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## NUMERICAL ANALYSIS OF THE SELF-SUSTAINING TRAVELING WAVE OF NUCLEAR FISSION PROPAGATED BY EPITHERMAL NEUTRONS IN URANIUM DICARBIDE MEDIUM<sup>1</sup>

This study investigates the self-sustaining traveling wave of nuclear fission in a uranium dicarbide medium by numerically solving a system of partial differential equations. The primary focus is on the neutron diffusion equation and nuclide balance equations, which are crucial for understanding the behavior of fission waves. By solving these equations, we aim to determine the propagation characteristics and assess the stability of nuclear fission waves in uranium dicarbide. Numerical analysis provides significant insights into the dynamics of neutron distribution and nuclide evolution, enhancing our understanding of the underlying physical processes and their implications for traveling wave reactor design.

**Keywords:** traveling wave reactor, epithermal neutrons, uranium dicarbide, neutron diffusion equation, reactor design, self-sustaining fission wave.

### 1. Introduction

The traveling wave reactor (TWR) represents an advanced nuclear reactor design with significant advantages over traditional models. In a TWR, the nuclear reaction front progresses through the fuel material, converting fertile material into fissile material as it advances. One of the main advantages of this design is the inherent safety of these reactors. This concept also offers the promise of improved fuel utilization and reduced waste generation compared to conventional reactor designs. Furthermore, it may enable the use of unconventional fuels such as depleted uranium or thorium, which are abundant and currently considered waste products in nuclear fuel cycles.

Research on traveling wave regimes of nuclear fission in fissile reactor media, prior to 2013, was conducted exclusively in the realm of fast neutrons (e.g., [1 - 31]). This focus was due to the criterion for traveling wave propagation, formulated in [1], which is satisfied only for fast neutrons. However, fast neutrons impose harsh conditions (~500 DPA) on the structural materials and the fuel of such reactors [24 - 26], which cannot be met in the foreseeable future.

A solution to the issue of radiation resistance in TWRs was proposed in [32]. The criterion for traveling wave propagation was studied for uranium fuel across a broad energy spectrum of neutrons (0.001 eV - 1 MeV), and it was found that the criterion is satis-

fied not only in the fast neutron energy region but also in the epithermal range (1 - 7 eV). Furthermore, [32] presented the results of simplified 1D modeling, demonstrating the feasibility of a traveling wave of nuclear fission in natural uranium driven by epithermal neutrons. It was suggested that future research efforts should focus on this direction. However, since then, only five studies [33 - 37] have been published that report on traveling wave regimes in fissile reactor media using non-fast neutrons.

This study investigates the propagation of a traveling wave of nuclear fission within a cylindrical uranium dicarbide (UC<sub>2</sub>) medium propagated by epithermal neutrons. UC<sub>2</sub> was selected for its effectiveness as a neutron moderator, facilitating the formation of the epithermal spectrum [38 - 39], as well as for its high thermal conductivity and robustness under high-temperature conditions. To initiate nuclear reactions, a neutron flux of  $10^{15} \text{ cm}^{-2}\text{s}^{-1}$  was chosen. According to [40, 41], this neutron flux density is representative of operational pulsed nuclear reactors. Additionally, [42] notes that compact pulsed nuclear reactors with even higher neutron flux densities have already been developed.

### 2. Governing equations

The neutron diffusion equation defines neutron behavior. Mathematically, its general form in the one-group approximation is:

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$$\frac{1}{v} \frac{\partial \phi(\vec{r}, t)}{\partial t} = \nabla \left[ D(\phi(\vec{r}, t), \vec{r}, t) \nabla \phi(\vec{r}, t) \right] - \phi(\vec{r}, t) \sum_m \Sigma_{a,m}(\vec{r}, t) + S(\phi(\vec{r}, t), \vec{r}, t), \quad (1)$$

where  $\phi(\vec{r}, t)$  is the neutron flux ( $\text{cm}^{-2}\text{s}^{-1}$ ),  $v$  is the neutron velocity ( $\text{cm/s}$ ),  $D(\phi(\vec{r}, t), \vec{r}, t)$  is the neutron diffusion coefficient ( $\text{cm}$ ),  $\Sigma_{a,m}(\vec{r}, t)$  is the macroscopic absorption cross-section of  $m$ -th nuclide ( $\text{cm}^{-1}$ ),  $S(\phi(\vec{r}, t), \vec{r}, t)$  is the neutron source term ( $\text{cm}^{-3}\text{s}^{-1}$ ).

