Neutronics in fusion devices

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Briefly about me…

- I am a chemical engineer from Mexico turned nuclear engineer.
- Before joining, PSU, I worked for 13 years at the National Polytechnic Institute in Queretaro, Mexico.
- I have been involved in fusion research since 1998, when I was a grad student at the University of Illinos.
- Current chair of the IEEE NPSS Fusion Technology Committee (until Dec 2022).
- I work mainly on the field of plasma-material interactions, and more recently I have started working in neutronics simulation for fusion devices.
- I am a cat person, I play squash and I put together Japanese mecha models.

Outline

- Fusion and neutrons.
- Why are neutrons important?
- Practical aspects of neutronics simulations of fusion devices
- Conclusions and final thoughts

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FUSION AND NEUTRONS

In 1935, during his research tenure at the legendary Cavendish Laboratory, the Australian physicist Mark Oliphant achieved the first fusion reactions on Earth.

Fusion energy is nuclear in origin

- Nuclear reactions produce or consume energy because some nuclear mass is lost or gained during the reaction.
- Mass lost ⟶ Energy is released
- Mass gained ⟶ Energy is absorbed

$$A + B \rightarrow C + D$$

$$\Delta m = m_C + m_D - (m_A + m_B)$$

$$\boxed{E = \Delta m\, c^2}$$

$$c = 3\times 10^8\, {}^{m}/_{s}$$

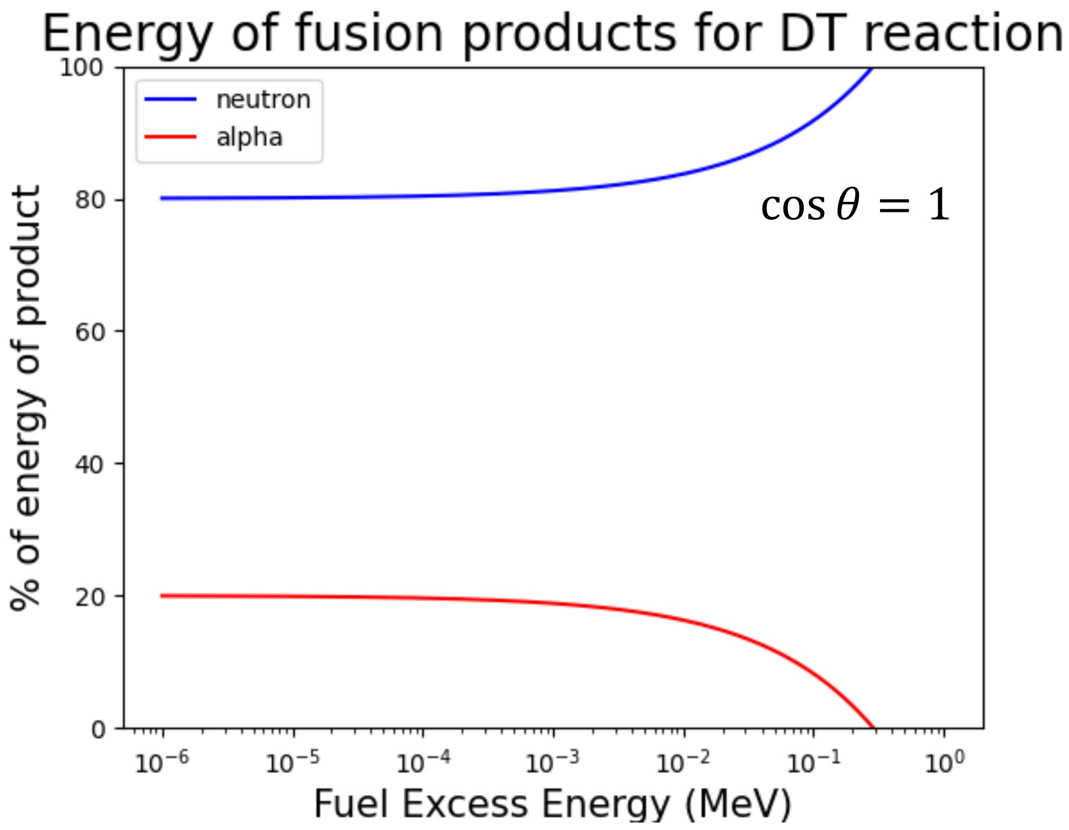
$\Delta m > 0$: Reaction is endothermic (requires energy to proceed)

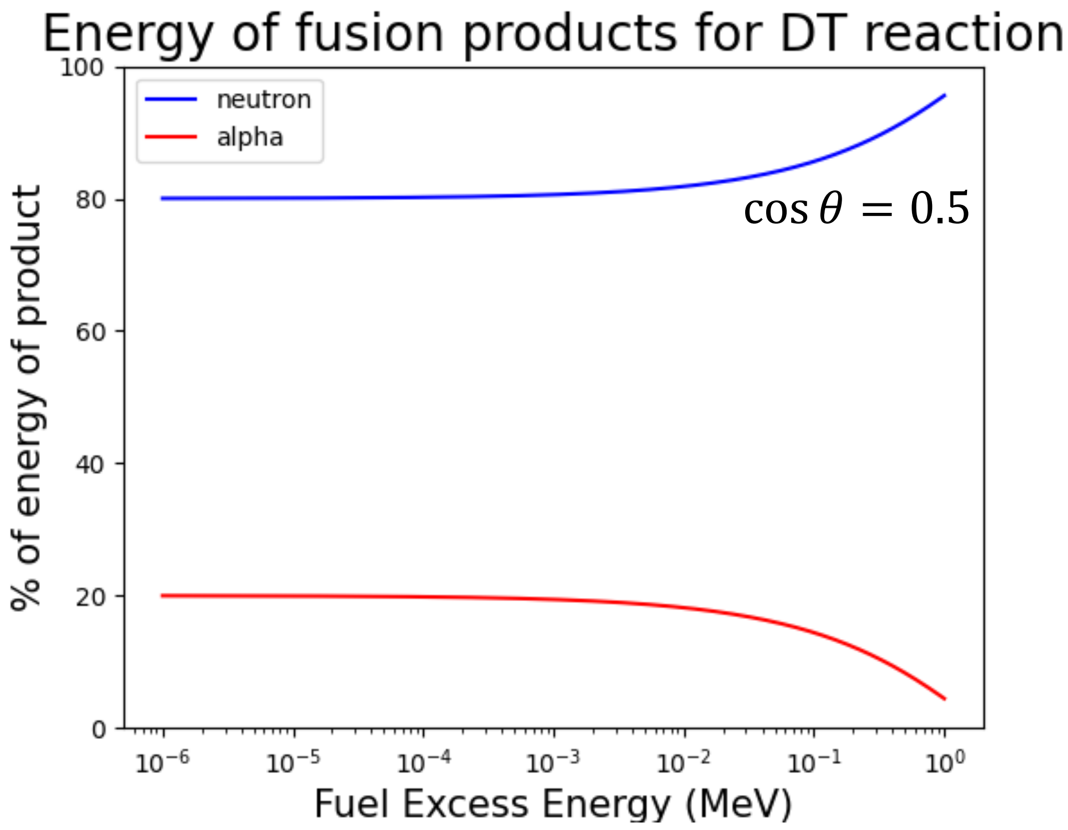
$\Delta m < 0$: Reaction is exothermic (releases energy when it proceeds)

