NEAMS Modeling and Simulation
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HTGR Existing/Legacy Tools and Gaps
Hans Gougar (INL)
Co-NTD – Advanced Reactor Technologies
General Picture of HTGR Analysis Tools

- **Physics and basic design and plant analysis approaches & physics** – were developed along with the 1st Generation HTGR technology developed in the US and Germany (70s-80s). Need to be validated and re-qualified.

- **Large safety margins** – afforded by the coated particle fuel, large thermal inertia of the graphite, and inert helium coolant allow large uncertainties in analysis results.

- **HTGR-dedicated codes and model development ceased** (more or less) after 1990 but general advances in neutron transport, CFD, etc. have been applied successfully.

- **New HTGR tools** – are slowly under development but are not ready for production work.

- **High fidelity multiphysics models** are not generally sought for design and safety analysis (licensing) but are useful for component design, investigation of complex or localized phenomena, reference solutions.

**Fort St. Vrain**
Benchmarks, Criticals, Engineering Demos

• **HTTR (Japan, 1998-)**
  – 30 MWt Engineering demo (prismatic), IAEA CRP-5 (TECDOC), OECD HTTR LOFC Project (on hold until restart) - Will be coupled to a gas turbine and hydrogen plant

• **HTR-10 (China, 2000-)**
  – 10 MWt Engineering demo (pebble bed), IAEA CRP-5

• **Critical Experiments**
  – ASTRA and VHTRC (CRP-5)
  – HTR Proteus (PSI)

• **Code-to Code Benchmarks** –
  – PBMR400 Coupled Code Benchmark (OECD TECDOC)
  – MHTGR Couple Code Benchmark (OECD – just finishing up)
  – CRP on Uncertainty Analysis in HTRs (IAEA in progress)

• **Some relevant experiments for which data is available**
  – SANA (pebble bed heat transfer)
  – NACOK – oxidation of graphite
  – TRISO Fuel benchmark (CRP-6), GIF VHTR Fuels PMB
  – HTTF (Oregon State) – Depressurized LOF – undergoing shakedown
  – NSTF (ANL) – Ex-core vessel heat removal
  – Fort St. Vrain?
  – GIF VHTR CMVB - HTR-PM startup and testing facilities?
• **Proof of Concept** – demonstrated ability to capture important physics; acceptable performance on analytical benchmarks and simplified ‘real-world’ models; minimal or no customer support.

• **Engineering Scale** – validated against experimental benchmarks; plausible results for more complex (‘real world’) applications; coherent user interface with some error checking; R&D level QA and configuration management; minimal customer support; nominal licensing requirements specified by BEA/DOE but otherwise freely distributed.

• **Production Scale** – acceptable performance against data from benchmarks and operational data; full documentation (Theory/Programmer/User Manuals); Formal customer support and software maintenance; Licensing options for different types of users
Modeling Areas

- Fuel Performance/Fission Product Transport within Fuel Matrix
- Neutronics & Depletion, Shielding
- Core Thermal-Fluidics at Power, System and Safety Analysis
- Chemistry/Corrosion, Source Term (outside of Fuel Matrix)
- Mechanical/Structural Analysis, PRA

Particles

Compacts

Fuel Elements

Prismatic Modular Reactor

Pebble Bed Reactor

Pyrolytic Carbon
Silicon Carbide
Uranium Oxycarbide Kernel

Coated Particle

Pebble
Fuel Performance/FP Transport

**PARFUME**

- **Technical Readiness:** Proof of Concept
- **Functionality:** Simulates the thermo-mechanical behavior of TRISO fuel particles and surrounding prismatic or pebble graphite fuel elements using steady-state and transient heat transfer. Computes TRISO particle failure probabilities given user-input geometry, fluence, temperature, and burnup histories. Evaluates fission product transport and release from TRISO particles and fuel elements based on temperature.
- **Validation Basis:** IAEA CRP6 benchmark (German, US, Japanese tests) . AGR PIE data. UO₂ and UCO TRISO fuel irradiation and safety tests through IAEA and GIF benchmarks.
- **Computational Requirements:** PC/Workstation (FORTRAN-77)
- **Gaps:** UCO applicability is limited by lack of data on UCO kernel properties; material properties not characterized at high fluence.
- **Owner Contact Info/Support Level/Availability:** INL (Blaise.Collin@inl.gov); minimal support; requests for software considered on an individual basis
- **Remarks:** The particle failure model is largely empirical and includes a 1-D stress analysis. 3-D effects are captured using correction factors generated separately with a 3-D stress analysis code (ABAQUS). Fission product releases are generally over-predicted given the lack of high quality data on particle layer diffusion coefficients.
- **Others:** PANAMA-FRESCO(FZ-Jülich), XFP-(X-Energy), ATLAS(Areva), BISON(INL)
Core Neutronics & Depletion - prismatic