The source term  $S(\phi(\vec{r}, t), \vec{r}, t)$  represents neutron production from fission, depending on factors like neutron flux, macroscopic fission cross-section, and delayed neutron contributions. Mathematically, the source term is expressed as:

$$S(\phi(\vec{r}, t), \vec{r}, t) = \phi(\vec{r}, t) \sum_l v_l \Sigma_{f,l}(\vec{r}, t) + \sum_g \sum_p \lambda_{p,g} C_{p,g}(\vec{r}, t), \quad (2)$$

where  $v_l$  is the average number of neutrons produced per fission of  $l$ -th nuclide,  $\Sigma_{f,l}(\vec{r}, t)$  is the macroscopic fission cross-section of  $l$ -th nuclide,  $\lambda_{p,g}$  is the decay constant and  $C_{p,g}(\vec{r}, t)$  is the concentration of the  $p$ -th delayed neutron precursor of  $g$ -th parent nuclide.

To simplify the numerical analysis, we assume a constant diffusion coefficient [32]

$$D = D(\phi(\vec{r}, t), \vec{r}, t) = 0.02 \text{ cm} \quad (3)$$

throughout the medium. While this maintains reasonable accuracy, it may introduce some errors, particularly if the medium's properties vary significantly. Future research could involve incorporating spatially and time-dependent diffusion coefficients to refine the model and address discrepancies arising from changes in the medium's properties.

In this study, the  $\text{UC}_2$  medium is modeled in cylindrical geometry, with the cylinder characterized by radius  $R$  and height  $H$ . We use cylindrical coordinates  $(\rho, \theta, z)$  to describe the spatial distribution of neutrons, where  $\rho$  is the radial distance from the central axis,  $\theta$  is the azimuthal angle,  $z$  is the axial coordinate.

Central symmetry is assumed, making neutron flux and related quantities independent of the azimuthal angle  $\theta$

$$\frac{\partial \phi(\rho, \theta, z, t)}{\partial \theta} = 0. \quad (4)$$

This reduces the problem from three spatial dimensions to just radial distance  $\rho$  and axial position  $z$ , simplifying the neutron diffusion equation and making it easier to solve numerically.

Thus, the neutron diffusion equation to be solved in cylindrical geometry with central symmetry and constant diffusion coefficient is:

$$\frac{1}{v} \frac{\partial \phi(\rho, z, t)}{\partial t} = D \nabla^2 \phi(\rho, z, t) - \phi(\rho, z, t) \sum_m \Sigma_{a,m}(\rho, z, t) + S(\phi(\rho, z, t), \rho, z, t), \quad (5)$$

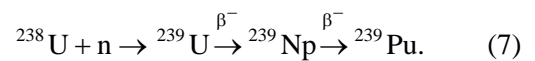
where  $\nabla^2 = \frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial}{\partial \rho} \right) + \frac{\partial^2}{\partial z^2}$  is Laplacian in cylindrical geometry with central symmetry.

In this study, the evolution of nuclide concentrations is modeled using nuclide balance equations, accounting for neutron-induced reactions, beta decay, and transmutation. For any  $i$ -th nuclide, the general form of the balance equation is:

$$\begin{aligned} \frac{dN_i(\rho, z, t)}{dt} = & -\sigma_{i,f} \phi(\rho, z, t) N_i(\rho, z, t) - \\ & -\sigma_{i,c} \phi(\rho, z, t) N_i(\rho, z, t) + \\ & + \sum_j \sigma_{j \rightarrow i} \phi(\rho, z, t) N_j(\rho, z, t) - \lambda_i N_i(\rho, z, t) + \\ & + \sum_k \lambda_k N_k(\rho, z, t), \end{aligned} \quad (6)$$

where  $N_i(\rho, z, t)$  is the concentration of  $i$ -th nuclide ( $\text{cm}^{-3}$ ),  $\sigma_{i,f}$  is the microscopic fission cross-section of  $i$ -th nuclide ( $\text{cm}^2$ ),  $\sigma_{i,c}$  is the microscopic neutron capture cross-section of  $i$ -th nuclide ( $\text{cm}^2$ ),  $\sigma_{j \rightarrow i}$  is the microscopic cross-section for the transmutation of  $j$ -th nuclide into  $i$ -th nuclide,  $\lambda_i$  is the decay constant of  $i$ -th nuclide ( $\text{s}^{-1}$ ),  $\lambda_k$  is the decay constant of  $k$ -th parent nuclide that decays into  $i$ -th,  $N_k(\rho, z, t)$  is the concentration of the parent  $k$ -th parent nuclide.

