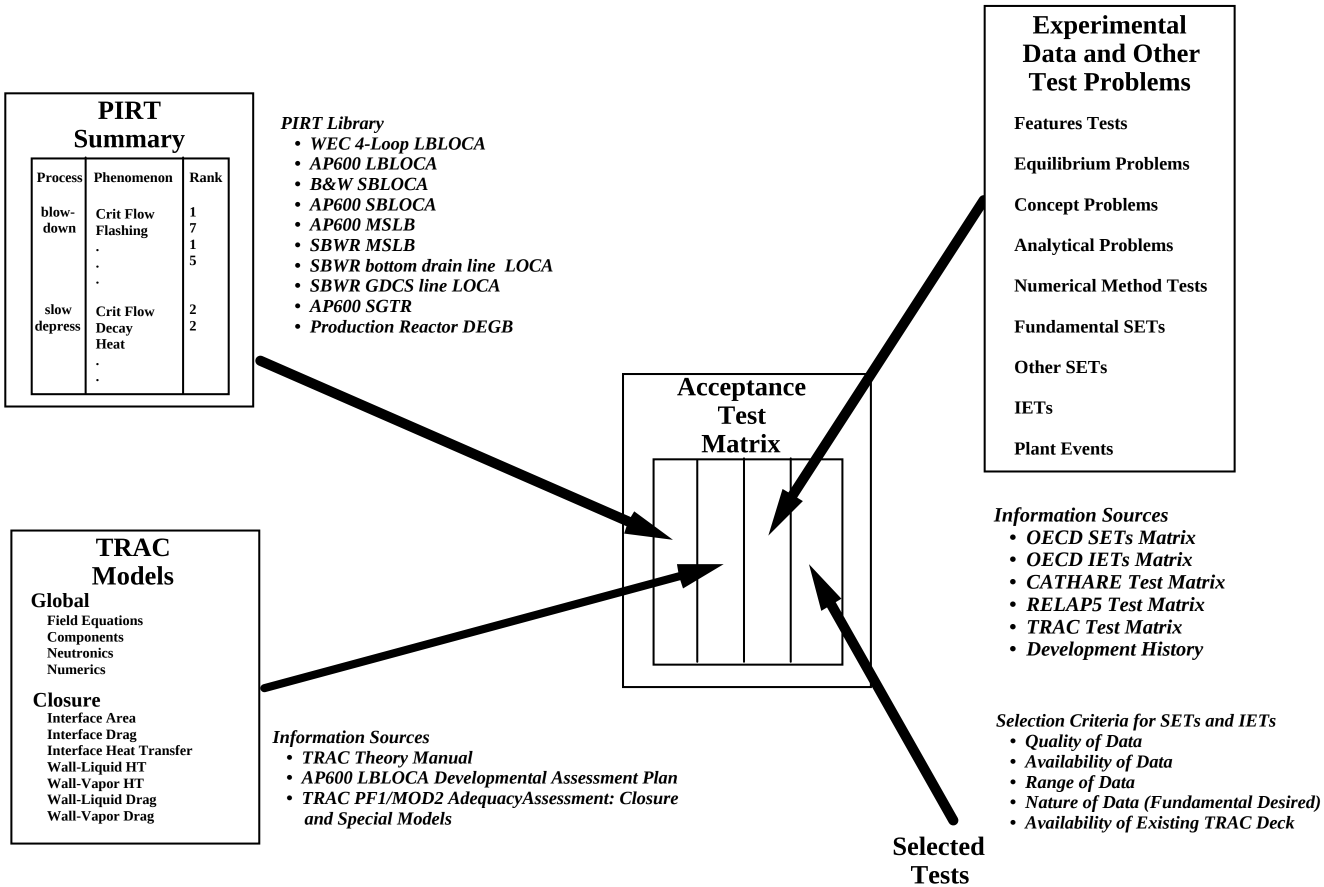
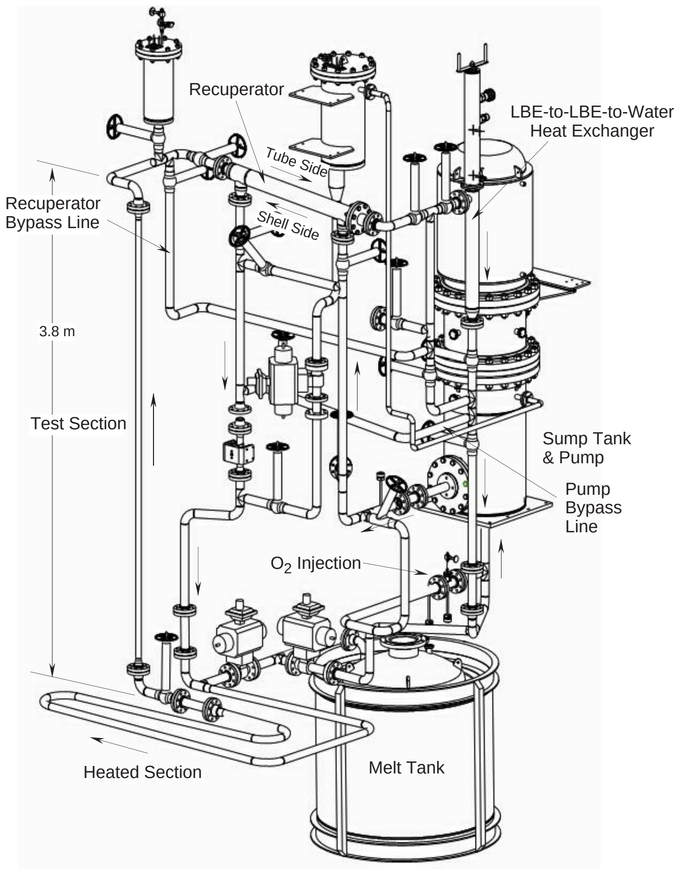


