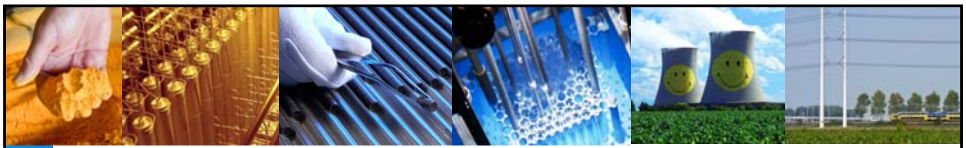

Coupled neutronics and thermal hydraulics calculations for MSR

4-11-2013

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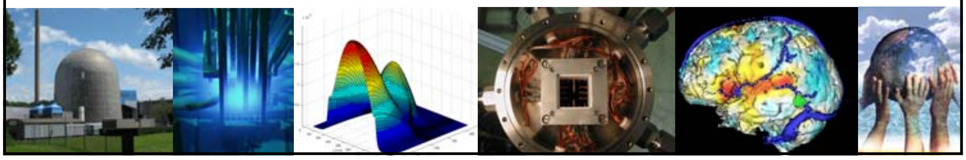
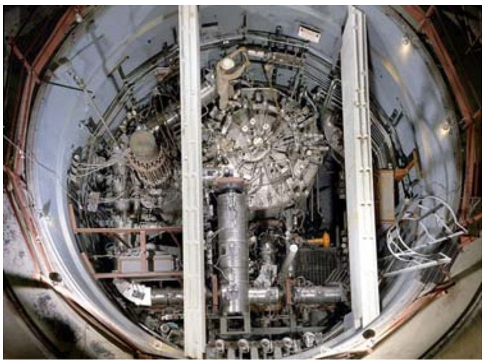


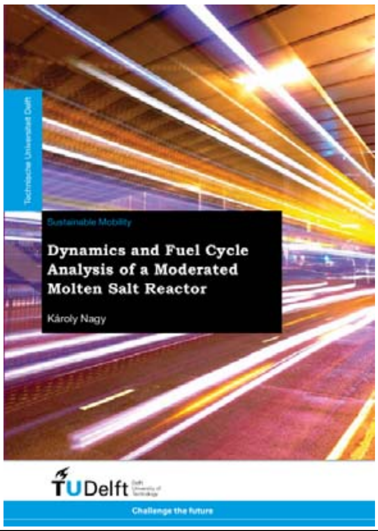
Three main concepts

- Molten Salt Reactor Experiment



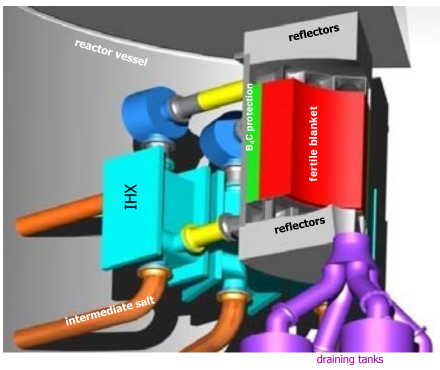
Three main concepts

- Molten Salt Self-Breeder Reactor (TU-Delft design)



Three main concepts

- Molten Salt Fast Reactor (Gen-IV design, CNRS)



Molten Salt Reactor Experiment

- Developing calculation scheme for MSR
  - 3D
  - time-dependent
  - feedback by coupling neutronics and thermal calculations
  - Model the MSRE
  - Keep programs general
- Assumptions
  - Fuel velocity field is input
  - Flow parallel to the axis of the core

Neutron diffusion code DALTON

DALTON used for simulations is a mature in-house developed neutronics code (pm 2001)

- Multigroup diffusion model
- Geometry: 2D (rz, xy), 3D (xyz, rθz)
- Eigenvalue (alpha + lambda modes)
- Steady-state and transient capabilities
- Precursors included
- Mostly used previously for coupled calculations in the field of HTR and MSR systems

$$\frac{1}{v_g}\frac{\partial \Phi_g}{\partial t} = \nabla \cdot D_g \vec{\nabla}\Phi_g - \Sigma_g^r \Phi_g + \sum_{g \neq g'}^{G} \Sigma_{g\to g'}^s \Phi_{g'} + \chi_p \sum_{g'}^{G} (1-\beta)\nu\Sigma_{g'}^f \Phi_{g'} + \sum_i^I \lambda_i \chi_d C_i$$

$$\frac{\partial C_i}{\partial t} = \sum_{g'}^{G} \beta_i \nu \Sigma_{g'}^f \Phi_{g'} - \lambda_i C_i - \nabla \cdot \left(C_i \vec{u}\right)$$

MSRE: Discretization of the precursor equation

- Pump transients can induce strong gradient of precursor concentration
- Discretization: $$\frac{\partial C}{\partial t} = -\nabla uC + \ldots$$

$$\Delta V \frac{\partial C_i}{\partial t} = u_{i-1/2}\Delta A_{i-1/2} C_{i-1/2} - u_{i+1/2}\Delta A_{i+1/2} C_{i+1/2} + \ldots$$

- Requires evaluation of the face value:

Upwind

$$C_{i+1/2} = C_i$$

TVD (total variation diminishing)

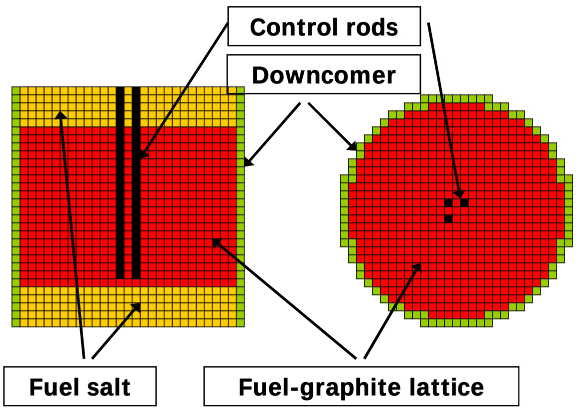
$$C_{i+1/2} = C_i + \frac{1}{2}\Psi\left(\frac{C_{i+1} - C_i}{C_i - C_{i-1}}\right)(C_i - C_{i-1})$$

$$\Psi(r) = \frac{r + |r|}{1 + r}$$

Reduces numerical dispersion

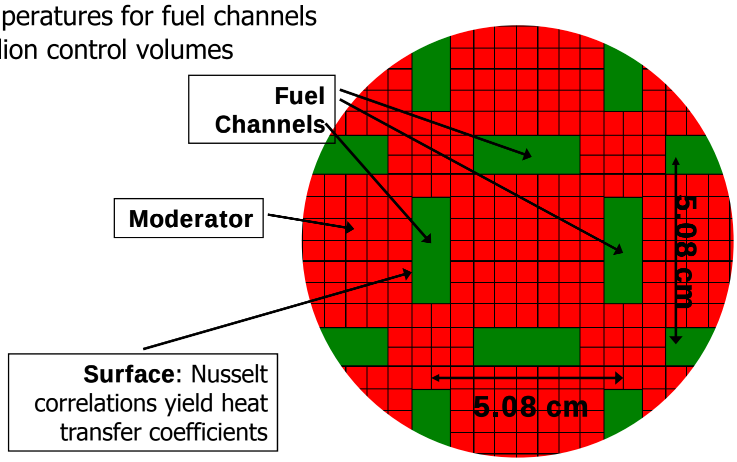
3D model of MSRE

- Approximating cylindrical reactor in X-Y-Z geometry
- 8 group cross section library by SCALE
- Internal albedo boundaries for control rods



3D model of MSR

- Fuel: Heat convection (vertical)
- Moderator: Heat conduction (3D)
- Individually calculating each fuel channel (1150 channels)
- Bulk temperatures for fuel channels
- ~1.5 million control volumes