The conversion of fertile  $^{238}\text{U}$  to fissile  $^{239}\text{Pu}$  is critical in sustaining a traveling wave of nuclear fission. The process involves neutron capture by  $^{238}\text{U}$  and subsequent beta decay of  $^{239}\text{U}$  and  $^{239}\text{Np}$ . The full reaction chain is described below:



In addition to  $^{238}\text{U}$ ,  $^{235}\text{U}$  also plays an important role in the reactor, providing a fissile material for initiating fission. To enhance the accuracy of our

model, we incorporate delayed neutron precursors for both  $^{235}\text{U}$  and  $^{239}\text{Pu}$ , using a 6-group approach.

The eventual equations governing the evolution of the nuclides involved in the reaction chain (7), along with  $^{235}\text{U}$ , are presented below:

$$\frac{dN_{\text{U-235}}}{dt} = -\sigma_{\text{U-235},f}\phi N_{\text{U-235}} - \sigma_{\text{U-235},c}\phi N_{\text{U-235}}, \quad (8)$$

$$\frac{dN_{\text{U-238}}}{dt} = -\sigma_{\text{U-238},c}\phi N_{\text{U-238}}, \quad (9)$$

$$\frac{dN_{\text{U-239}}}{dt} = \sigma_{\text{U-238},c}\phi N_{\text{U-238}} - \lambda_{\text{U-239}}N_{\text{U-239}}, \quad (10)$$

$$\frac{dN_{\text{Np-239}}}{dt} = \lambda_{\text{U-239}}N_{\text{U-239}} - \lambda_{\text{Np-239}}N_{\text{Np-239}}, \quad (11)$$

$$\begin{aligned} \frac{dN_{\text{Pu-239}}}{dt} = & \lambda_{\text{Np-239}}N_{\text{Np-239}} - \\ & -\sigma_{\text{Pu-239},f}\phi N_{\text{Pu-239}} - \sigma_{\text{Pu-239},c}\phi N_{\text{Pu-239}}. \end{aligned} \quad (12)$$

Using a 6-group approach, we model delayed neutron precursors from the fission of  $^{235}\text{U}$  and  $^{239}\text{Pu}$ . Each  $p$ -th precursor of the  $g$ -th parent nuclide ( $^{235}\text{U}$  and  $^{239}\text{Pu}$ ) has its own decay constant  $\lambda_{p,g}$  and delayed neutron fraction  $\beta_{p,g}$ .

The balance equation for the  $p$ -th delayed neutron precursor of the  $g$ -th parent nuclide is given by:

$$\begin{aligned} \frac{\partial C_{p,g}(\rho, z, t)}{\partial t} = & \beta_{p,g}\sigma_{g,f}\phi(\rho, z, t)N_g(\rho, z, t) - \\ & -\lambda_{p,g}C_{p,g}(\rho, z, t), \end{aligned} \quad (13)$$

where  $C_{p,g}(\rho, z, t)$  is the concentration of the  $p$ -th delayed neutron precursor of the  $g$ -th parent nuclide.

For the parent nuclide  $^{235}\text{U}$ , the balanced equation for the  $p$ -th delayed neutron precursor is:

$$\frac{\partial C_{p,\text{U-235}}}{\partial t} = \beta_{p,\text{U-235}}\sigma_{\text{U-235},f}\phi N_{\text{U-235}} - \lambda_{p,\text{U-235}}C_{p,\text{U-235}}. \quad (14)$$

For the parent nuclide  $^{239}\text{Pu}$ , the balance equation for the  $p$ -th delayed neutron precursor is:

$$\frac{\partial C_{p,\text{Pu-239}}}{\partial t} = \beta_{p,\text{Pu-239}}\sigma_{\text{Pu-239},f}\phi N_{\text{Pu-239}} - \lambda_{p,\text{Pu-239}}C_{p,\text{Pu-239}}. \quad (15)$$

The full system of equations – combining the neutron diffusion Eq. (5), nuclide balance Eqs. (8) - (12), and delayed neutron precursor Eqs. (14) and (15) – describes the evolution of neutron flux and nuclide concentrations in the  $\text{UC}_2$  medium. Solving this system offers valuable insights into the propagation and stability of the traveling wave of nuclear fission.

### 3. Numerical model setup

The modeled system consists of a cylindrical fuel medium composed of  $\text{UC}_2$ . The cylinder is initially enriched with 15 %  $^{235}\text{U}$ , while the remaining 85 % consists of  $^{238}\text{U}$ . The fuel composition is treated as a homogeneous mixture of  $^{235}\text{U}$ ,  $^{238}\text{U}$ , and carbon.