Fig. 2-3. Information sources supporting creation of the Validation Test Matrix.

TRACE Applications

- Analysis applications enhance understanding of key processes
  - Accidents and transients
  - Licensees' calculations (auditing)
  - Test planning
  - Test assessment
  - Design performance
- Applications have included PWRs, BWRs, heavy-water reactors, experimental facilities, and accelerator facilities

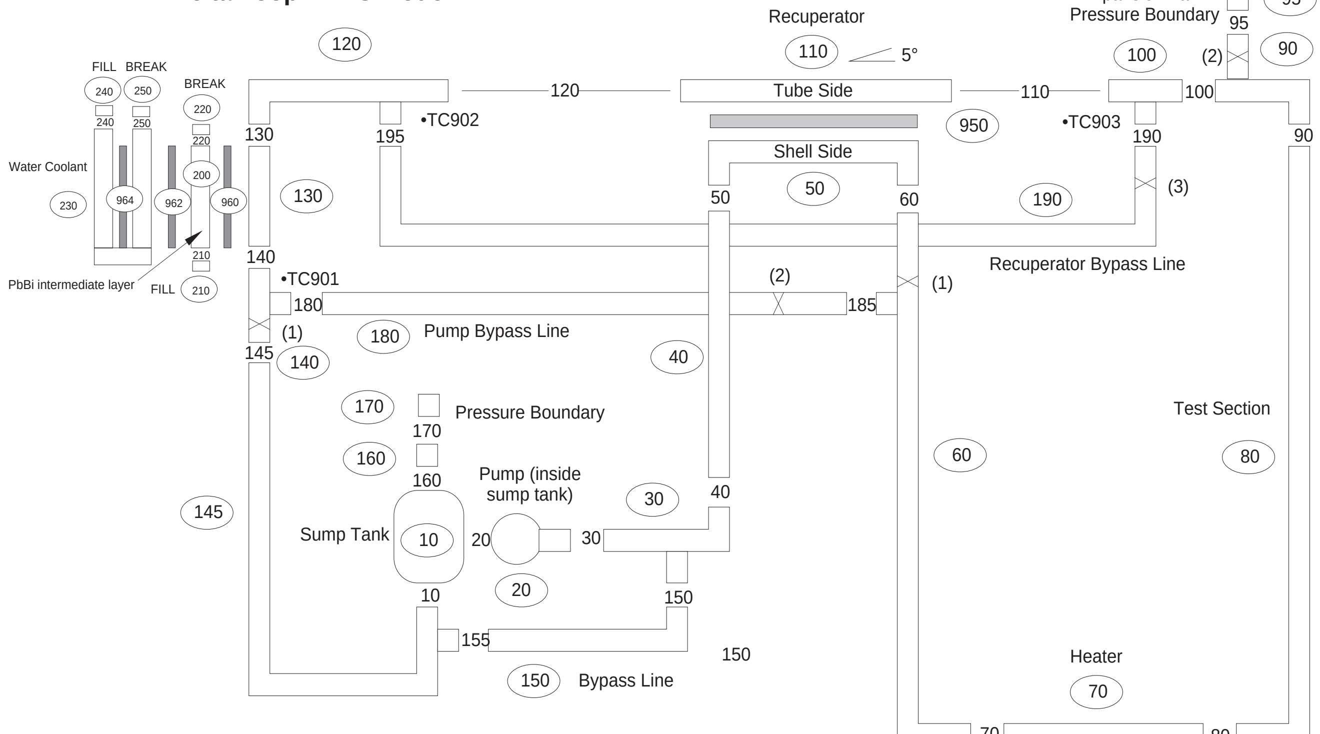
DELTA Loop Facility
(Liquid Lead-Bismuth Materials Test Loop)



