Xe-100 Licensing Topical Report Mechanistic Source Term Approach

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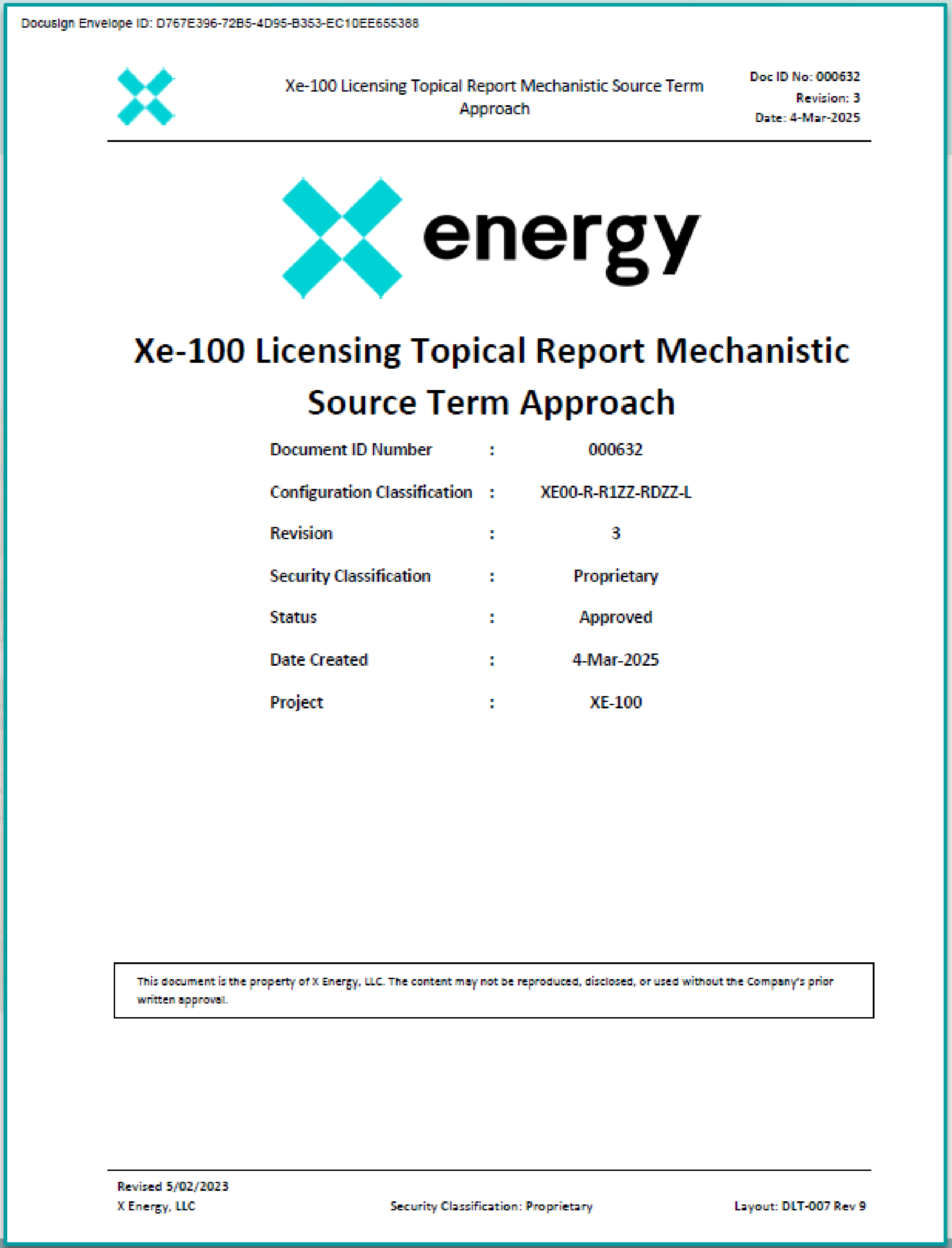
Outline

- X-energy's Mechanistic Source Term (MST) Approach
- Mechanistic Source Term Models
- Q&A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Mechanistic Source Term (MST) Approach

- **Scope:**
  - **Included:** Description of MST models used to determine radionuclide transport phenomena and estimate mechanistic source terms used to support the preliminary analysis and evaluation of the Xe-100
  - **Excluded:** Actual implementation evaluation cases and outputs (included in a future XSTERM Topical Report)

- **Interfacing Documents:**
  - Risk-Informed Performance-Based Licensing Basis Approach for the Xe-100 Reactor (ML21196A071)
  - Xe-100 Licensing Topical Report: Transient and Safety Analysis Methodology (ML25077A285)
  - Xe-100 Principal Design Criteria Licensing Topical Report (ML24047A310)
  - Xe-100 Licensing Topical Report TRISO-X Pebble Fuel Qualification Methodology (ML22216A179)
  - Xe-100 Licensing Topical Report Atmospheric Dispersion and Dose Calculation Methodology (ML23268A456)

Mechanistic Source Term (MST) Approach

- Xe-100 MST methodology is part of the implementation of a **risk-informed, performance-based design and licensing basis** according to the Nuclear Energy Institute (NEI) 18-04 and Nuclear Regulatory Commission (NRC) Regulatory Guide (RG) 1.233

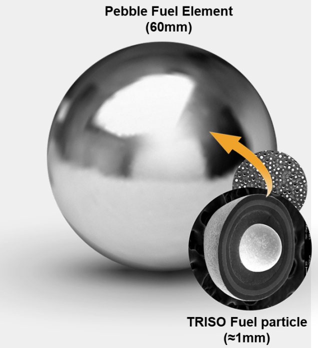
- **Regulatory Guidance (SECY-93-092):**
  - Reactor and fuel performance under normal and off-normal operating conditions is sufficiently well understood to permit a mechanistic analysis.
  - Sufficient data should exist on the reactor and fuel performance through the research, development, and testing programs to provide the adequate confidence in the mechanistic approach.
  - Transport of fission products can be adequately modelled for all barriers and pathways to the environs, including specific consideration of containment design. The calculations should be as realistic as possible so that the values and limitations of any mechanism or barrier are not obscured.
  - Events considered in the analyses to develop the set of source terms for each design are selected to bound severe accidents and design-dependent uncertainties.

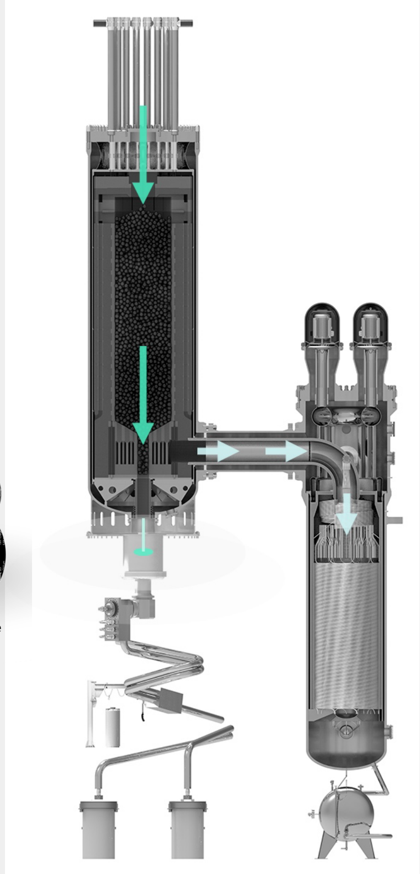
Mechanistic Source Term (MST) Approach

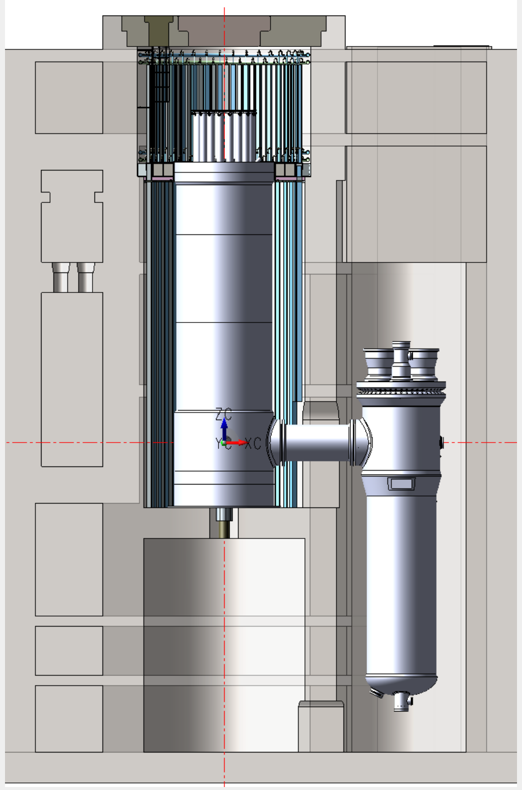
➢ **Xe-100 source terms** are:

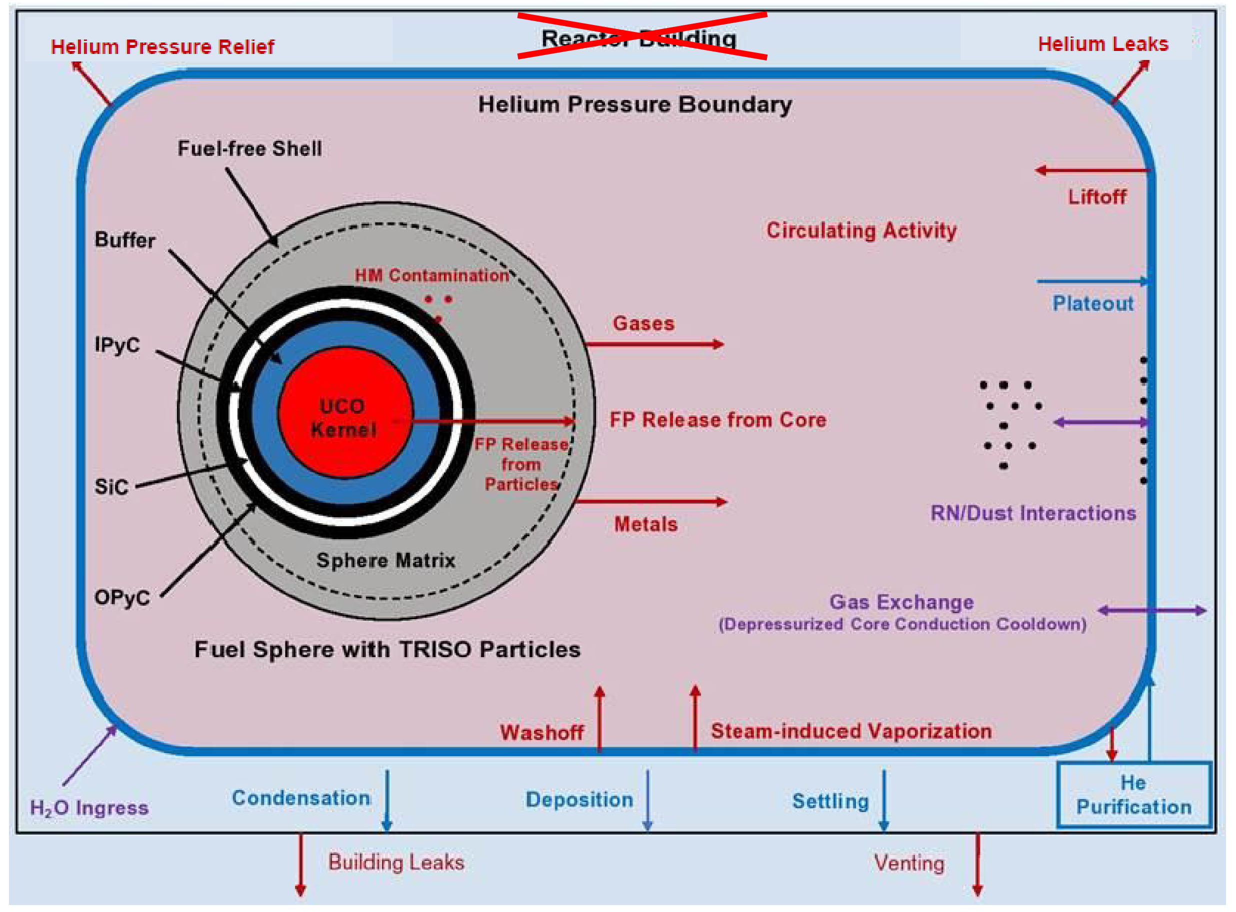
- Event-specific
- Determined mechanistically using models of fission product (FP) generation and transport
- Accounting for the reactor's inherent and passive design features and the performance of FP release barriers that constitute the functional containment
- Inclusive of the quantities, timing, physical and chemical forms, and thermal energy of the release
- Different from light water reactor source terms based on severe core damage event(s)