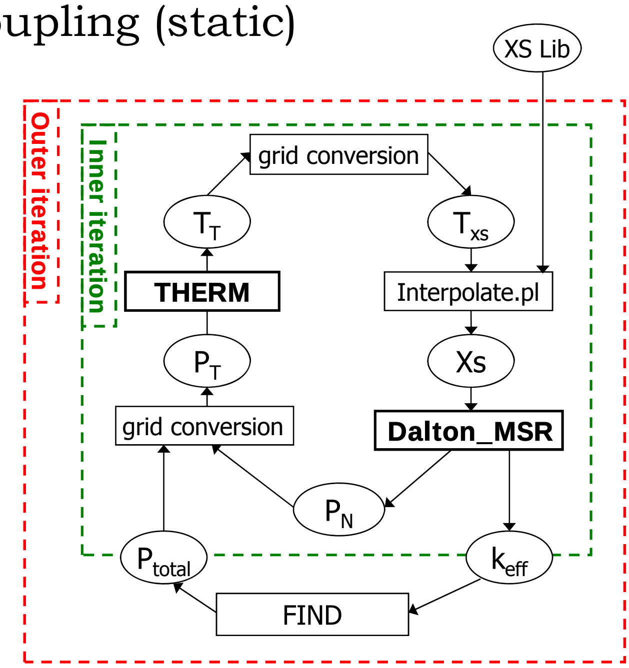
MSRE: Coupling (static)

Nested iterations

- obtain k_{eff} for a given power
- obtain power for $k_{eff} = 1$

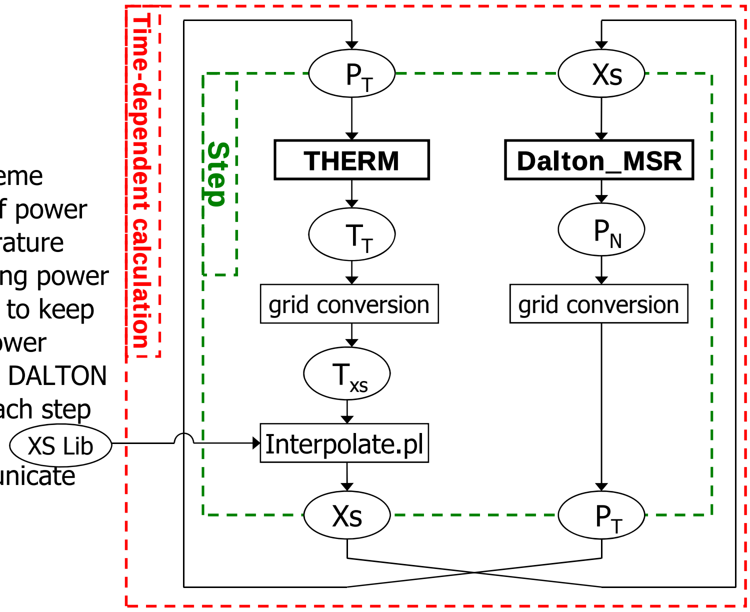
Temperature step of base XS library:
ΔT=100°C

Interpolation by SCALE/ICE



MSRE: Coupling (dynamic)

- Explicit scheme
- Exchange of power and temperature
- Renormalizing power distribution to keep the total power
- THERM and DALTON calculate each step separately and communicate afterwards

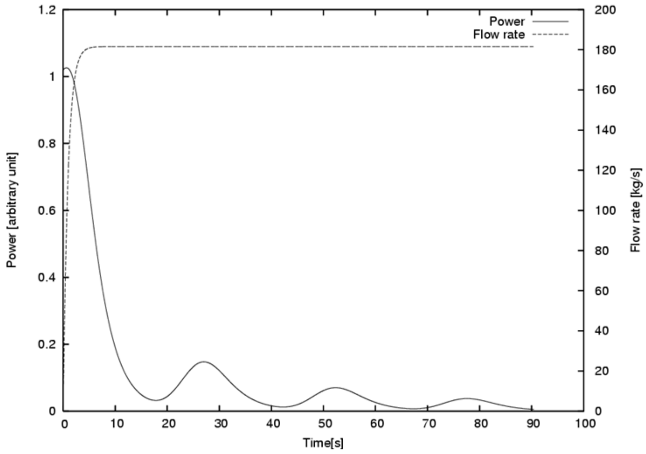


MSRE: Feedback Coefficients

	Fuel temp. coeff. α_f	Moderator temp. coeff. α_m
Calculation	-9.77 pcm/K	-6.31 pcm/K
Measurement (MSRE)	-8.46 pcm/K	-4.68 pcm/K
Difference	14 %	26 %

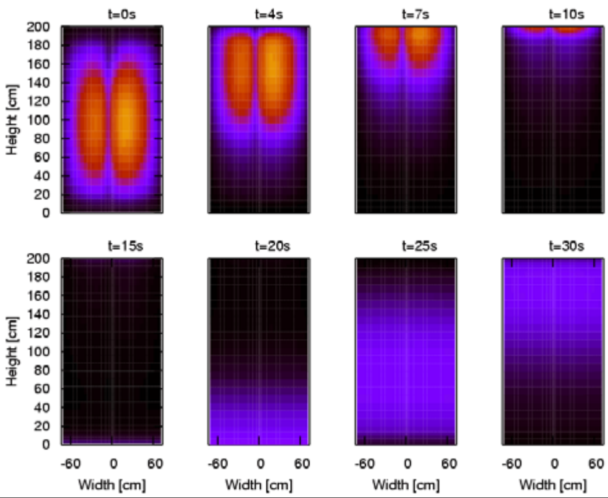
MSRE: Pump start up

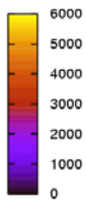
- Typical fluid-fuel transient
- Power: 1W
  no feedback
- Beginning:
  - fuel stationary
  - k_{eff} = 1
- Starting fuel pump



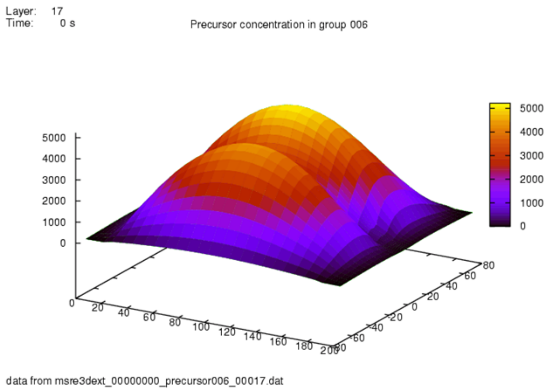
MSRE: Pump start up

Precursor concentration group 6 (longest $T_{1/2}$)



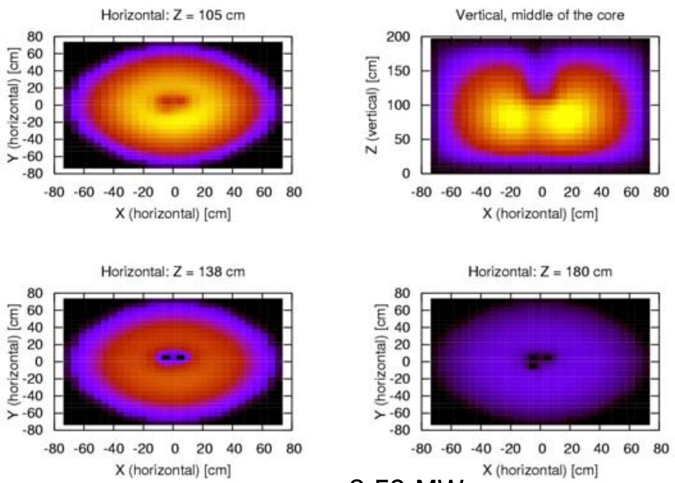


MSRE: Pump start up



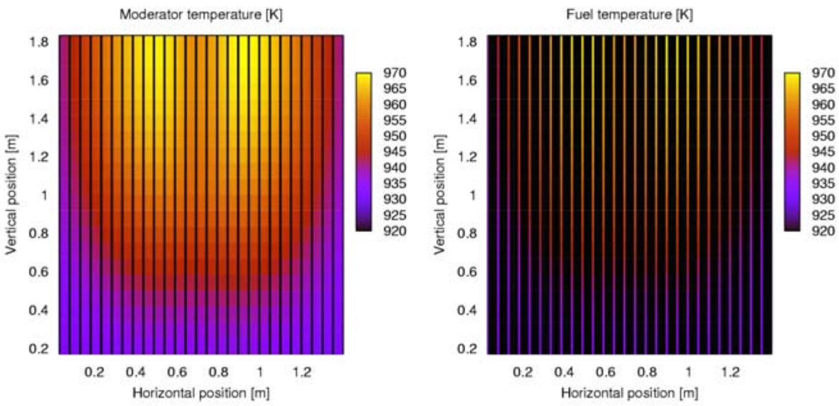
Precursor concentration group 6 (longest half-life)