- 60kW Heat Input
- 58 gpm pump flow
- Recuperator
- LBE-to-LBE-to-H2O Heat Exchanger
- 2” 316SS Piping
- 1” Piping in Test Section
- Recuperator and Pump Bypass Lines
- Oxygen Control System
- Initial Tests - Late 2001
- 48-h Test - August 2002

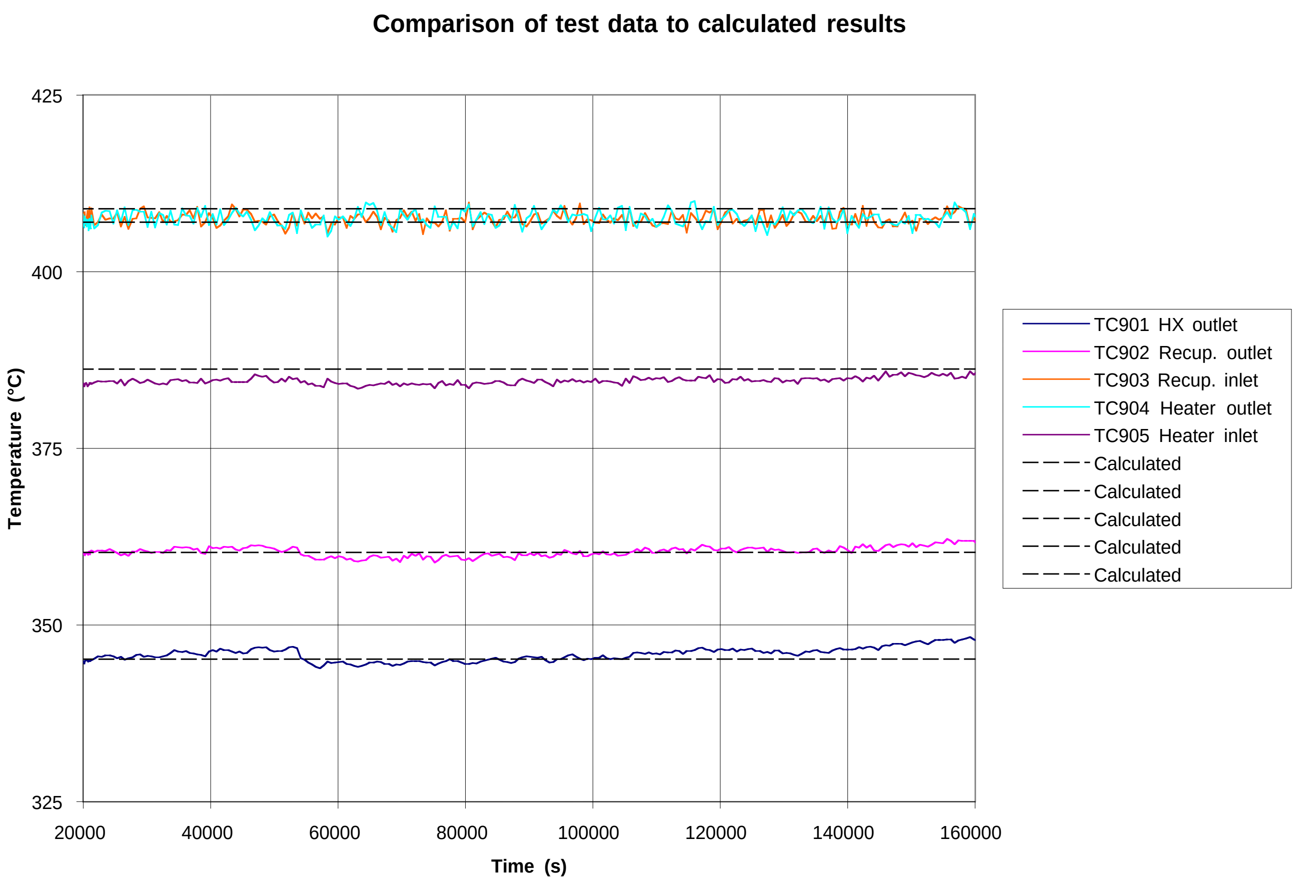
Delta Loop TRACE Model

Delta Loop TRAC Model



Valve positions:
(1) open for normal operation, closed for natural convection operation
(2) closed for normal operation, open for natural convection operation
(3) normally closed for both normal and natural convection operation but
can be opent to bypass recuperator for natural convection operation

48-h Test Data Comparison



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TRACE Applications for the LANSCE-1L Test Facility Safety Study

