Theory of reactor operation Short lecture in reactor physics for the participants of the 2023 ARIEL Hands-on school on nuclear data from Research Reactors

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- 1 Physical model of neutron propagation
- 2 Fundamental concepts
- 3 Balance of neutrons Transport equation

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- 4 Neutron diffusion
- 5 Reactor kinetics

#### 6 Burnup

## Random walk

Physical model of neutron propagation

- point particle
- flying in space
- ocassionally colliding with nuclei
  - absorption
  - scatter
  - etc
- sequence of collisions to absorption
- subject of laws of probability
- random walk



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## Deterministic approach

Physical model of neutron propagation

- quantities of engineering interest
  - reaction rates for heat generation, burnup, etc
  - multiplication factor
- we don't care about fluctuations
- taking ensemble average
- instead of particles: fluid-like representation



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## Phase space

Fundamental concepts

#### State of a neutron

- It's traveling
  - at location r,
  - in direction  $\Omega$ ,
  - and at energy E

#### Phase space

- Possible states of any neutron
- Quantities are functions of these independent variables (r, Ω, E)



Fundamental concepts

Neutron density
$$n(\mathbf{r}, \Omega, E) \quad \left[\frac{n}{\mathrm{cm}^3 \, \mathrm{St} \, \mathrm{eV}}\right]$$

#### Interpretation

Number of neutrons per unit volume of the phase space (unit volume, unit solid angle, and unit energy)



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## Flux and cross sections

Fundamental concepts

#### Reaction rates are proportional to

- number (density) of neutrons
- their velocity
- number (density) of nuclei
   Proportionality constant:
   microscopic cross section

$$R_{\rm x} = \sigma_{\rm x}(E)N({\rm r},E)v(E)n({\rm r},\Omega,E)$$

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## Flux and cross sections

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$$R_{x} = \sigma_{x}(E)N(r, E) \quad v(E)n(r, \Omega, E)$$
$$R_{x} = \sum_{x}(r, E) \quad \varphi(r, \Omega, E)$$

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## Flux and cross sections

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Angular flux	Macroscopic cross section
$\varphi(r,\Omega,E) = v(E)n(r,\Omega,E)$	$\Sigma_{\rm x}({ m r},E)=\sigma_{\rm x}(E)N({ m r},E)$
Interpretation	Interpretation
Number of neutrons crossing at a	"Probability" of reaction per unit

small surface, in direction  $\Omega$  distance travelled

## Scalar flux and current

Fundamental concepts

#### Scalar flux

$$\Phi(\mathsf{r}, E) = \int_{4\pi} \varphi(\mathsf{r}, \Omega, E) \,\mathrm{d}\Omega$$

Flux of neutrons flying in any direction

#### Net current

$$\mathsf{J}(\mathsf{r}, E) = \int_{4\pi} \Omega \varphi(\mathsf{r}, \Omega, E) \,\mathrm{d}\Omega$$

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Net number of neutrons crossing a surface

How many neutrons leave a small volume around r?

- Number of neutrons crossing surface f
   f · Ωφ(r, Ω, E)
- Number of neutrons leaving V $L_V = \oint_F f(\mathbf{r}) \cdot \Omega \varphi(\mathbf{r}, \Omega, E) d\mathbf{r}$
- Apply Gauss's theorem  $L_V = \int_V \Omega \cdot \nabla \varphi(\mathbf{r}, \Omega, E) \, \mathrm{d}\mathbf{r}$
- Streaming loss at r:  $L = \lim_{V \to r} \frac{L_V}{V} = \Omega \cdot \nabla \varphi(\mathbf{r}, \Omega, E)$



## Gain and loss of neutrons

Balance of neutrons

#### Balance of neutrons in a point of phase space

$$\frac{\partial n}{\partial t}(\mathbf{r},\Omega,E,t) = \frac{1}{v}\frac{\partial \varphi}{\partial t}(\mathbf{r},\Omega,E,t) = \text{source} - \text{loss}$$

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What's loss?

streaming

 $\Omega \cdot \nabla \varphi(\mathbf{r}, \Omega, E, t)$ 

collision

 $\Sigma_t \varphi(\mathbf{r}, \Omega, E, t)$ 

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## Gain and loss of neutrons

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#### What's source?

