Multiphysics Simulation Of 2nd Generation
\(^{238}\text{Pu}\) Production Designs Using COMSOL®

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COMSOL
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Outline

- Background and Objective
- Target Holder Flow Validation
  - Purpose, Flow Regions, Results
- Experiment Safety Analysis
  - Eccentric Flow
  - Thermal-Structural
  - Accident Transients
- Summary and Future Work
Background and Objective

The $^{238}$Pu Supply Project at the High Flux Isotope Reactor

- $^{238}$Pu is the fuel source for RTGs that power NASA deep space missions
- This presentation discusses the safety analyses required for irradiation of production targets at the High Flux Isotope Reactor (HFIR) at ORNL
- Target Qualification at the HFIR: Four phase test program complete
  - Post-irradiation examination (PIE) results from each phase serve as a hold point for the following irradiations
- PIE Characteristics:
  - pellet dimensional changes
  - fission gas release %
  - heat generation rates
  - pellet clad interaction
  - $^{236}$Pu production
  - product yields
Background and Objective
Experiment Qualification at the High Flux Isotope Reactor

• Target qualification at HFIR requires a safety review that assures target cooling in off-normal and nominal reactor operating conditions

• Target cooling is maintained such that:
  - No material melting: $T_{\text{max}} < T_{\text{melt}}$
  - No surface burnout: $T_{\text{surf-max}} < T_{\text{saturation}}$
  - Clad stress/strains below yield: $\sigma_{\text{clad}} < \sigma_{\text{yield}}$, $\varepsilon_{\text{clad}} < \varepsilon_{\text{break}}$
  - Target axial forces on welds: $F_{\text{axial}} < F_{\text{target-failure}}$

• Off-normal safety review includes the following cases:
  - Steady-State Analysis in COMSOL
    • 50% reduced flow
    • 130% overpower $\leftarrow$ Bounding safety condition
  - Transient Analysis (now) in COMSOL:
    • Small break LOCA $\leftarrow$ Bounding safety condition
    • Loss of offsite power (LOOP)
Background and Objective  
Overview of COMSOL Models

- Five models include physics interfaces of computational flow dynamics (CFD), heat transfer, solid mechanics, and pipe flow
- Additional equations for flow coupling operators, gap/contact conductance, fission gas release, irradiation-driven dimensional changes
- Two thermal hydraulic models (CFD & Heat Transfer)
  - Full Target Holder used for Flow Validation
  - Eccentric Geometry for asymmetric flow positions
  - Address steady-state surface burnout
- Two thermal-structural models (Solid Mechanics & H.T)
  - 2-D R-Z model of entire target pin
  - 3-D model of limiting pellet and adjacent clad
  - Address steady-state melting and structural integrity
- Transient model (Non-Isothermal Pipe Flow & H.T.)
  - Address accident transient surface burnout
Target Holder Flow Validation Model

Flow Impact of New 2nd Generation Target Holder

- Compute the 3-D Flow Distributions in 2nd Generation Target Holder
  - Import CAD geometry and use COMSOL features to simplify flow paths (see target holder, right)
  - Slice geometry to take advantage of holder symmetry
  - Address asymmetric flow channels (see right)
  - Multiple flow rate cases to compare to conducted flow test measurements (see table below)
  - Cases to optimize existing design drawings for orifice flow control and connecting slot size/location

<table>
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<th>Model</th>
<th>Case</th>
<th>Description</th>
<th>Flows (gpm)</th>
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<td>Flow Test Geometry</td>
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Inlet Region: From top plenum to just before connecting slot
Outlet Region: Exit orifices to bottom plenum
Target Region: From upper to lower connecting slots (or upper to lower welds on targets).
Target Holder Flow Validation Model

**Inlet Flow Region**

- **Inlet Flow Region**
  - 1/6\textsuperscript{th} slice geometry
  - Central target inlet restricted
  - ~10 psi drop
  - Side inlets to periphery

- **Finned Flow Region**
  - 1/6\textsuperscript{th} slice geometry
  - Connecting slot size/location chosen to allow sufficient flow to central target
  - Asymmetric flow in periphery channel

- **Outlet Flow Region**
  - 1/3\textsuperscript{rd} slice in outlet region
  - End cap geometry on test vs. design requires reduced orifice diameter

\[ \text{X-Y Flow area at top end caps (right)} \]

\[ \text{Flow Velocity Streamlines (bottom right)} \]
Target Holder Flow Validation Model

**Finned Target Flow Region**

- **Inlet Flow Region**
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- **Outlet Flow Region**
  - 1/3rd slice in outlet region
  - End cap geometry on test vs. design requires reduced orifice diameter