- **LANSCE-1L test facility primary cooling system design study.**
  - **The main objective is to study the effect of the piping connections among the window, upper target, and lower target on the beam shutdown resulting from melting of the window.**
  - **Three piping layouts were studied.**
    - **Parallel connection outside the crypt (current layout).**
    - **Series connection outside the crypt.**
    - **Series connection inside the crypt.**
- **Loss-of-pump with beam on accident Analysis.**

Risk-Consequence Policy for LANL

	Likelihood				
Severity	**Frequent** usual occurrence to likely occurrence, reasonably expected	**Probable** likely occurrence to irregular occurrence, infrequent	**Occasional** irregular occurrence, infrequent to slight chance of occurrence	**Improbable** slight chance of occurrence to highly unlikely occurrence	**Remote** highly unlikely occurrence to extremely unlikely occurrence
Catastrophic: death, severe injury/ occupational illness, severe environmental harm or liability, or severe property damage	High	High	High	Medium	Low
Critical major injury/ chronic impairment or occupational illness, major environmental harm or liability, or major property damage	High	High	Medium	Low	Minimal
Moderate minor injury/ temporary impairment or occupational illness, minor environmental harm or liability, or minor property damage	High	Medium	Low	Minimal	Minimal
Negligible less than minor injury or occupational illness, less than minor environmental harm or liability, or less than minor property damage	Low	Minimal	Minimal	Minimal	Minimal

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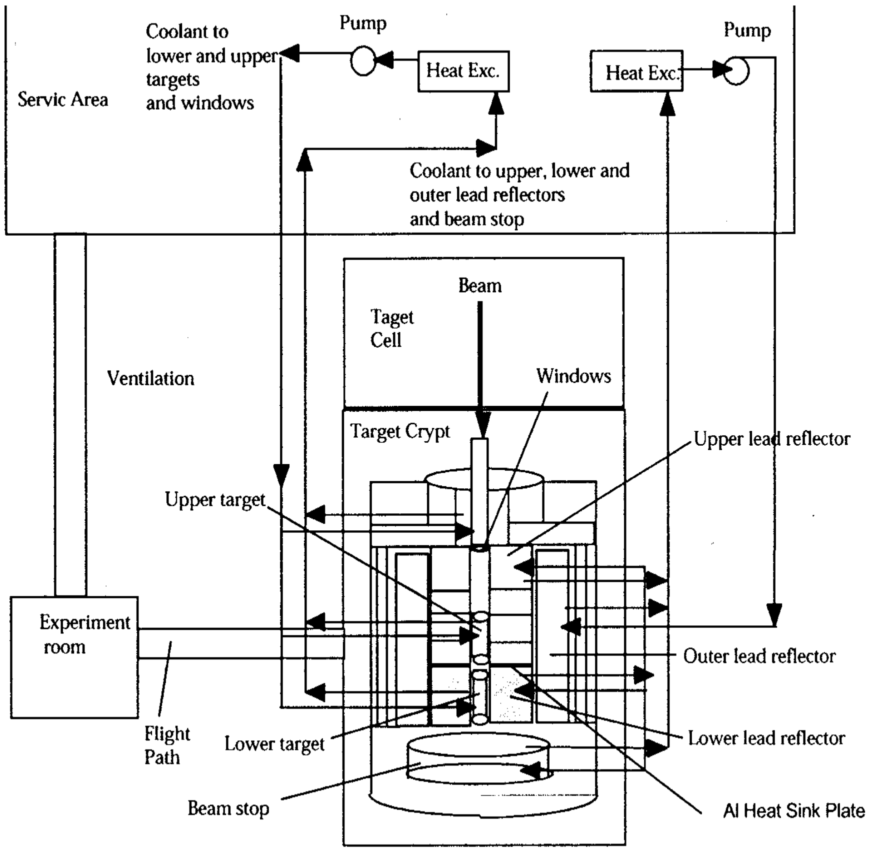
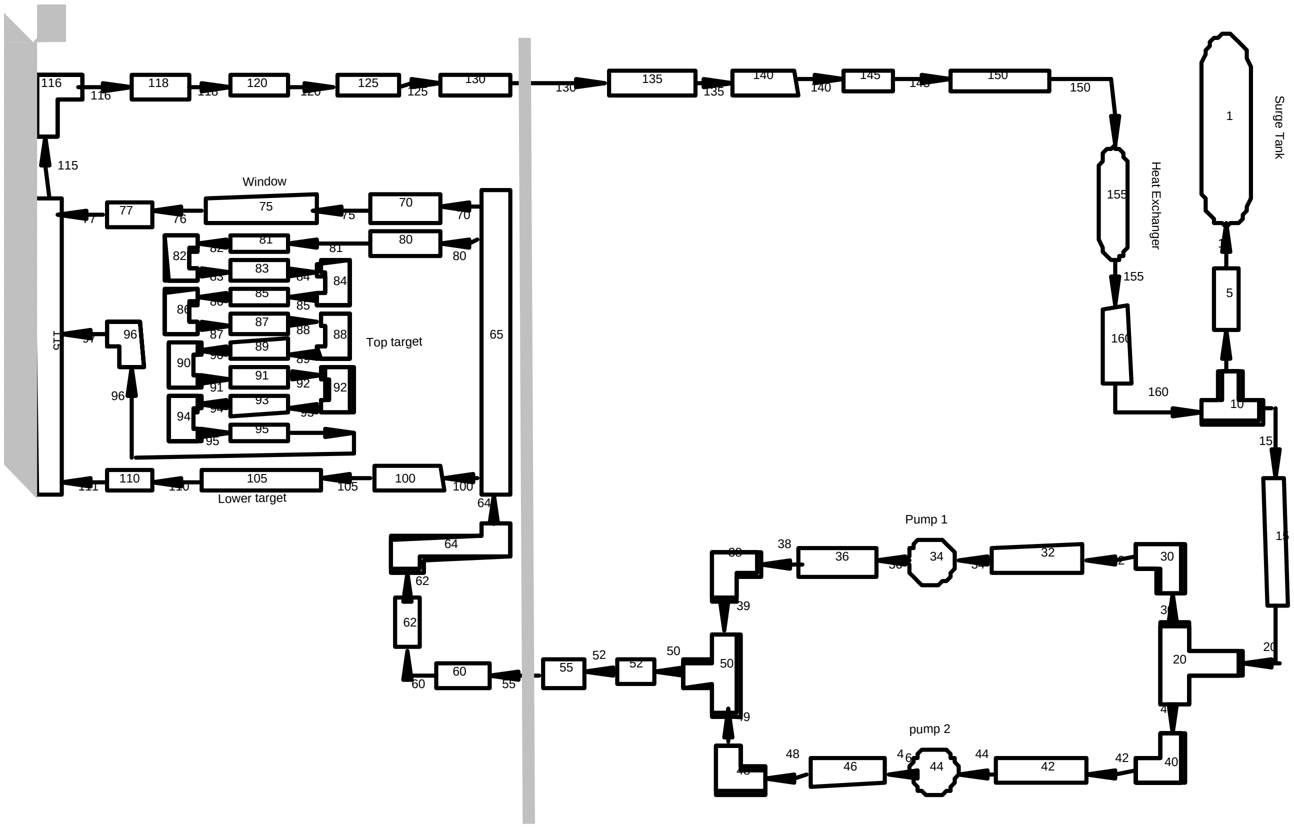
Target Cooling System Sketch



