WANDA Session Summary: Predictive Codes for Isotope Production

Session Co-Chairs: *Susan Hogle (ORNL), Ellen O'Brien (LANL), Andrew Voyles (LBNL)*

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The DOE Isotope Program Perspective on Nuclear Data

Dr. Ethan Balkin: DOE Program Manager for Isotope R&D

- The DOE Isotope Program has, and will continue to have **significant nuclear data needs** requiring investment in its R&D portfolio.
  - The need for reliable evaluated nuclear data is true across all user communities, but isotope production is not limited to neutron-induced reactions.
  - This is underpinned by the need for **accurate** predictive codes.
- The DOE IP is funding ongoing measurements for high energy protons and neutrons, photonuclear reactions, and low energy reaction pathways.
- **Pathways exist for programs to partner with us to accelerate and/or add scope to our ongoing activities.**

The Predictive Power of TALYS

Nuclear Data Section, IAEA: Arjan Koning

- Applications for fundamental nuclear physics research and produced nuclear data for applications.
  - Streamline to input all important nuclear (reaction) physics into one code scheme.
  - Projectiles: neutron, photon, proton, deuteron, triton, Helium-3, alpha particle.
  - Targets: Z= 3-124, A=5-339.
  - Incident energy: 1 meV - 1 GeV.
- **Needs:**
  - Efficient access to **all** experimental data is essential. A curated & evaluated selection of this data is also needed in order to establish quality.
  - Multiple pre-equilibrium and level density models are what we need to tune to improve predictive power. We need a nuclide-by-nuclide TALYS parameter adjustment
    - Quality experimental data for this adjustment is ***essential.***

EMPIRE-3.2: Nuclear Reaction Code System

LANL: Mike Herman

- Application Space:
  - Incident energies up to ~150 MeV with projectiles: n, p, d, t, ^{3}He, ^{4}He, γ, and Heavy Ions (HI).
  - Provides: reaction cross sections, residual production cross sections, angular distributions, spectra (incl. PFNS), angle-energy distributions of reaction products.
  - Predictive power is ~30% globally.
- Needs:
  - Level densities
    - Collective enhancements at higher energies (unexplored)
    - D_0 off of stability line
    - Spin distributions
  - Multiple pre-equilibrium emission for > ~30 MeV
  - Reliable theoretical models for going off of the stability line or experimental data to calibrate phenomenological input parameters.

ALICE 2021

Marshall Blann & M.Maiti, Dept. of Physics, Indian Institute of Technology

- ALICE is a Monte Carlo code using the Weisskopf-Ewing evaporation and GDH precompound decay models.
- Required inputs - mass and charge of target and projectile, and projectile energies.
- **Needs:**
  - Benchmarking of the NLD models near shell closure would be valuable in making recommendations for best choices versus shell proximity and help predictive power. Would also show regions where more data is needed.
  - Do code outputs from new models have improvement in shape and position for peak yields or are they just a reproduction error in experiments?
    - Recommend that recent codes based on the Hauser-Feshbach formulation be used both for the better physics of HF, and because these codes are currently maintained.

CoH_3: The Coupled-Channels and Hauser-Feshbach Code

LANL, Theoretical Division: Toshihiko Kawano

- Statistical Model Code for Compound Nuclear Reactions
  - A main tool for calculating nuclear reactions for A > 20, E > 1 keV (above resolved resonance region).
  - Provides complete information of nuclear reactions: reaction cross sections and energy and angular distributions of secondary particles.
- **Needs:**
  - Pre-equilibrium reaction
    - Exciton model works when phenomenological parameters are well-tuned, but crude approximations are always involved.
    - New development of quantum mechanical models ongoing and have capability for large improvement.
  - Nuclear level densities
    - Most important physical quantity for predicting unknown IP cross sections, and could have largest uncertainties in high energy reactions.
    - Experimental data of nuclide production in the vicinity of target reactions is essential.

Predicting Isotopes with FLUKA

INFN: Alfredo Ferrari

- FLUKA is a general purpose tool for calculations of particle transport and interactions with matter.
- Code can compute excitation functions, can work from thermal energies to very high energies.
- Built-in capability for evolution and buildup of induced activity. Fully coupled build-up and decay, up to 5 different decay channels per isotope.
- **Needs:**
  - Experimental Nuclear Data: low energy neutron transport, charged particle reactions nuclear reactions, inventory evolution, and dose rate predictions – all impossible without reliable nuclear data.
  - Nuclear Structure Data: populating near drip lines so mass, levels, spin, parity, and decay data for these exotic isotopes are important.