MSRE: Thermal flux (static)



power 8.59 MW

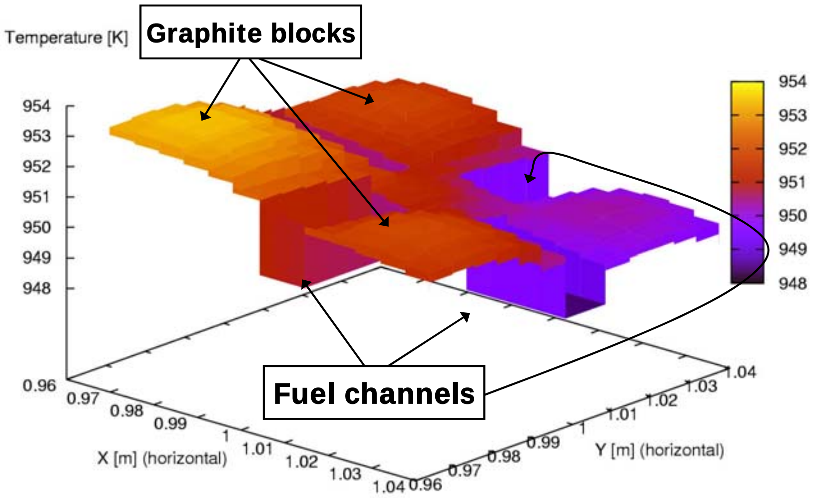
MSRE: Temperature field (static)



power 8.59 MW

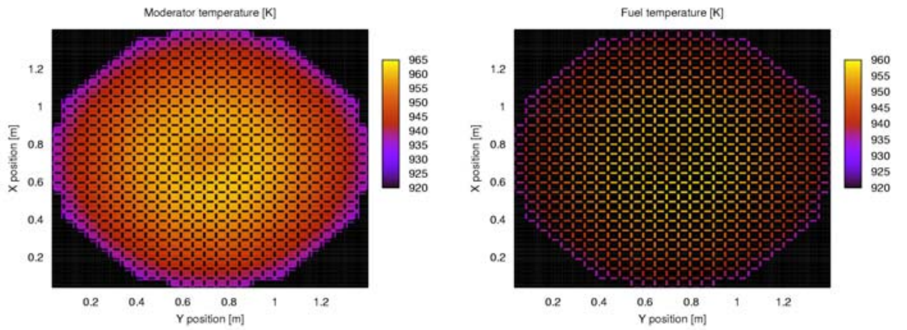
MSRE: Temperature field close up

High resolution calculation to determine the surface temperature of the graphite and the heat transfer



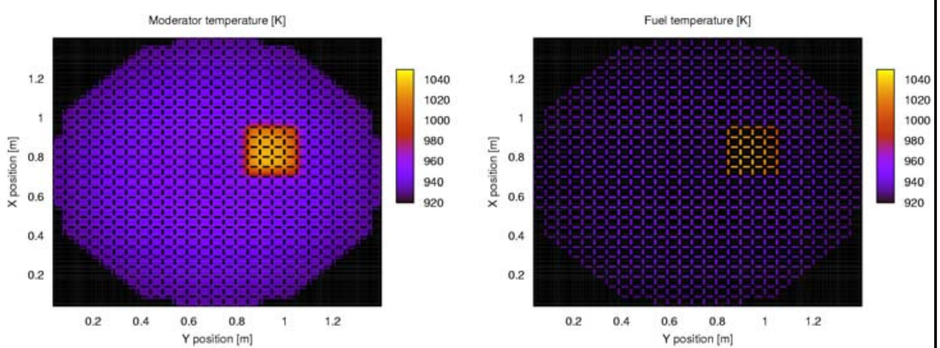
MSRE: Temperature field (static)

Horizontal cross-sectional of temperature fields at the middle of the core



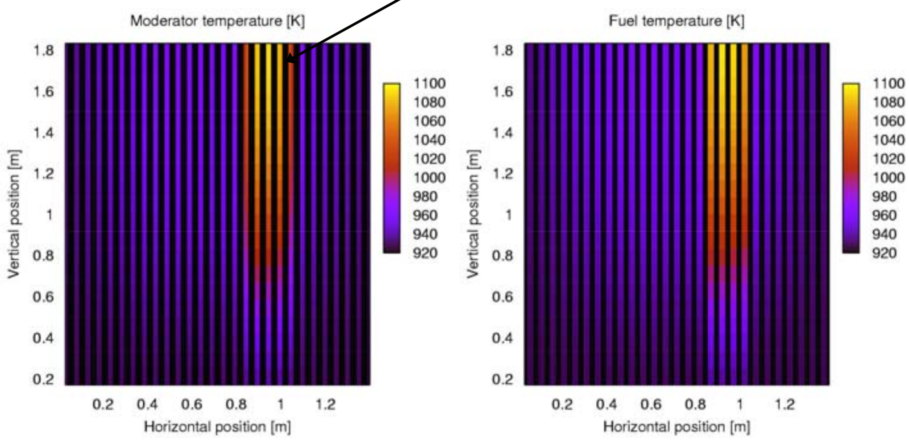
MSRE: Debris accident

- Debris gets into primary loop
- Blocks some of the fuel channels - mass flow reduced by 80%
- Total mass flow maintained
- Power reduces: 8.59 MW → 8.32 MW

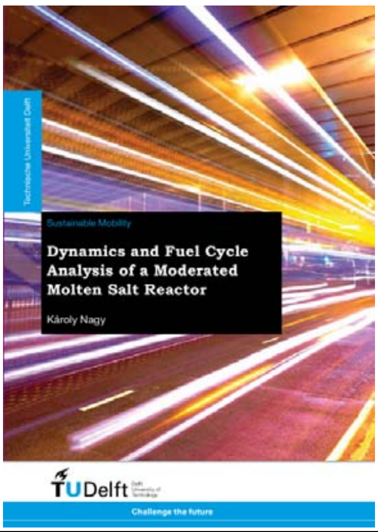


MSRE: Debris incident

Graphite conducts the heat from blocked channels

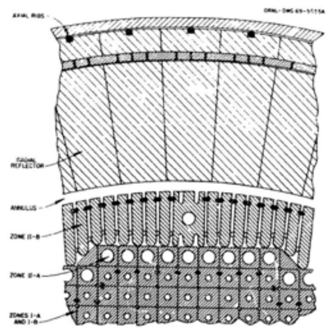


Molten Salt Self-Breeder Reactor



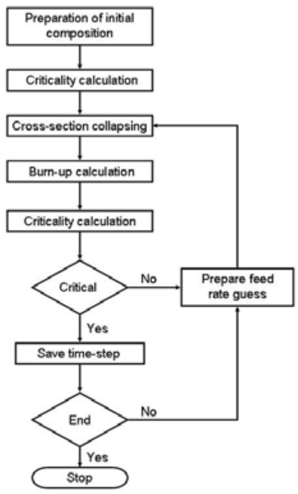
Molten Salt Breeder Reactor

- ORNL design from the late 1960s
- 1000 MWe, breeder MSR
- Single fuel, single pass, moderated
- Salt composition: $LiF\text{-}BeF_2\text{-}ThF_4\text{-}UF_4$
- The project was canceled in 1970
- The volume of the primary loop had to be processed in 10 days
- The global temperature feedback coefficient of the MSBR was positive



Optimization methodology

- Calculate 50 years of full power operation
- Core radius: 2.5 m
- Core height: 5 m
- Salt composition: $LiF\text{-}BeF_2\text{-}ThF_4\text{-}UF_4$
- Channel arrangement: triangular lattice
- Number of fuel channels: varies
- Channel diameter: varies (6 cm)
- Thorium concentration: varies (12 mol%)
- Volume ratio: varies (3)
- Power density: varies (5 MW/m^3)



Sensitivity to channel diameter

Homogeneous core: high Pa production, but high U-233 load.

