Application and development of tools for HTR neutronics and thermal hydraulics analysis at IKE

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General Objectives: Development of an Integrated Tool for the Analysis of Stationary and Dynamic Behavior of HTRs

- Neutronics reactor design (stationary and transient).
- In-Core Thermal-hydraulics and fuel thermal behavior.
- Modeling of components and dynamics of Power Conversion Unit (PCU).
HTR applications

• Neutronics stationary
• Neutronics transient
• Thermal hydraulics
• PCU simulation
Codes available

- ZIRKUS, KIND
- THERMIX/KONVEK
- ANISN/DORT/TORT (1D-3D $S_N$-transport)
- Monte Carlo: MCNP(X)/KENO
- NJOY (Cross section preparation)
- RSYST (IKE), general reactor physics applications
- MICROX-2
- RESMOD (IKE), multicell spectral code
- FLOWNEX (M-Tech), system code
ZIRKUS

- Modular system with functional modules and data base system
- Restricted to pebble bed HTR types
- Flexibility high, but rather complex
- Several adaptations to PBMR like systems (annular core) were made together with simplifications of input structure
Main modular ZIRKUS sequence for stationary neutronics - thermal hydraulics calculations

- **KUGEL**: Definition of spherical fuel element
- **WQRFL**: Cross-sections for reflectors (temperature, density, impurity)
- **NIVERM**: Number densities initialisation/shuffling
- **NEWA**: Dancoff factors
- **MICROX**: Cross section resonance treatment and spectral calculation (microscopic XS for spectral zones)
- **MAGRU**: Macroscopic cross sections for burnup zones
- **HBLOCK**: 2D diffusion calculation, variable group numbers, Xe distribution
- **VORNEK**: Power density calculation
Main modular ZIRKUS sequence for stationary neutronics - thermal hydraulics calculations

- **ZBUCK**: Bucklings for spectral zones derived from diffusion calculation
- **SBURN**: Depletion calculation for all burnup zones
- **NZW**: Decay heat calculation
- **NZWAUS**: Interface decay heat data
- **LDTHERMI**: Interface ZIRKUS-THERMIX
- **THERMIX**: Thermal hydraulic calculation
- **TZIRK**: Interface THERMIX-ZIRKUS
- **DIFK**: Diffusion constants for cavity region
ZIRKUS-features

- first core
- transition core
- equilibrium core
- flow pattern of pebbles
- reload strategy
- fuel/moderator elements
- 2 D representation for burn up
- 3 D stationary calculations (burnup distribution 2D) with Monte-Carlo codes MCNP and/or KENO
- temperature coefficients
- water ingress
- xenon reactivity
- flexibility, connection to other codes possible
Typical ZIRKUS/THERMIX applications

- Cross-section Database
- MICROX/ MCNP
- FIRST-CORE TRANSITION CORE EQUILIBRIUM CORE
- Calculation of Reactivity Coefficients. Database for Transients Monte Carlo, $S_N$-Transport
- ZIRKUS Database
- Thermal-hydraulic analysis
- LOFC
- DLOCA
ZIRKUS options

- SINGLE MODULE INPUTS
- SEQUENCE OF MODULES
- EXECUTION OF SINGLE MODULES AND SEQUENCES
- ARCHIVING OF CALCULATIONAL RESULTS
- RESTART-OPTION
- INTERFACE TO THERMAL HYDRAULICS
- INTERFACE TO TRANSPORT PROGRAMS
- INTERFACE TO TRANSIENT CODES KIND; RZ KIND
ZIRKUS modular chain

- KUGEL, DIFK
  - WQRFL
    - NIVERM
      - NEWA
        - MICROX
          - MAGRU
            - HBLOCK
              - VORNEK
  - ZBUCK
    - SBURN
      - NZW
        - NZWAUS
          - LDTHERMI
            - THERMIX
              - TZIRK
Simulation platform

Universität Stuttgart
Institut für Kernenergetik und Energiesysteme

Main Simplot Page
Requests
Check Server Status
Info Session

Info Pebble Bed Master
New Pebble Bed Master

Reactor
Fuel Element
Simulation Model

Start Simulation

Info Session

Simulation platform

Virtual Power Plant - PBMR

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next Fuel Element

Main Simplot Page
Requests
Check Server Status
Info Session

Info Pebble Bed Master
New Pebble Bed Master

Reactor
Fuel Element
Simulation Model

Start Simulation

The PBMR-400 Core Design - 2nd Workshop - OECD/NEA, Issy les Moulineaux - 26-27 January 2006
Cross section data base and spectral code

- Data evaluations: JEFF 3.1
- MICROX-2 spectral code
- RESMOD spectral code
- MCNP(X) Monte Carlo
- Thermal neutron scattering laws for graphite
MICROX-2 for detailed calculation of spectra in fast, resonance and thermal range