Mechanistic Source Term (MST) Approach









Radionuclide Release Barriers

Mechanistically Modelled Radionuclide Transport Phenomena

MST Models

LTR Appendix	Model	Scope	Codes implementing similar capability
A	FPM	Fuel Performance (particle failure fractions)	PARFUME (INL), PANAMA, STACY
B	THM	Thermodynamics	VSOP-THERMIX-KONVEK, AGREE (UMich), STAR-CCM+ (Siemens)
C	SOLM	Time-dependent radionuclide production, transport & release from fuel elements	PARFUME (INL), GETTER, FRESCO, STACY
D	GASM	Steady-state gaseous fission product release	PARFUME (INL), NOBLEG, STACY
E	DUSTM	Graphite / metallic dust production	N/A
F	HPBM	Dust, fission and activation product behavior in primary circuit	DAMD (PBMR), PADLOC (GA), RADAX, SPATRA, RADC (GA), MELCOR (Sandia)
G	CORRM	Air/water Ingress, fuel materials corrosion rates	OXIDE-4 (GA), TINTE, GRACE (FE), STAR-CCM+ (Siemens), Fluent (ANSYS)
	KSIM	Plant simulator using point-kinetics core model with spatial and thermo-dynamics coupling	MGT / TINTE, AGREE (UMich), RELAP-7 (INL), Flownex (M-Tech)
	TRITM	Tritium plant mass balance	TRITGO (GA), THYTAN (JAEA), TPAC (INL), TMAP (INL), ORIGEN-S (ORNL)
	Dispersion/Dose	Off-Site doses	MACCS (Sandia), HotSpot (LLNL), RASCAL (NRC), ADDAM (AECL)

→ *Xe-100 Licensing Topical Report, Atmospheric Dispersion and Dose Calculation Methodology* (ML23268A456)

XSTERM

US-DOE Code

German (Legacy) Code

Commercial NQA-1 Code

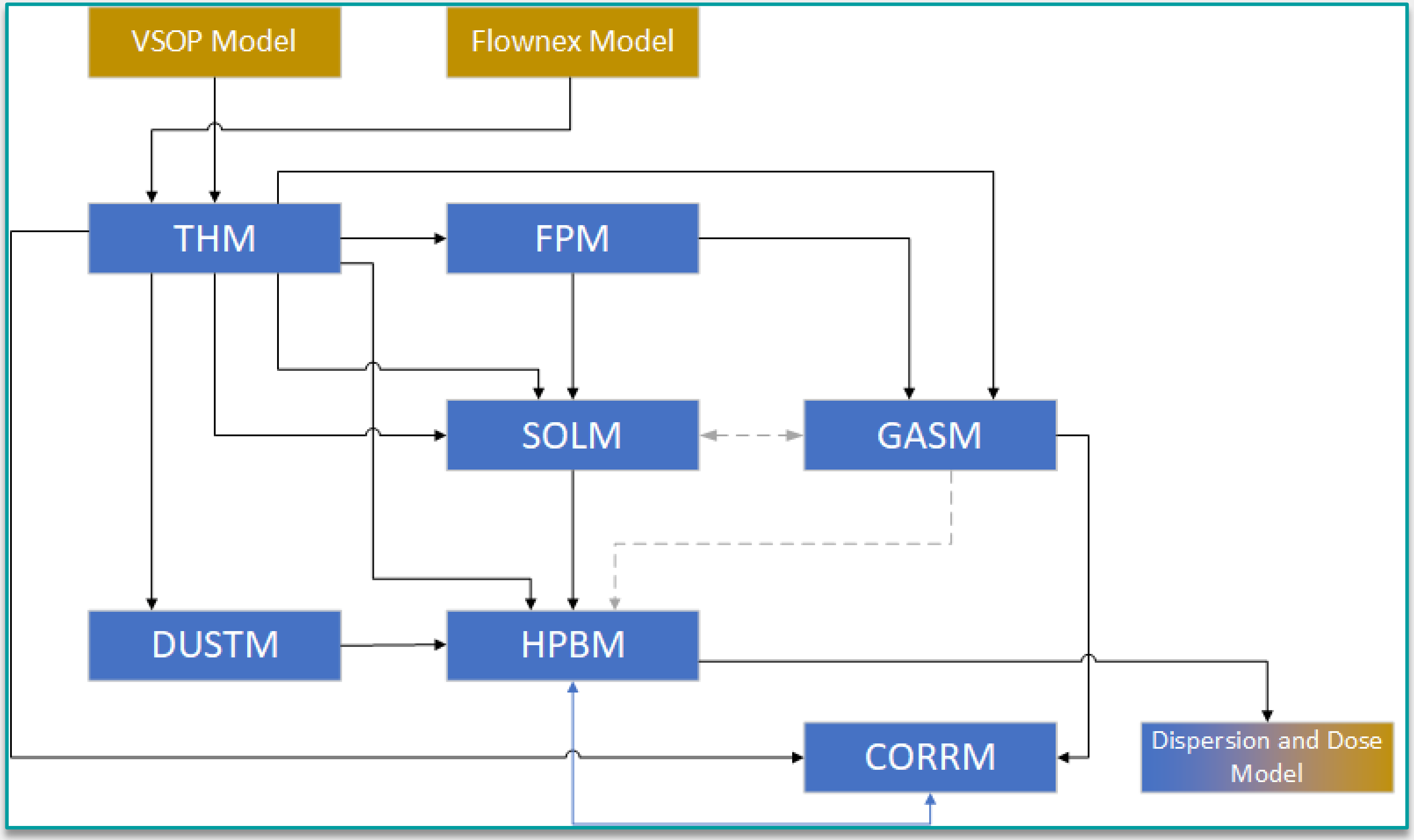
Other

XSTERM Code

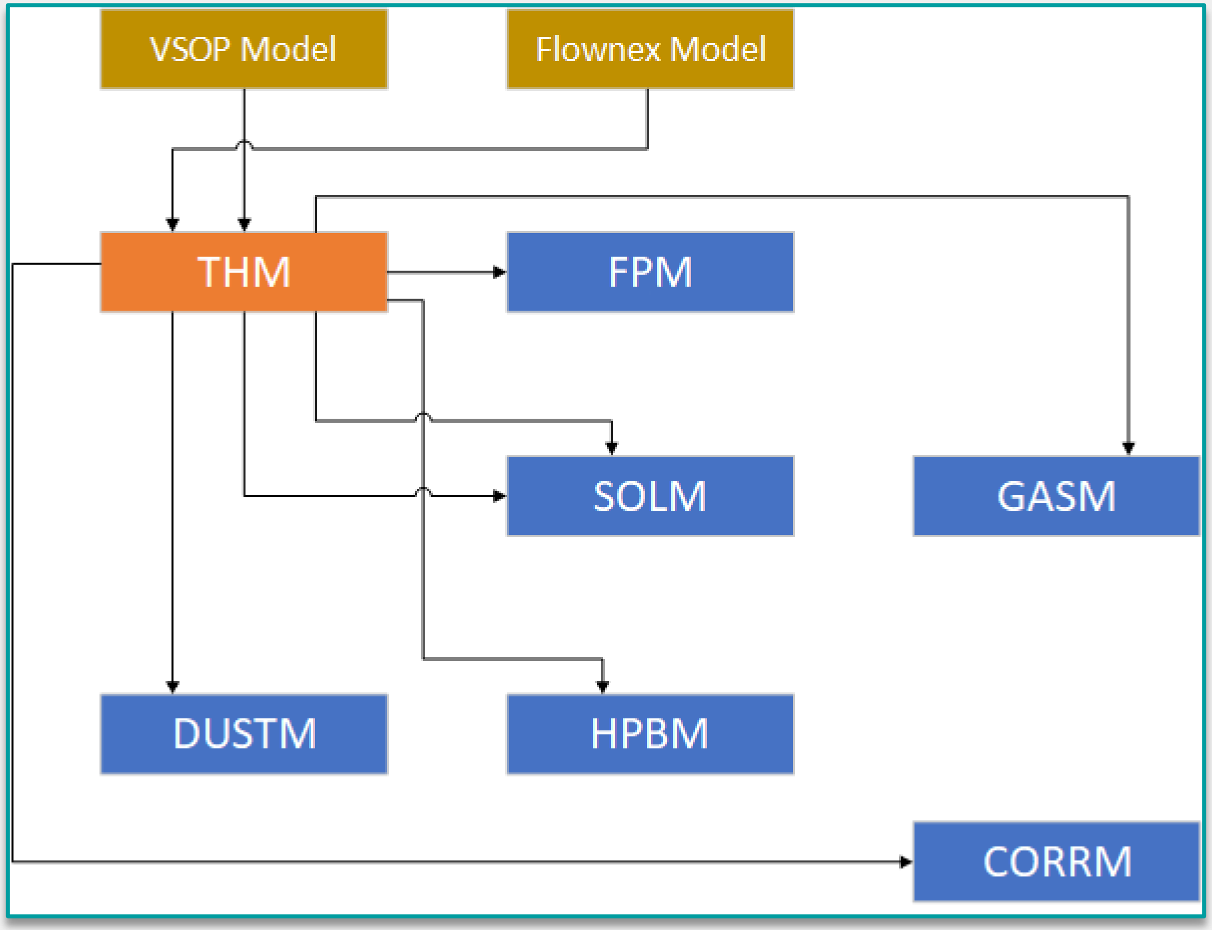
- **Evaluation Model for the quantification of Xe-100 source terms and dose calculations**
- Implementation of the MST models presented in this TR, part of X-energy safety analysis code suite
- Developed under X-energy Quality Assurance Program
- Goal: NQA-1 qualification

- **Verification and Validation, Uncertainty Quantification** in progress
  - Line-by-line code verification, comparison with analytical solutions, automated testing in the continuous-integration framework
  - Phased validation – each phase aims at validating a set of medium and high ranked phenomena from the Xe-100 Safety Analysis PIRT
    - Phase 1: Activity Release and Transport (FPM, GASM, SOLM, HPBM)
    - Phase 2: Reactor Temperature and Power (TDM, KSIM)
    - Phase 3: Dust Production (DUSTM)
    - Phase 4: Exposure to Oxidating Environments (CORRM, TRITM)
  - Uncertainty Quantification Plan based on the Xe-100 Safety Analysis PIRT