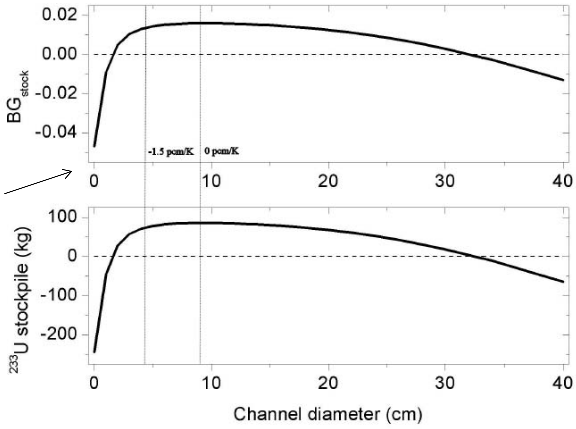


Figure 4.2: Effect of the variation of the channel diameter on the breeding gain. Th concentration: 12 mol%, power density: 5 MW/m^3, volume ratio: 3. The temperature feedback coefficient of the core increases as the channel diameter increases. The -1.5 pcm/K and 0 pcm/K points are shown in the figure.

Sensitivity to volume ratio

High Pa production, but high U-233 load.

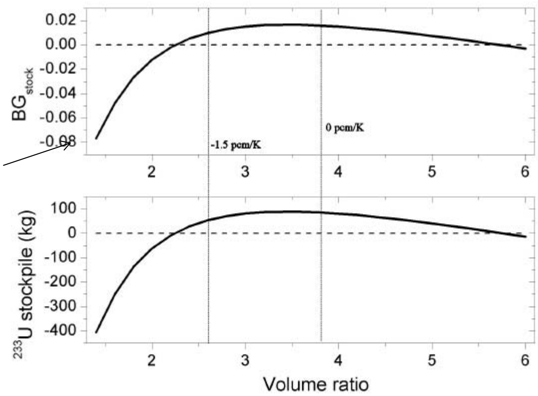
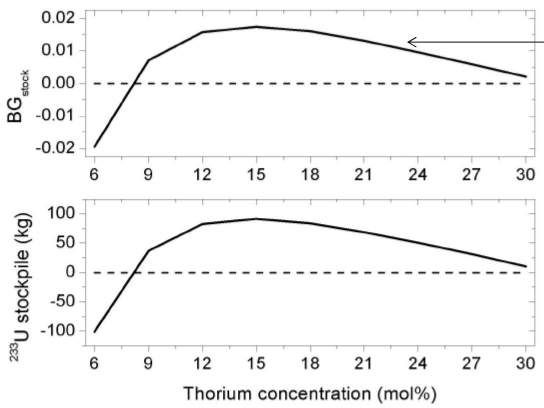


Figure 4.3: Effect of the variation of the volume ratio on the breeding gain. Th concentration: 12 mol%, power density: 5 MW/m^3, channel diameter: 6 cm. The temperature feedback coefficient of the core increases as the volume ratio increases. The -1.5 pcm/K and 0 pcm/K points are shown in the figure.

Sensitivity to thorium concentration

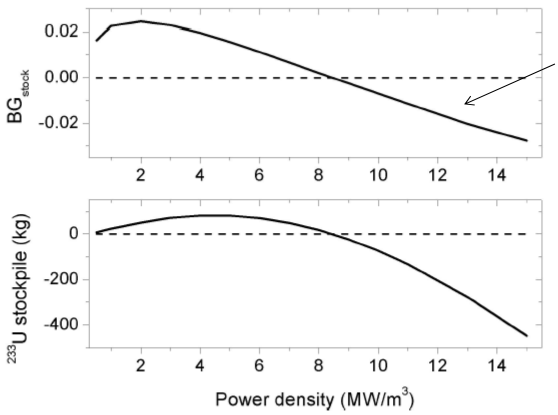


Harder spectrum; higher critical load

Remark: Th substitutes light elements in the salt

Figure 4.4: Effect of the variation of the thorium concentration on the breeding gain. Channel diameter: 6 cm, power density: 5 MW/m^3, volume ratio: 3.

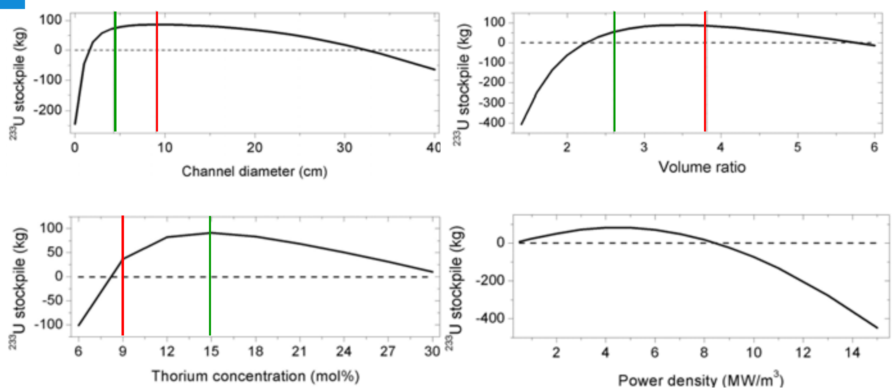
Sensitivity to power density

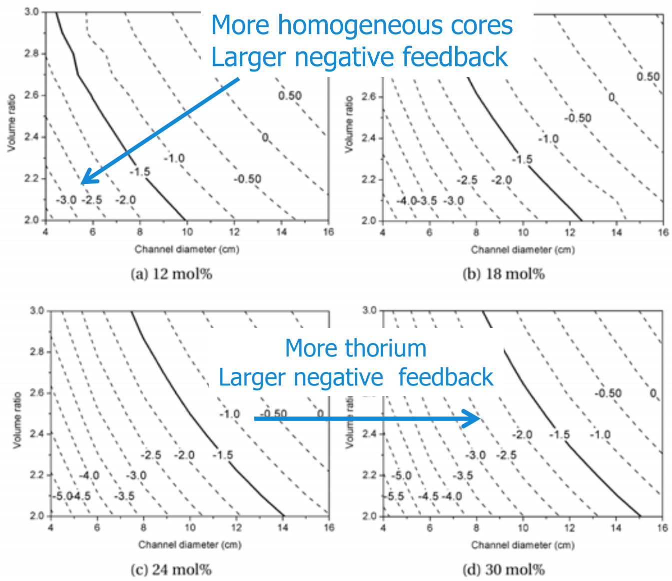


Power up
BG down

Figure 4.5: Effect of the variation of the power density on the breeding gain. Th concentration: 12 mol%, channel diamter: 6 cm, volume ratio: 3.

Effects of the parameter variation





Final optimization results

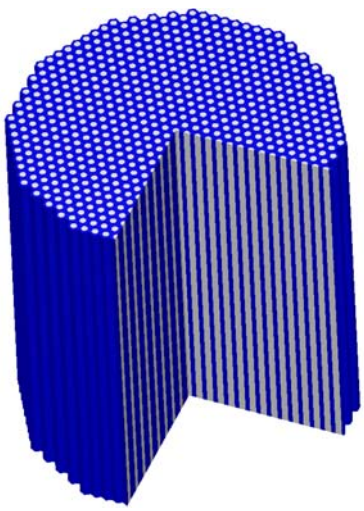
Table 4.4: Power density and corresponding graphite lifetime for self-breeder cores