$$c^2 = 931.5\, \frac{MeV}{amu} = 9\times 10^{16}\, \frac{J}{kg}$$

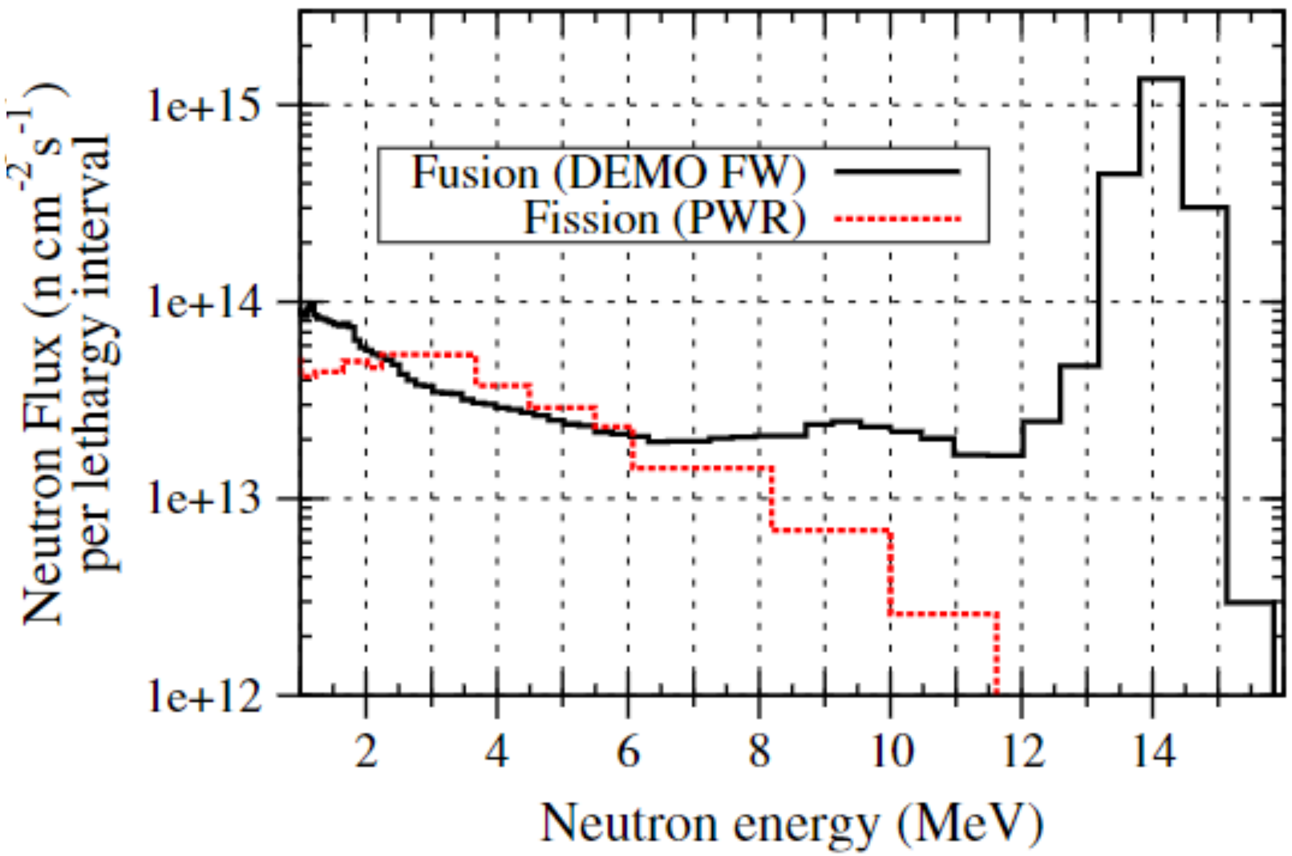
Energy of DT fusion products

$$^2H + \, ^3H \rightarrow \, ^4He + n \quad Q = 17.6\, MeV$$





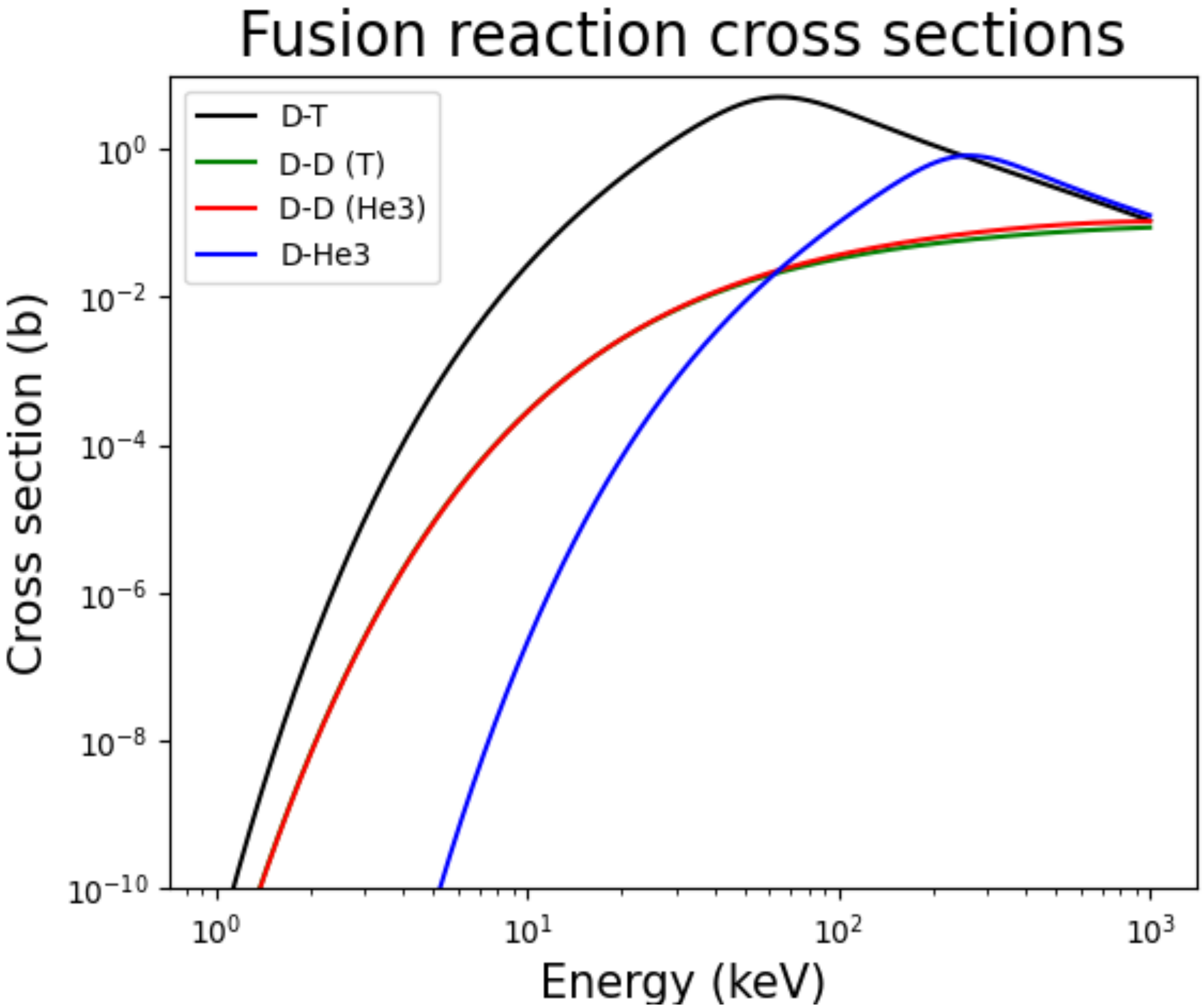
Neutron energy spectrum: fission vs fusion



M.R. Gilbert et al. J. Nuc. Mat. **442** S755–S760 (2013)

Fusion cross sections

- The cross section is proportional to the probability of fusion happening at a given energy.
- It is derived from quantum mechanical calculation given the effective potential previously described.
- There are semiempirical fits to the measured and calculated cross sections that are quite useful to make numerical calculations of fusion power.
- This document contains such fits for different fusion reactions.



This is why the DT reaction is preferred: it has the highest cross section at any given temperature

Collision frequency

- Consider particles A in motion colliding with particles B stationary (or very low energy).
- The average distance λ traveled by an A particle with velocity v before it interacts with B is given by:

$$\langle \lambda \rangle = \frac{1}{n_B \sigma(v)}$$

n_B is the particle density of species B

- Therefore, the average time elapsed between two consecutive interaction events is given by:

$$\langle \tau \rangle = \frac{\langle \lambda \rangle}{v} = \frac{1}{n_B \sigma(v) v}$$

- And the collision frequency "per particle A" is therefore:

Greek letter "nu"

Letter "v"

$$\nu = \frac{1}{\langle \tau \rangle} = n_B \sigma(v) v$$

Reaction rate for a given velocity

- So, the volumetric interaction rate r is just the particle density of A (n_A) within the volume times the fusion frequency:

$$r(v) = n_A n_B \sigma(v) v$$

- And the total reaction rate R is given by the following volume integral:

$$R = \int r(v) dV = \int n_A n_B \sigma(v) v dV$$

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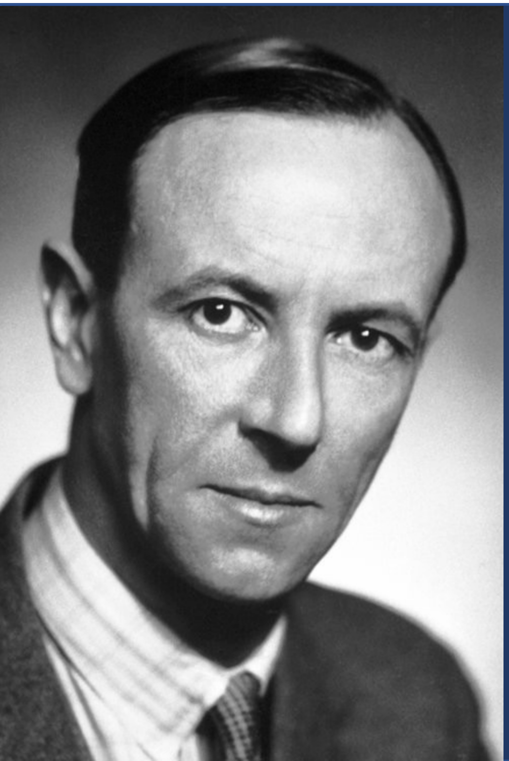
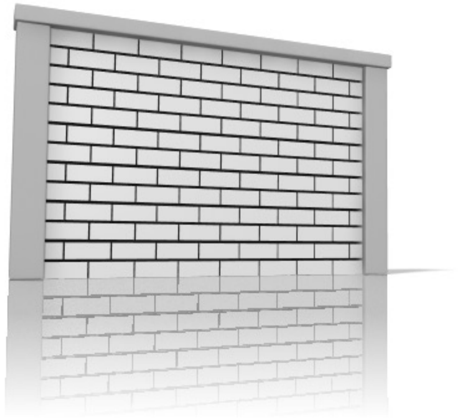
Why are neutrons important?



James Chadwick, a British scientists at the Cavendish Laboratory, discovered the neutron in 1932. This was a giant leap in the understanding of atomic and nuclear physics.

The importance of neutrons in fusion devices

- Neutrons deposit energy.
- Neutrons do damage.
- Neutrons produce tritium.

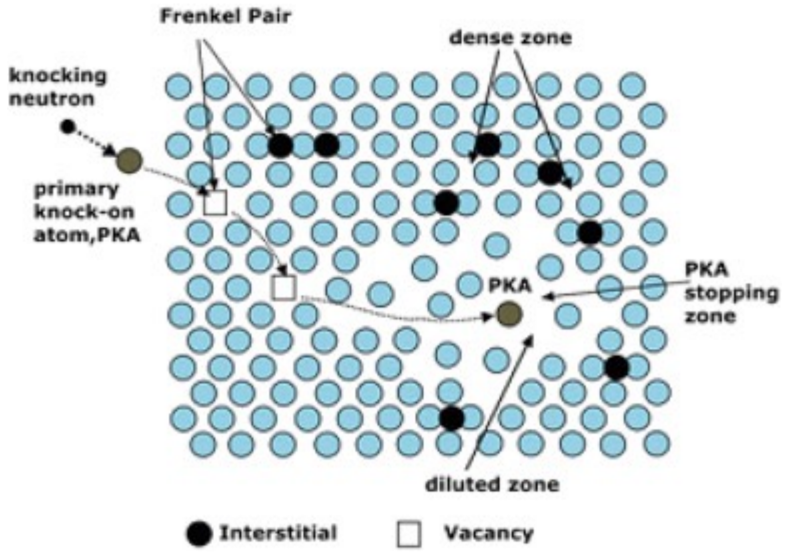


- All these processes involve *interaction* of neutrons with its environment

Some neutrons interactions

Interaction	Medium	Result	Relevance
Elastic scattering	Liquid	Heat transfer	Energy extraction from fusion reactor
Elastic scattering	Solid	Defect formation	Material lifetime reduction
Absorption	Solid/Liquid	Formation of radioactive isotopes	Activation of materials, beta and gamma emission
Nuclear reaction	Solid/Liquid	Formation of helium/hydrogen Fission	Tritium breeding, material swelling, additional energy production from fission

Neutron damage in solids



PKA: primary knock-on atom

$$R_d = n \int_{E}^{\hat{E}} \phi(E_\mathrm{i})\sigma_\mathrm{D}(E_\mathrm{i})\mathrm{d}E_\mathrm{i}$$

n: material atomic density
ϕ: energy-resolved neutron flux
σ_D: displacement cross section

$$\sigma_\mathrm{D}(E_\mathrm{i}) = \int_{T_{min}}^{T_{max}} \sigma_s(E_\mathrm{i}, T)\nu(T)\mathrm{d}T$$

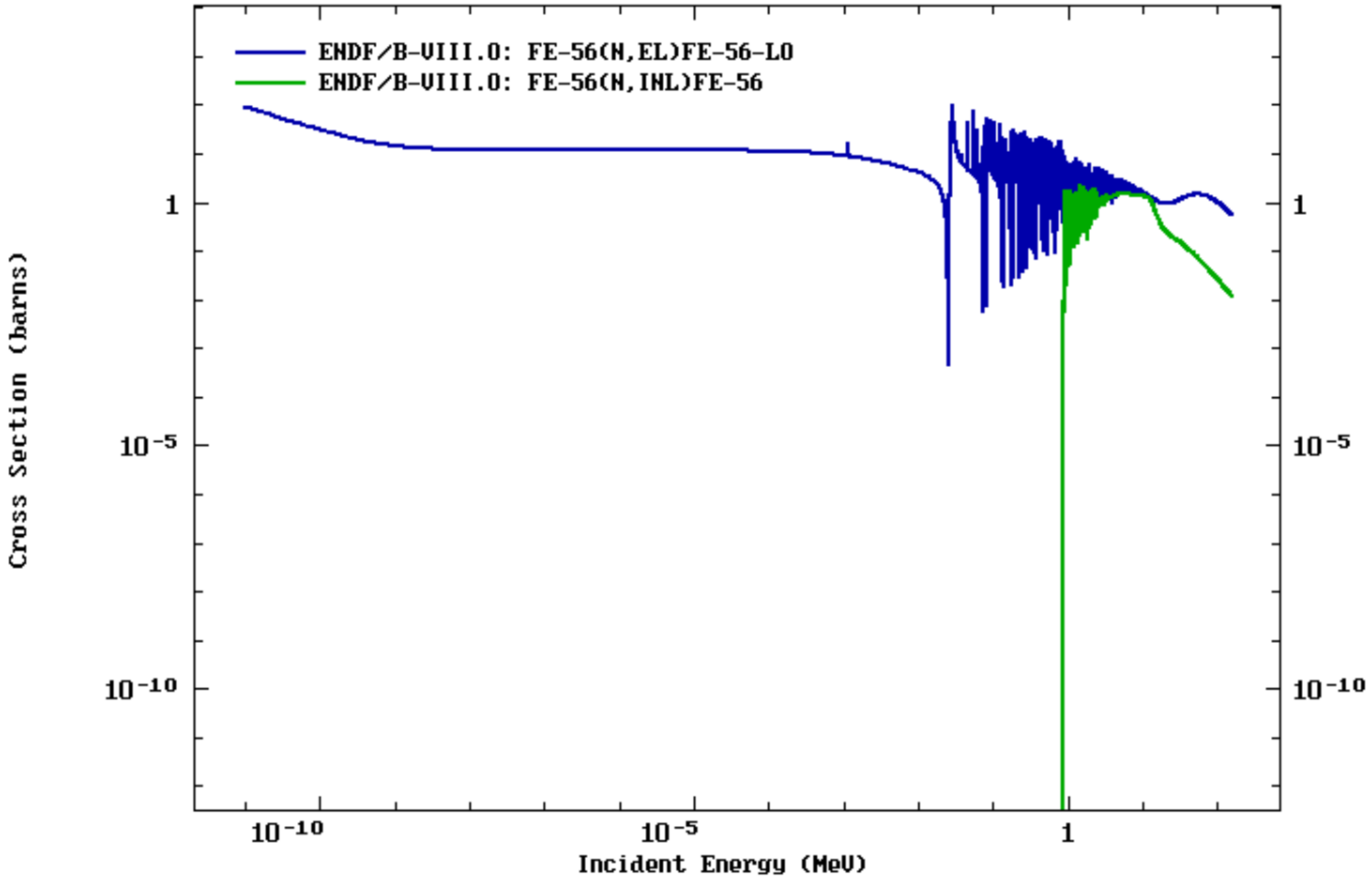
ν : PKAs per collision
σ_s: elastic scattering cross section

$$R_d = n\sigma_\mathrm{s}\left(\frac{\gamma \overline{E}_\mathrm{i}}{4E_\mathrm{d}}\right)\phi, \qquad \gamma = \frac{4A}{(1+A)^2}$$

n: material atomic density
ϕ: neutron flux above E_d
E_d: displacement energy
E_i: neutron energy