Core MST Models Relationship

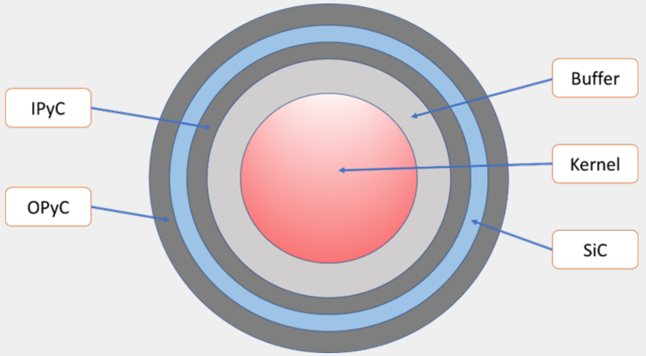


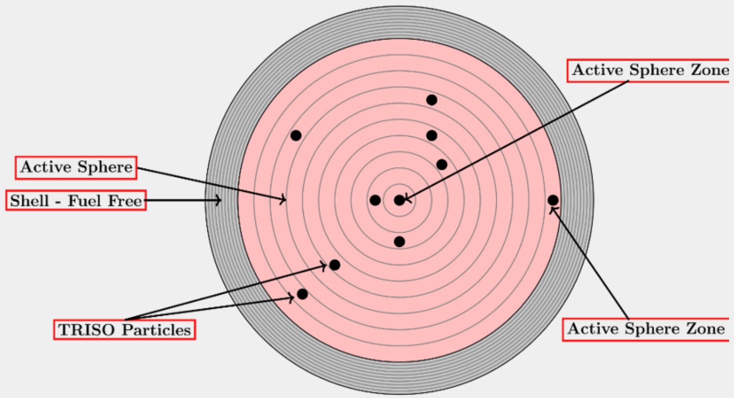
THM: Thermodynamics Model

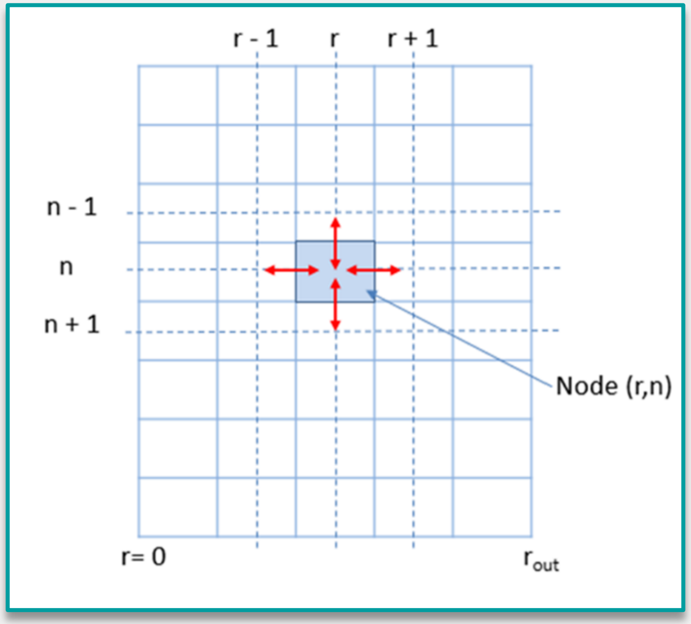


THM: Application Domain

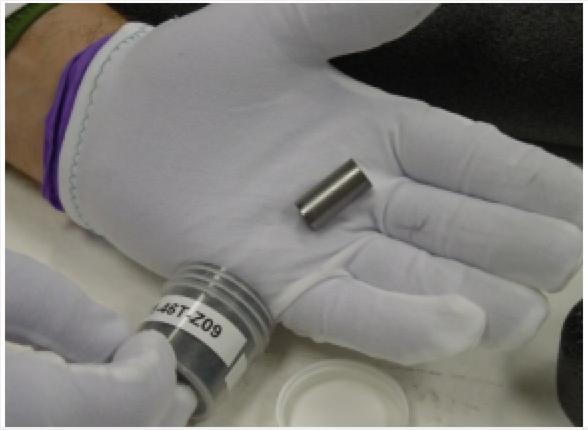
Xe-100 Single-Pebble / Core Calculations

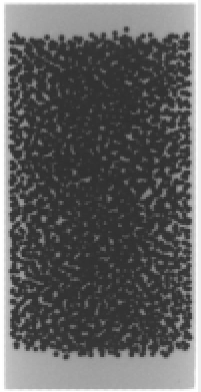


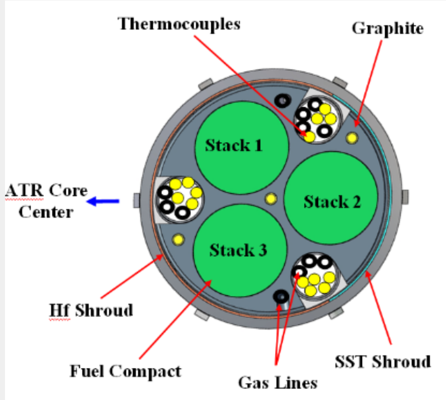




Fuel Compact Calculations (Validation)







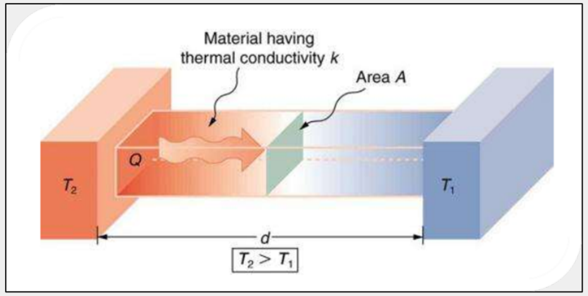
THM: Phenomena Modelled

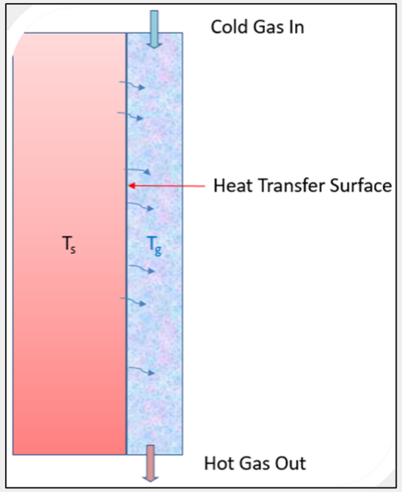
- Conductive Heat Transfer: Fourier law of heat conduction with space-, temperature- and dose-dependent conduction coefficients
  - Zehner-Bauer-Schlünder model in the pebble bed

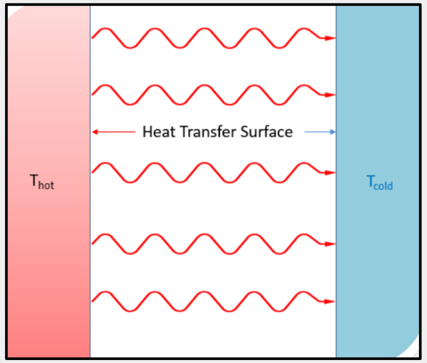
$$\lambda_{pb} = \lambda_{sc} + \lambda_r + \lambda_f$$

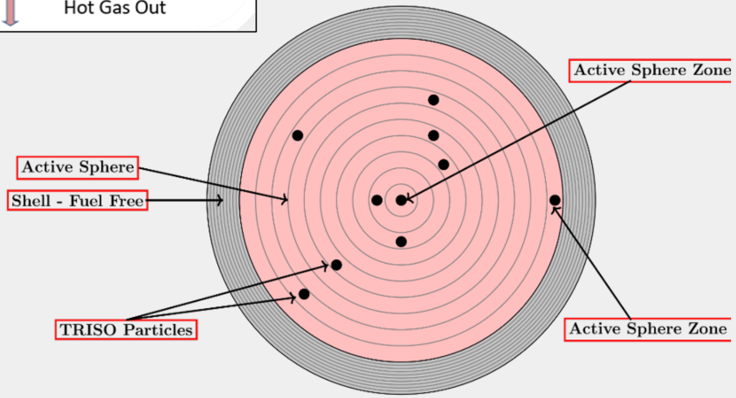
  - Reflector graphite model based on research of G. Haag
- Convective Heat Transfer: Kugeler-Schulten correlation
- Radiative Heat Transfer: Stefan-Boltzmann law
- Heat Sources: fission, gamma, decay heat (DIN-25485 standard)

- Pebble temperatures: 1D-radial heat conduction through pebble mesh zones with core node temperature as boundary condition – semi-analytic
- Particle temperatures: 1D-radial heat conduction through particle mesh zones with pebble zone temperature as boundary condition – semi-analytic
- Compact temperatures: 2D-axisymmetric heat conduction through compact zones with prescribed outer temperature – finite-difference discretization + successive-over-relaxation iterative method