At the start of the simulation, the neutron flux within the medium is set to zero  $\phi(\rho, z, t)|_{t=0} = 0$ . To initiate the fission wave, a steady neutron current density of  $10^{15} \text{ cm}^{-2}\text{s}^{-1}$  is applied at one end of the cylinder (referred to as the injection base) for a duration long enough to allow the system to reach a self-sustaining state.

The boundary condition at the injection base for the neutron current density is:

$$J_0 = -D \frac{\partial \phi}{\partial z} \Big|_{z=0} = 10^{15} \text{ cm}^{-2}\text{s}^{-1}. \quad (16)$$

This high-intensity neutron source is necessary to generate sufficient  $^{239}\text{Pu}$  through neutron capture by  $^{238}\text{U}$ , enabling the fission wave to become self-sustaining after the source is removed.

Heat exchange is assumed to occur through the side surface of the cylinder and will be addressed in future work. For this surface, we introduce the concept of an abstract protective shell:

$$\frac{1}{\phi_R} \frac{\partial \phi}{\partial \rho} \Big|_{\rho=R} = -\frac{1}{d}, \quad (17)$$

where  $R$  is the radius of the modeled cylinder and  $d$  is known as the extrapolated length. Conceptually, it separates the fissile medium from the coolant, allowing for simplification of the mathematical model while still accounting for neutron losses from the fissile medium.

The injection base, where the external neutron source is removed after initiation, is treated as a reflective boundary

$$\frac{\partial \phi}{\partial z} \Big|_{z=0} = 0 \quad (18)$$

that prevents neutron leakage. Similarly, the opposite base (referred to as the termination base) of the cylinder, which does not interact with the neutron source, is also modeled as a reflector

$$\frac{\partial \phi}{\partial z} \Big|_{z=H} = 0, \quad (19)$$

where  $H$  is the height of the modeled cylinder.

Table 1. Key constants to model nuclide evolution

Nuclide	Microscopic fission cross-section $\sigma_f$ , b	Microscopic absorption cross-section $\sigma_a$ , b	Decay constant $\lambda$ , 1/s
$^{235}\text{U}$	136.43	57.61	—
$^{238}\text{U}$	—	252.5	—
$^{239}\text{U}$	—	4.8	$492.53 \cdot 10^{-6}$
$^{239}\text{Np}$	—	—	$3.4 \cdot 10^{-6}$
$^{239}\text{Pu}$	473.43	286.15	—

Table 2. Key constants to model delayed neutron precursor evolution

Delayed neutron precursor		Decay constant $\lambda_p$ , $\text{s}^{-1}$	Delayed neutron fraction $\beta_p$
Parent nuclide	Number		
$^{235}\text{U}$	1	0.0124	0.000215
	2	0.0305	0.001424
	3	0.111	0.001274
	4	0.301	0.002568
	5	1.14	0.000748
	6	3.01	0.000273
$^{239}\text{Pu}$	1	0.01231	0.0000072
	2	0.03	0.000626
	3	0.12375	0.000444
	4	0.325352	0.000685
	5	1.117741	0.000180
	6	2.66538	0.000093

For the simulation, we employed specific microscopic cross-sections and decay constants for the key nuclides involved in the fission process, along with the decay constants and delayed neutron fractions for each precursor group associated with  $^{235}\text{U}$  and  $^{239}\text{Pu}$ , as presented in Tables 1 and 2, respectively, with values sourced from [32].

#### 4. Numerical method

In this study, we use the control volume formulation (CVF) to numerically solve the neutron diffusion equation in a cylindrical  $\text{UC}_2$  medium. CVF discretizes

the domain into finite control volumes and integrates the governing equations over each, resulting in algebraic equations that approximate the original partial differential equations. By applying finite differences for flux and its derivatives, CVF efficiently solves for the neutron flux distribution  $\phi(\rho, z, t)$ . This method is particularly effective for conservation laws like neutron diffusion.

The neutron diffusion equation is integrated over the control volume of the node ( $\rho_j = j\Delta\rho$ ,  $z_k = k\Delta z$ ) and over the time interval from  $t_i$  to  $t_{i+1} = t_i + \Delta t$ :