scatter

$$\int_{0}^{\infty} \int_{4\pi} \Sigma_{s} \left( \mathsf{r}, \Omega' \to \Omega, E' \to E \right) \varphi(\mathsf{r}, \Omega', E', t) \, \mathrm{d}\Omega' \, \mathrm{d}E'$$

fission

$$\frac{f(E)}{4\pi}\int_0^{\infty}\int_{4\pi}\nu\Sigma_f\left(\mathsf{r},E'\right)\varphi(\mathsf{r},\Omega',E',t)\,\mathrm{d}\Omega'\,\mathrm{d}E'$$

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## Transport equation

Balance of neutrons

#### The (first order differential form of the) transport equation

$$\frac{1}{v}\frac{\partial\varphi}{\partial t}(\mathbf{r},\Omega,E,t) = -\Omega\cdot\nabla\varphi(\mathbf{r},\Omega,E,t) - \Sigma_t\varphi(\mathbf{r},\Omega,E,t) + Q(\mathbf{r},\Omega,E,t)$$

#### Generalised source

$$Q(\mathbf{r}, \Omega, E, t) = \int_{0}^{\infty} \int_{4\pi} \Sigma_{s} \left( \mathbf{r}, \Omega' \to \Omega, E' \to E \right) \varphi(\mathbf{r}, \Omega', E', t) \, \mathrm{d}\Omega' \, \mathrm{d}E' + \frac{f(E)}{4\pi} \int_{0}^{\infty} \int_{4\pi} \nu \Sigma_{f} \left( \mathbf{r}, E' \right) \varphi(\mathbf{r}, \Omega', E', t) \, \mathrm{d}\Omega' \, \mathrm{d}E' + S(\mathbf{r}, \Omega, E, t)$$

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Very hard to solve because

- complicated dependence on energy E (resonances, thermalisation)
- lack of theoretical understanding (singular solutions)
- number of independent variables  $\rightarrow$  combinatorial explosion

Possible routes out of the trouble

- simplification
- numerical methods needed
- but usually both of them

Ideas and approaches

- $\blacksquare$  Point kinetics  $\rightarrow$  focus on time dependence
- $\blacksquare$  Diffusion  $\rightarrow$  get rid of the angular variable  $\Omega$
- Discrete ordinates  $\rightarrow$  discretise everything in (r,  $\Omega, E$ )
- $\blacksquare$  Collision probabilities  $\rightarrow$  connect everything to everything

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- $\blacksquare \text{ Monte Carlo} \rightarrow \text{simulate random walk}$
- Multigroup/fewgroup approximation
- Resonance shielding, cross section weighting

## Diffusion theory

Neutron diffusion

#### Idea

For ease of life, flux could be approximated with linear expansion:

$$arphi(\mathsf{r},\Omega,E)pproxrac{1}{4\pi}\Phi(\mathsf{r},E)+rac{3\Omega}{4\pi}\mathsf{J}(\mathsf{r},E)+\ldots$$

#### Assumptions

Severe and restrictive conditions

- dominant reaction is scatter
- no strong absorbers
- spatial flux variation is weak
- angular dependence of flux is mild

### Getting rid of $\Omega$ Neutron diffusion

#### What you do

- Substitute the linear flux expansion into the transport equation
- Integrate the equation for  $\Omega$

#### What you get

$$\frac{1}{v}\frac{\partial\Phi}{\partial t}(\mathbf{r}, E, t) = -\nabla \mathsf{J}(\mathbf{r}, E, t) - \Sigma_t \Phi(\mathbf{r}, E, t) + Q_0(\mathbf{r}, E, t)$$

- $Q_0(\mathbf{r}, E, t)$  is the isotropic part of the generalised source
- Balance of neutrons, irrespective of their direction of flight
- One equation for two unknowns:  $\Phi(r, E, t)$ , J(r, E, t)
- One more equation is needed

How to get connection between the flux  $\Phi(r)$  and the J(r) current?

- $\blacksquare$  multiply the transport equation with  $\Omega,$  and integrate again
- neglect time derivative of the current  $\left(\frac{\partial J}{\partial t}(\mathbf{r}, E, t) \approx 0\right)$
- neglect energy change in the anisotropic part of the scatter

#### Fick's Law

$$\mathsf{J}(\mathsf{r}, E, t) = -D(\mathsf{r}, E)\nabla\Phi(\mathsf{r}, \mathsf{E}, \mathsf{t})$$

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- diffusion coefficient  $D(\mathbf{r}, E) = \frac{1}{3\Sigma_{tr}(\mathbf{r}, E)}$ ,  $\Sigma_{re}(\mathbf{r}, E) = \Sigma_{t}(\mathbf{r}, E) - \operatorname{avg}(\cos \theta)\Sigma_{s}(\mathbf{r}, E)$
- eliminate J(r, E, t) from the previous equation