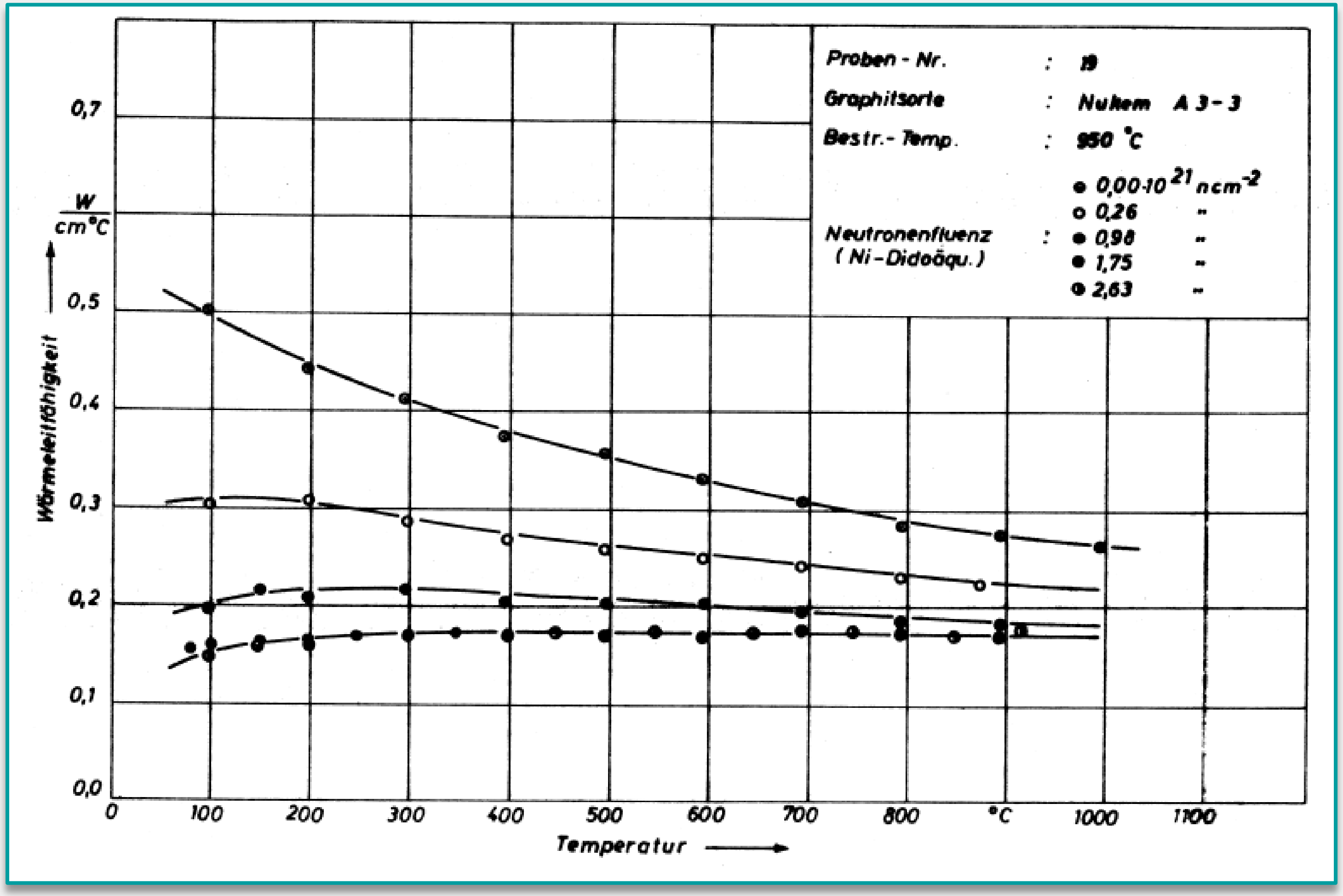






THM: Material Properties

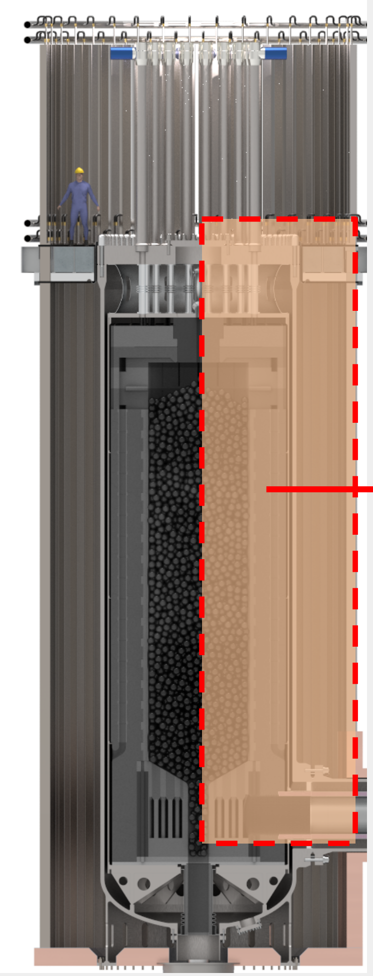
- Explicit correlations or data fits
- Generally temperature-dependent => iterations



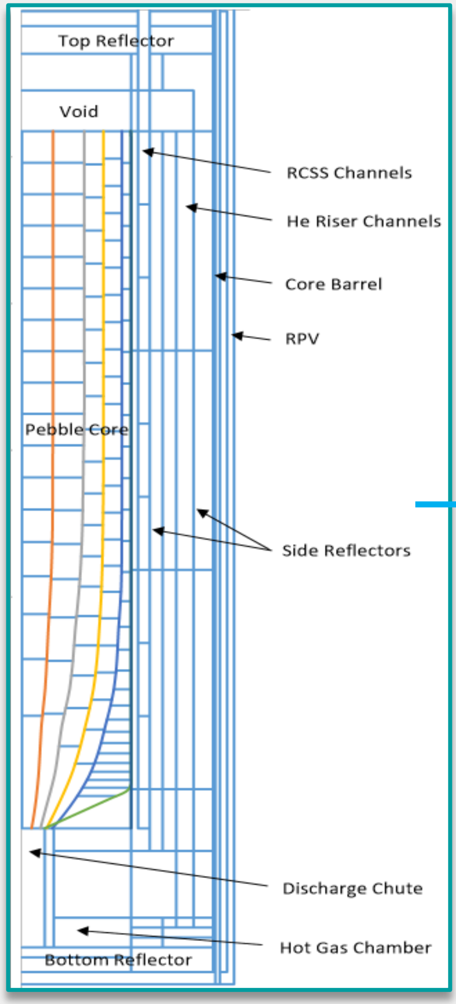
THM: Input Data and Boundary Conditions

- Second order least-squares mapping from VSOP grid to simplify heat transfer calculations

Xe-100 Reactor



VSOP Model



MST Model

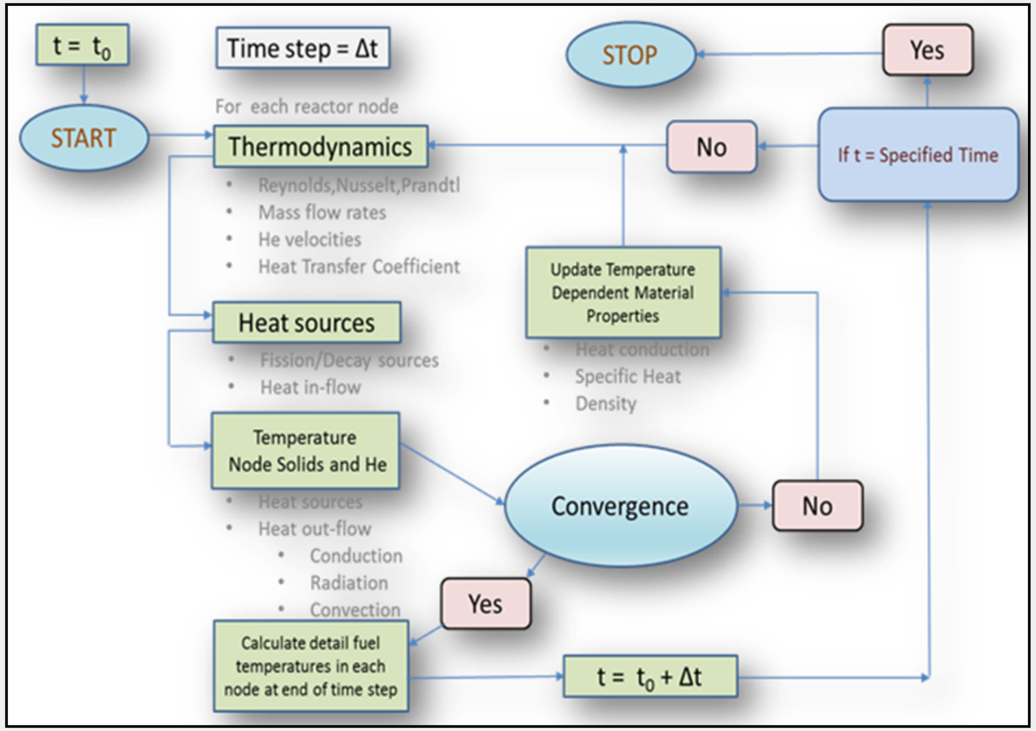
Fuel 1	Fuel 2	Fuel 3	Fuel 4	Fuel 5	Reflector 1	Reflector 2	Reflector 3	Ref3/Barrel	Barrel	RBCS	RP
297.7	295.5	292.3	297.6	299.4	283.1	275.7	268.7	266.1	260.2	256.2	208.
337.3	332.4	326.0	332.4	347.3	300.6	285.9	275.9	270.2	265.4	259.5	213.
376.0	368.6	359.1	369.4	394.5	318.9	295.0	281.2	274.2	269.1	262.8	217.
417.4	407.5	395.2	410.3	439.8	341.3	307.0	287.4	278.5	272.6	263.7	218.
461.6	449.4	433.8	450.3	478.3	364.4	319.8	293.7	283.0	275.9	264.0	219.
503.3	488.7	471.7	488.8	510.9	386.9	332.9	300.3	287.4	279.4	264.4	219.
543.3	526.5	508.5	525.3	537.7	409.5	347.0	307.5	292.5	283.3	265.0	219.
581.2	562.4	543.5	557.4	559.7	431.3	361.0	314.7	297.6	287.2	265.6	220.
615.6	594.8	575.6	587.1	577.7	451.6	374.6	321.7	302.5	291.0	266.1	220.
646.6	624.2	605.7	613.2	593.0	469.9	387.1	328.3	307.2	294.7	266.6	221.
674.6	650.7	633.4	636.6	605.8	487.5	399.5	334.8	311.9	298.3	267.1	221.
699.8	674.5	657.4	657.3	616.6	502.9	410.5	340.7	316.1	301.5	267.6	222.
722.6	696.2	679.3	675.4	625.9	516.7	420.7	346.2	319.9	304.5	267.9	222.
742.2	714.7	699.1	690.9	634.4	530.1	430.6	351.5	323.8	307.5	268.3	222.
759.3	730.8	716.7	704.1	642.2	540.8	438.7	355.9	326.8	309.8	268.6	222.
774.4	745.3	732.5	715.6	649.4	551.0	446.3	360.0	329.8	312.1	268.8	223.
787.9	758.1	746.0	725.8	656.1	560.4	453.5	363.9	332.6	314.3	269.1	223.
799.2	769.1	757.7	734.6	662.6	568.1	459.2	367.0	334.8	316.0	269.2	223.
808.9	778.7	768.5	742.2	668.1	575.4	464.8	370.0	337.0	317.7	269.3	223.

Total core mass flow rate (Flownex)

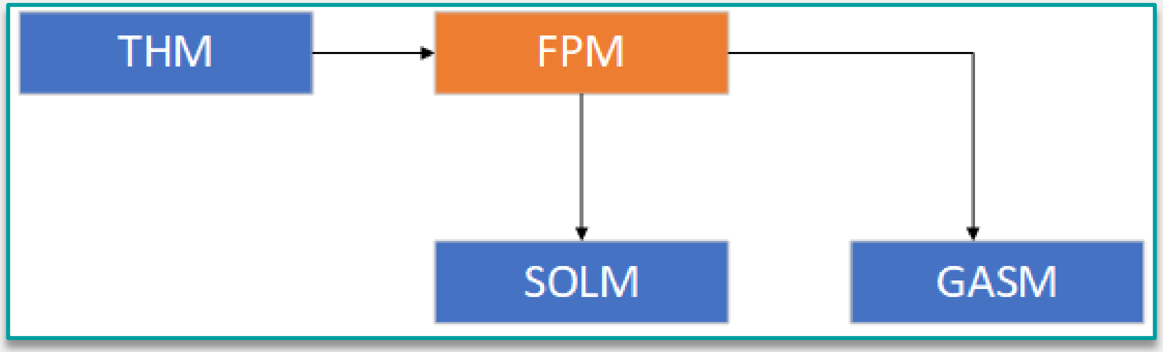
Disclaimer: Values shown above only for illustrative purposes

THM: Time-Stepping Algorithm

- Backward Implicit/Explicit Iterative Method
- Iterative calculation to converge reactor and coolant temperatures in each time-step
- Transient simulations
- Establishing steady state