Volumetric rate of displacement production

Neutron damage to ^{56}Fe



$n = 8.5\times10^{23}\ \text{cm}^{-3}$

$E_i = 14\ \text{MeV}$

$E_d = 25\ \text{eV}$

$\sigma_s = 2\times10^{-24}\ \text{cm}^2$

$\phi = 1\times10^{13}\ \text{cm}^{-2}\text{s}^{-1}$

$\gamma = 0.07$

$$\frac{R_d}{n} = \sigma_s\left(\frac{\gamma\overline{E}_\text{i}}{4E_\text{d}}\right)\phi = 2\times10^{-6}\,\frac{\text{dpa}}{\text{s}} = 63\ \text{dpa/yr}$$

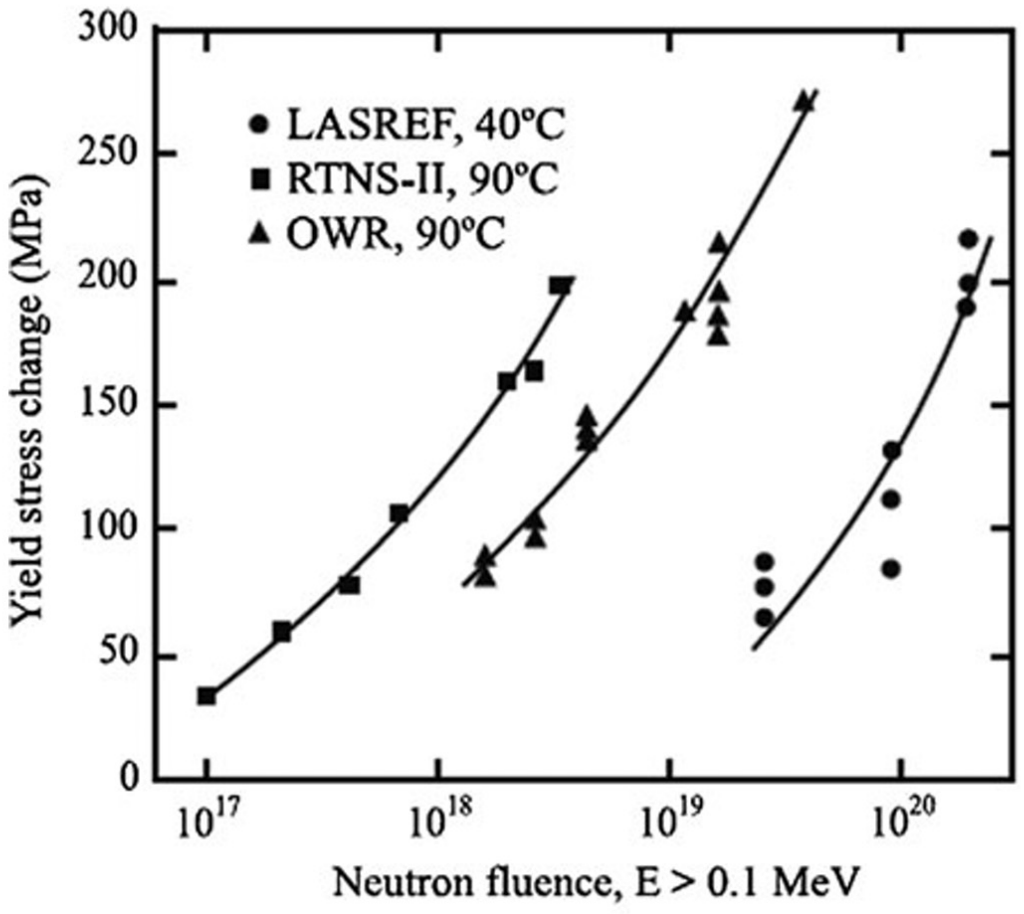
Twice the value of a fast nuclear reactor!

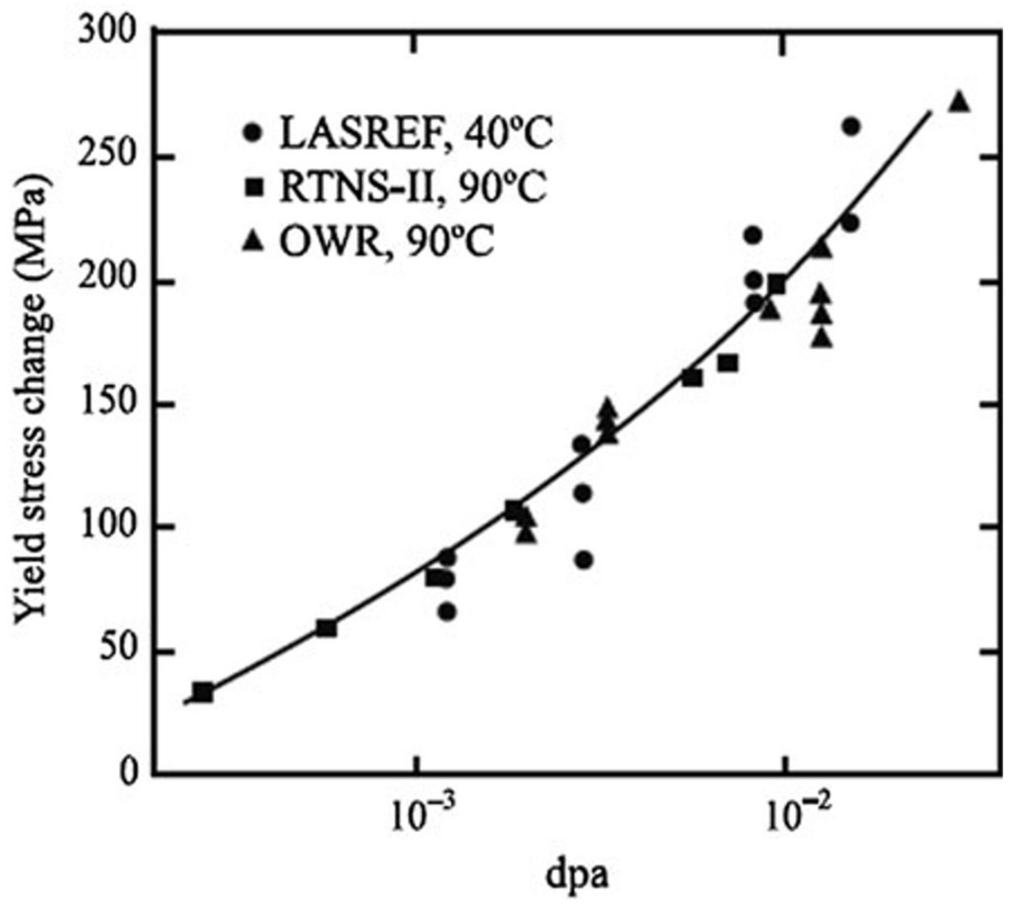
Neutron damage in solids

Los Alamos Spallation Radiation Effects Facility (LASREF)

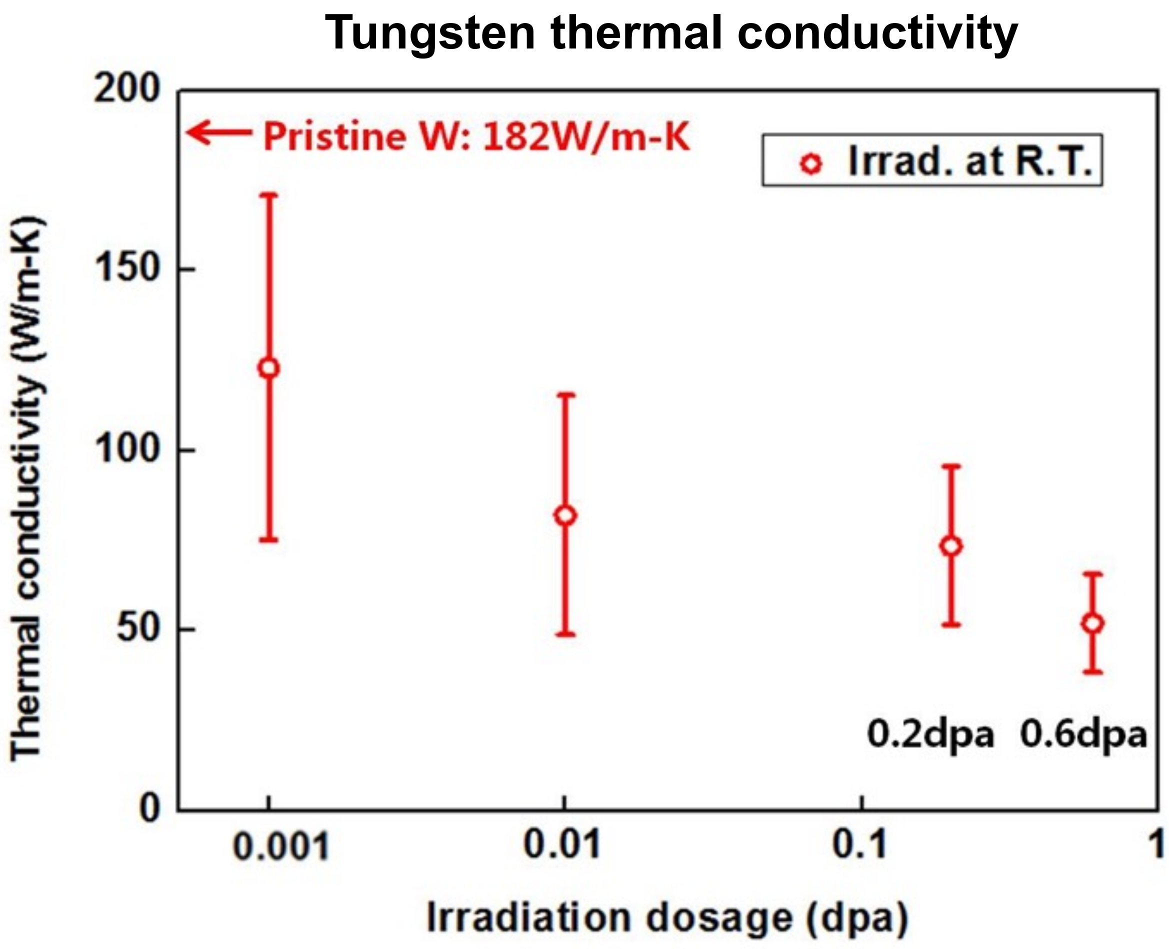
Omega West Reactor (OWR)

Rotating Target Neutron Source II (RTNS-II)