## The diffusion equation

Neutron diffusion

#### Finally the diffusion equation

$$\frac{1}{v}\frac{\partial\Phi}{\partial t}(\mathsf{r},E,t) = \nabla D(\mathsf{r},E)\Phi(\mathsf{r},\mathsf{E},t) - \Sigma_t\Phi(\mathsf{r},E,t) + Q_0(\mathsf{r},E,t)$$

generalised source:

$$\begin{aligned} Q_0(\mathbf{r}, E, t) &= \int_0^\infty \Sigma_{s0} \left( \mathbf{r}, E' \to E \right) \Phi(\mathbf{r}, E', t) \, \mathrm{d}E' + \\ f(E) \int_0^\infty \nu \Sigma_f \left( \mathbf{r}, E' \right) \Phi(\mathbf{r}, E', t) \, \mathrm{d}E' + S(\mathbf{r}, E, t) \end{aligned}$$

- much-much easier to solve
- analytical and numerical solution methods are available

# The physics behind Fick's law Neutron diffusion

- Plenty of neutrons here, they will migrate to the neigbour region
- No neutrons in the neighbour, they can't migrate to here

#### Figuratively

Neutrons are rolling down from the flux hill.



# Criticality and $k_{\rm eff}$

#### The diffusion equation

$$\mathbf{0} = \frac{1}{v} \frac{\partial \Phi}{\partial t}(\mathbf{r}, E, t) = \nabla D(\mathbf{r}, E) \Phi(\mathbf{r}, E, t) - \Sigma_t \Phi(\mathbf{r}, E, t) + Q_0(\mathbf{r}, E, t)$$

balancing the equation with the multiplication factor

$$Q_{0}(\mathbf{r}, E, t) = \int_{0}^{\infty} \Sigma_{s0} \left( \mathbf{r}, E' \to E \right) \Phi(\mathbf{r}, E', t) dE' + \frac{f(E)}{k_{\text{eff}}} \int_{0}^{\infty} \nu \Sigma_{f} \left( \mathbf{r}, E' \right) \Phi(\mathbf{r}, E', t) dE' + S(\mathbf{r}, E, t)$$

eigenvalue equation instead of time dependence

rather general, can be done to the transport equation as well

- Primarily, we would like to know the reactor power as a whole
- time dependent neutron transport/diffusion models are complicated
- too much detail  $\rightarrow$  too much work
- seeking some simple approach
- trying to compute overall number of neutrons N(t)
- without considering phase space variables  $(r, \Omega, E, t)$

#### Point kinetic equation

$$\varphi(\mathbf{r},\Omega,E,t) = N(t)\Phi(\mathbf{r},\Omega,E)$$

separating time dependence and shape function

- fission neutron lifetime is short, 10 - 100 μs
- small deviation from k<sub>eff</sub> = 1.0 results rapid increase reactor power
- fission products have excess neutrons
- strong  $\beta^-$  decay
- some fission neutrons are produced after one or more decay
- time scale 0.1 *s* − 100 *s*, i.e. significantly later



- divided into six groups
- $\lambda_i$  decay constants
- $\beta_i$  delayed n, fractions

## Overall balance of neutrons

Reactor kinetics

How is the number of neutrons changing during the average life time  $\tau_n$  of a neutron?

$$N(t+\tau_n) = \frac{k_{\text{eff}}(1-\beta)N(t)}{k_{\text{eff}}(1-\beta)N(t)} + \sum_{i=1}^{6} \lambda_i C_i(t) \tau_n + \frac{S(t)}{\tau_n} \tau_n$$

• 
$$k_{\text{eff}}(1-\beta)N(t)$$
 increase from chain reaction

- $\sum_{i=1}^{6} \lambda_i C_i(t) \tau_n$  emitted by decaying delayed neutron precursors
- **S**(*t*)  $\tau_n$  introduced by external source

## Balance of delayed neutron precursors

Reactor kinetics

Further equations are needed for the delayed precursors

$$C_i(t+ au_n) = C_i(t) + \frac{\kappa_{\mathsf{eff}}\beta_i N(t)}{\kappa_{\mathsf{eff}}\beta_i N(t)} - \frac{\lambda_i C_i(t)}{\lambda_i C_i(t)} au_n, \quad \mathsf{where} \quad i=1\dots 6$$

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*k*<sub>eff</sub>β<sub>i</sub>N(t) precursors produced by fission
 λ<sub>i</sub>C<sub>i</sub>(t) τ<sub>n</sub> precursors decaying to delayed neutrons