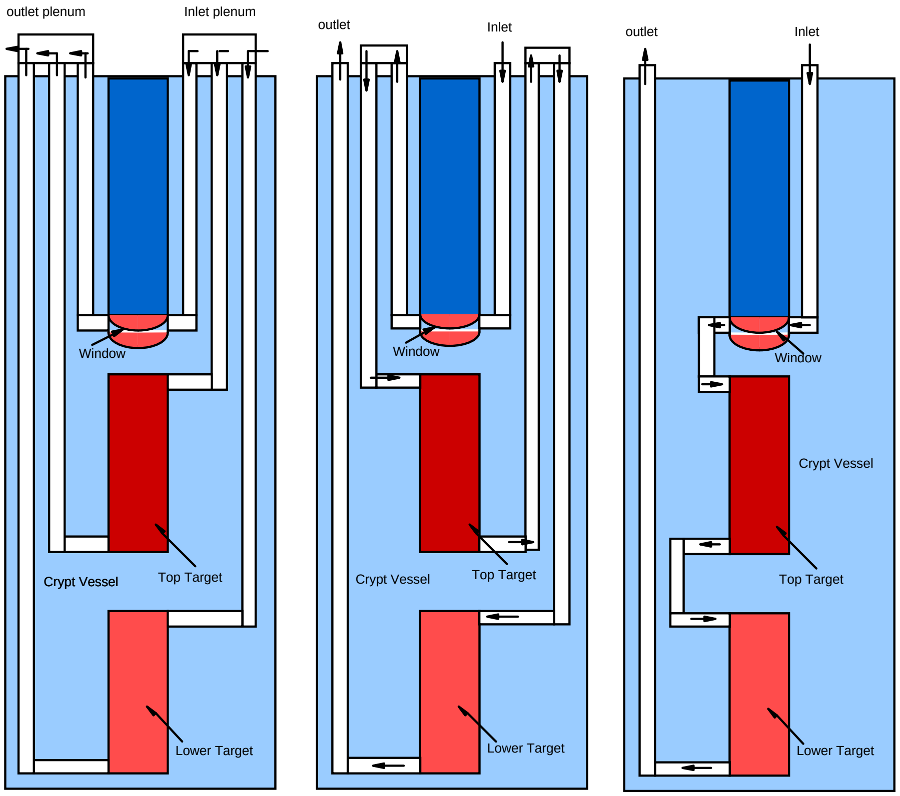
LANSCE-1L Test Facility Layout

- LANSCE 1L-area target crypt consists of an upper target, a lower target, two windows, a lower reflector, an upper reflector, outer reflectors, beam stop, and hydrogen moderator.
- The lower and upper targets and the window are cooled by a closed loop cooling system.
- The lower and upper reflectors and the beam stop are cooled by a separate closed loop cooling system.