Neutron damage in solids



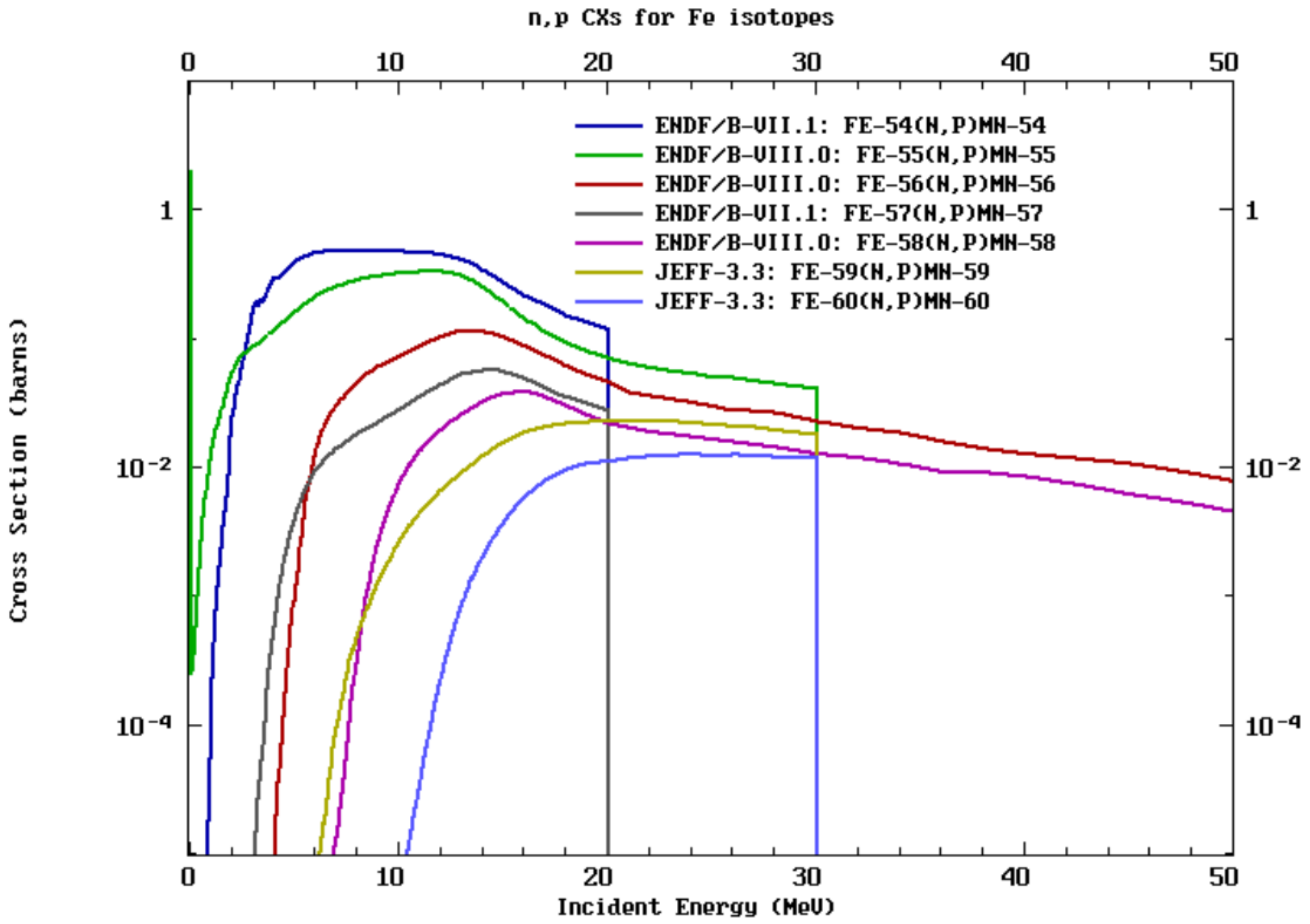
Tungsten becomes a poorer heat conductor as damage increases!

G. Tynan. 26th IAEA Fusion Energy Conference, paper MPT/P5-1G (2016)

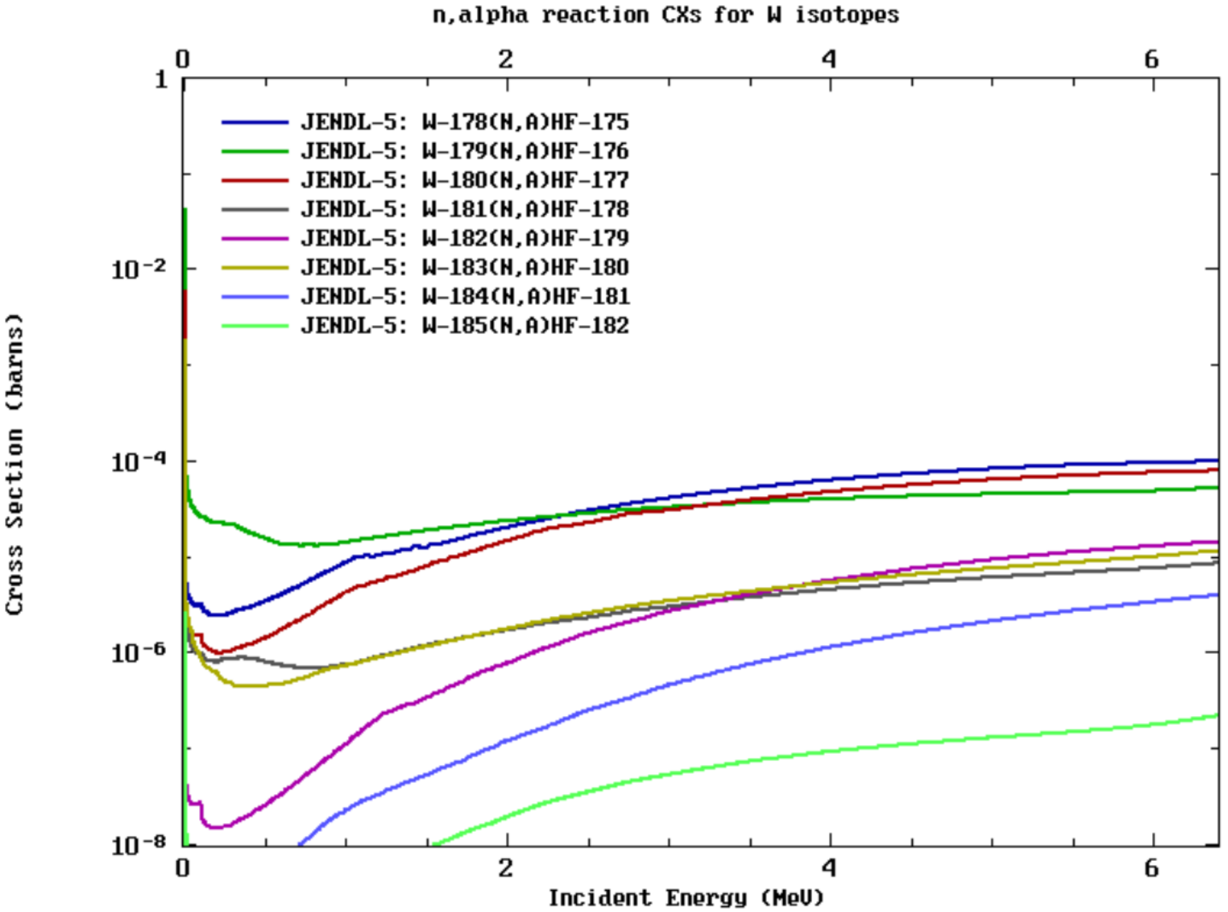
Neutron reactions

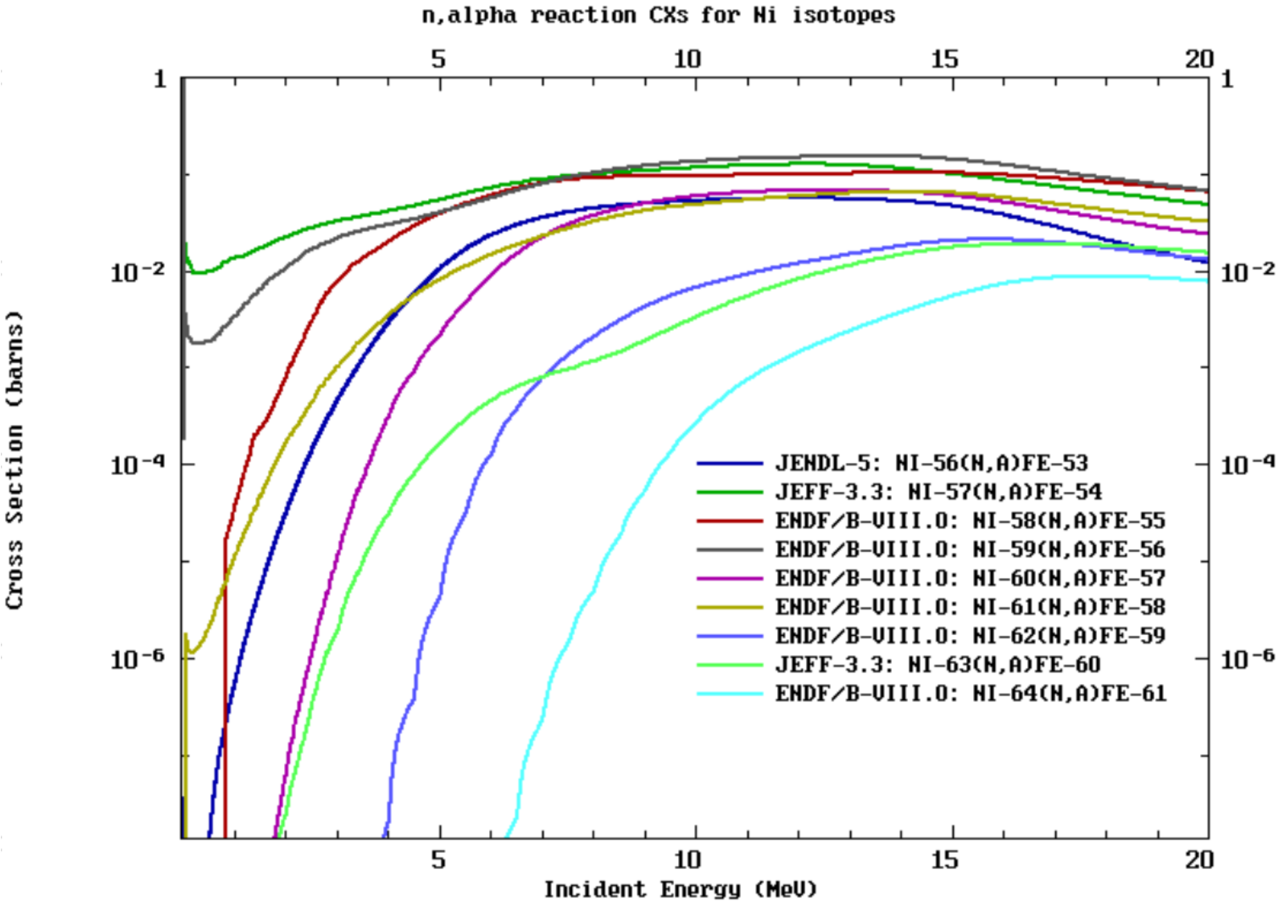
- Besides the collisional damage associated with neutron scattering, other stuff can happen:
  - Nuclei can capture a neutron and become radioactive, emitting alpha, gamma or beta radiation. **Activation**
  - If the neutron reaction generates a proton or an alpha particle, the material will start accumulating gases (hydrogen and helium, respectively) **Swelling**