*X-Y Flow area at finned region (right)*

*Streamline velocities at connecting slot (bottom)*

*Velocity Profile (bottom right)*
Target Holder Flow Validation Model

Outlet Flow Region

- **Inlet Flow Region**
  - 1/6th slice geometry
  - Central target inlet restricted
- **Finned Flow Region**
  - 1/6th slice geometry
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X-Y Outlet Flow Velocity & Paths (right)

**Flow Velocity Streamlines (bottom right) for flow test and design**

- **Around Cup**
- **Bottom Cup Flow**
- **Side Exit Flow**
- **Closed Flow Path**
- **Open Flow Paths**

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Oak Ridge National Laboratory
High Flux Isotope Reactor
Spallation Neutron Source
Target Holder Flow Validation Model

Validation Results

• Comparison to Flow Test Results
  – Flow test measured pressures and holder flow
  – Model results compare well against the experiment results
  – Flow degradation in central target for reduced connecting slot size confirmed

• Design-Study
  – Assessed effect of connecting slot size and locations
  – Assessed increased flow for updated design
  – Prescribed orifice diameter for desired design flow

**Flow degradation in central channel (top right)**

**Pressure drop vs. flow comparison (bottom right) for flow test and models**
Experiment Safety Analysis

Thermal-Hydraulic Models

- Thermal hydraulic analysis
  - Non-isothermal flow multiphysics coupling of turbulent flow and heat transfer interfaces
  - Solved for k-ε and k-Ω turbulence models
  - 1.3 – 4.4 million mesh

- Full target holder
  - Solved at EOC-1 and EOC-3 for nominal and 50% flow conditions at 100% power

- Eccentric model
  - Fully revolved finned region, extrusion coupling operators used to transpose boundary flow conditions
  - Four eccentric flow positions analyzed for central and “hot pin” or pin 1 peripheral target at 130% overpower conditions
  - Limiting steady-state burnout results identified at pin 1 eccentric flow position shown on right

Temperature (top) and velocity (bottom) profiles for nominal (left) and eccentric (right) flow position cases.
Experiment Safety Analysis
Thermal-Structural Models

- Two thermal-structural models developed
  - 2-D R-Z representation of entire target pin
  - 3-D of limiting pellet and adjacent clad (to incorporate asymmetric flow)
  - Address steady-state overpower melting and structural integrity limits

- 2-D R-Z Target Pin
  - Simulations ran at EOC-1, 2, and 3 for pins 1 and 7
  - Pin 1 is limiting, where burnup-driven swelling/densification drives temperature maxima and stress

- 3-D Pellet/Clad
  - Pin 1 symmetric convective cooling inputs used as function of azimuthal angle
  - Small decrease in safety margin from 2-D R-Z reference
  - 1-2 million DOF

Pellet Stack Temperature Profiles
Asymmetric convective cooling (left) and 3-D pellet temperature profile (right)
Experiment Safety Analysis

Transient Analysis

• Uses non-isothermal pipe flow (1-D target holder flow paths) and heat transfer in solids (3-D target cladding)

• Coupled using general extrusion operators and antiderivative approximation

\[ F(x) = \int_{a}^{x} u(x')dx' = \int_{a}^{b} u(x') \ast [x' \leq dest(x)]dx' \]

• Accident transients include SBLOCA and LOOP (see right, top and bottom, respectively)

• Use plant model time-dependent boundary conditions

• SBLOCA, Pin 1 is more limiting, compares well to previous analysis in 1-D thermal hydraulics code RELAP5

Transient results of SBLOCA (top) and LOOP (bottom) accidents for surface burnout.
Simulation Models of 2\textsuperscript{nd} Generation Target
Summary and Future Work

• Conclusions
  – Five high fidelity models developed spanning four COMSOL physics modules
  – Good comparison of COMSOL CFD simulations to experiment flow tests
  – Characterization of 3-D CFD allowed asymmetric flow channels
  – Utilized pipe flow module and new use of coupling operators
  – Target cooling and structural integrity maintained for steady-state and transient conditions

• Future COMSOL work in the $^{238}$Pu Project
  – Assess conservatisms in safety analysis models and utilize further to:
    • Increase neptunium loading
    • Allow reduced target holder flow (for flow diversion)
  – Thermal-structural analysis of permanent beryllium (by M. Crowell)
    • Assess optimized permanent beryllium design for $^{238}$Pu production
    • Investigate end-of-life flow degradation
The High Flux Isotope Reactor is located on the Oak Ridge National Laboratory campus.

The High Flux Isotope Reactor is a US DOE Office of Science User Facility.

HFIR Activities:
- Cold and thermal neutron scattering
- Isotope production
- Materials irradiation
- Neutron activation analysis
- Gamma irradiation
- Neutrino research

Thank you!

Questions?