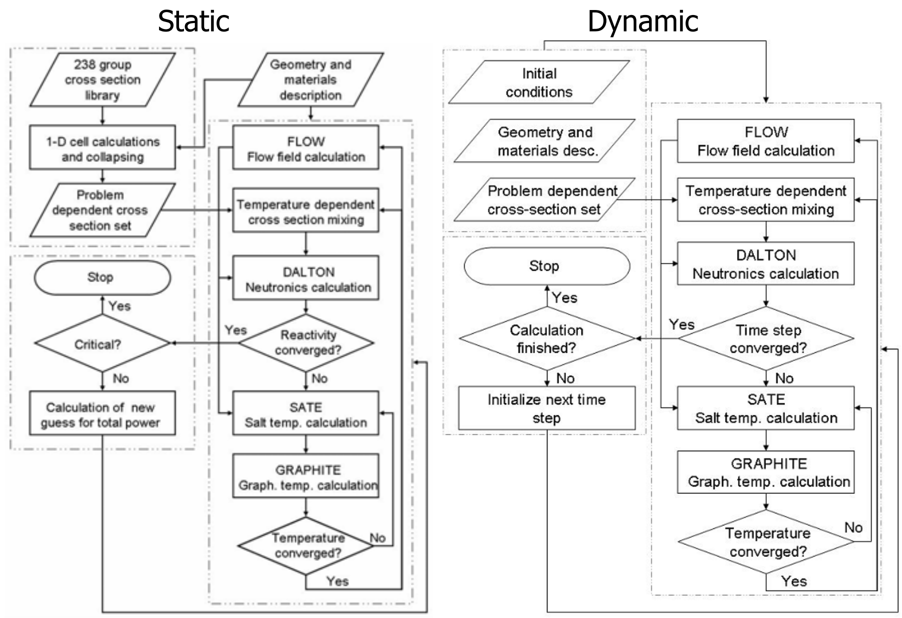
Th	(mol%)	Channel diameter (cm)						
		3	4	5	6	7	8	9
12	Volume ratio	3.5	3.1	2.8	2.6	2.4	2.25	2.1
	BOL load (kg)	1067	1172	1273	1347	1445	1527	1628
	Power density (MW/m^3)	8.52	8.22	7.84	7.55	7.04	6.55	5.8
	Flux level($\cdot 10^{14}/cm^2s$)	2.02	1.89	1.75	1.65	1.51	1.38	1.20
	Lifetime (PP)	13.1	13.5	14.1	14.5	15.4	16.4	18.3
	Lifetime (AP)	20.9	21.5	22.4	23.1	24.6	26.2	29.4
15	Volume ratio	4	3.5	3.15	2.85	2.65	2.45	2.3
	BOL load (kg)	1112	1242	1356	1484	1580	1702	1805
	Power density (MW/m^3)	9.75	9.5	9.19	8.71	8.25	7.71	7.11
	Flux level($\cdot 10^{14}/cm^2s$)	2.28	2.13	2.00	1.84	1.74	1.56	1.42
	Lifetime (PP)	11.2	11.4	11.7	12.2	12.7	13.6	14.6
	Lifetime (AP)	17.8	18.2	18.7	19.6	20.2	21.8	23.3

PP - Peak Power
AP - Average Power
Lifetimes are given in full power years

Description of the final design

- Vessel radius 3 m
- Core radius 2.4 m
- Vessel height 6.9 m
- Core height 5 m
- Plenum height 0.2 m
- Number of fuel channels 1327
- Channel diameter 0.07 m
- Salt composition LiF - BeF_2 - ThF_4 - UF_4
- Thorium conc. 15 mol%
- Mass flow rate 5395 kg/s
- Length of primary loop 30 m
- Power production 792 MW



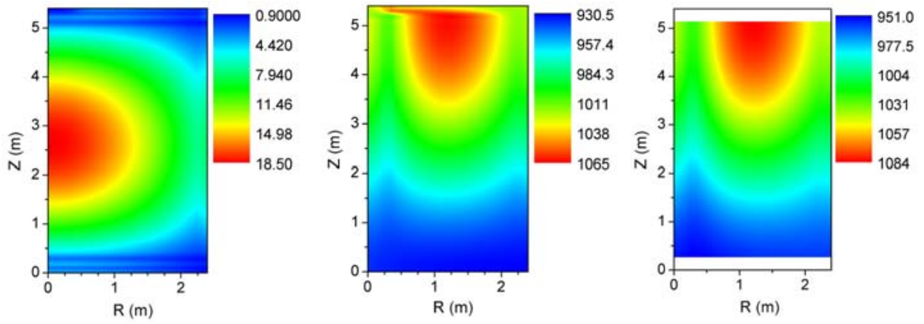


Building blocks of the calculations

- Salt temperature calculation:
  1-D channels, 2-D plena and 1-D primary loop
- Graphite temperature calculation:
  3-D finite element calculation on the whole volume
- Flow field calculation:
  2-D porous media
- Reactor physics calculation:
  2-D diffusion calculation

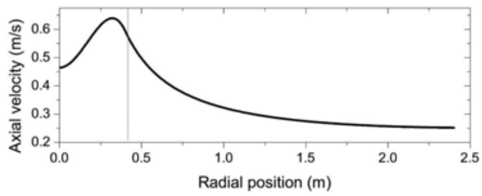
Results of steady-state calculations

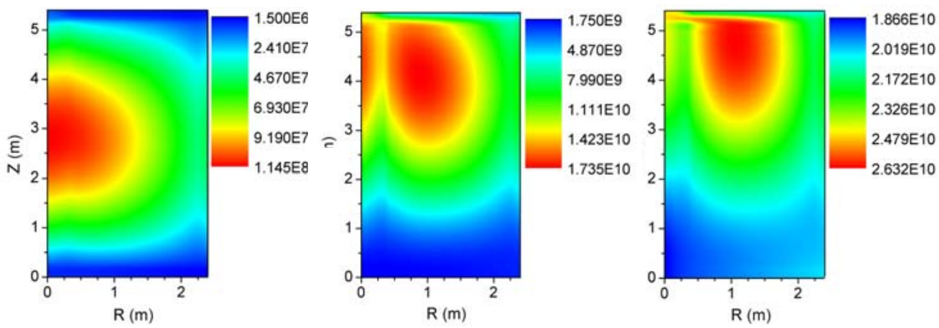
- Feedback coefficient of the salt: -3.86 pcm/K
- Feedback coefficient of the graphite: 2.16 pcm/K



Power density [MW/m^3]   Salt temp [K]   Graphite temp [K]

