# Calculation and Interpretation of Higher Order Flux Modes in the KUCA A-Core ADS

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# 1. Introduction

The authors are involved with a multi-year research project targeting the analysis and design of an Accelerator Driven System as a future Minor Actinide (MA) transmutation system. In this research, measurement data is used from the Kyoto University Critical Assembly (KUCA) A-core ADS facility. This ADS facility consists of a zero-power, subcritical core into which neutrons are injected, either from a DT-source, or from a spallation source driven with 100 MeV protons. The subcritical core has a thermal neutron spectrum. For ADS the online monitoring of the reactivity is crucial to ascertain a safe operating margin to criticality. In an ADS, a pulsed neutron experiment is the obvious choice. In this case, the so-called prompt  $\alpha$ -mode of the reactor is important. Development of related theory and analysis tools is important for ADS development.

#### 2. Theory

The basic equation describing the behaviour of a nuclear reactor is the time-dependent transport equation. In the case of time dependence, a distinction must be made between the prompt fission neutrons and the delayed neutrons, hence the equations are, in operator notation:

$$\begin{aligned} \frac{1}{v} \frac{\partial \psi}{\partial t} + \nabla \cdot \hat{\mathbf{\Omega}} \psi + \mathbf{T} \psi &= \mathbf{S} \psi + (1 - \beta) \chi_p \mathbf{F} \psi \\ &+ \sum_j \lambda_j \chi_{d,j} c_j \\ \frac{\partial c_j}{\partial t} &= \beta_j \mathbf{F} \psi - \lambda_j c_j \end{aligned}$$

where **T** is the collision operator, **S** is the scatter operator, and **F** is the fission operator. If the operators are not time dependent, the solution to this equation has the form  $\psi(\mathbf{r}, E, \hat{\mathbf{\Omega}}, t) = e^{\alpha t} \Psi(\mathbf{r}, E, \hat{\mathbf{\Omega}})$ , and similar for the precursor concentrations [1]. The transport equation becomes:

$$\frac{\alpha}{v}\Psi + \nabla \cdot \hat{\Omega}\Psi + \mathbf{T}\Psi = \mathbf{S}\Psi + (1-\beta)\chi_p \mathbf{F}\Psi + \sum_j \lambda_j \chi_{d,j} C_j \quad (1)$$

$$\alpha C_j + \lambda_j C_j = \beta_j \mathbf{F} \Psi \tag{2}$$

Boundary conditions determine the admissible  $\alpha_j$  (the eigenvalues) and the corresponding spatial shape functions

 $\Psi_{\alpha_j}$  (the so-called  $\alpha$ -modes). From elementary mathematics, the transport operator has one real eigenvalue  $\alpha_0$  which is the least negative, or even positive, of all eigenvalues. After a sufficiently long time, the flux in the reactor is thus given as  $\psi = e^{\alpha_0 t} \Psi_{\alpha_0}$ , with the special case  $\alpha_0 = 0$  corresponding to a *critical* reactor.

In a different type of analysis, the time dependence of the neutron flux is removed by introducing an artificial steady state, by replacing  $\nu$  with  $\nu/k$  in the fission operator. The critical transport operator then becomes:

$$abla \cdot \mathbf{\hat{\Omega}}\Psi + \mathbf{T}\Psi = \mathbf{S}\Psi + rac{1}{k}\chi\mathbf{F}\Psi$$

Similar to the  $\alpha$ -modes, admissible values of  $k_j$  are determined by the boundary conditions, and (for historical reasons) the corresponding flux shape functions  $\Psi_{\lambda}$  are called  $\lambda$ -modes. As long as the precursors do not move, there is no need to distinguish between prompt and delayed neutrons in the case of  $\lambda$ -modes.