**PHISICS**

- **Technical Readiness:** Proof of Concept
- **Functionality:** Computes the time-dependent flux and power distribution in the core. Depletes and shuffles fuel elements.
- **Validation Basis:** ??
- **Computational Requirements:** PC/Workstation (FORTRAN-90), HPC Cluster
- **Gaps:** Somewhat limited ability to treat localized absorbers
- **Owner Contact Info/Support Level/Availability:** INL (Cristian.Rabiti@inl.gov); minimal support; requests for software considered on an individual basis
- **Remarks:** User-specified $P_n$ nodal transport (INSTANT). Coupled to RELAP5-D for thermal-fluid analysis. Rod-following under development. Experimental SPH treatment under development. Diffusion codes may work if the cross sections are properly prepared using a lattice code that captures all layers of heterogeneity including spectral penetration between blocks. Monte Carlo codes are suitable for steady state design and high fidelity reference solutions (SERPENT, MCNP-ORIGEN, MONTEBURN)
- **Others:** PARCS (NRC), DIF3D-REBUS(ANL), APOLLO-CRONOS (AREVA)
Core Neutronics & Depletion – pebble bed

**PEBBED**

- **Technical Readiness:** Proof of Concept
- **Functionality:** Computes the equilibrium flux and power distribution in the core. Depletes and shuffles fuel elements.
- **Validation Basis:** HTR-PROTEUS, HTR-10 Initial Criticality
- **Computational Requirements:** PC/Workstation (FORTRAN-90), HPC Cluster
- **Gaps:** Time-dependence (for transients and pre-equilibrium core states)
- **Owner Contact Info/Support Level/Availability:** INL ([Hans.Gougar@inl.gov](mailto:Hans.Gougar@inl.gov)); minimal support; requests for software considered on an individual basis
- **Remarks:** Coupled diffusion-depletion with pebble shuffling. Coupled to THERMIX-KONVEK for steady state thermal-fluid analysis. Online cross-section generation with COMBINE7. Monte Carlo codes (SERPENT, MCNP-ORIGEN, MONTEBURN) are suitable for steady state design and high fidelity reference solutions but depletion codes lack the algorithm for treating moving/recirculating fuel elements. Transient analysis does not require fuel
- **Others:** VSOP (FZ-Jülich)
Pebble Bed Dynamics

PEBBLES

- Technical Readiness: Proof of Concept
- Functionality: Simulates pebble flow (and dust production).
- Validation Basis: ANABEK and more recent pebble flow experiments (mostly not under prototypical conditions)
- Computational Requirements: PC/Workstation (FORTRAN-90), HPC Cluster
- Gaps: Full physics can be computationally demanding
- Owner Contact Info/Support Level/Availability: INL (joshua.cogliati@inl.gov); minimal support; publicly available
- Remarks:
- Others: LAMMPS (Sandia), PFC3D (Itasca)
Lattice Physics/ Cross Section Generation

**SCALE 6.2**

- **Technical Readiness:** Production
- **Functionality:** Multiple transport solvers, include 2D SN unstructured mesh for prismatic designs, 1D SN for pebble designs, 3D Monte Carlo. ORIGEN for depletion.
- **Validation Basis:** HTR-PROTEUS, HTR-10 Initial criticality, VHTRC, HTTR
- **Computational Requirements:** nominal (v6.2 has parallelized Monte Carlo
- **Gaps:** ??
- **Owner Contact Info/Support Level/Availability:** RSICC
- **Remarks:** Recent upgrade (6.2) treats double heterogeneity, annular fuel elements. Problem-dependent Doppler broadening (inc. graphite). Coupled to the PARCS full core simulator. TSUNAMI SUSA, SERPENT (VTT)
Shielding