TRACE Model for the Target Cooling System



Three Piping Layouts in the Crypt



Parallel Connection outside the crypt vessel

Series Connection outside the crypt vessel

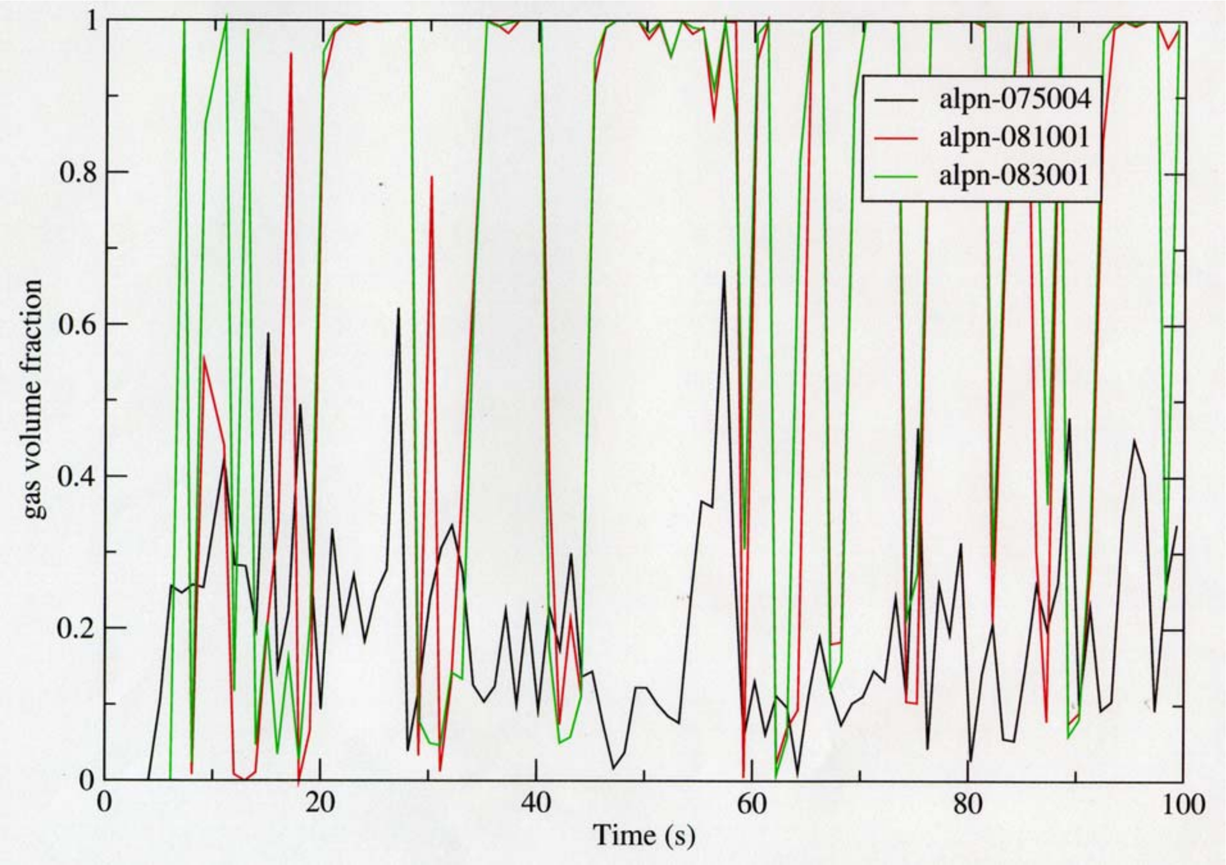
Series connection inside the crypt vessel

TRACE Results

- For a loss-of-pump accident, the TRACE results show that the window will remain cool even with the beam on throughout the transient.
- Window performance is independent of the piping layouts in the crypt. The idea of passively shutting down the beam based on melting the window will not work.
- The flow channel of the window never dries out and the gas volume fraction oscillates about 0.2.
- The window is heated to about 490 K but the upper target is heated to 3200 K at 100 s.