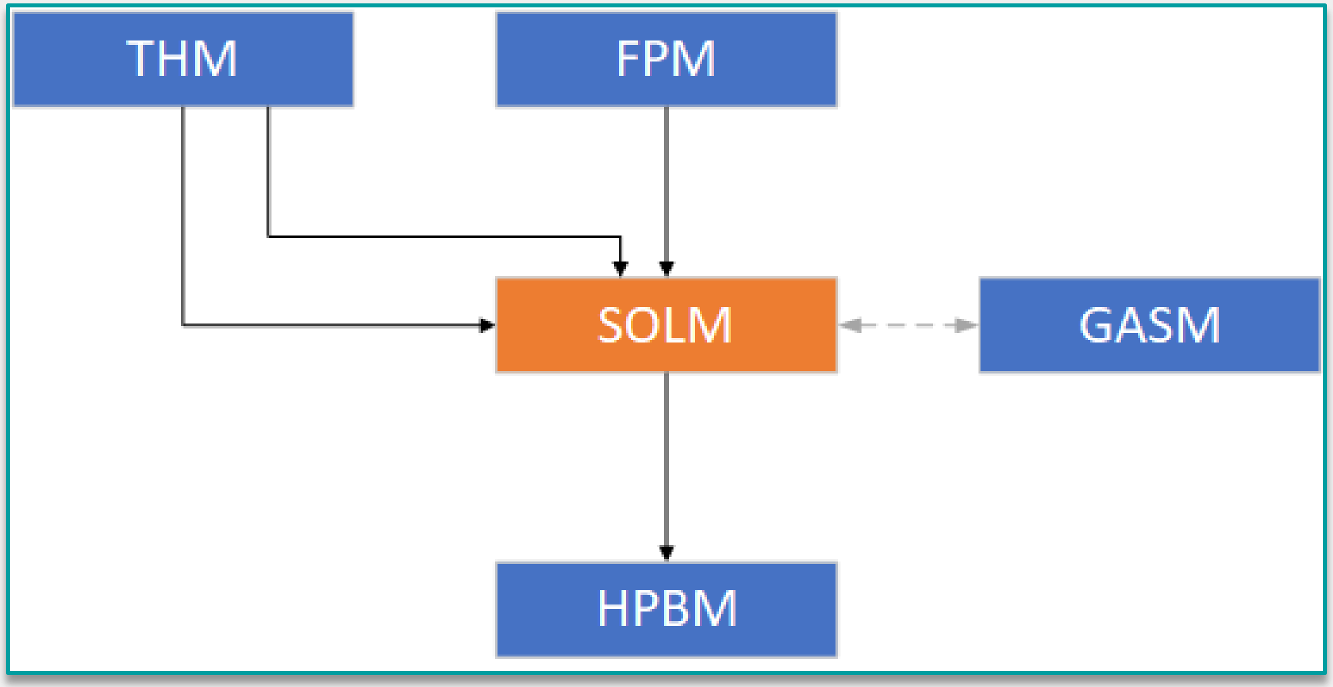
FPM (Particle Failure Probability Model)



FPM: Phenomena Modelled

- **Pressure vessel failure** of TRISO particles
  - effects of pyro-carbon (PyC) irradiation-induced creep on the effective stress of the silicon-carbide (SiC) layer
  - Irradiation-Induced dimensional change of PyC layer
  - Fission gas pressure
  - Kernel irradiation swelling
  - Kernel thermal expansion
- **Kernel migration** (Amoeba)
- **Fission product corrosion**
- **SiC thermal decomposition**
- **Manufacturing defects**
  - Exposed kernel (i.e., defect of all coating layers)
  - SiC defect (i.e., defect of the SiC layer with at least one other coating layer intact)
  - Inner PyC layer defect
  - Dispersed heavy metal fraction

SOLM (Fission Product Transport Model)



SOLM: Phenomena Modelled

- Fission product **production** by **direct fission** in kernels, **recoil** from kernels to the buffer layer, **decay** and **activation**

- Fission product **removal** by means of **decay** and **activation**

- **Transport and release** of fission products from particles and fuel elements by means of **diffusion**

- Effects on isotope transport and retention from **as-manufactured particle defects**, **contamination** and **particle failures** that may occur during operation

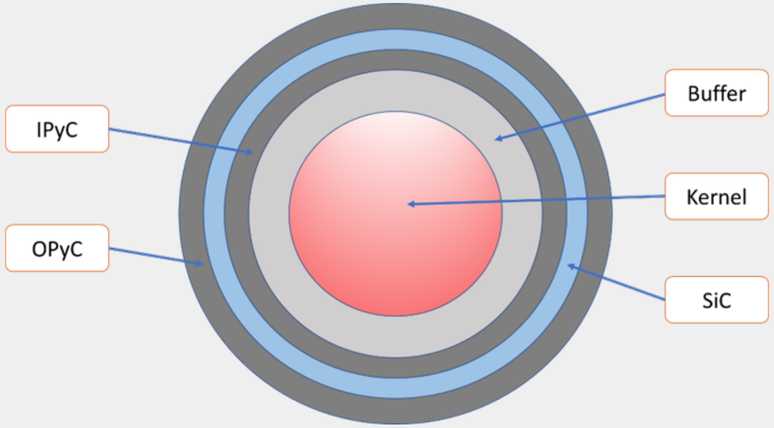


Table 4-2. Classes of radionuclides of interest for HTGR design.

Radionuclide Class	Key Nuclide	Form in Fuel	Principal In-Core Behavior	Principal Ex-Core Behavior
Tritium	H-3	Element (gas)	Permeates intact SiC; sorbs on core graphite	Permeates through heat exchangers
Noble gases	Xe-133	Element (gas)	Retained by PyC/SiC	Removed by helium purification system
Halogens	I-131	Element (gas)	Retained by PyC/SiC	Deposits on colder metals
Alkali metals	Cs-137	Oxide-element	Retained by SiC; some matrix/graphite retention	Deposits on metals/dust
Tellurium group	Te-132	Complex	Retained by PyC/SiC	Deposits on metals/dust
Alkaline earths	Sr-90	Oxide-carbide	High matrix/graphite retention	Deposits on metals/dust
Noble metals	Ag-110m	Element	Permeates intact SiC	Deposits on metals
Lanthanides	La-140	Oxide	High matrix/graphite retention	Deposits on metals/dust
Actinides	Pu-239	Oxide-carbide	Quantitative matrix/graphite retention	Retained in core

SOLM: Modelling Scope

- Calculate **isotope concentrations** in fuel elements and particles
  - **for all core meshes**, following the multi-pass re-loading scheme to reach desired burnup to create an isotope library with the concentration distributions (initial condition for steady-state inventory and transient calculations)
  - **for a single sphere/compact** to model irradiation and safety (annealing) experiments (validation) and isolated fuel element calculations
- Calculate the **release over birth (R/B) ratios** for steady-state irradiations and **fractional releases** for transients

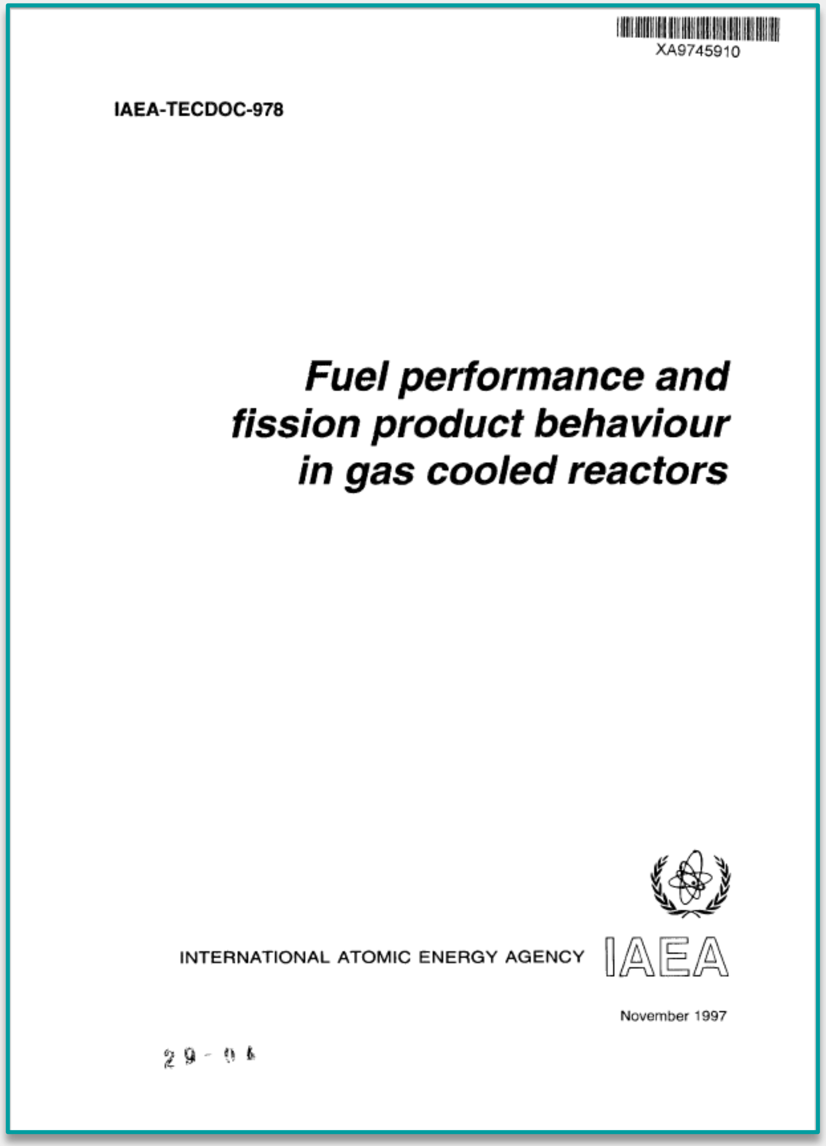
SOLM: Methodology

- Time-dependent heat conduction equation with temperature-dependent **effective diffusion coefficients**

$$D_{eff} = D_1 exp\left\{-\frac{Q_1}{RT}\right\} + D_2 exp\left\{-\frac{Q_2}{RT}\right\}$$

- 1D radial (pebbles) or 2D axi-symmetric (compacts)

- Boundary conditions: **Zero surface concentration** or **sorption transfer** via iso-thermic exchange between pebble surface and thin gas layer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IAEA-TECDOC-978

Fuel performance and fission product behaviour in gas cooled reactors

INTERNATIONAL ATOMIC ENERGY AGENCY IAEA

November 1997

SOLM: Numerical Solution

- **Implicit Euler method** for time-stepping for pebbles and compacts, or **backward-difference method (BDF2)** for compacts

- At each time step, a **system of linear algebraic equations** arising from the **finite difference discretization** of the diffusion and source terms is solved:

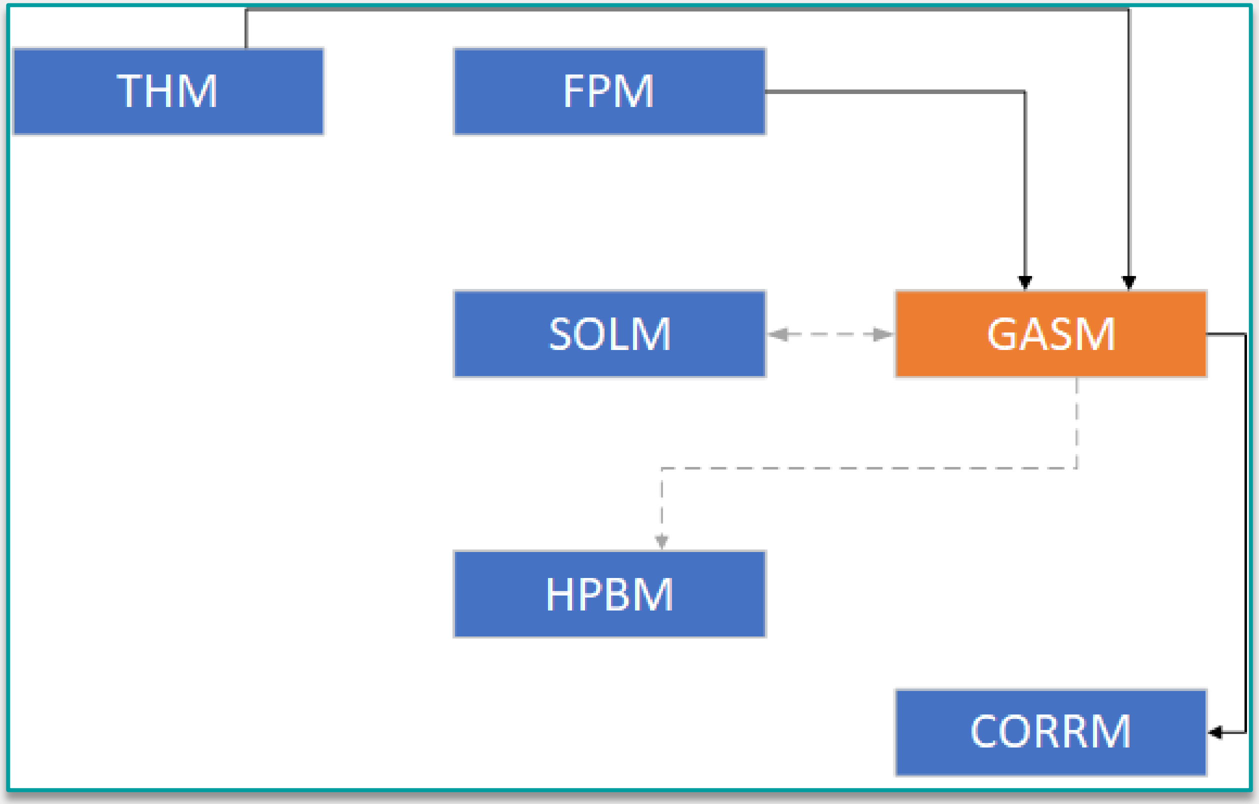
  $\Rightarrow$ 3-diagonal matrix system for pebble geometries