- FDCTAPE: 92 groups, fast range
- GARTAPE: Pointwise, Resolved, Resonance, range
- GGTAPE: 101 groups, thermal range
- Geometry of cell, temperature, Dancoff factor, buckling
- Zonewise Nuclide composition
- Condensed microscopic cross sections
### Present MICROX-2 Library based on JEFF-3.1

**158 Nuclides**

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Frequency distributions of graphite

The graph shows frequency distributions of graphite with different symbols and lines:
- **GA**: Solid magenta line
- **ORNLS**: Dashed blue line
- **NCSU**: Dotted green line

The x-axis represents the energy in eV, ranging from 0.00 to 0.25, and the y-axis represents the density of states (Rho(Omega)) in 1/eV, ranging from 0.00 to 40.
Comparison of measured and calculated spectra

- Experiment GAC-5A 274 K
- GAC-5a : GA model
- GAC-5a : ORNL model
- GAC-5a : NCSU model
- Experiment GAC-5F 600 K
- GAC-5f : GA model
- GAC-5F : ORNL model

Neutron Energy (eV)

E_{\text{Phi}}(E) (arbitrary units)
Transient calculations

⇒ ZKIND and
⇒ RZKIND codes

Both are neutron kinetic/dynamic codes for the pebble bed core primarily developed for the HTR-MODUL reactor.

The Tasks are: calculation of

• time dependent power distributions and reactivity effects
• temperature distributions
Thermal-hydraulic Models

Different models to simulate the heat production and temperature distribution in fuel

- Macro Model (2D RZKIND)
- Macro and Micro Model (1D ZKIND)
- enhanced Micro Model (1D PKIND)
Macro and Micro model of Heat conduction

Macro Model:

In RZKIND at the time a homogeneous model is implemented. The Fuel spheres are subdivided into several shells but the fuel temperature is assumed to be identical to the graphite temperature in the corresponding shell. The fuel temperature calculated for reactivity feedback is averaged over all shells containing fuel (except outer shell). The moderator temperature is the average of graphite temperatures of all shells.
Thermal-hydraulic Models used in KIND codes

$\langle T \rangle$ : average Temperature over the fine structure

$\tau$ : Temperature increase in the particle

$\langle T \rangle$ : average Temperature over the fine structure

$\tau$ : Temperature increase in the particle
Data Flow to RZKIND

- **ZIRKUS**
  - Geometry
  - Cross Section data

- **User’s Input File**

- **RZKIND**
  - Condensation of cross sections
  - ZIRKUS-Geometry
    - RZKIND-Geometry
    - ZKIND

- **VPF**
  - Polynomial fit of cross sections

- **OUTPUT FILE**

- **RZKIND Data-Library**
Features of the KIND Codes

Simulate

• Inlet temperature disturbances
• Mass flow disturbances
• Changes in power
• Reactivity disturbances
• Control rod movement or SAS insertion
• Xenon effects
• External reactivity effects
Example: Control rod withdrawal
(2D RZ-KIND calculation for HTR Modul)

(a) first scram works at 120% neutron flux
(b) second scram works if average He coolant outlet Temperature exceeds limit
(c) neither 1. Scram nor 2. scram works control rods withdraw to the maximum upper end position (-100cm)
Influence of detailed fuel temperature model
(control rod velocity: 100 cm/s)

Withdrawal of all rods with 100 cm/s

(blue) 2D RZ-KIND calculation

(red) 1D ZKIND particle model calculation

Extreme differences between the two models
Fast transient calculation

ZKIND (Particle model)

- 100 cm/s
Thermal hydraulics

General Objectives:

- Reliable and flexible integrated tool for analysis of static and dynamic behavior of HTRs:
- Emphasis on detailed description of in-vessel behavior, especially coupling of thermal-hydraulics and neutronics
- Existing tools as starting point for further development
- Present code THERMIX
HTR with annular core [PBMR]

Design of PBMR with annular core and compact central column

- Thermal power: 400 MW
- System pressure: 85 bar
- Inlet temperature: 500 °C
- Outlet temperature: 900 °C

Initial steady state temperature distribution

Examples of analyses and applications
Results for Annular Core Reactor

LOFC with depressurization

Solid temperature development

LOFC without depressurization:

Solid temperature development

Gas temperature and velocity (annular core only)
Further developments

- 3D calculations in ZIRKUS
- Improved treatment of streaming in cavities for diffusion calculations
- New 2D/3D thermal hydraulics module
- Extensions of the space time kinetics modules
  - more energy groups
  - more flexible mesh grid
  - coupling to new thermal hydraulics code
  - detailed heat transfer model for coated particles embedded into graphite matrix for 2D version
 Benchmark PBMR 400
Neutronics/Thermal hydraulics