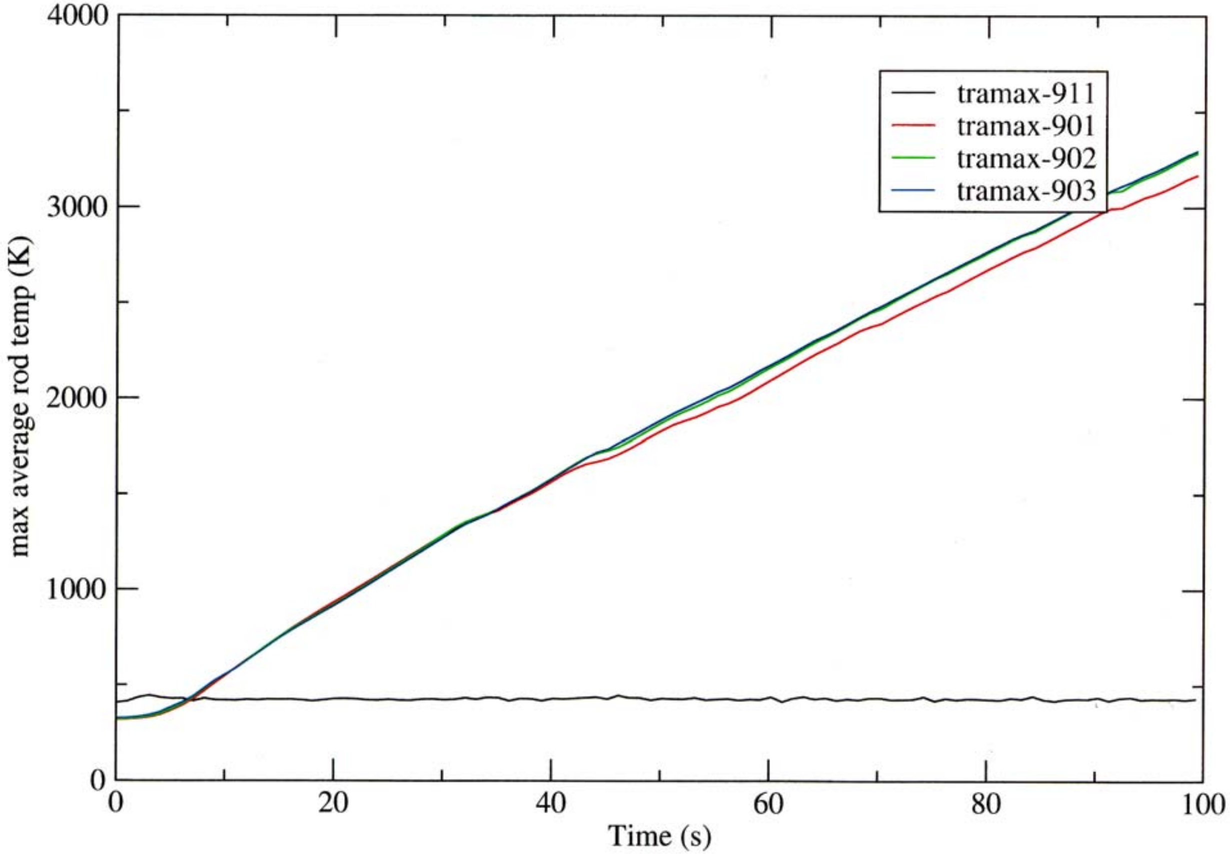
TRACE Results

Gas Volume Fraction (alpn-075004: window, alpn-081001 and alpn-083001: top-two-flow channels of the upper target)