  – solved by Gaussian elimination

  $\Rightarrow$ 5-diagonal matrix system for compact geometries

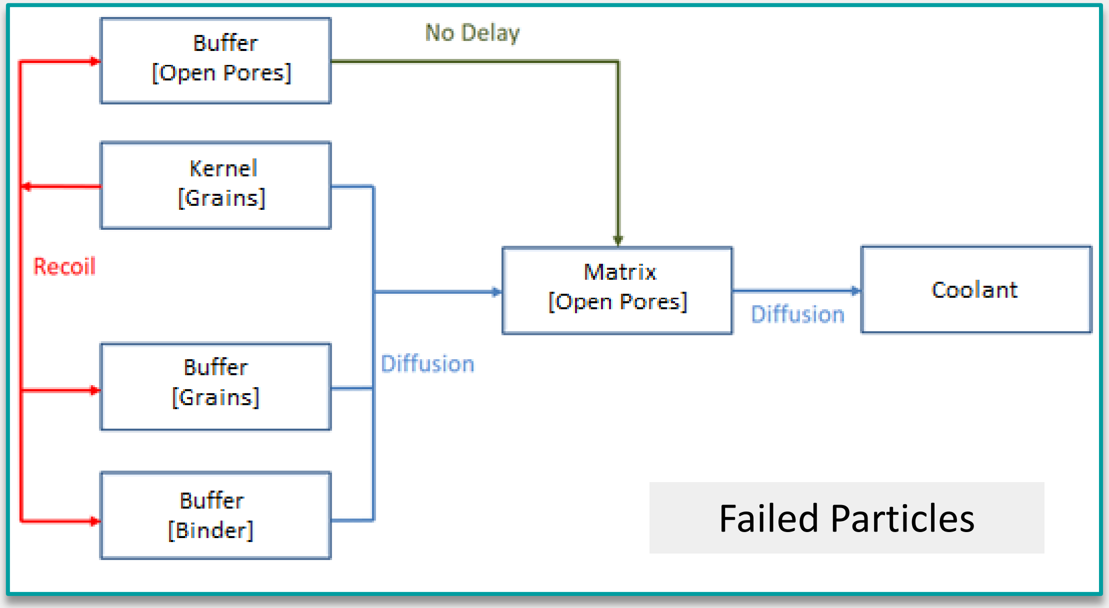
  – solved by the Gauss-Seidel iterations

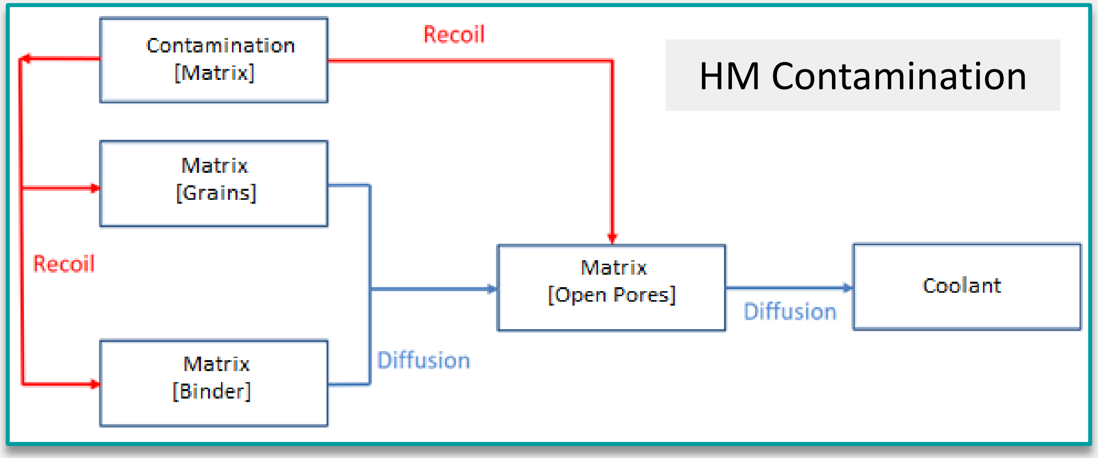
GASM (Gaseous Fission Product Transport Model)



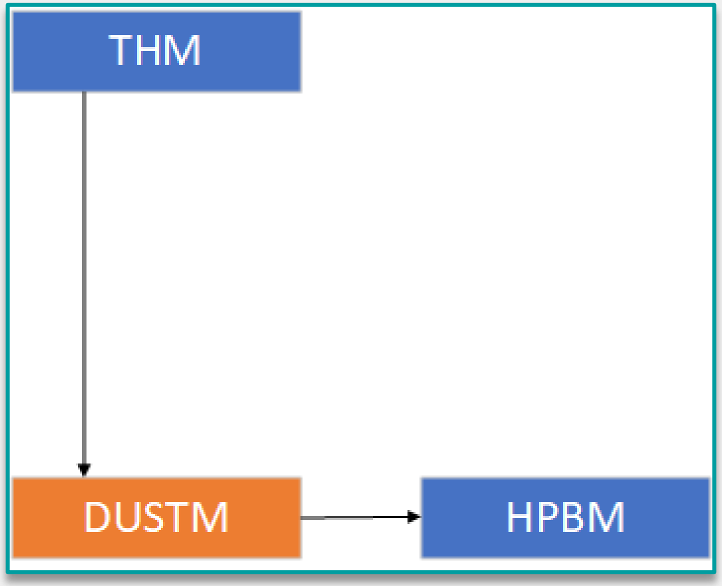
GASM: Phenomena Modelled

- Steady-state gaseous fission product (FP) release from particles and pebbles (R/B ratios)
- Short half-lives of the gas isotopes => transport from the fuel kernel through intact coatings can be neglected
- FP sources:
  - heavy metal (HM) contamination of matrix/outer PyC layers of particles
  - failed particles
- Two models dynamically switching based on fuel temperature: **Röllig Model** and **Richards Model**





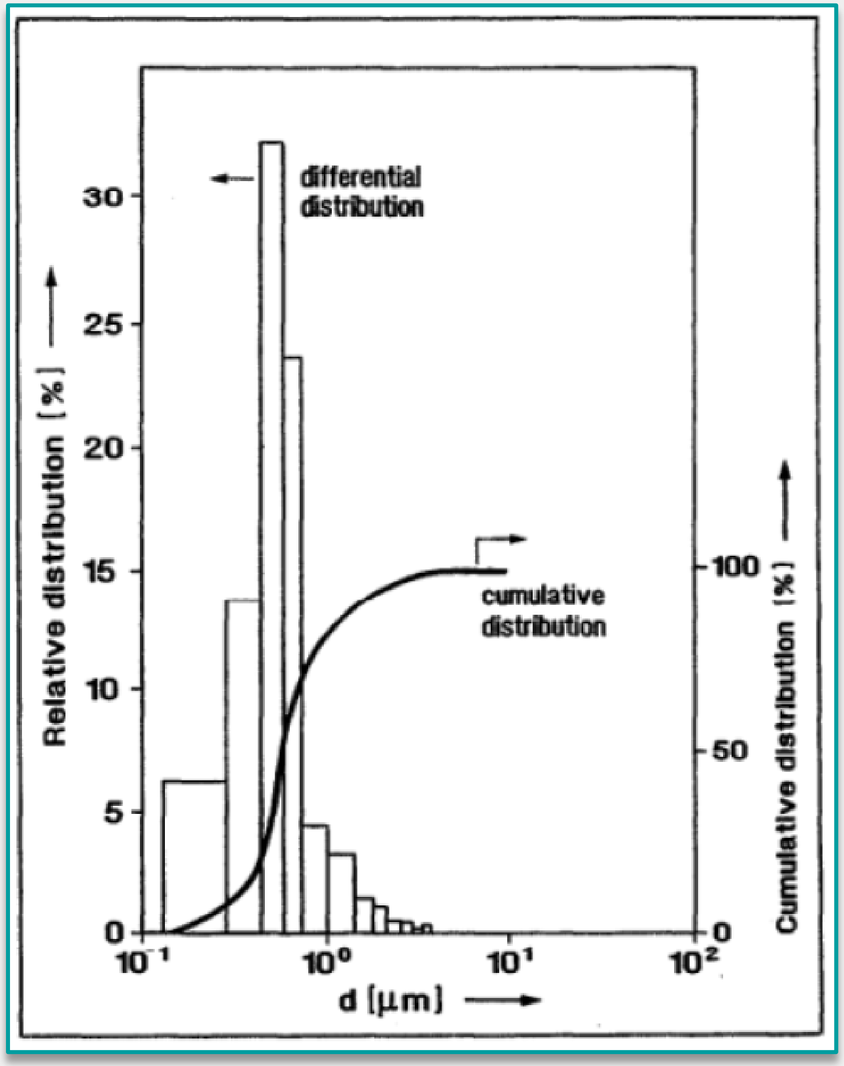
DUSTM: Dust Production



DUSTM: Phenomena Modelled

- Graphite and metallic dust production from
  - pebble-pebble and pebble-reflector abrasion
  - pebble abrasion during its transport through the fuel handling system (FHS) piping
  - control rod abrasion during its movements over the operating period