Hydrogen producing reactions examples

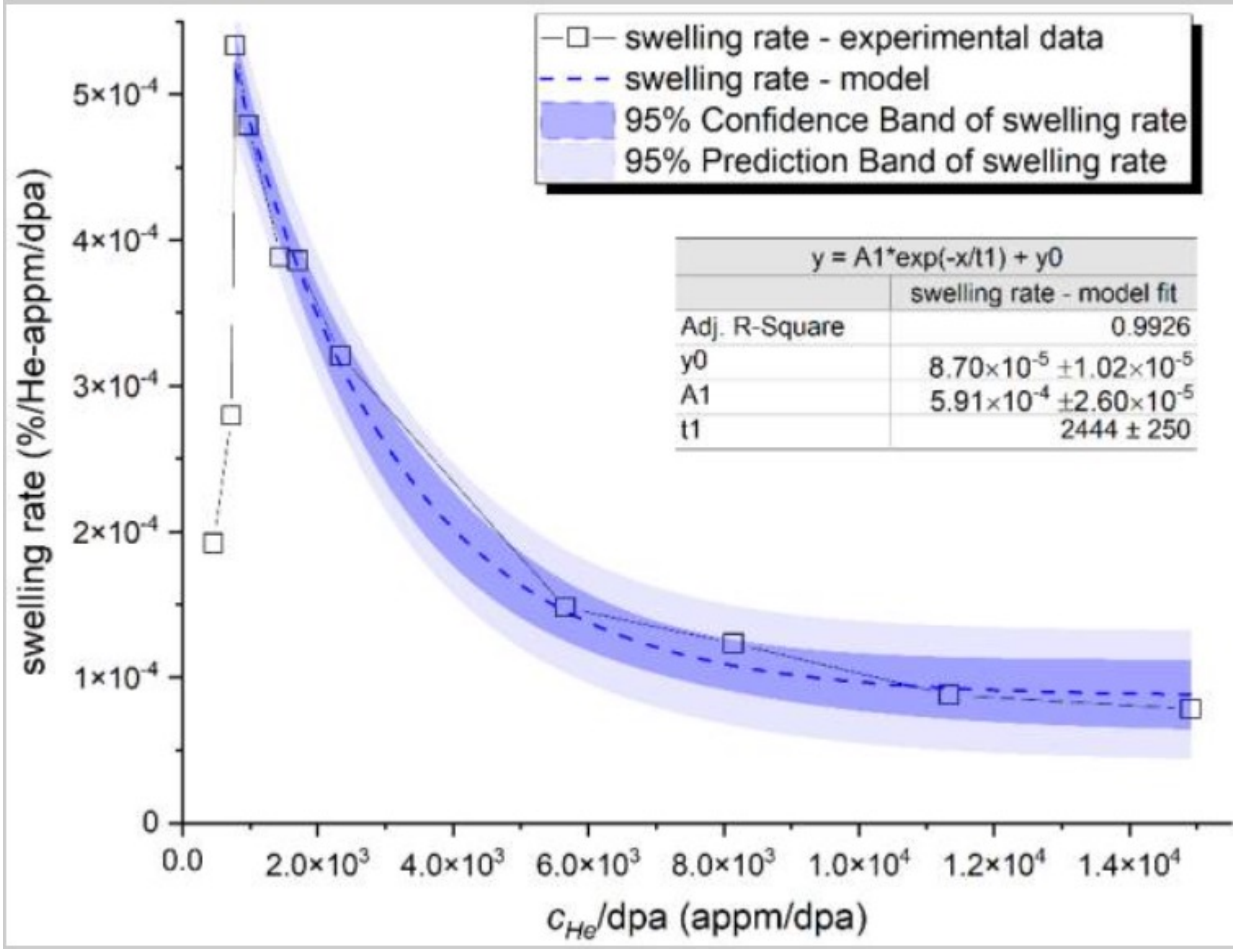


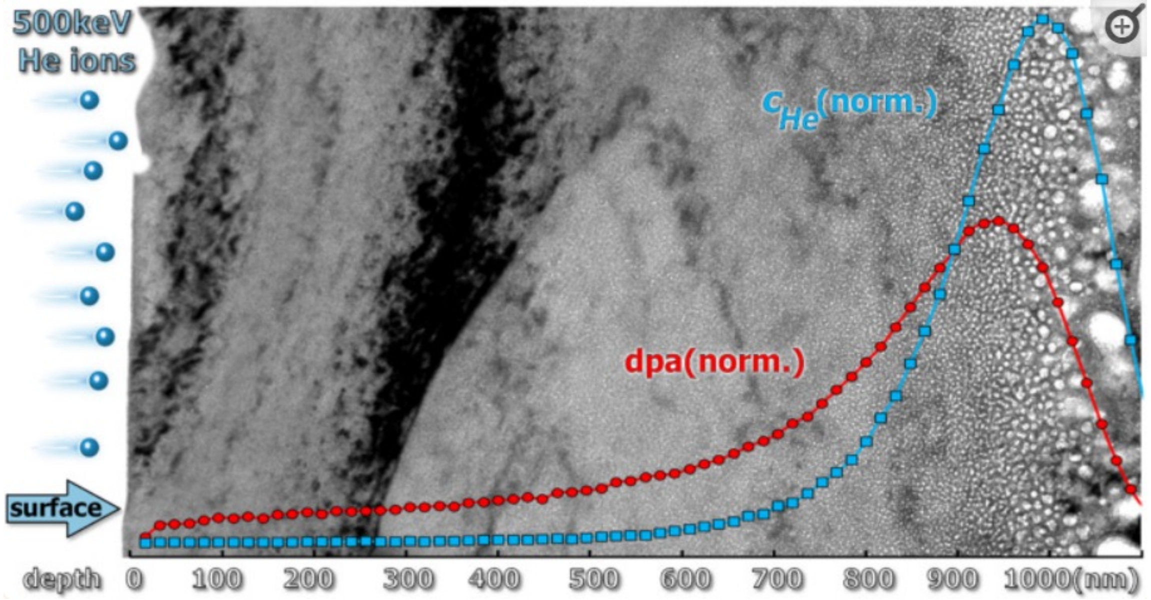
Helium production reaction examples





Stainless steel swelling vs irradiation damage



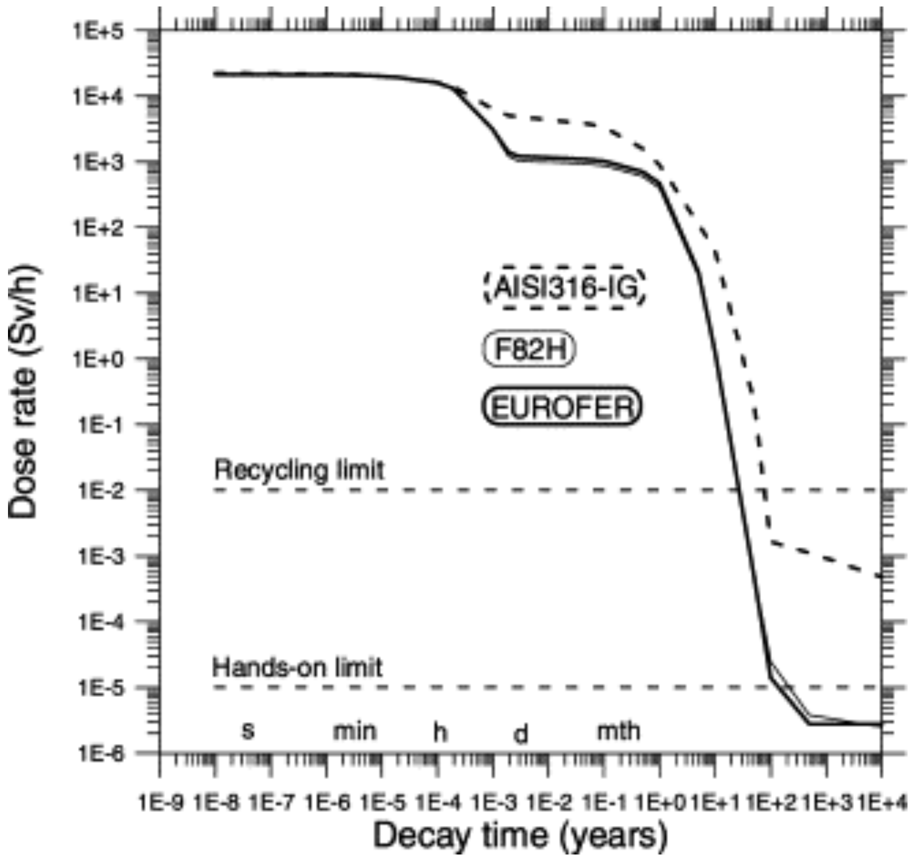


S. Sojak et al. Materials (Basel, Switzerland) 14, n. 11, p. 2997 (2021)

Development of low activation steels

$$^{59}\mathrm{Co} \xrightarrow{(n,\gamma)} {}^{60}\mathrm{Co}$$

$$^{59}\mathrm{Co} \xrightarrow{(n,\gamma)} {}^{60m}\mathrm{Co} \xrightarrow{(IT)} {}^{60}\mathrm{Co}$$



K. Seidel et al. J. Nucl Mater 307:1037–1041 (2002)

Element	AISI 316L	EUROFER
Fe	67.91	89.4
C	0.02	0.11
Si	0.5	<0.05
Mn	1.71	0.11
Cr	16.2	8.8
Ni	11	0.01
Mo	2.18	0.005
Cu	0.35	0.01
N	0.07	0.007
P	0.03	0.003
S	0.02	0.005
W	---	1.1
V	---	0.19
Ta	---	0.12
Co	0.01	0.006
Ti	---	0.004
Cu	---	0.01
Al	---	0.05

Tritium requirements

- Currently, to operate large nuclear fusion experiments with tritium, it is obtained as a byproduct from fission reactors, nuclear fuel reprocessing facilities or from decommissioned nuclear weapons.
- This tritium can be used as start-up material for experimental fusion reactors, but the expectation is that a commercial fusion reactor should produce its own tritium.
- The tritium self-sufficiency of a fusion device is measured by the tritium breeding ratio (TBR), which is equal to 1 if each neutron from the reactor produces a tritium nucleus.
- Since tritium decays relatively fast (12.5 years), some irreversible tritium losses occur if tritium is not recovered immediately.
- Also, any tritium recovery technology will not 100% efficient.
- This means that more than one tritium be formed per emitted neutron.
- Factors such as tritium burnup fraction in the plasma, the size of the planned tritium reserve and the first wall material choices affect the value of the required TBR to achieve self-sufficiency, but a value of 1.15 is often quoted as a reasonable figure to ensure self-sufficiency.

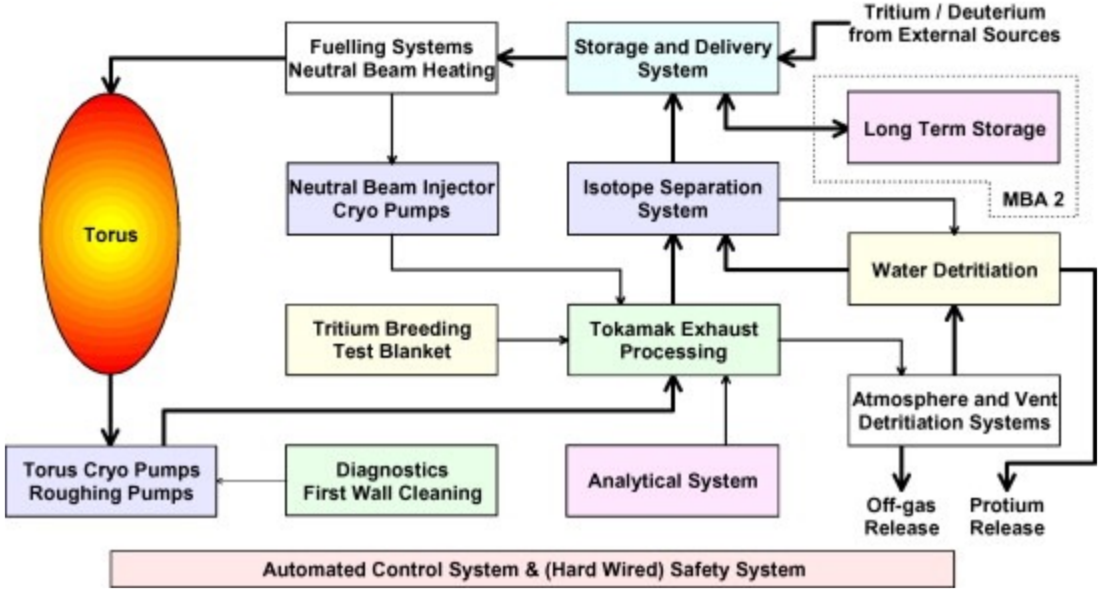
Tritium requirement

$$\dot{m}_T = 0.192P$$

P : neutron power (MW)
$\dot{m}_T$: tritium consumption (g/day)

A 250 MW neutron power (312.5 MW total) fusion device needs to produce 48 g of tritium per day.