### **2.1.** Relation between $\alpha$ -modes and $\lambda$ -modes

In the case of  $\alpha$ -modes, a distinction must be made between long time scales, where the delayed neutrons have an influence, and short time scales where only the prompt neutrons play a part. Let  $\alpha_l$  be an eigenvalue and  $\Psi_l$ ,  $C_l$  the corresponding shape functions. Then, using Eqs. (1) and (2) we find the *delayed*  $\alpha$ -modes:

$$\frac{\alpha_l}{v}\Psi_l + \nabla \cdot \hat{\mathbf{\Omega}}\Psi_l + \mathbf{T}\Psi_l = \mathbf{S}\Psi_l + \left[(1-\beta)\chi_p + \sum_j \frac{\lambda_j \chi_{d,j}\beta_j}{\alpha_l + \lambda_j}\right]\mathbf{F}\Psi_l \quad (3)$$

If the effect of delayed neutrons is ignored, the *prompt*  $\alpha$ -modes are found:

$$\frac{\alpha_l^p}{v}\Psi_l^p + \nabla \cdot \hat{\mathbf{\Omega}}\Psi_l^p + \mathbf{T}\Psi_l^p = \mathbf{S}\Psi_l^p + (1-\beta)\chi_p \mathbf{F}\Psi_l^p \quad (4)$$

Finally, for reference, the  $\lambda$ -modes satisfy the equation:

$$\nabla \cdot \hat{\mathbf{\Omega}} \Psi_{\lambda_m} + \mathbf{T} \Psi_{\lambda_m} = \mathbf{S} \Psi_{\lambda_m} + \frac{1}{k_m} \chi \mathbf{F} \Psi_{\lambda_m} \qquad (5)$$

For delayed  $\alpha$ -modes,  $|\alpha_l| < 1.0$ , so that the leading factor  $\alpha_l/v$  can be neglected. The result is that the form of the equations for the  $\alpha$ - and  $\lambda$ -mode are similar. In fact,  $\Psi_l$  and  $\Psi_m$  are identical if

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$$(1-\beta)\chi_p + \sum_j \frac{\lambda_j \chi_{d,j} \beta_j}{\alpha_l + \lambda_j} = \frac{\chi}{k_m}$$

Under certain idealized cases, this equation will be satisfied for J different values of  $\alpha_l$ ; the  $\alpha$ - and  $\lambda$  modes are then identical. In general the conclusion is that for certain values of  $\alpha_l$ , there is a correspondence between the delayed  $\alpha$ -modes and the  $\lambda$ -modes.

If the reactor is below prompt critical, there will be one least negative eigenvalue  $\alpha_0^p$ ; any other eigenvalue  $\alpha^p$  is more negative than  $\alpha_0^p$ .  $\alpha^p$  has a large magnitude as it is related to the decay of the prompt neutrons. If a prompt mode  $\Psi_l^p$  is substituted in Eq. (3), it would almost "fit" Eq. (3), except for the delayed neutron term. However, this delayed neutron term is divided by the (large)  $\alpha^p$  and hence its influence is small. We therefore conclude that for any prompt  $\alpha$ -mode there is a corresponding (nearly identical) delayed mode:  $\Psi_l^p \approx \Psi_l$ , and  $\alpha_l^p \approx \alpha_l$ .

A note must be made here on energy dependence of the modes. The  $\alpha$ -modes include the term  $\alpha/v$ , with v the neutron speed. For high energy neutrons, this term will be much smaller than for thermal neutrons. Thus the correspondence between  $\alpha$ -modes and  $\lambda$ -modes is also energy dependent.