$$\begin{aligned} \frac{1}{V} \int_{t_i}^{t_{i+1}} \int_{z_{k-\frac{1}{2}}}^{z_{k+\frac{1}{2}}} \int_{\rho_{j-\frac{1}{2}}}^{\rho_{j+\frac{1}{2}}} \rho \frac{\partial \phi(\rho, z, t)}{\partial t} d\rho dz dt = D \int_{t_i}^{t_{i+1}} \int_{z_{k-\frac{1}{2}}}^{z_{k+\frac{1}{2}}} \int_{\rho_{j-\frac{1}{2}}}^{\rho_{j+\frac{1}{2}}} \rho \left[ \frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial \phi(\rho, z, t)}{\partial \rho} \right) + \frac{\partial^2 \phi(\rho, z, t)}{\partial z^2} \right] d\rho dz dt - \\ - \int_{t_i}^{t_{i+1}} \int_{z_{k-\frac{1}{2}}}^{z_{k+\frac{1}{2}}} \int_{\rho_{j-\frac{1}{2}}}^{\rho_{j+\frac{1}{2}}} \rho \phi(\rho, z, t) \sum_m \Sigma_{a,m}(\rho, z, t) d\rho dz dt + \int_{t_i}^{t_{i+1}} \int_{z_{k-\frac{1}{2}}}^{z_{k+\frac{1}{2}}} \int_{\rho_{j-\frac{1}{2}}}^{\rho_{j+\frac{1}{2}}} \rho S(\phi(\rho, z, t), \rho, z, t) d\rho dz dt, \end{aligned} \quad (20)$$

where the integral of the source term is

$$\begin{aligned} \int_{t_i}^{t_{i+1}} \int_{z_{k-\frac{1}{2}}}^{z_{k+\frac{1}{2}}} \int_{\rho_{j-\frac{1}{2}}}^{\rho_{j+\frac{1}{2}}} \rho S(\phi(\rho, z, t), \rho, z, t) d\rho dz dt = \int_{t_i}^{t_{i+1}} \int_{z_{k-\frac{1}{2}}}^{z_{k+\frac{1}{2}}} \int_{\rho_{j-\frac{1}{2}}}^{\rho_{j+\frac{1}{2}}} \rho \phi(\rho, z, t) \sum_l \nu_l \Sigma_{f,l}(\rho, z, t) d\rho dz dt + \\ + \sum_g \sum_p \lambda_{p,g} \int_{t_i}^{t_{i+1}} \int_{z_{k-\frac{1}{2}}}^{z_{k+\frac{1}{2}}} \int_{\rho_{j-\frac{1}{2}}}^{\rho_{j+\frac{1}{2}}} \rho C_{p,g}(\rho, z, t) d\rho dz dt. \end{aligned} \quad (21)$$

We approximate the integral (20) using the following discrete analog:

$$-a_{i,j,k}^p \phi_{j-1,k}^{i+1} + b_{i,j,k} \phi_{j,k}^{i+1} - c_{i,j,k}^p \phi_{j+1,k}^{i+1} = d_{i,j,k}^p, \quad (22)$$

where

$$b_{i,j,k} = j\Delta\rho^2\Delta z + 2jD\Delta t\Delta z + 2\frac{Dj\Delta\rho^2\Delta t}{\Delta z} + j\Delta\rho^2\Delta z\Delta t \sum_m \sum_{a,m}^{i,j,k}, \quad (23)$$

$$a_{i,j,k}^p = D\Delta t\Delta z \left( j - \frac{1}{2} \right), \quad (24)$$

$$c_{i,j,k}^p = D\Delta t\Delta z \left( j + \frac{1}{2} \right), \quad (25)$$

$$a_{i,j,k}^z = \frac{Dj\Delta\rho^2\Delta t}{\Delta z}, \quad (26)$$

$$\bar{b}_{i,j,k} = j\Delta\rho^2\Delta z + j\Delta\rho^2\Delta z\Delta t \sum_l \nu_l \sum_{f,l}^{i,j,k}, \quad (27)$$

$$\bar{c}_{i,j,k}^z = \frac{Dj\Delta\rho^2\Delta t}{\Delta z}, \quad (28)$$

$$d_{i,j,k}^p = a_{i,j,k}^z \phi_{j,k-1}^{i+1} + \bar{b}_{i,j,k} \phi_{j,k}^i + \bar{c}_{i,j,k}^z \phi_{j,k+1}^i + d_{i,j,k}, \quad (29)$$

$$d_{i,j,k} = j\Delta\rho^2\Delta z\Delta t \sum_g \sum_p \lambda_{p,g} C_{p,g}^{i,j,k}. \quad (30)$$