For reference, a CANDU reactor (the main source of tritium currently) produces tritium at a rate around 0.27 g/day.



M. Glugla et al. Fus. Eng. Des. 82, pp. 472-487 (2007)

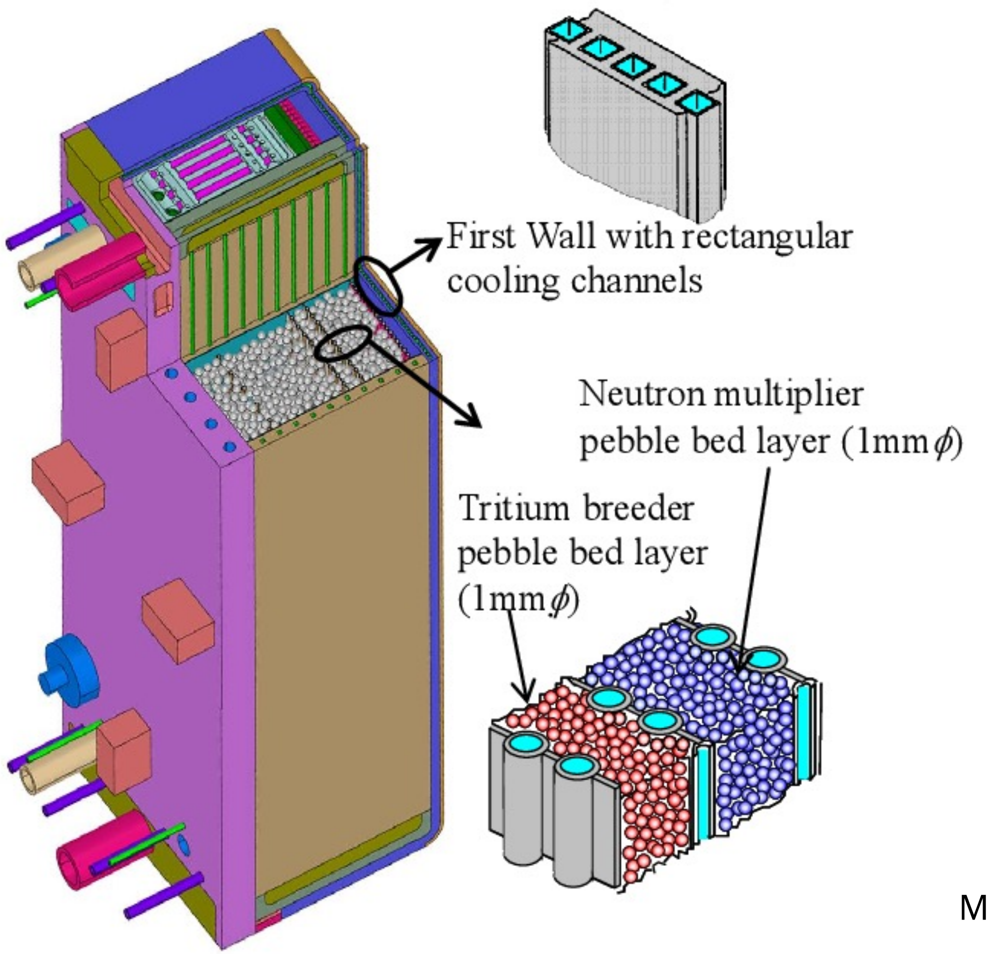
Tritium production in fusion devices

- By far the most popular route for producing tritium is the reaction between a neutron and the ^{6}Li isotope:

$$^{6}Li + n \longrightarrow {}^{3}H + {}^{4}He$$

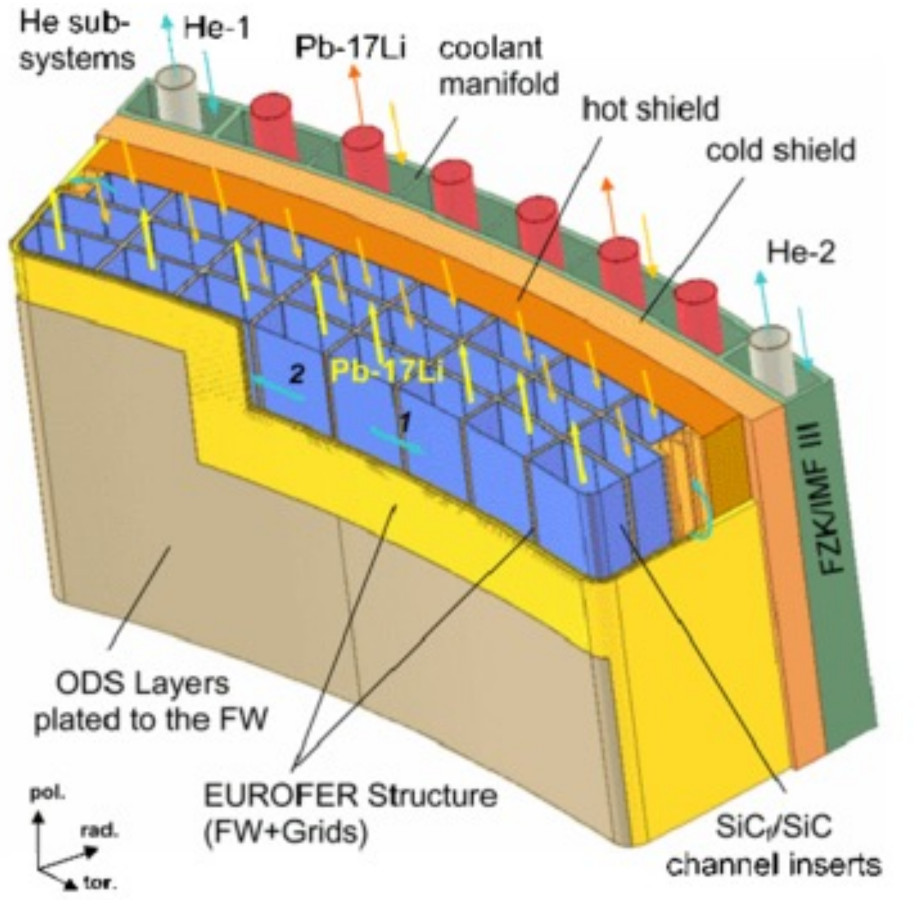
- Both solid and liquid breeding materials have been proposed.
- Li ceramics are the most popular solids.
- Molten Li, Pb-Li and FLiBe are the most popular liquids.

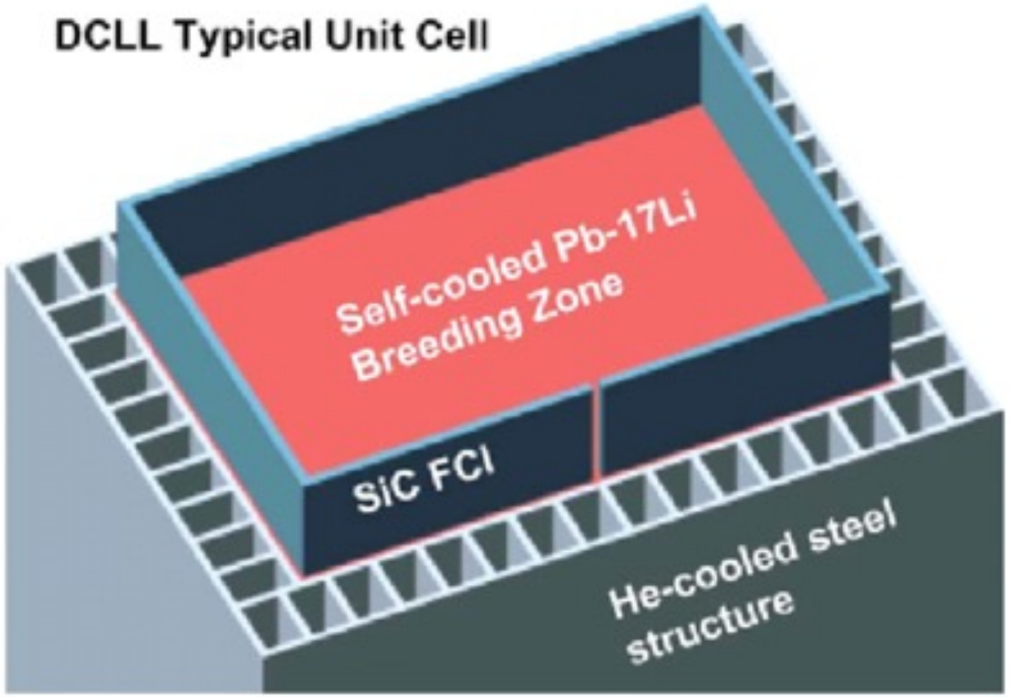
A solid breeder blanked design example



M. Enoeda et al. Proc. 21st Int. Conf. on Fusion Energy (Chengdu, China, 2006)

A liquid breeder blanket module design example





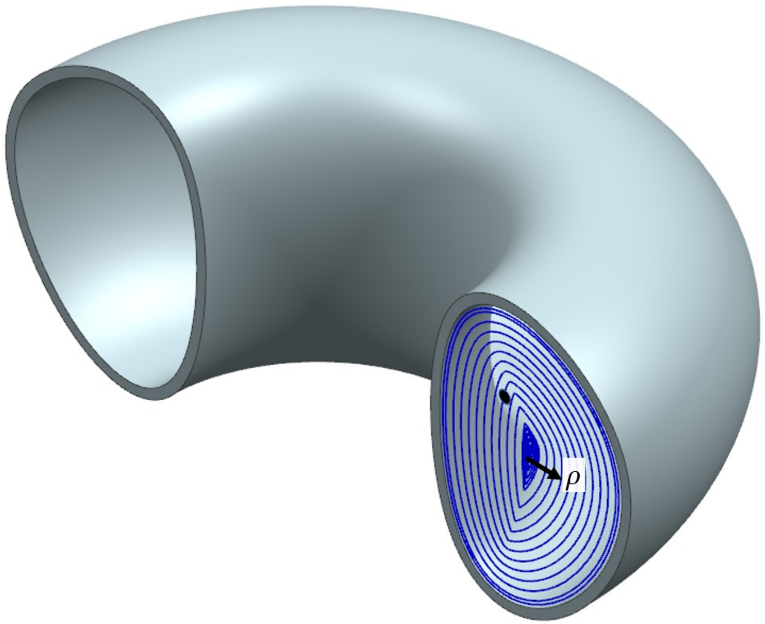
Practical aspects of neutronics simulations in fusion devices

Stanislaw Ulam, a Polish-American mathematician and physicist, developed what we now know as the Monte Carlo method while working at Los Alamos National Laboratory in the Manhattan Project. Monte Carlo methods are key in the simulation of neutron transport

Key elements

- A volumetric, non-homogeneous fixed neutron source with a complex shape.
- Regions of space with various compositions.
- A neutron reaction database for every material present in the system at any given time.
- Values of the neutron flux everywhere within the system at all times.