## 3. Calculation of the Modal Shapes

For the calculation of the mode shapes, some simplifications and approximations are introduced. First, diffusion theory is used instead of transport theory; energy is discretized into energy groups and space is discretized into finite volumes. With these discretizations, all operators in the aforegoing equations are matrices, and all continuous function become vectors. The solution is found as the eigenvalues and eigenfunctions of a matrix. Let **D** denote the diffusion operator. For the prompt  $\alpha$ -modes, one obtains:

$$\frac{1}{\alpha}\boldsymbol{\phi} = \left[\mathbf{D} + \mathbf{T} - \mathbf{S} - (1 - \beta)\chi_p \mathbf{F}\right]^{-1} \left(-\frac{1}{V}\boldsymbol{\phi}\right)$$

For the delayed  $\alpha\text{-modes},$  one finds after some manipulations:

$$\frac{1}{\alpha}\boldsymbol{\phi} = \left[\mathbf{D} + \mathbf{T} - \mathbf{S} - (1 - \beta)\chi_p + Z\mathbf{F}'\right]^{-1} \left(-\frac{1}{V}\boldsymbol{\phi} - \boldsymbol{\chi}_d \boldsymbol{c}\right)$$

where  $\mathbf{F}'$  is a modified fission operator, and for the  $\lambda$ -modes:

$$k\phi = [\mathbf{D} + \mathbf{T} - \mathbf{S}]^{-1} \chi \mathbf{F} \phi$$

All these equations have the form of a generalized eigenvalue equation, i.e.  $\mathbf{B}^{-1}\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$ , and can be solved on a digital computer. The solution strategy is as follows:

- 1. Select a trial vector  $\phi_A$ .
- 2. Depending on the type of mode under evaluation, calculate a source term:
  - For prompt  $\alpha$ -modes  $q_{\alpha^p} = -\phi_A/V$
  - For delayed  $\alpha$ -modes  $oldsymbol{q}_{lpha} = oldsymbol{\phi}_A / oldsymbol{V} oldsymbol{\chi}_d oldsymbol{c}_A$
  - For  $\lambda$ -modes  $q_{\lambda} = \chi \mathbf{F} \phi_A$ .
- 3. Solve a fixed source problem:

$$\left[\mathbf{D}+\mathbf{T}-\mathbf{S}_{s}
ight] \boldsymbol{\phi}_{D}=\left[\mathbf{S}_{d}+\mathbf{S}_{u}+\mathbf{K}
ight] \boldsymbol{\phi}_{D}+\mathbf{q}$$

where the matrix **K** depends on the type of eigenvalue to be computed. The scatter operator has been separated into a self-scatter contribution, an upscatter contribution and a downscatter contribution. The solution  $\phi_D$  is calculated with an iterative algorithm.

4. Based on the solution vector  $\phi_D$ , adjust the trial vector  $\phi_A$  and repeat until  $\phi_D$  is a valid eigenvector with corresponding eigenvalue.

# 3.1. Adjoint equations

For many applications, the adjoint modes are required, and thus these adjoint modes need to be calculated. The adjoint modes are solutions to the adjoint equations. The adjoint equations are found using the "rules for adjointness" for each operator in the equations. If the diffusion equation is discretized into a matrix equation as above, the matrices are real and thus the adjoint counterparts are found by taking the transpose of all relevant matrices.

## 3.2. Computer analysis

In the present research, the DALTON computer code [2] is used for investigations into the properties of the  $\alpha$ - and  $\lambda$ -modes of a nuclear reactor. DALTON is a 3D multigroup diffusion code which can calculate the prompt and delayed  $\alpha$ -modes, the  $\lambda$ -modes, as well as fixed source and time dependent problems. Eigenvalues and -modes are determined with the ARPACK software [3].

## 4. Results

In the first stage of this research, the properties of the prompt and delayed  $\alpha$ -modes are investigated. A slightly subcritical 1D test case was devised. The core has two regions, fuel and reflector, and there are 12 energy groups (8 below 4 eV). The fuel is a mixture of HEU and poly-ethylene (PE), and the reflector is pure PE, similar to the materials used in the KUCA-A ADS, although fuel fraction and core size are adjusted to find a slightly subcritical 1D system. In Figure 1a are given the fundamental prompt  $\alpha$ -mode, delayed  $\alpha$ -mode, and  $\lambda$ -mode. In this case,  $\alpha_0$  is relatively small and all modes are similar, except at very low energies where the term  $1/v^g$  is relatively large. As an illustration, in Figure 1b are given the 4<sup>th</sup> order modes. In this case,  $\alpha_p$  is large and as a result the prompt  $\alpha$ -modes differ from the other two modes.