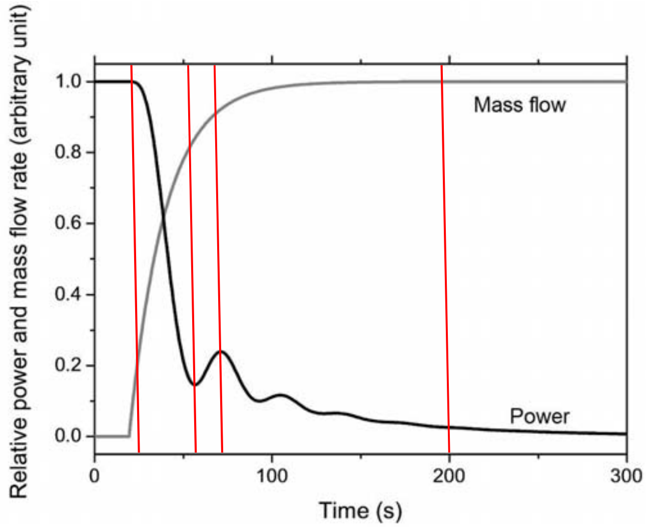
Distribution of precursors

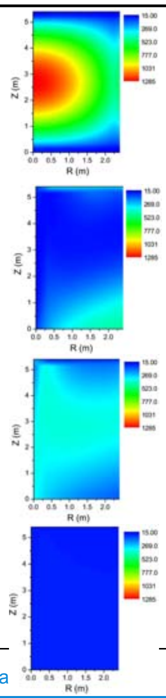




T=0.2 s   T=5 s   T=54 s

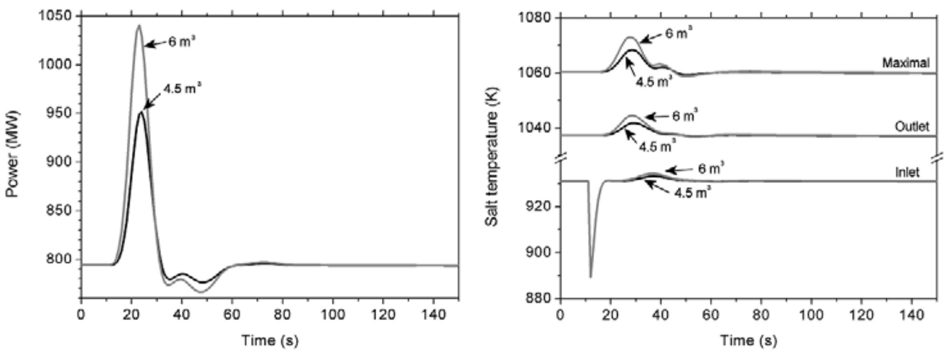
Zero-power pump start





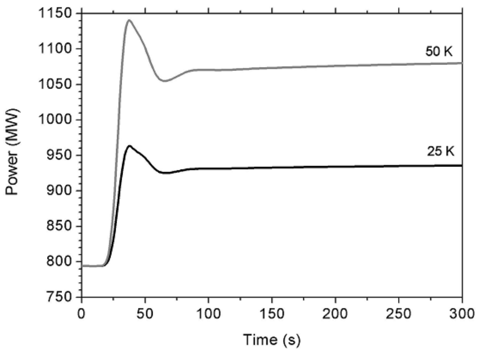
Slug flow transient

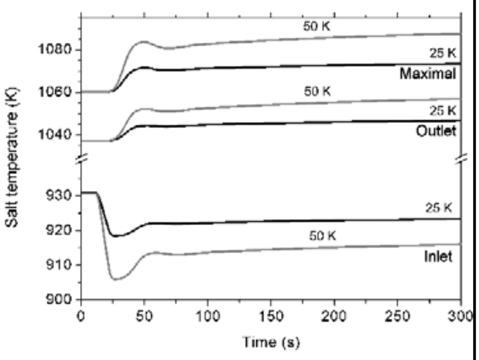
Insertion of cold salt (T-50 K) to the primary loop



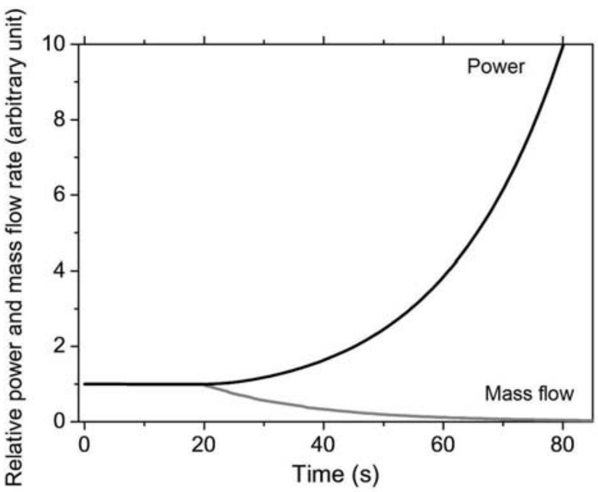
Overcooling transient

Temperature decrease secondary site heat exchanger

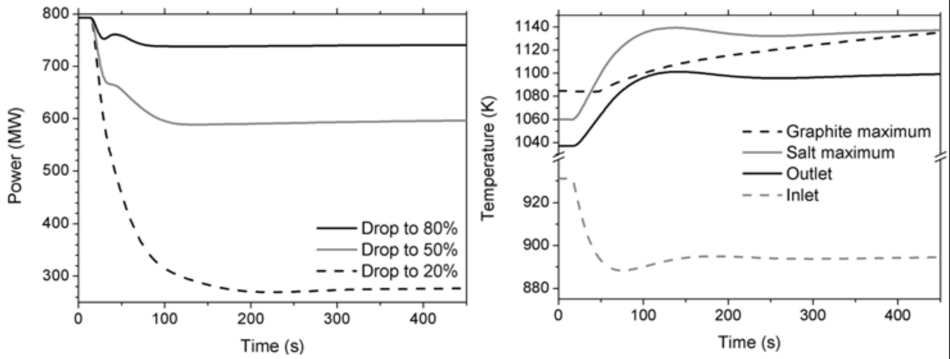




Pump coast-down at zero power



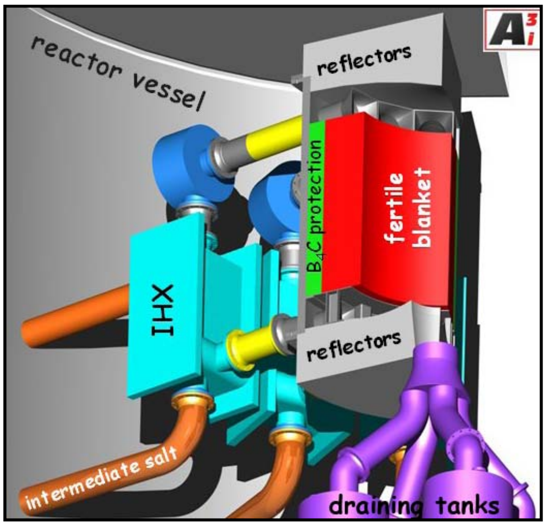
Pump coast-down at full power



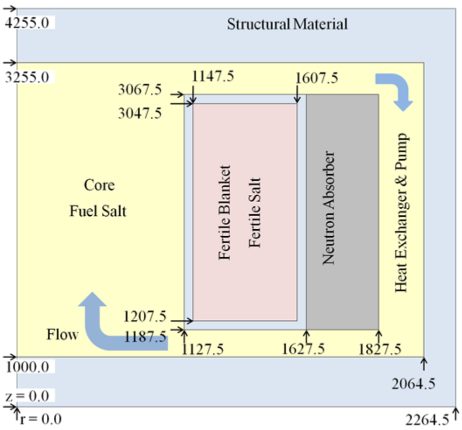
Conclusions

- It is possible to design a moderated Molten Salt Reactor with
  - Capacity for self-breeding
  - Sufficiently large negative temperature feedback coefficient
  - Sufficiently long graphite life time
- The negative feedback of the salt quickly stabilizes the reactor in the presented transients without excessive temperatures

Molten Salt Fast Reactor



Geometry and physics includes



Modeling:

- No heat transfer in blanket, reflectors and absorber regions
- Fresh fuel
- No flow in blanket
- Complete rz models for neutronics and heat transfer and fluid dynamics
- Properties from benchmark description (except 'Boussinesq' and some simplified materials)

Neutronics model

A special version of DALTON, i.e. DALTON-MSR has previously been developed to explicitly account for precursor transport.

Here, transport based on convection-diffusion model (effective viscosity)

$$\frac{\partial C_i}{\partial t} + \boldsymbol{u} \cdot \nabla C_i = \nabla \cdot (\mu + \mu_t) \nabla C_i + \beta_i \sum_g \nu \Sigma_g^f \phi_g - \lambda_i C_i$$

Input from CFD

Additonal difficulties in numerical solution:

- For stationary fuel, precursor densities are eliminated from flux equations and afterward updated without further error
- For moving fuel, they require explicit solution

Fluid-dynamics and thermal model

In-house developed code (HEAT) used for flow and heat transfer

- Navier-Stokes like model
- Geometry: 2D (rz, xy)
- Turbulence modeling: standard two-equation k-ε model (eddy viscosity) combined with wall treatment near solid walls
- Boussinesq approximation for gravity, good validity up to hundreds of degrees variation
- HEAT based on PETSc solvers, relieves from coding issues

$$\rho \left(\frac{\partial \boldsymbol{u}}{\partial t} + \nabla \cdot \boldsymbol{uu} \right) = -\nabla p - \nabla \cdot \boldsymbol{\tau} + \rho \boldsymbol{g} \beta (T - T_{ref})$$

$$\boldsymbol{\tau} = -(\mu + \mu_t) \left(\nabla \mathbf{u} + \nabla \mathbf{u}^T \right) + \frac{2}{3} \rho k \boldsymbol{I}$$

- Pump modelled by momentum source in down comer channel (pressure-drop as volumetric momentum source)

Fluid-dynamics and thermal model

Modelling of the heat transfer in the salt is based on a standard approach compatible with the CFD turbulence model. It includes models for:

- Fission heat source
- Model for losses to heat exchanger
- Turbulent heat diffusion (based eddy-diffusivity)

$$\rho C_p \left(\frac{\partial T}{\partial t} + \boldsymbol{u} \cdot \nabla T \right) = \nabla \cdot (\lambda + \frac{\mu_t}{\Pr}) \nabla T + \varepsilon_{fiss} \sum_g \nu \Sigma_g^f \phi_g - h_{hx}(T - T_{hx})$$

Cross section generation

Based on the SCALE package

- Self shielding based on infinite homogeneous medium approach (large fuel regions)
- A 1D axial and 1D radial computation are performed using transport for collapsing (66 radial zones and 39 axial zones) to account for spectral changes
- Cross sections generated for 200-2100K (100K increments)
- 9 neutron groups

- NOTE: fresh fuel case, no burnup

Cross section mapping

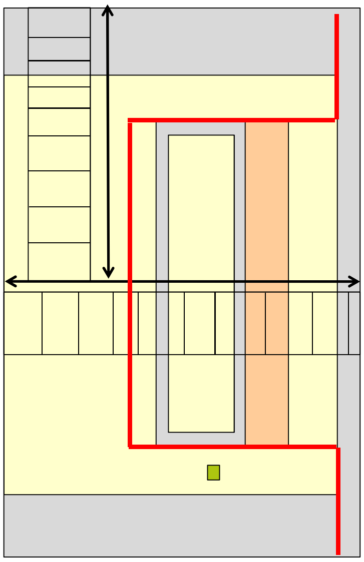
Cross sections depend on space through the temperature as well

Map needed to select proper xs set

Each mesh cell corresponds to specific cross section library and subsequently interpolated for temperature

A point either belongs to the axial set (left of red line) or to the radial set (right of red line)

Remains "fingerspitzengefühl"



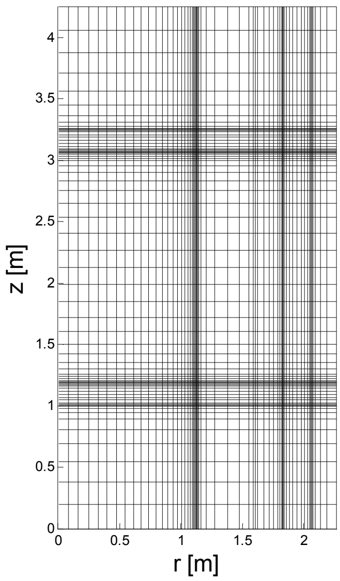
Mesh generation

Computational mesh for neutronics 66x78

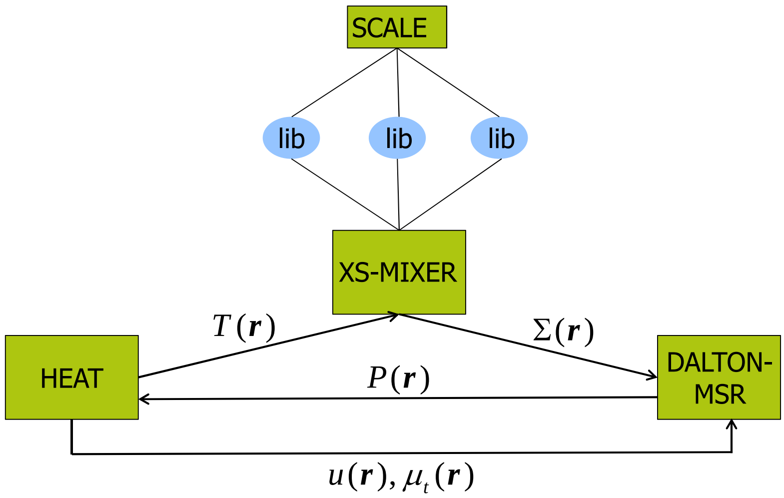
CFD mesh twice as fine in each direction (132x156). Has proper width near walls for correct behavior of turbulence model, i.e. y+ values (friction, turbulence)

Meshes overlap for simplicity where CFD dictates refinement near walls

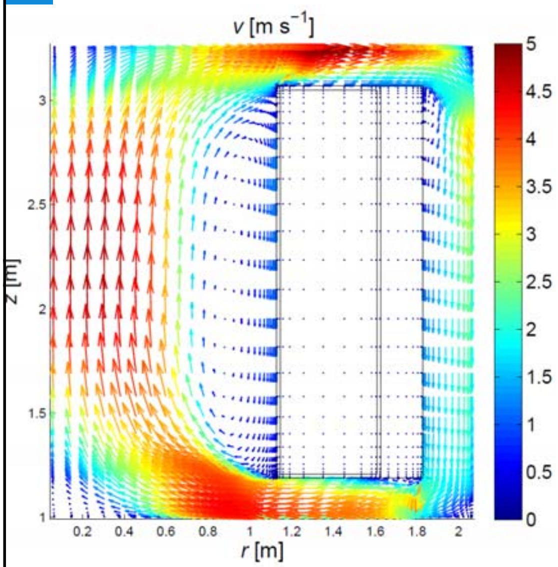
Interpolations required for data transfer between codes (conservation issue)



Computational scheme

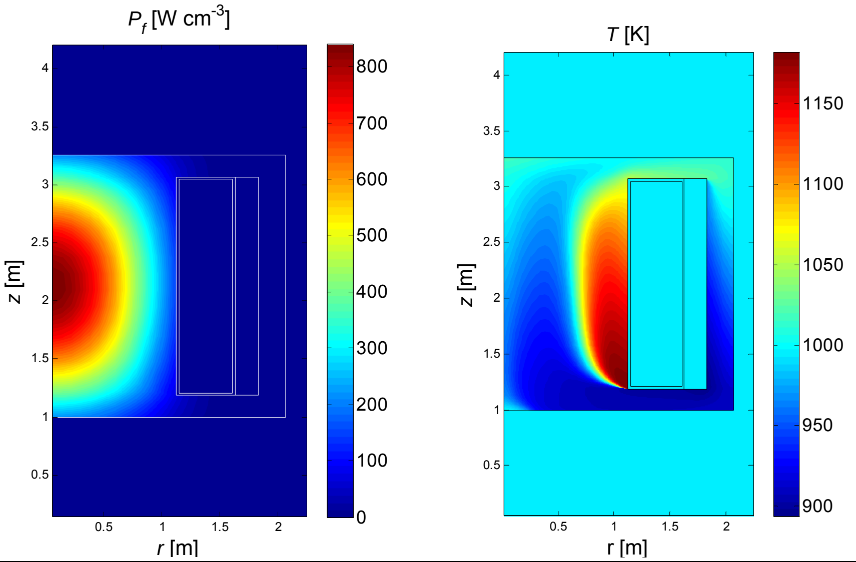


Steady state results: mean flow

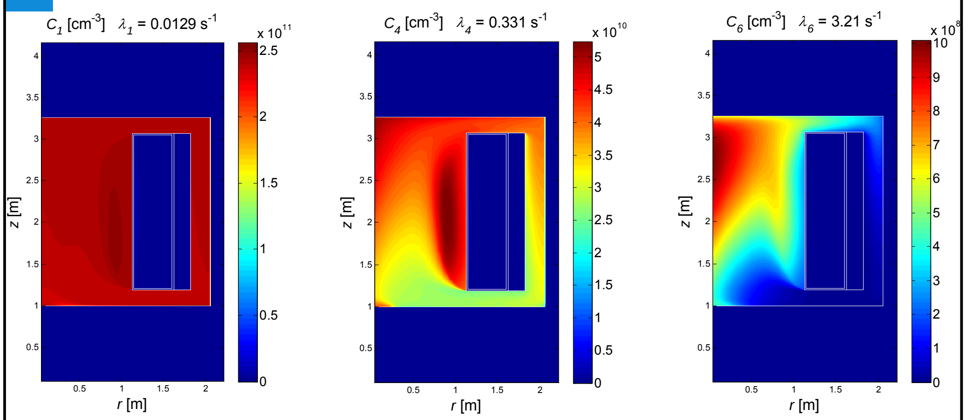


- Main recirculation loop: disadvantage for temperature field
- Small secondary flow in corner regions
- Results based on τ = 3.0 s circulation time
- ≈3 percent additional U-233 required for criticality