With the discrete analog (22), we form a tridiagonal system of algebraic equations, which in matrix form is represented as:

$$\begin{bmatrix} b_{i,0,k} & -c_{i,0,k}^p & 0 & \dots & 0 & 0 & 0 \\ -a_{i,1,k}^p & b_{i,1,k} & -c_{i,1,k}^p & \dots & 0 & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & -a_{i,j,k}^p & b_{i,j,k} & -c_{i,j,k}^p & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & -a_{i,N_R-1,k}^p & b_{i,N_R-1,k} & -c_{i,N_R-1,k}^p \\ 0 & 0 & 0 & \dots & 0 & -a_{i,N_R,k}^p & b_{i,N_R,k} \end{bmatrix} \begin{bmatrix} \phi_{0,k}^{i+1} \\ \phi_{1,k}^{i+1} \\ \vdots \\ \phi_{j,k}^{i+1} \\ \vdots \\ \phi_{N_R-1,k}^{i+1} \\ \phi_{N_R,k}^{i+1} \end{bmatrix} = \begin{bmatrix} d_{i,0,k}^p \\ d_{i,1,k}^p \\ \vdots \\ d_{i,j,k}^p \\ \vdots \\ d_{i,N_R-1,k}^p \\ d_{i,N_R,k}^p \end{bmatrix} \quad (31)$$

for each  $k$ -th layer of the cylinder along  $Oz$ -axis. This allows for an efficient numerical solution, as tridiagonal systems can be solved using specialized algorithms such as the Thomas algorithm, which reduces computational complexity. The solution for each  $k$ -layer is sequentially obtained based on the results from the previous  $(k-1)$ -layer, ensuring that the propagation of the traveling wave of nuclear fission is accurately modeled.

The numerical solution for the nuclide balance equation can be achieved more easily than for neutrons, but it provides an important criterion for selecting the time step  $\Delta t$ . A first-order Taylor approximation is applied:

$$N(\rho_j, z_k, t_{i+1}) = N_{j,k}^{i+1} = N_{j,k}^i + \frac{\partial N}{\partial t} \Big|_{\substack{\rho=\rho_j \\ z=z_k \\ t=t_i}} \Delta t. \quad (32)$$

By demanding that calculated concentrations

remain non-negative  $N_{j,k}^i + \frac{\partial N}{\partial t} \Big|_{\substack{\rho=\rho_j \\ z=z_k \\ t=t_i}} \Delta t \geq 0$ , we

derive the following criterion for the time step:

$$\Delta t \geq -N_{j,k}^i / \frac{\partial N}{\partial t} \Big|_{\substack{\rho=\rho_j \\ z=z_k \\ t=t_i}}. \quad (33)$$

## 5. Results and discussion

In this section, we present the results of our 3D numerical simulations of the traveling wave of nuclear fission, focusing on its propagation characteristics and dynamics. The Figures below demonstrate how key quantities within the medium evolve over time, providing valuable insights into the stability and fuel efficiency of the TWR.

Two numerical experiments were conducted: the first as an initial trial and the second with more detailed settings, as outlined in Table 3.

Table 3. Simulation parameters for numerical experiments

Parameter	Experiment 1	Experiment 2
Diameter		10 cm
Height	15 cm	20 cm
Radial step		1 mm
Axial step	1 cm	1 mm
Time step		0.1 s
External source duration	20 days	10 days

In Experiment 1, a larger axial step size  $\Delta z$  - 1 cm was used. The results demonstrated a self-sustaining traveling wave of nuclear fission, with fluctuations observed at approximately 5-day intervals, linked to the accumulation and subsequent rapid burnout of  $^{239}\text{Pu}$ .

Experiment 2 was conducted using a 10-times

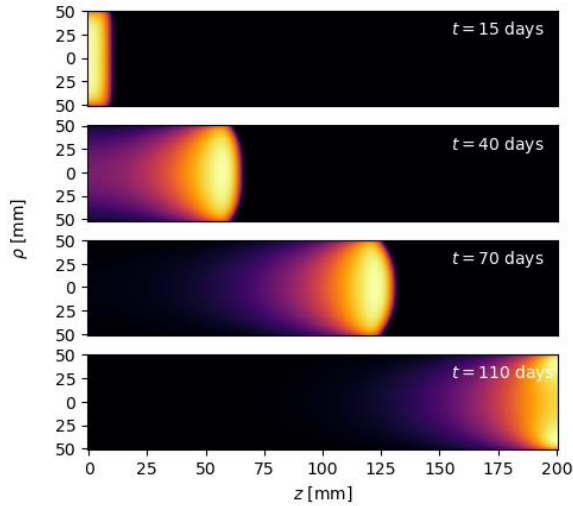


Fig. 1. 2D neutron dynamics along the central cross-section of the cylinder in Experiment 2. (See color Figure on the journal website.)