Figure 1:  $\alpha$ - and  $\lambda$ -modes in 1D geometry.

A 2D test case was also devised: a rectangular core (HEU and PE), surrounded by a thick PE reflector. The system is deliberately asymmetrical to avoid problems with degeneration of the eigenvalues. The same 12-group energy structure is used. In this case also the general similarity between delayed  $\alpha$ -modes and  $\lambda$ -modes was confirmed. The prompt  $\alpha$ -modes can be markedly different from the  $\lambda$ -modes, as illustrated in Figure 2 where the 4<sup>th</sup>  $\lambda$ -mode and prompt  $\alpha$ -mode are shown.

Ultimately, the  $\alpha$ - and  $\lambda$ -modes are only useful if their application to a real reactor gives useable results. In the present work, it was decided to analyze the KUCA ADS benchmark [4], Case I-1. In this core, a slightly subcritical configuration was created and a pulsed neutron exper-



Figure 2: The 4<sup>th</sup> prompt  $\alpha$ -mode as returned by ARPACK and the corresponding  $\lambda$ -mode in 2D geometry.

iment was performed. Results are listed in Table I. A full 3D, time-dependent analysis was performed with the DAL-TON code of a pulsed neutron experiment with a pulse width  $\Delta t_p = 100 \,\mu\text{s}$  and a repetition width  $\Delta t_r = 20 \,\text{ms}$ . In Figure 3 is given the time-dependent neutron flux in group 11 (thermal flux), roughly in the center of the core. The flux shape corresponds to the theoretical expectation. After the source pulse, many  $\alpha$ -modes are excited, but ultimately only the fundamental prompt  $\alpha$ -mode ( $\alpha_0^p$ ) remains, and indeed, the flux decays as a simple exponential once the higher modes have died away.

Table I: Results for KUCA Case I-1.

	Measured	Calculated
k <sub>eff</sub> [ - ]	0.995	0.991524
$\alpha_0^p  [\mathrm{s}^{-1}]$	-266	-297

Theoretically, the flux shape in the reactor during the period of exponential decay should be the mode shape of the fundamental prompt  $\alpha$ -mode. In Figure 4 the calculated mode shape for  $\alpha_0^p$  is compared with the flux shape during



Figure 3: Simulation of pulsed neutron experiment in KUCA (benchmark case I-1).

the exponential decay period. While detailed investigations are ongoing, the flux shapes appear very similar.



(a) Calculated prompt  $\alpha$  mode



(b) Flux shape during exponential decay

Figure 4: The calculated mode shape corresponding to  $\alpha_0^p$  and the flux shape obtained in the exponential decay period.

Further investigations are ongoing, concerning the distribution of the precursors in the system. If the flux decays as a pure exponential, as predicted by theory, the precursor distribution is determined by the prompt  $\alpha$ -mode. However, during a short time following the source pulse, many higher modes are excited, and these higher modes all cause the presence of precursors. As a result the precursor distribution is not quite in the fundamental mode and as a result, the clean exponential decay curve has a contamination from these precursors. The influence of the contamination on the count rate of a detector is a key issue in the determination of the reactivity of the system.

# 5. Conclusion and Outlook

The theory behind prompt and delayed  $\alpha$ -modes and  $\lambda$ -modes was presented and the similarity properties of these modes were shown. Trial calculations in 1D and 2D have shown the general properties of the various modes in a simple model of a nuclear reactor. The goal of the present work is the analysis of the KUCA ADS experiments with deterministic codes. In the present work, one case (I-1) was analyzed and while the results are not yet fully investigated, preliminary results indicate a good correspondence between theory and experiment. In the future, the influence of the higher order alpha modes will be investigated in order to realize a reliable estimation of reactivity.

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