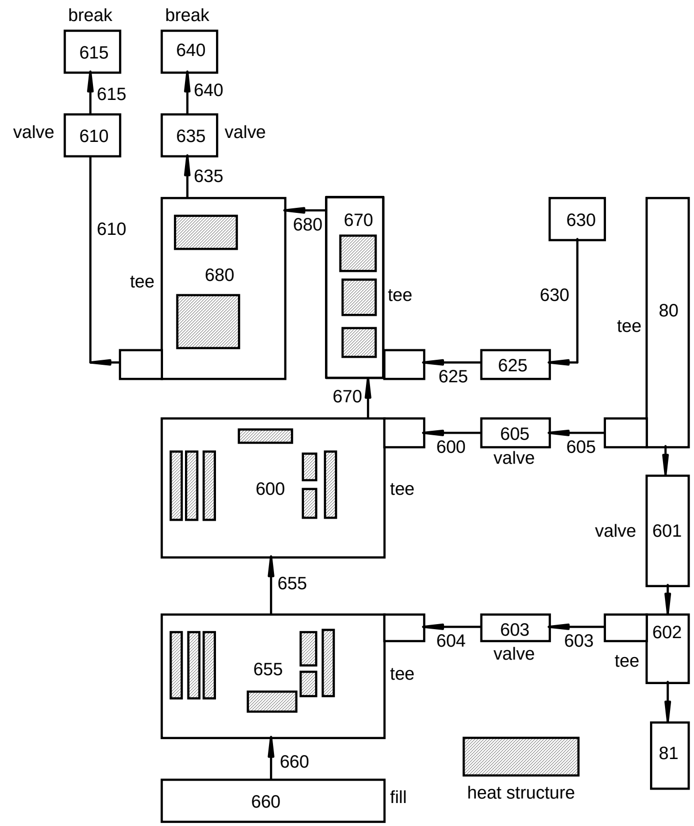
TRACE Results

Maximum average rod temperature (tramax-911: window, tramax-901, tramax-902 and tramax-903: target-top-three plates)



Loss-of-Pump Accident with Beam On Analysis

TRACE Crypt Model:



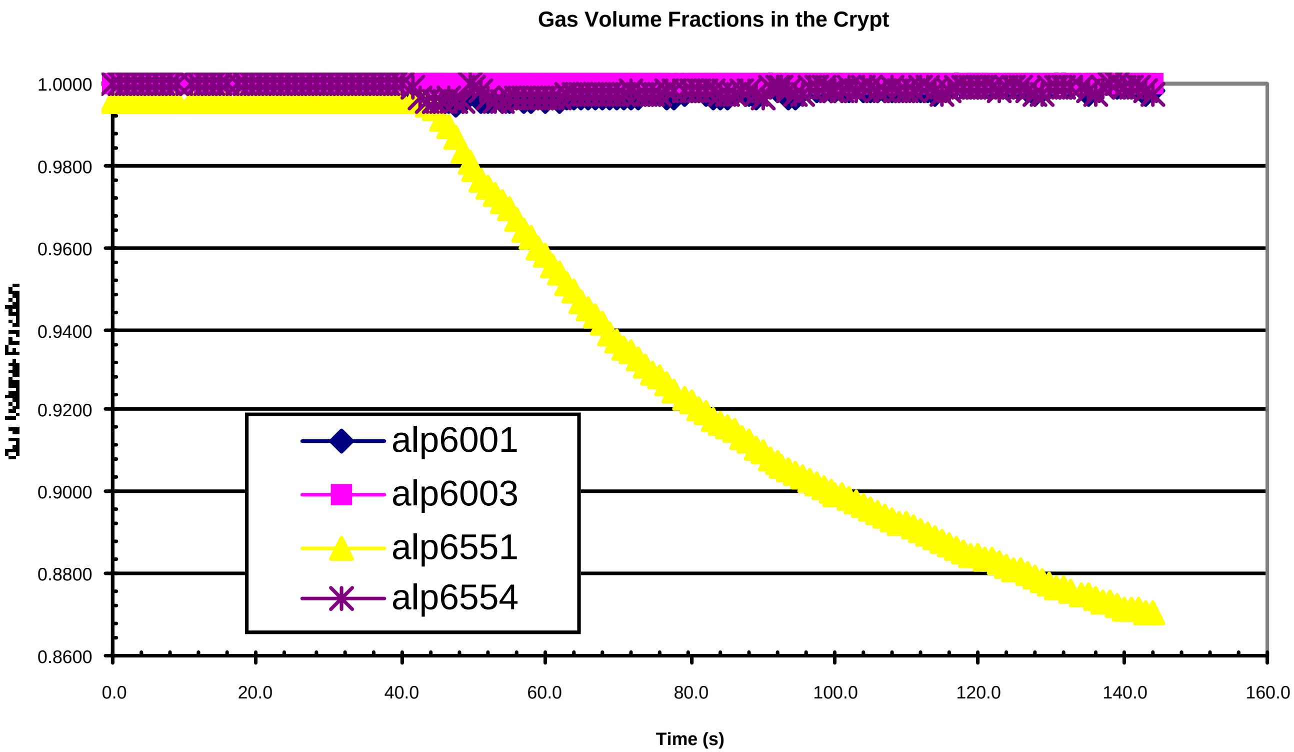
*The overall TRACE model consists of the system model shown previously, and the crypt model shown here.

TRACE Results

- The upper target canister reaches the melting temperature (1500 K) at about 41s.
- The cooling system is completely drained at about 140 s
- After the cooling system is completely drained, the target would be cooled by radiation to the cool outside reflectors.
- A TRACE radiation model was developed and the preliminary results show that the upper target reaches about 3200 K at about 300 s and keeps at that temperature throughout the transient.

TRACE Results

Gas volume fractions in the crypt (alp6551: bottom, alp6554: middle, alp6001 and alp6003: top-two levels)



TRACE Results

Surface temperatures (rft812: lumped upper steel plate, rft901: upper target, rft910: lower target)