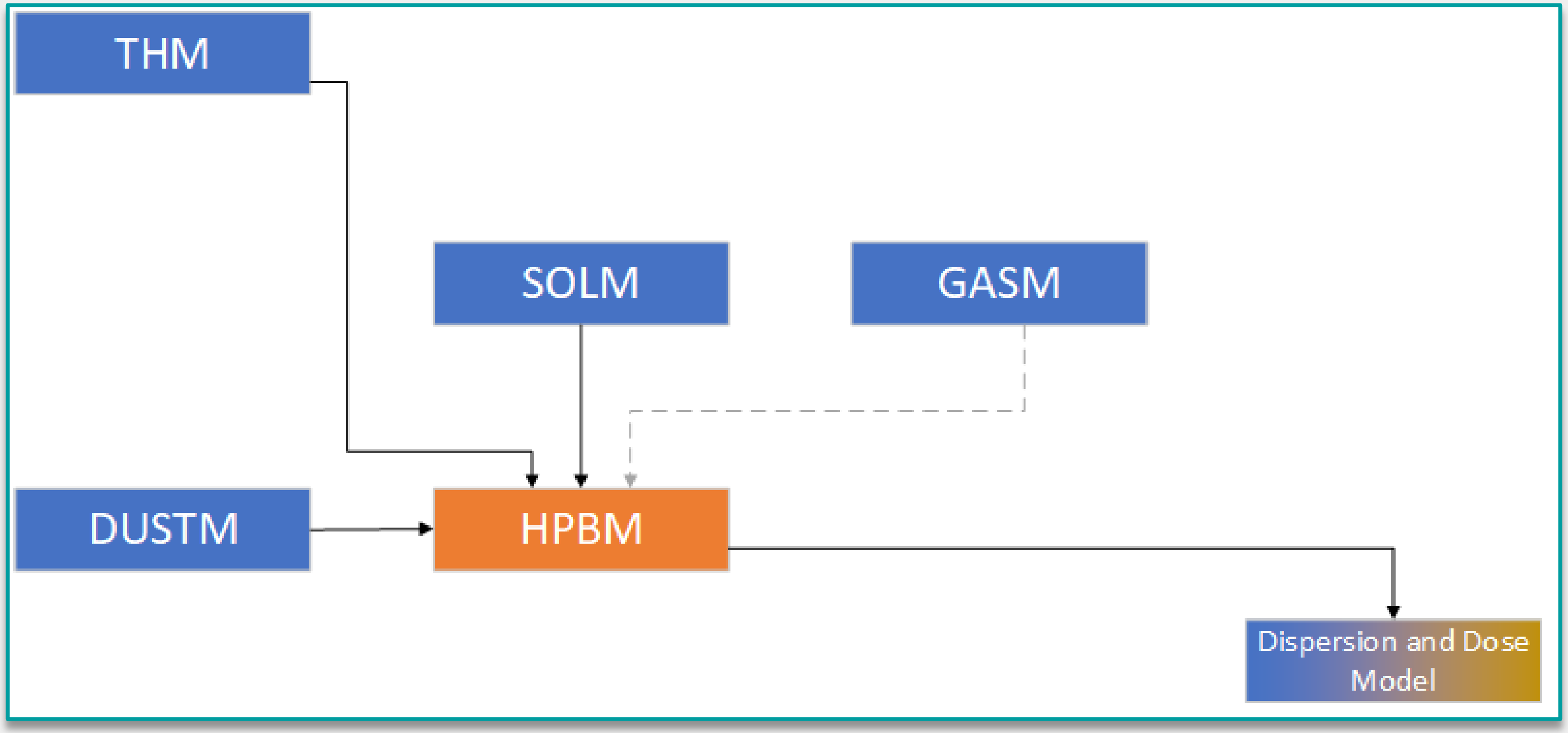
- Dust particle size spectrum lumped into bins, based on the historical measurements from the German pebble-bed reactor AVR



DUSTM: Methodology

- In-Core dust production
    - Wear from friction based on the theory of asperity contact
    - Total dust production proportional to geometry-dependent **dust production rate parameter** and **frictional force**
    - Frictional force proportional to temperature-dependent **friction coefficient** and height-dependent load pressure on the pebbles
    - **Load pressure** on the pebbles computed by modified Janssen's silo pressure formula including the effects of pressure drop
- Dust production in fuel handling system (FHS)
    - Proportional to empirically determined dust generation rate per meter of pebble movement in the FHS, number of fuel passes and length of the FHS pipe
- Dust production in the reactivity control system (RCS)
    - Proportional to empirically determined dust generation rate per meter of RCS rod motion and the total RCS rod distance travelled during the operation time
- **Dust production rate parameter** determined by applying the model on the AVR reactor operation data and adjusting the parameter to yield the measured total lifetime dust in AVR
    - Graphite/metallic dust ratio obtained from the Vampyr II experiment data

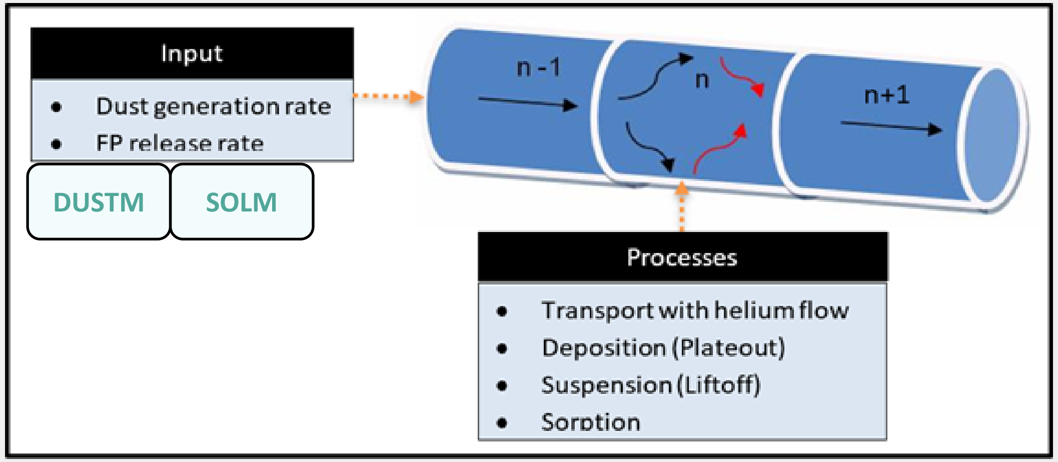
HPBM: Helium Pressure Boundary Model

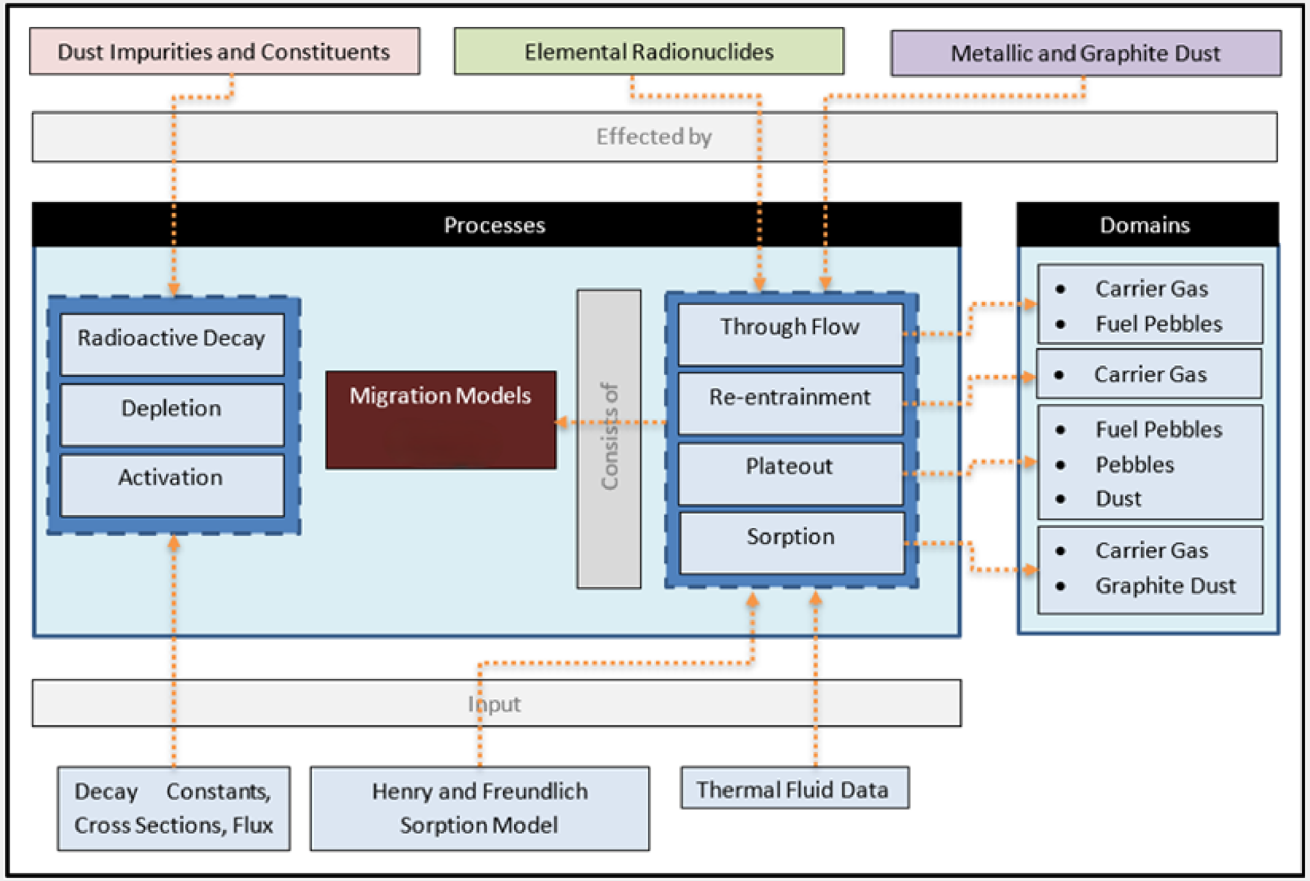


HPBM: Phenomena Modelled

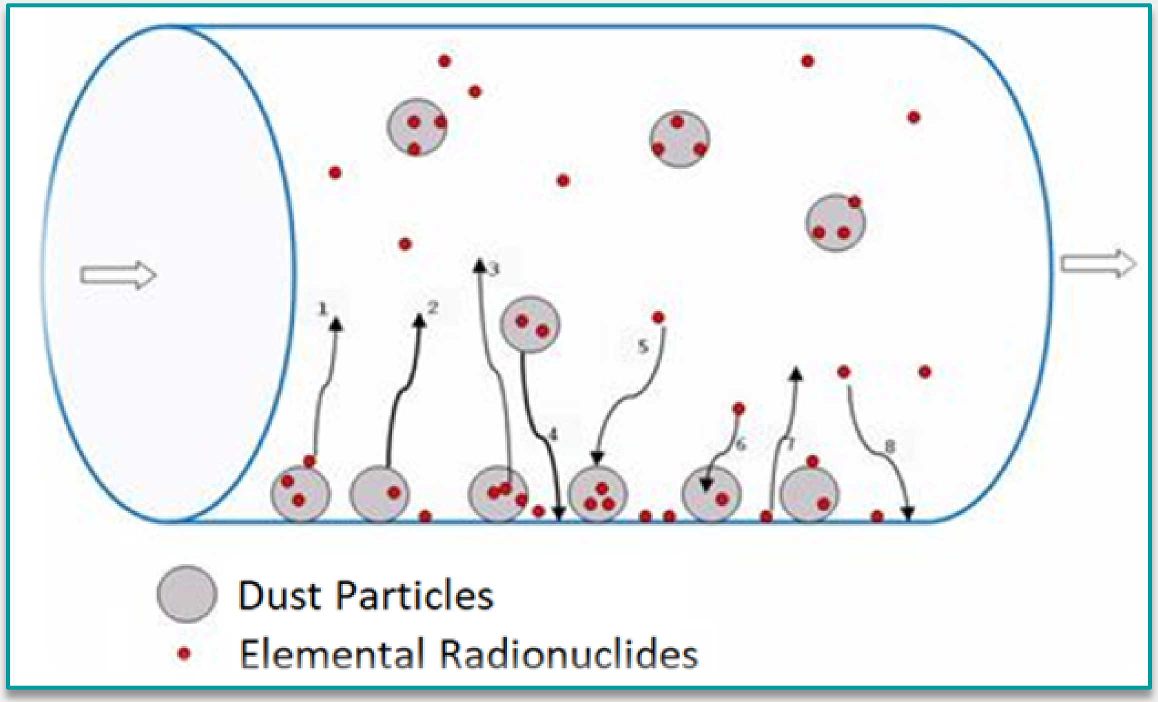
- radionuclide (RN) release from pebbles,
- deposition on component surfaces (RN, dust),
- plate-out on dust (RN)
- re-entrainment into circulating He (RN, dust),
- intra- and inter-component transport (RN, dust),
- RN transmutation through activation and radioactive decay
- RN removal through radioactive decay
- RN sorption into the graphite dust and de-sorption into circulating helium