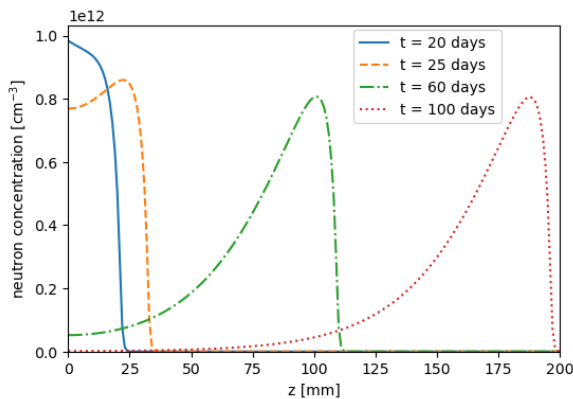


Fig. 3. Neutron propagation along the central axis ( $\rho = 0$ ) of the cylinder in Experiment 2. (See color Figure on the journal website.)

It is clear that the larger axial step size of 1 cm is too coarse for modeling processes with parameters on the scale of 1 cm or smaller. A finer axial step, around 0.1 mm, would be more appropriate, though it would require significant computational resources.

The power generated by the self-sustaining traveling wave of nuclear fission in  $\text{UC}_2$  was monitored throughout the simulation. Fig. 5 shows the power as a function of time, illustrating an initial rise during the early phase of fission wave propagation, with the power peaking at approximately 140 MW. After this peak, the power output stabilized, indicating the onset of a steady-state regime where the fission wave continued to propagate at a constant rate, sustaining the nuclear reaction without significant fluctuations, as long as fertile material remained available.

smaller axial step  $\Delta z$  - 1 mm, resulting in more accurate data. A self-sustaining traveling wave of nuclear fission was observed. Shortly after formation, the wave stabilized and became steady, with no fluctuations detected (Figs. 1 - 4). The wave's propagation velocity is approximately 2 - 3 mm/day, or around 1 m/year, with a fission front width of about 2 cm.

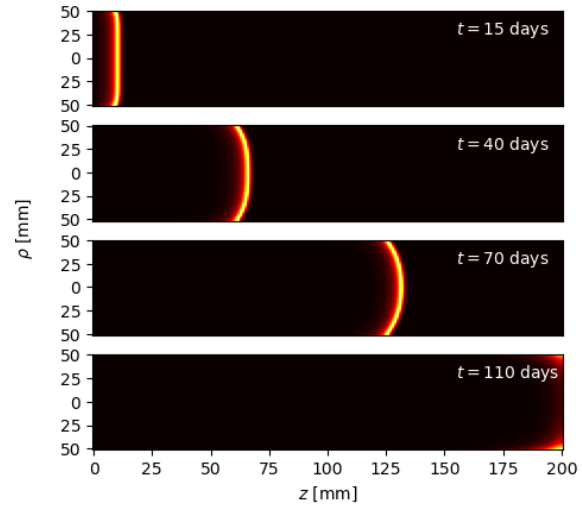


Fig. 2. 2D  $^{239}\text{Pu}$  dynamics along the central cross-section of the cylinder in Experiment 2. (See color Figure on the journal website.)

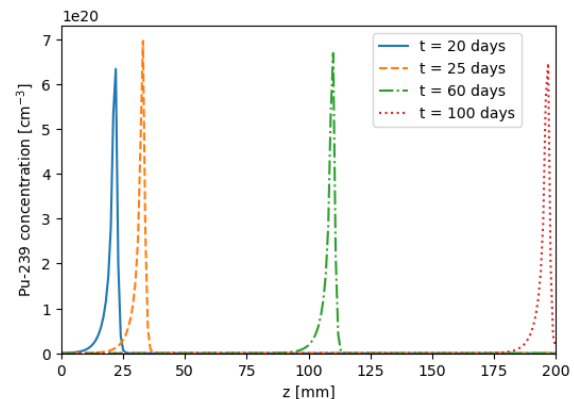


Fig. 4.  $^{239}\text{Pu}$  propagation along the central axis ( $\rho = 0$ ) of the cylinder in Experiment 2. (See color Figure on the journal website.)

Further research is needed to explore heat transfer and material behavior under these conditions of such high-power production. Nevertheless, the high-power output is a promising result, positioning TWRs as a highly competitive option in advanced nuclear reactors.

As shown in Fig. 5, once the fission wave is formed, the burnout of  $^{239}\text{Pu}$  begins to play the dominant role in energy production, contributing 100 MW compared to approximately 40 MW from  $^{235}\text{U}$ . In Fig. 6, we can observe that once the fission wave stabilizes,  $^{239}\text{Pu}$  produces roughly 2.5 times more neutrons than  $^{235}\text{U}$ , which was initially used for enrichment to facilitate wave formation and further propagation.