• ZIRKUS and DORT model (exercise 1)
• THERMIX and KONVEK model (exercise 2)
### Mesh and media assignment : Steady State Exercise 1

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</table>

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The PBMR-400 Core Design - 2nd Workshop - OECD/NEA, Issy les Moulineaux - 26-27 January 2006
Compositions for Benchmark Model (THERMIX-Konvek)
Results neutronics exercise 1

- Calculations performed with the Diffusion code of ZIRKUS (2D)
  - Cavities treated via direction dependent diffusion coefficients
- For comparisons: DORT 2D $S_N$-calculations $P_0$- transport corrected
  - Cavities treated as vacuum

<table>
<thead>
<tr>
<th>Value</th>
<th>ZIRKUS/Diffusion</th>
<th>DORT-S16</th>
<th>DORT-S12</th>
<th>DORT-S8</th>
<th>DORT-S6</th>
<th>DORT-S4</th>
<th>DORT-S2</th>
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<tr>
<td>$k$-eff</td>
<td>1.003488</td>
<td>0.992842</td>
<td>0.991904</td>
<td>0.99383</td>
<td>0.997045</td>
<td>0.99376</td>
<td>0.995983</td>
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<tr>
<td>Maximum fast flux (n/cm$^2$/s)</td>
<td>2.005E+14</td>
<td>2.041E+14</td>
<td>2.045E+14</td>
<td>2.045E+14</td>
<td>2.043E+14</td>
<td>2.046E+14</td>
<td>2.052E+14</td>
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<tr>
<td>Maximum thermal flux (n/cm$^2$/s)</td>
<td>3.055E+14</td>
<td>3.141E+14</td>
<td>3.153E+14</td>
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<tr>
<td>Leakage from core (% per lost neutron)</td>
<td>15.40</td>
<td>15.24</td>
<td>15.28</td>
<td>15.20</td>
<td>15.06</td>
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<td>Leakage from domain (% per lost neutron)</td>
<td>0.209</td>
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<td>0.211</td>
<td>0.213</td>
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Fast flux density PBMR-400 exercise 1
DORT S16

The PBMR-400 Core Design - 2nd Workshop - OECD/NEA, Issy les Moulineaux - 26-27 January 2006
Thermal flux density PBMR-400 exercise 1
DORT- S16
Relative difference DORT S8 to S16 reference solution (fast group)
Relative difference DORT S8 to S16 reference solution (thermal group)
Relative difference DORT S2 to S16 reference solution (fast group)
Relative difference DORT S2 to S16 reference solution (thermal group)
Fission neutron source distribution (DORT) S-16 calculation for exercise 1
Relative difference in fission neutron source distribution between S-8 and S-16 calculation
Relative difference in fission neutron source distribution between S-2 and S-16 calculation
Exercise 2

Heat flow to surface cooling system 974.5 kw!

Maximum fuel temperature 996.7 °C!

<table>
<thead>
<tr>
<th>Description</th>
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<tr>
<td>Inlet helium temperature (°C)</td>
<td>500</td>
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<td>Outlet helium temperature (°C)</td>
<td>998.2</td>
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<td>Inlet Pressure (MPa)</td>
<td>9.33944</td>
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<td>Outlet Pressure (MPa)</td>
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<td>Total pressure drop (kPa) - Inlet to outlet</td>
<td>339.44</td>
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<td>Pebble bed pressure drop (kPa) - Top / bottom fuel</td>
<td>278</td>
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<td>Average fuel temperature (°C)</td>
<td>815.28</td>
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<td>Average moderator temperature (°C)</td>
<td>796.5</td>
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<tr>
<td>Average helium temperature in core (°C)</td>
<td>740.61</td>
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Pebble surface temperature distribution exercise 2
Flow field exercise 2
Remarks exercise 1

- $k_{\text{eff}}$ strongly dependent from diffusion constants in cavity over pebble bed core for diffusion method
- $k_{\text{eff}}$ about 1% lower for $S_N$ (DORT) method, depending from SN order
- $S_N$ order from influence of fluxes at outer boundaries and cavities
- For $S_N$ calculations the absorber cross sections should be adopted
- transport correction for $P_0$ calculation adequate?
- Treatment of cavities well defined for $S_N$ calculations
Remarks exercise 2

- Spatial discretisation could be refined
- fuel, moderator and reflector temperatures seem to be adequate for steady state cases
Remarks exercise 3

• A reproduction of the reference cross section data was not possible
• Coupled calculations with interpolated cross sections led to inconsistent results
• Some interpolated data should be compared