HPBM: Phenomena Modelled





HPBM: Particle Mass Transfer



(1) Liftoff of elemental radionuclide from plated-out dust

(2) Liftoff of plated-out dust from component surface

(3) Sorption of elemental radionuclide from plated-out dust into helium

(4) Plateout of entrained dust onto component surface

(5) Plateout of entrained elemental radionuclide onto plated-out dust

(6) Sorption of entrained elemental radionuclide into plated-out dust

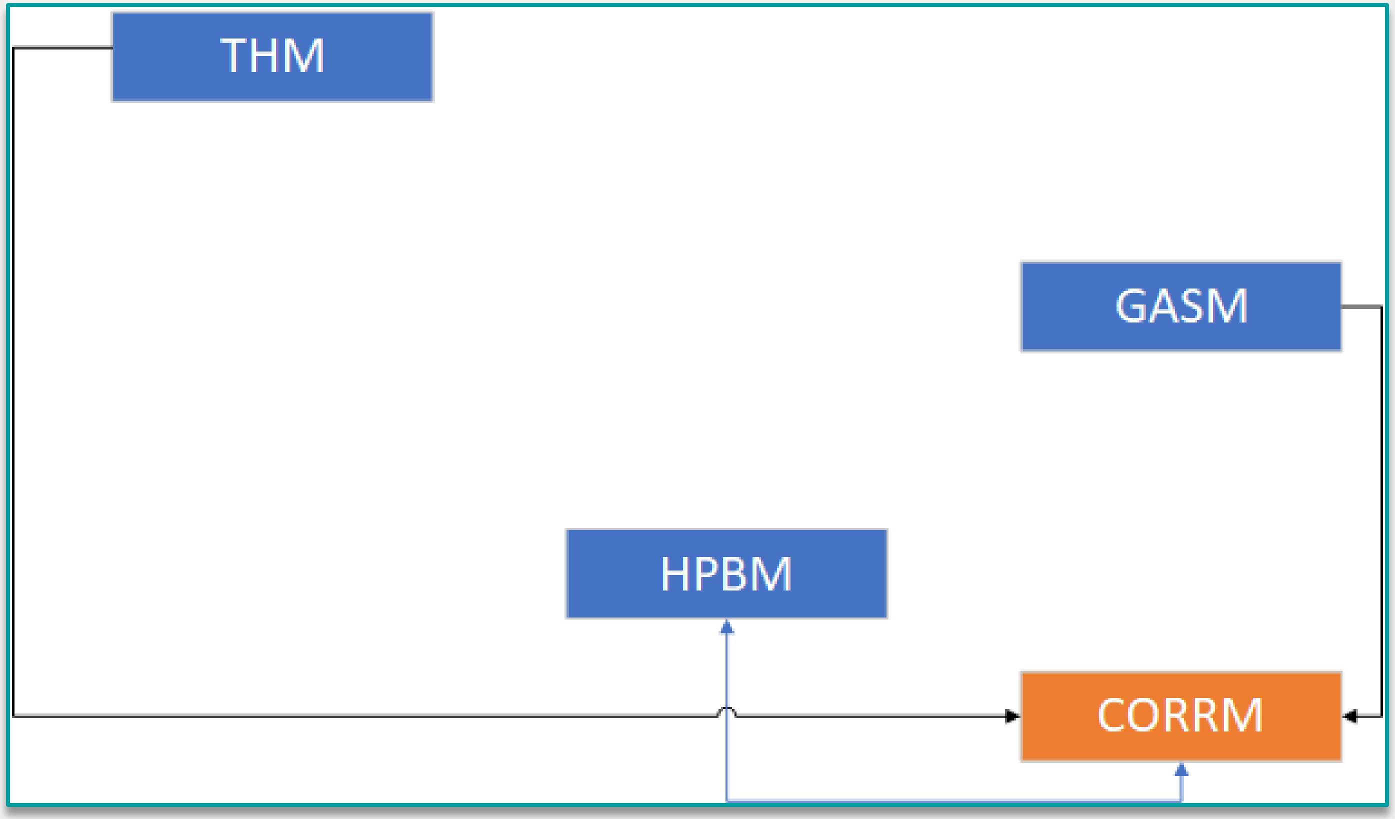
(7) Liftoff of elemental radionuclide from component surface

(8) Plateout of elemental radionuclide onto component surface

HPBM: Numerical Solution

- Coupled set of 2D partial differential equations for multi-phase flow and mass balance
- Phases:
  1. Helium gas
  2. Circulating dust
  3. Deposited dust
  4. Circulating isotopes
  5. Deposited isotopes
- Finite volume + Backward Implicit-Explicit Method (IMEX) discretization

CORRM: Core Corrosion Model



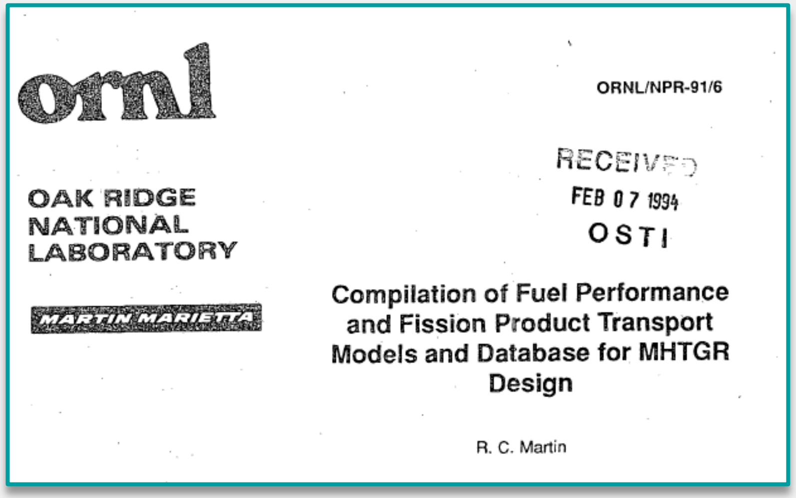
CORRM: Methodology

$$\text{Corrosion Rate} = \frac{(\text{Kinetic Factor})(\text{Driving Force})}{(\text{Adsorption Term})}$$

with temperature-dependency of kinetic factor and adsorption terms modelled by Arrhenius-type correlation

- Applied to fuel element graphite materials to determine the radionuclide release enhancement due to corrosion
- Based on correlation for H-451 fuel element graphite investigated at General Atomics

Material	State	Atmosphere
UCO kernel	Normal	Trace H_2O
	DLOFC	Air/He
PyC coating	H_2O ingress	H_2O/He
“US A3-3” matrix	Normal	Trace H_2O
	DLOFC	Air/He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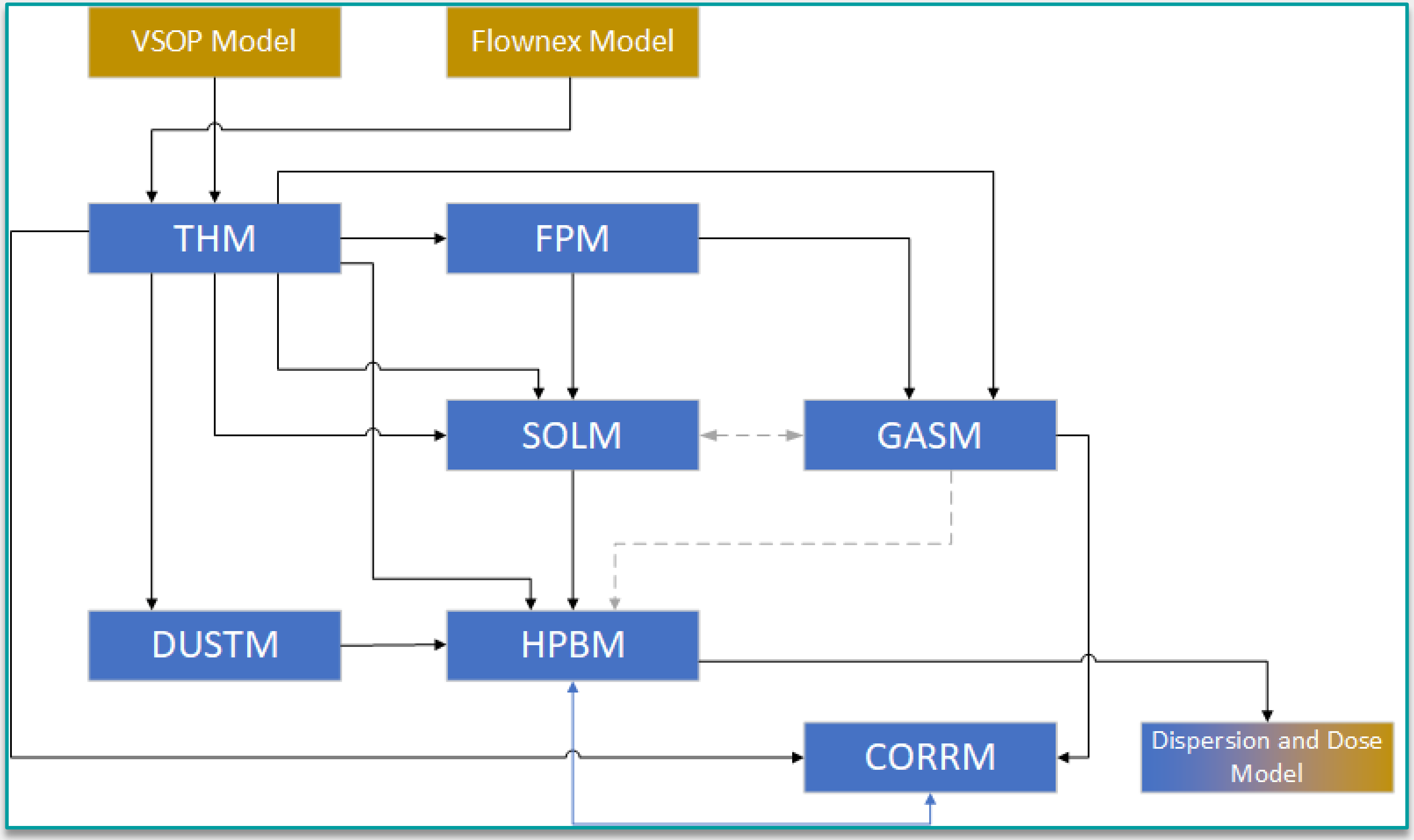
MARTIN MARIETTA

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design

R. C. Martin

Overall Mechanistic Source Term Calculation



Q & A

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List of Acronyms

CORRM	Corrosion model	**PyC**	Pyrolytic-carbon
DLOFC	Depressurized loss of forced cooling	**Q&A**	Questions & answers
DOE	Department of Energy	**R/B**	Release to birth ratio
DUSTM	Dust production model	**RCS**	Reactivity control system
FHS	Fuel handling system	**RG**	Regulatory Guide
FP	Fission product	**RN**	Radionuclide
GASM	Gaseous FP release model	**SiC**	Silicon-Carbide
HM	Heavy metal	**SOLM**	RN diffusion and release model
HPBM	Helium pressure boundary model	**THM**	Thermo-hydraulics model
HTGR	High Temperature Gas-cooled Reactor	**TR**	Topical Report
KSIM	Neutron kinetics & plant simulation model	**TRISO**	Tristructural-Isotropic
MST	Mechanistic source term	**TRITM**	Tritium release model
NQA	Nuclear Quality Assurance	**UCO**	Uranium Oxycarbide
PIRT	Phenomena identification and ranking table	**XSTERM**	X-energy's mechanistic source term code suite