Recent and Future Improvements to MCNP6 for Isotope Production Applications

LANL, Monte Carlo Codes, XCP-3: Michael E. Rising

- MCNP6 is the LANL general purpose, continuous-energy Monte Carlo radiation transport code.
- Activation/Depletion: code coupling efforts
  - MCNP + CINDER, MONTEBURNS, MCNP + ORIGEN, MCNP + FISPACT
- Future Improvements:
  - Event record – histp (history file) – deprecate in favor of PTRAC-based capability.
  - Collision Physics
    - Proton data and model physics
  - Production/Depletion
    - Make CINDER (activation/depletion code) a callable library for use in coupled calculation.

Recent and Future Improvements to MCNP6 for Isotope Production Applications

LANL, Monte Carlo Codes, XCP-3: Michael E. Rising

- **Future Work/Needs:**
  - Ongoing method developments
    - Code improvements relevant to charged-particle transport.
    - Data and model physics updates as necessary.
  - Method verification (comparisons to analytic results)
    - Charged-particle/condensed history algorithm verification.
    - Production/depletion method verification.
  - Validation
    - Need benchmark experiments and models that integrate collision physics data and models, residual nuclide calculations, and production/depletion.
  - Make CINDER a callable library - can be coupled to other codes.

Isotope Production Calculations Using FISPIN

UK National Nuclear Laboratory: Beth Slingsby

- FISPIN is a standard code used in the UK over the last 60 years to calculate the composition and evolution of irradiated nuclear fuel and related waste streams.
  - FISPIN11, has been in development for approximately 4 years and was a complete rewrite of the FISPIN solution method to include nuclear reaction data for accelerators.
  - Key assumptions –thin targets, neutron only sources
  - Methodology for handling accelerator based neutron energy spectrum
- **Needs:**
  - Models are no longer limited by computational capabilities, but by the uncertainties in nuclear data – quality of underpinning nuclear data is essential.
    - Decay data
    - Neutron transmutation cross-sections

HFIRCON: A Neutronics Toolkit for HFIR Multi-Cycle Depletion Analyses

ORNL: Charles Daily

- Toolkit to automate many HFIR irradiation calculations
  - Materials testing, isotope production, target and/or core design.
  - Multi-cycle neutronics/depletion analysis toolkit.
  - Couples enhanced MCNP5 to ORIGEN with ADVANTAG variance reduction.
  - Transport uses ENDF/B-VII.0 and ENDF/B-VII.1 cross sections supplemented with gamma production data from JEFF3.1.2, JENDL4.0u, CENDL3.1, and TENDL-2013.
  - Depletion uses SCALE-ORIGEN data.
- **Needs:**
  - Reaction cross sections for isotope production campaigns and ORIGEN depletion.
    - Full evaluation with scattering and secondary particle production not needed for ORIGEN.
  - Gamma production data (GPD)
    - Local heat generation rates can be off significantly.

LISE^{++}

FRIB/MSU: Oleg Tarasov

- Predicts intensities and purities of rare isotope beams for the planning of future experiments with in-flight separators.
  - Essential for tuning of rare isotope beams where results can be quickly compared to on-line data.
- Applicable to low, medium, and high-energy facilities (fragment- and recoil-separators with electrostatic and/or magnetic selection).
- Reliance on databases for ionization energies, experimental production cross sections (exotic nuclei are important), compound materials, and fission barriers.
- **Needs:**
  - Atomic masses, isomeric states database, fission barriers, production cross sections, and fragment momentum distributions.
  - Detailed information is needed for excitation energy of fissile nuclei after abrasion.

Recommendations

Nuclear Level Densities

1. Targeted campaigns to obtained level density information for compound nuclei of interest to the isotope production community.
    - Combination of partnering with astrophysics groups that already do level density measurements or more directly encouraging these measurements.
    - With established detector array and analysis code, process involves approximately 1 week of continuous beam time to probe 20 – 30 MeV wide region of level density.

Level densities will globally improve predictive capabilities for all residual products coming out of that compound nucleus.

Residual Production Data & Evaluation

1. Residual production cross section data – needed for all reaction channels on target materials of interest.
   - Currently funded to collect proton-, photon-, and high energy neutron-induced cross section data for targets of interest to DOE IP. It is recommended that this be expanded to heavy ions as well.
   - Data for co-production of stable nuclides is also needed - this is equally valuable for improving predictive capabilities.
   - Selection of which cross sections need to be measured should be guided by both isotope production needs, and an informed and guided connection between experimentalists and theorists.

2. A concerted effort is needed to evaluate existing and future experimental nuclear data in order to generate an evaluated database or input into an existing database structure.
   - Recommendation: add a charged-particle evaluation subcommittee to CSWEG in order to keep this as a sustained focus.

Benchmarking & Validation

1. Validation of measured nuclear data against code predictions.

2. Need benchmark experiments and models that integrate collision physics data and models, residual nuclide calculations, and production/depletion.
   - Representative geometries are essential.

3. Validation of charged-particle stopping powers is vital for coupling reaction physics to transport and multiphysics codes