**MCNP**

- **Technical Readiness:** Production
- **Functionality:** Computes fluence, damage, and heating rates for deep shielding problems
- **Validation Basis:** numerous
- **Computational Requirements:** Nominal, highly scalable
- **Gaps:** ??
- **Owner Contact Info/Support Level/Availability:** RSICC
- **Remarks:** NA
- **Others:** SERPENT (VTT)
Thermal Fluidic Analysis

**RELAP5-3D**

- **Technical Readiness:** Production
- **Functionality:** System analysis code: computes core-wide coolant and fuel temperatures, coolant flow rates and pressure. Balance-of-plant modules
- **Validation Basis:** Extensive LWR validation. HTR-relevant data being used to validate models of HTTF and NSTF experiments.
- **Computational Requirements:** Nominal
- **Gaps:** ??
- **Owner Contact Info/Support Level/Availabilty:** INL (james.wolf@inl.gov)
- **Remarks:** Recently coupled to PHISICS for prismatic reactor steady-state and transient analysis. CFD is used to investigate local behavior and complex phenomena but whole core transient analysis with CFD is still out of range. Higher resolution models are desirable.
- **Others:** GRSAC (ORNL), FLOWNEX (flownex.com), RELAP-7(INL), AGREE(NRC), MGT (FZ-Jülich), THERMIX-DIREKT (FZ-Jülich)
High Fidelity Thermal Fluidic Analysis

- **Technical Readiness**: Production
- **Functionality**: High fidelity analysis of local or complex phenomena
- **Validation Basis**: Limited for HTRs
- **Computational Requirements**: HPC
- **Gaps**: Owner Contact Info/Support Level/Availability: Varies
- **Remarks**: Whole-core analysis is not yet feasible. Look at coarse mesh methods or coupling to a low order simulation
- **Others**: FLUENT, STAR-CCM, NEK5000
Chemistry/Corrosion

**RELAP5-3D?**

- **Technical Readiness:** Production
- **Functionality:** System analysis code: computes core-wide coolant and fuel temperatures, coolant flow rates and pressure. Balance-of-plant modules
- **Validation Basis:** minimal for graphite oxidation
- **Computational Requirements:** Nominal
- **Gaps:** Graphite oxidation model needs to be upgraded and tested
- **Owner Contact Info/Support Level/Availability:** INL (james.wolf@inl.gov)
- **Remarks:** Graphite oxidation solver can be updated to use oxidation models recently developed. Will have to address the production of CO and other products of graphite-oxygen reactions.
- **Others:** MGT(FZ-Jülich)
Source Term/Severe Accident

**MELCOR**

- **Technical Readiness**: Production
- **Functionality**: Integral analysis of severe accident progression and releases
- **Validation Basis**: LWR
- **Computational Requirements**: Nominal
- **Gaps**: Dust interactions (need isotherms and aerosol properties), graphite oxidation models
- **Owner Contact Info/Support Level/Availability**: Sandia NL
- **Remarks:**
- **Others**: XSTERM(X-Energy), SPATRA(?).
Structural/Seismic Analysis

**Commercial tools**

- **Technical Readiness:** Production
- **Functionality:** Thermo-mechanical analysis of components, graphite, seismically-vulnerable structures
- **Validation Basis:** All type of power plants
- **Gaps:** Graphite creep may require model updates using data currently being generated. Seismic analyses for nuclear applications in general are due for modernization
- **Others:** ANSYS, ABAQUS, etc.

- Grains shrink parallel to planes and grow in perpendicular direction
  - **Overall volume shrinkage**

  Cracks formed during fabrication accommodate swelling – *for a while*
Commercial tools

- Technical Readiness: Production
- Functionality: Thermo-mechanical analysis of components, graphite, seismically-vulnerable structures
- Validation Basis: All type of power plants
- Computational Requirements: ??
- Gaps: ??
- Owner Contact Info/Support Level/Availability: Woody.com
- Remarks: NA
- Others: RISKMAN, RAVEN(INL), DAKOTA(Sandia)