Power density/temperature



Precursor concentrations



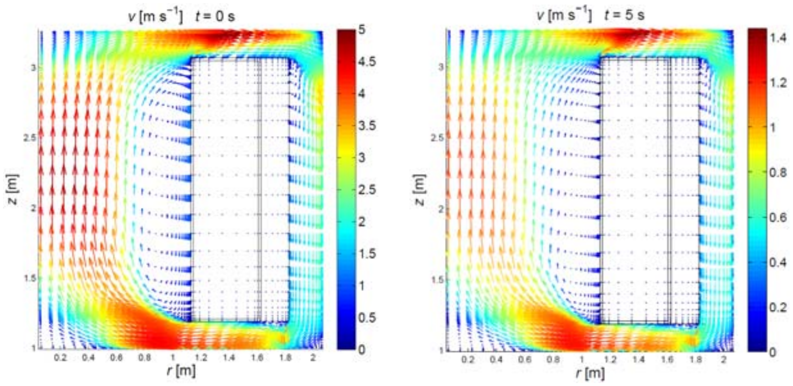
- Long lifetimes: homogeneous distributions and decay. Complete decay in down comer
- Short lifetimes: local balance between production and decay. Only slight shift in spatial distribution.
- Intermediate lifetimes: mixed …

Transient behavior: simulations done

System failure (power loss):
- Heat-exchanger Failure (h=0)
- Pump Failure (Δp=0)
- Simultaneous Pump and heat-exchanger failure (h=0; Δp=0)

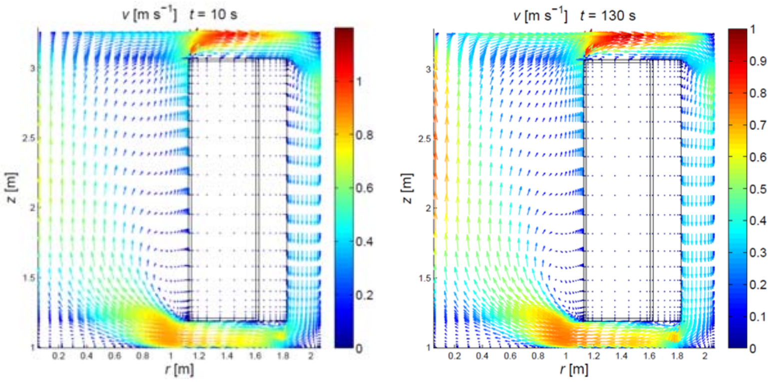
Instantaneous reactivity insertions (control issues):
- 48 pcm 0.1% extra U-233
- 102 pcm 0.2%
- 156 pcm 0.3%
- 265 pcm 0.5%
- 533 pcm 1.0%

Transient 1: pump failure



- Rapid initial decay of flow rate within first 5 seconds

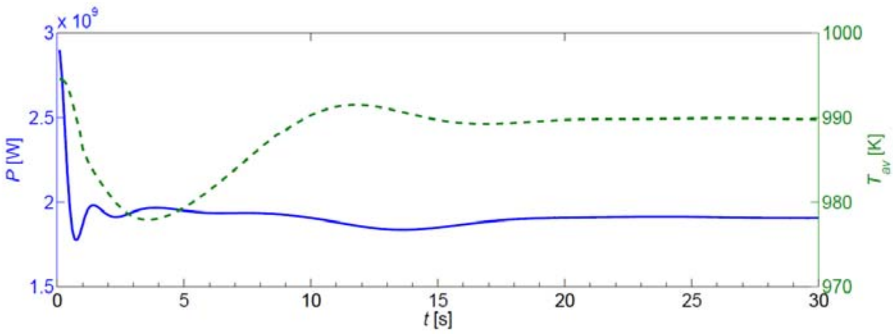
Transient 1: pump failure



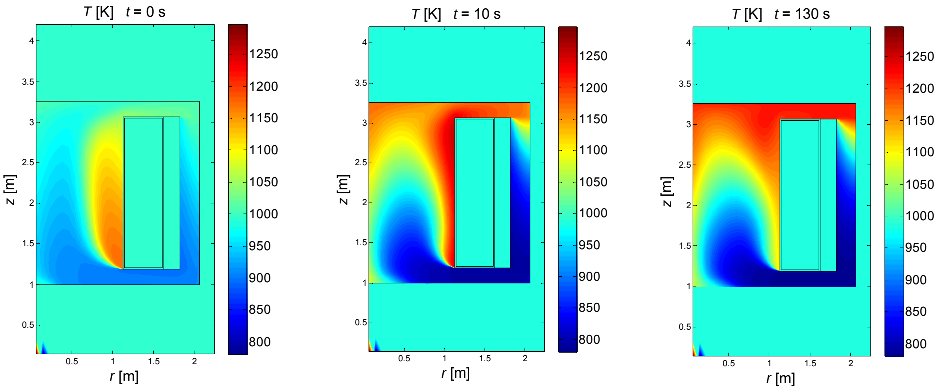
- Flow almost steady state after 130 seconds
- Flow rate decreased by factor 6 compared to steady-state
- Pure natural convection with different structure of recirculation zone
- Complex interplay between flow and buoyancy

Transient 1: pump failure

Sequence of events
- Flow drops due to friction
- Core salt heats up and creates feedback causing power decrease
- HX remains equally effective (constant h = model flaw) -> average T drops while core T is in fact higher
- Flow changes structure at later times and reaches new steady state
- $P(\infty)=1.9\ GW_{th}$
- NOTE: T in HX reaches solidification … T is near T_external



Transient 1: pump failure

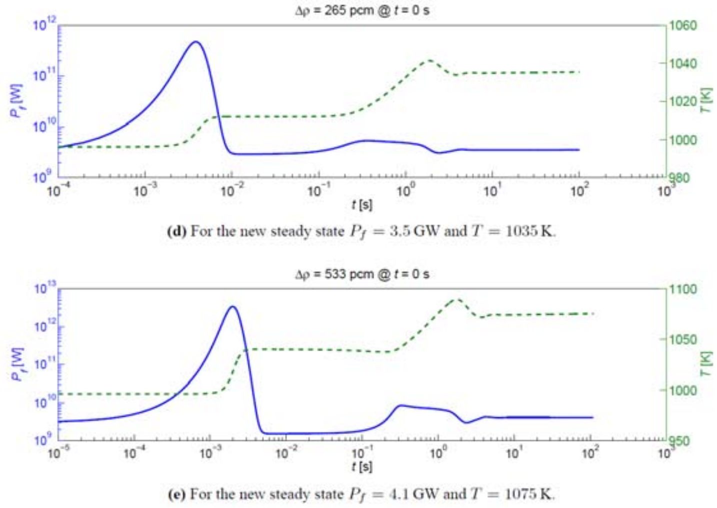


Transient 2: reactivity insertion

Sequence of events

- Reactivity is instantaneously added by increasing U-233 density
- Prompt jump occurs, where feedback limits the growth
- Delayed effects from precursors
- Complex interplay of hot and cold fluid exiting and entering the core region cause some further transients until final steady state is reached
- The final power in steady state is slightly larger than the initial power to compensate for the external reactivity

Transient 2: reactivity insertion



Conclusions MSFR

- Complete multi-physics model describing coupled neutronics-fluid-dynamics and heat transfer.
- Steady state temperatures reach maximum of T < 1200 K in core recirculation zone (probably sensitive to turbulence modelling).
- The MSFR is a very stable and safe reactor due to the high fuel salt specific heat capacity and high negative reactivity coefficient.

General conclusions MSR modelling

- Fuel temperature and density have a strong influence on the power profile and production in fluid fuel reactors
- Thermal hydraulics and thermal calculations modelled from simple models in MSRE to full CFD in MSFR
- Meanwhile added:
  - ☑ Modelling of fuel burnup
  - ☑ Improved decay heat model
- More to come:
  - ❑ More advanced geometries
  - ❑ Modelling of chemical processes
  - ❑ …

Downloads

- http://www.nera.rst.tudelft.nl/en/publications/phd-theses/
  - thesis of Karoly Nagy (2012)
- http://www.nera.rst.tudelft.nl/en/publications/msc-theses/
  - thesis Lodewijk Frima (2013)
  - thesis Erik van der Linden (2012)