Finally using the Taylor expansions  $N(t + \tau_n) \approx N(t) + \tau_n \frac{dN}{dt}(t) + \dots$  and  $C_i(t + \tau_n) \approx C_i(t) + \tau_n \frac{dC_i}{dt}(t) + \dots$  to get  $\cdots$ 

### Point kinetic equations

Reactor kinetics

#### Point kinetic equations

$$rac{\mathrm{d}N}{\mathrm{d}t}(t) = rac{
ho-eta}{\Lambda}N(t) + \sum_{i=1}^6\lambda_iC_i + S(t)$$
 $rac{\mathrm{d}C_i}{\mathrm{d}t}(t) = rac{eta_i}{\Lambda}N(t) - \lambda_iC_i(t)$ 

#### With

Reactivity

$$\rho = \frac{k_{\rm eff}-1}{k_{\rm eff}}$$

#### Generation time

$$\Lambda = \frac{\tau_n}{k_{\rm eff}}$$

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## Solution of the point kinetic equations

Reactor kinetics

#### Assuming S(t) = 0, the solution can be written as

#### Ansatz

$$N(t) = N^0 \exp(\omega t)$$
$$C_i(t) = C_i^0 \exp(\omega t)$$

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Substituting this into the point kinetic equations a formula for period  $\omega$  can be obtained.

## Inhour equation

Reactor kinetics

#### Charachteristic polynomial of the system

Relation between reactivity and reactor period

$$\frac{\rho}{\beta} = \frac{\Lambda}{\beta}\omega + \omega \sum_{i=1}^{6} \frac{\beta_i/\beta}{\lambda_i + \omega}$$

one eigenvalue can be positive or negative, depending on reactivity



#### Full solution of the point kinetic equations Reactor kinetics

The full solution can be written as the sum of 7 modes

$$egin{aligned} \mathcal{N}(t) &= \sum_{j=0}^6 \mathcal{N}_j^0 \exp(\omega_j t) \ \mathcal{C}_i(t) &= \sum_{j=0}^6 \mathcal{C}_{i,j}^0 \exp(\omega_j t) \end{aligned}$$

 $N_i^0$  and  $C_{i,i}^0$  can be tuned to fit initial condition.

# Reactivity jump

- critical reactor
- sudden increase in reactivity
- sum of 7 exponentials

• 
$$\omega_0 > 0 > \omega_j$$
, where  $j = 1 \dots 6$ 

#### Dominant mode

 $\omega_0 > 0$  assymptotic behaviour



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## Subcritical neutron multiplication

Reactor kinetics

- subcritical reactor with source
- number of neutrons in the core  $N = \tau_n \left(S_0 + S_0 k_{eff} + S_0 k_{eff}^2 + \dots\right)$ geometric series  $N = \frac{S_0 \tau_n}{1 k_{eff}} = \frac{S_0 \Lambda}{-\rho}$ m'crit m''crit m''

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estimation of critical mass, rod position, etc

## Change of composition

Burnup

- nuclear reactions transmute isotopes from one into another
- composition of the reactor slowly changing
- main processes
  - fission into mid-size nuclei, e.g.  $^{235}$ U + n  $\rightarrow$  fission products
  - $\label{eq:states} \begin{array}{l} \bullet \mbox{ build up of transuranium } \\ \mbox{ isotopes } \\ e.g. \ ^{238}\mbox{U} + n \rightarrow \ ^{239}\mbox{Np} \rightarrow \\ ^{239}\mbox{Pu} + n \rightarrow \ ^{240}\mbox{Pu} + n \rightarrow \\ ^{241}\mbox{Pu, etc} \end{array}$
  - Activation of structural materials



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# Mathematical treatment of burnup

Equation for the number density (Bateman equations)

$$\frac{\mathrm{d}N_i}{\mathrm{d}t}(t) = -\left(\sigma_i^{\mathsf{a}}\Phi + \lambda_i\right)N_i(t) + \sigma_j^{\mathsf{c}}\Phi N_j(t) + \lambda_k N_k(t)$$

- balance equation of rates of production and loss
- system of ordinary differential equations
- a few dozen or hundred of coupled equations
- at afirst glance, this is an easy job

#### Reality kicks in

- 1. spatial dependence
- 2. cross sections and flux are changing in time
- 3. for real life reactors  $\rightarrow$  bloody hard job  $\rightarrow$  more in later lectures

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## The End

Thank you for your attention