Plasma transport



Mass, momentum and energy conservation

$$\frac{1}{V'}\left(\frac{\partial}{\partial t}-\frac{\dot{B}_0}{2B_0}\frac{\partial}{\partial\rho}\rho\right)(V'n_e)+\frac{1}{V'}\frac{\partial}{\partial\rho}\Gamma_e=S_e$$

$$\frac{3}{2}\left(\frac{1}{V'}\right)^{-5/3}\left(\frac{\partial}{\partial t}-\frac{\dot{B}_0}{2B_0}\frac{\partial}{\partial\rho}\rho\right)\left[(V')^{5/3}n_ek_BT_e\right]+\frac{1}{V'}\frac{\partial}{\partial\rho}\left(q_e+\frac{5}{2}k_BT_e\Gamma_e\right)=P_e$$

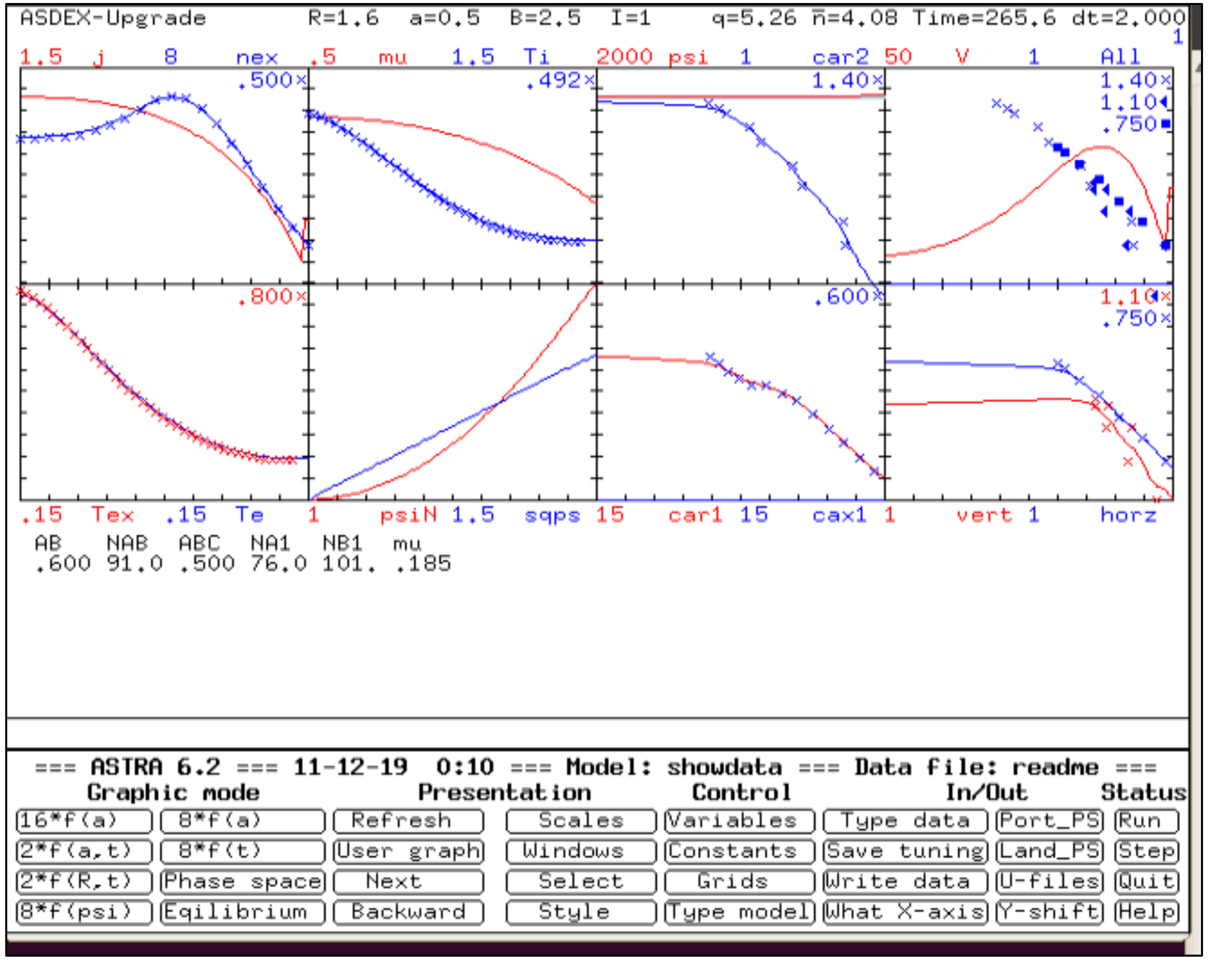
$$\frac{3}{2}\left(\frac{1}{V'}\right)^{-5/3}\left(\frac{\partial}{\partial t}-\frac{\dot{B}_0}{2B_0}\frac{\partial}{\partial\rho}\rho\right)\left[(V')^{5/3}n_ik_BT_i\right]+\frac{1}{V'}\frac{\partial}{\partial\rho}\left(q_e+\frac{5}{2}k_BT_i\Gamma_i\right)=P_i$$

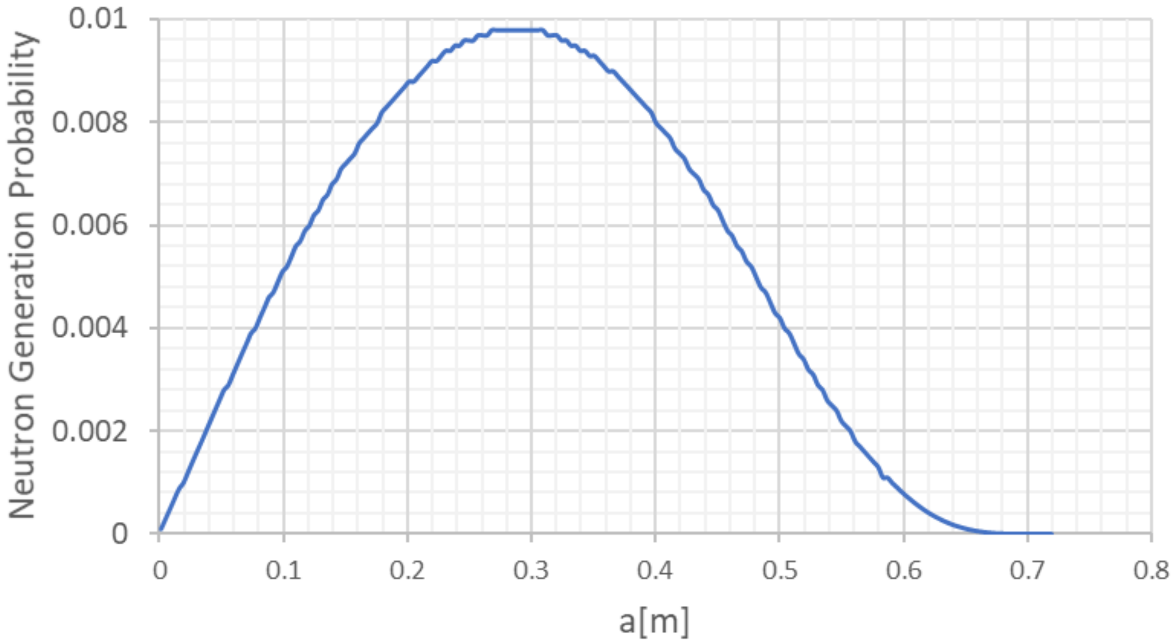
Mechanical equilibrium

$$\sigma_\parallel\left(\frac{\partial\psi}{\partial t}-\frac{\rho\dot{B}_0}{2B_0}\frac{\partial\psi}{\partial\rho}\right)=\frac{J^2R_0}{\mu_0\rho}\frac{\partial}{\partial\rho}\left(\frac{G_2}{J}\frac{\partial\psi}{\partial\rho}\right)-\frac{V'}{2\pi\rho}(j_{BS}+j_{CD})$$

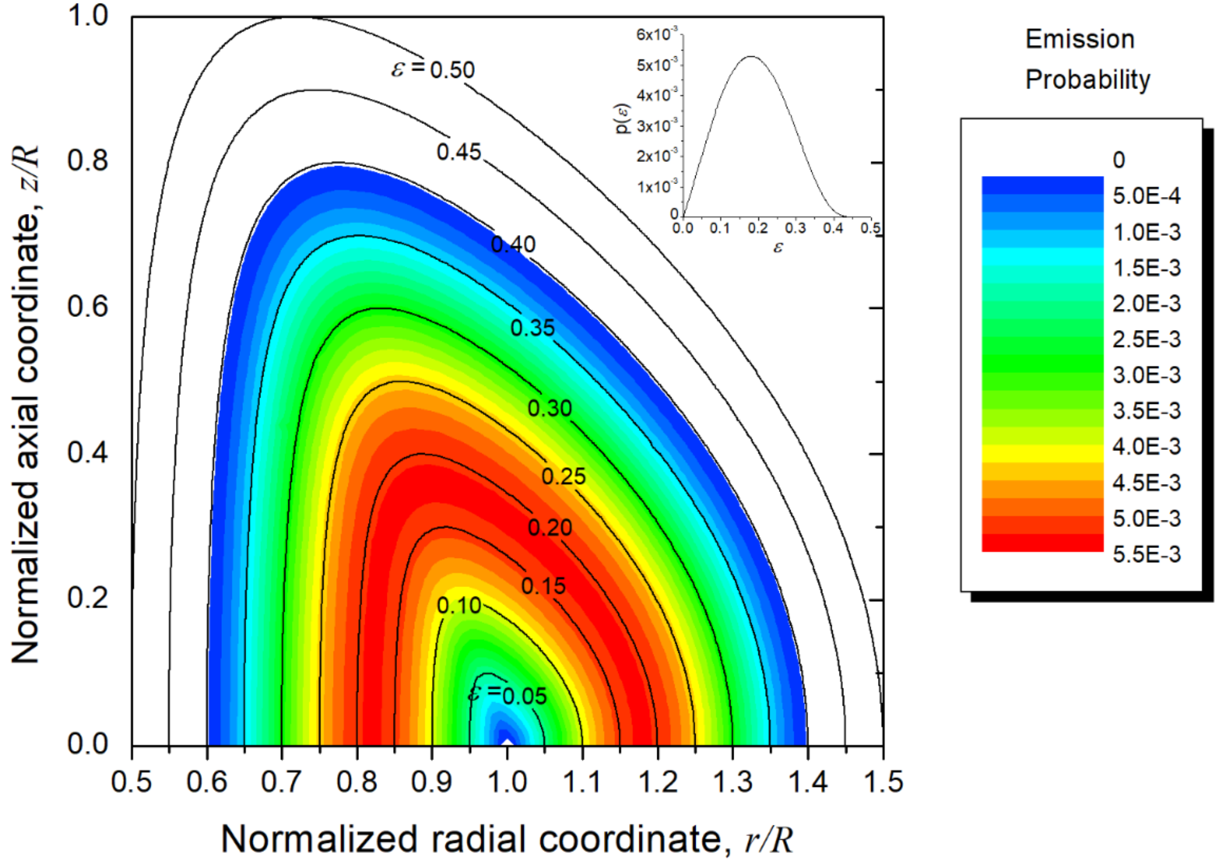
A numerical code is required to obtain density and temperature profiles as a function of machine parameters (geometry, plasma current, magnetic field, transport coefficients, auxiliary heating, etc…)

ASTRA simulations





Source strength



$$r_{DT}(\rho) = k_{DT}(kT_i)\frac{n^2}{4}$$

$$S_{TOT} = \int_{Vol} r_{DT}(\rho)dV = \int_0^{\varepsilon_{max}} r_{DT}(\rho)\frac{dV}{d\rho}d\rho$$

$$P(\rho) = \frac{S(\rho)}{S_{TOT}} = \frac{\int_0^{\rho} r_{DT}(\rho)\frac{dV}{d\rho}d\rho}{\int_0^{\rho_{max}} r_{DT}(\rho)\frac{dV}{d\rho}d\rho}$$

$$p(\rho) = \frac{dP}{d\rho} = \frac{r_{DT}(\rho)\frac{dV}{d\rho}}{S_{TOT}}$$

H. Salazar-Cravioto et al. IEEE Trans. Plas. Sci. 48, pp. 1810-1816 (2020)

Neutron flux calculation

- The multigroup neutron diffusion equation coupled set needs to be solved to find the energy-resolved neutron flux within the system:

Out-scattering

Fission

$$-D_g\nabla^2\phi_g + \left(\Sigma_{ag} + \sum_{g'\neq g}^{G} \Sigma^{s}_{g\to g'}\right)\phi_g = S_g + \chi_g \sum_{g'=1}^{G} \upsilon\Sigma_{fg'}\phi_{g'} + \sum_{g'=1}^{G} \Sigma^{s}_{g'\to g}\phi_{g'}$$

Diffusion leakage

Absorption

External source

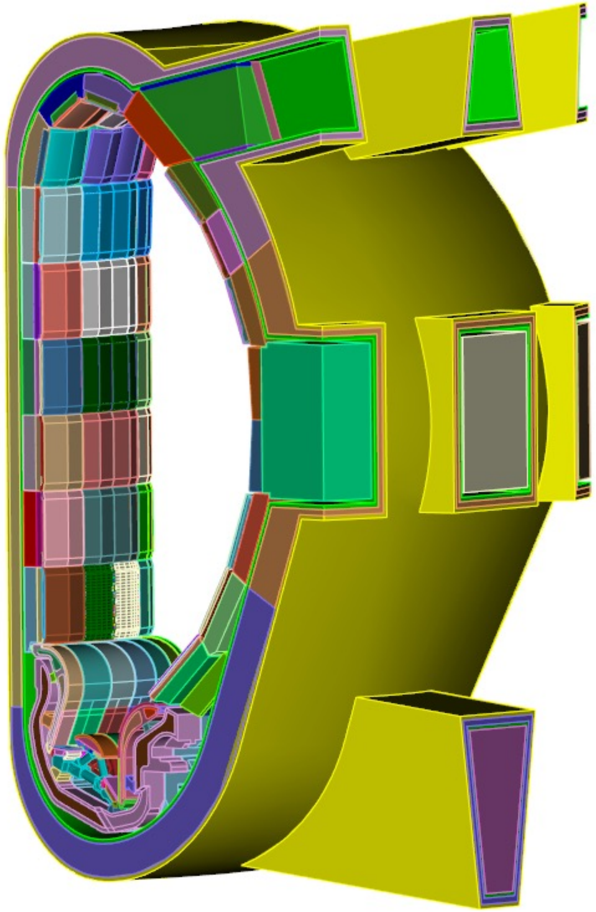
In-scattering

Neutro … such as KENO, SERPENT, M … solve t … tron diffusion equation for "f … n using the Monte Carlo method, with up to 256 groups

These macroscopic cross sections and diffusion coefficients are composition-dependent.

Coupling neutron transport and CAD

- Important efforts are currently underway for linking Monte Carlo neutron transport simulations with CAD geometry specification.
- This departs radically from the cumbersome constructive geometry definitions typical of most neutronics codes
- Constructive geometry is sufficient for rough/exploratory modeling, CAG is necessary for detailed accurate modeling.



A. M. Ibrahim et al. Nuclear Technology 175, pp. 251-258 (2011)

P. Wilson et al. Fusion Eng. Des., 83, pp. 824 (2008)

Nuclear reaction kinetics

Removal flow

Consumption to produce other isotopes

Decay

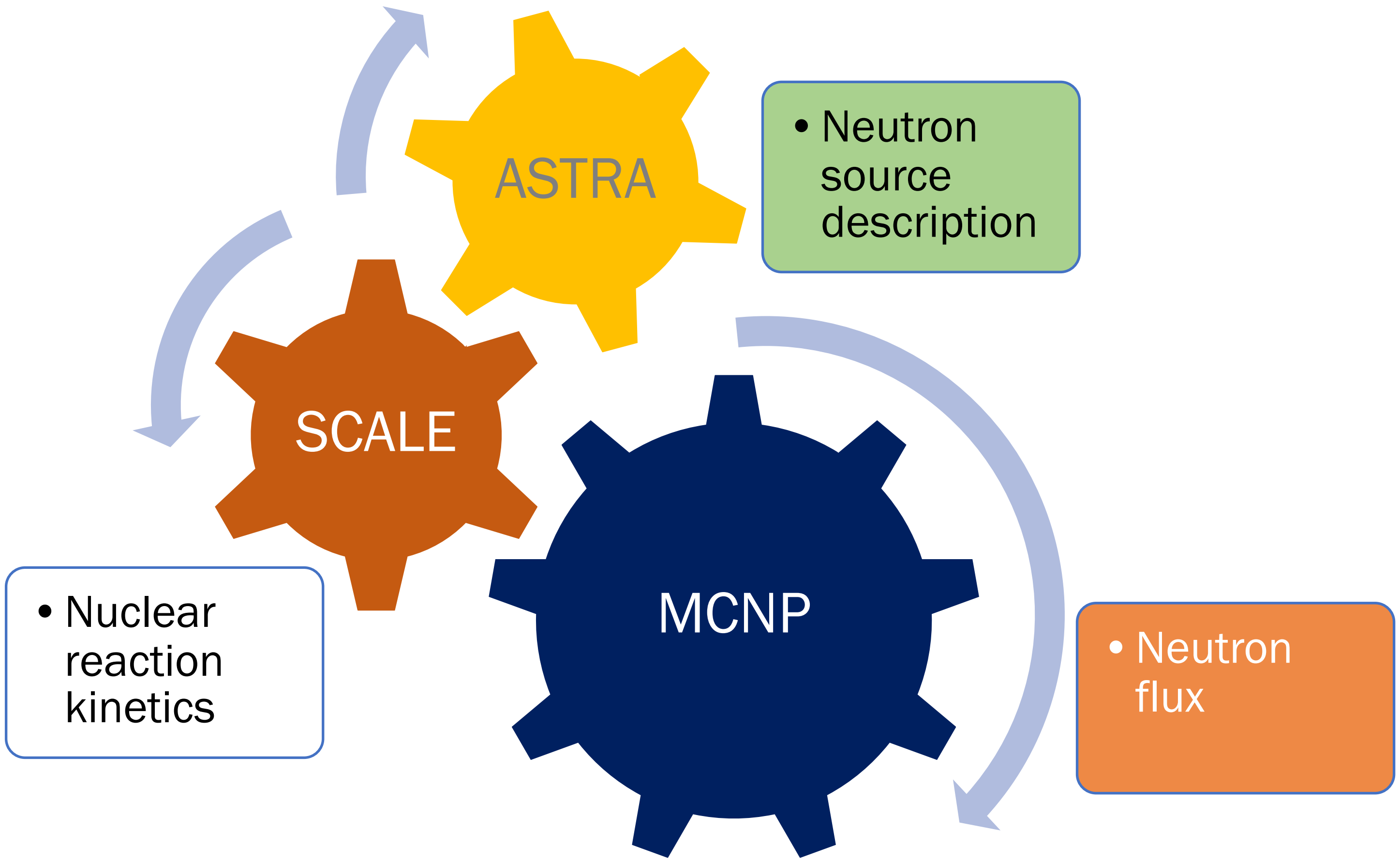
$$\frac{d(Vn_i)}{dt} = \dot{N}_{i,in} - \dot{N}_{i,out} + \sum_{g=1}^{G} \int \left[\left(\sum_{\substack{j=1 \\ j \neq i}}^{N} \sigma_{j \to i} n_j - \sum_{\substack{j=1 \\ j \neq i}}^{N} \sigma_{i \to j} n_i \right) \phi_g + \sum_{\substack{j=1 \\ j \neq i}}^{N} d_{ji} \lambda_j n_j - \lambda_i n_i \right] dV$$

Feed flow

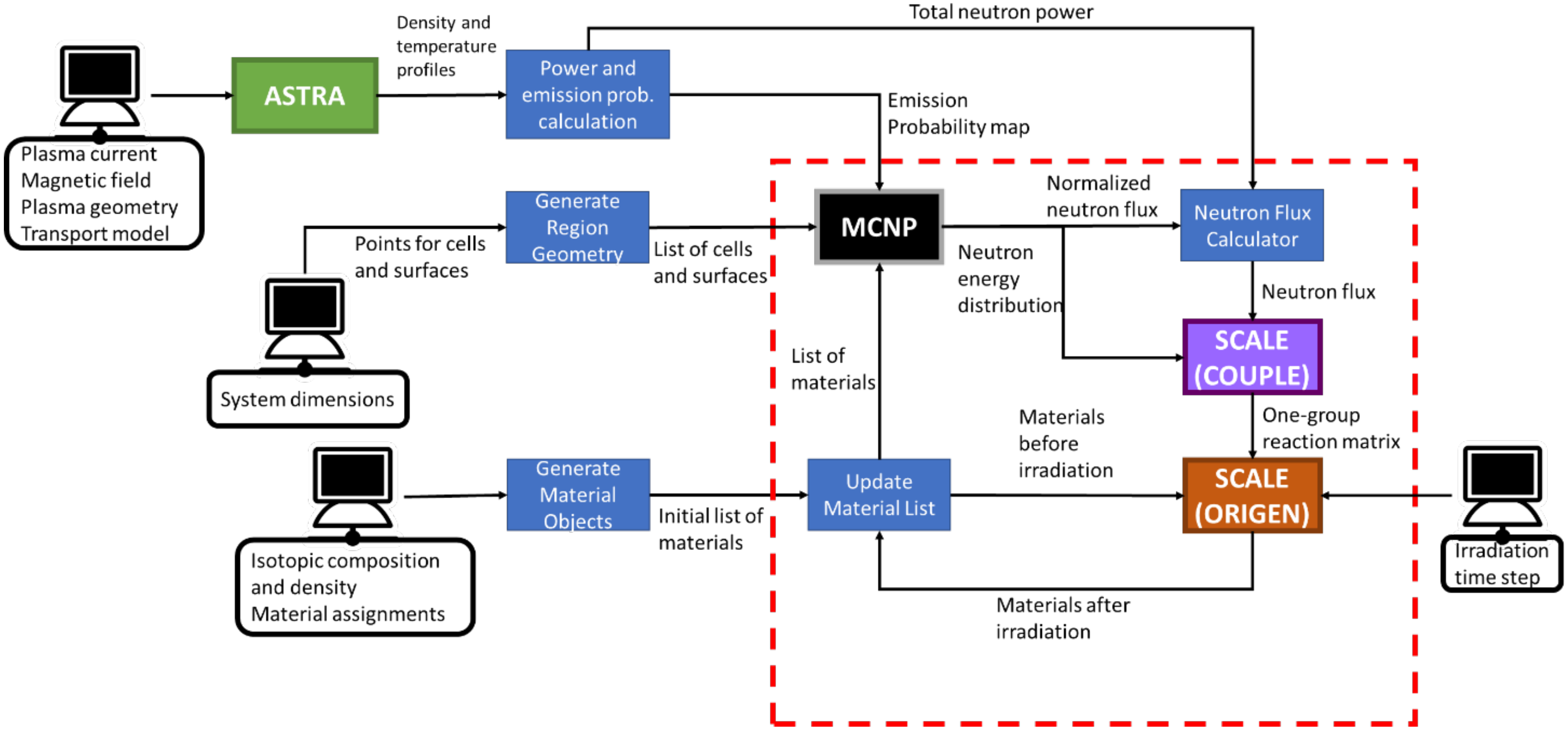
Production from isotope j

Generation by decay of other isotopes

Fusion system neutronics simulations



Code interlinking scheme



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Conclusions and final thoughts

Final thoughts

- Neutronics in fusion devices is important, since neutrons damage materials, activate stuff and produce tritium.
- Simulation of neutronics for fusion devices requires:
  - Neutron transport calculations (OpenMC, MCNP, KENO)
  - Plasma equilibrium Calculations (ASTRA, CORSICA)
  - Nuclear reaction kinetics (ORIGEN, FISPACT)
  - Advanced CAD processing for meshing and geometry definition (SW, AutoCAD, CAD-processing libraries).
- Information from these codes requires a coordination and processing effort to ensure adequate information flow.

Find out more!

- G. S. Was. "Fundamentals of Radiation Material Science". ISBN 978-1-4939-3438-6
- Y. Wu. "Fusion Neutronics". ISBN 978-981-10-5469-3
- UW Neutronics Center for Excellence
- LANL MCNP Home
- ORNL ORIGEN Home
- Plasma equilibrium codes from Woodruf Scientific

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