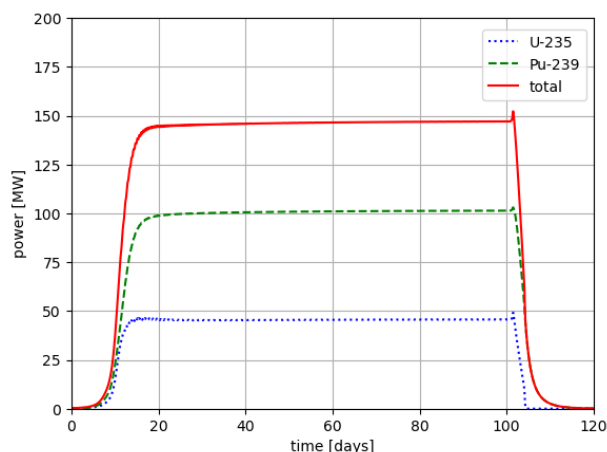


Fig. 5. Power output during fission wave propagation. (See color Figure on the journal website.)

Although a high enrichment level of 15 % was applied in our initial simulations, the fission of  $^{239}\text{Pu}$  still dominates the propagation of the nuclear fission wave through the  $\text{UC}_2$  medium (Figs. 5 and 6). This suggests that the initial enrichment could potentially be lowered, possibly even to depleted uranium levels. However, further research is needed to determine the optimal conditions. Additionally, now that we understand the properties of a steady fission wave and the conditions required for its propagation, we can prepare a startup zone to make the process self-sustaining as quickly as possible, minimizing the need for a powerful external neutron source.

## 6. Conclusions

In this work, we presented the methodology and results of 3D numerical simulations of a traveling wave of nuclear fission in a cylindrical  $\text{UC}_2$  medium. Given that many nuclear reactors are designed with cylindrical symmetry, this model is highly relevant for practical applications. We report, for the first time,

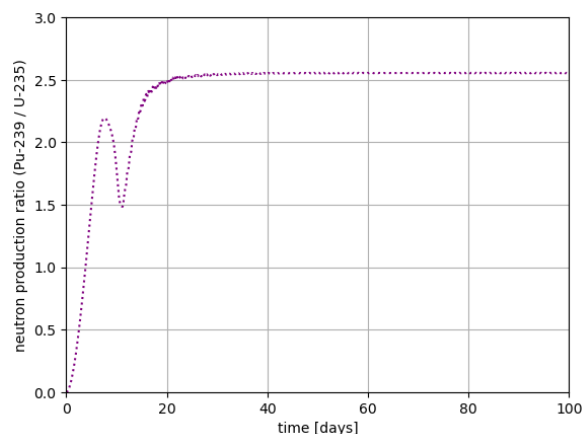


Fig. 6. Neutron production ratio of  $^{239}\text{Pu}$  to  $^{235}\text{U}$  during fission wave propagation. (See color Figure on the journal website.)

results from a numerical experiment where the external neutron source was turned off after the formation of a stable, self-sustaining traveling wave.

By employing the CVF, we achieved a robust numerical solution to the neutron diffusion equation, offering valuable insights into the propagation and stability of these waves in the  $\text{UC}_2$  medium.

The simulations demonstrated significant nuclide burnout and efficient power production, meeting key criteria expected for TWRs, including fuel efficiency, waste reduction, resistance to nuclear proliferation, and enhanced safety.

While the current model is simplified – focusing solely on the active zone and excluding structural materials, moderators, and coolant – it provides a solid foundation for further development. Future research will enhance the model by incorporating additional nuclides interacting with neutrons and extending the neutron diffusion equation to include specific coolants and protective shells. This iterative approach ensures steady progress toward a comprehensive and realistic model.

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**ЧИСЛОВИЙ АНАЛІЗ САМОЖИВИЛЬНОЇ РУХОМОЇ ХВИЛІ ЯДЕРНОГО ПОДІЛУ,  
ПРОПАГОВАНОЇ НАДТЕПЛОВИМИ НЕЙТРОНАМИ В СЕРЕДОВИЩІ УРАНУ ДІКАРБІДУ**

Досліджено саможивильну рухому хвилю ядерного поділу в середовищі урану дікарбиду через чисельне розв'язання системи диференціальних рівнянь. Основна увага приділяється рівнянню дифузії нейтронів та рівнянням балансу нуклідів, які є ключовими для розуміння поведінки хвиль поділу. Метою дослідження є визначення характеристик поширення та перевірка стабільності хвиль ядерного поділу. Числовий аналіз надає глибокі уявлення про динаміку розподілу нейтронів та зміну нуклідного складу, що є корисним у проектуванні реакторів рухомої хвилі ядерного поділу.

*Ключові слова:* реактор рухомої хвилі ядерного поділу, надтеплові нейтрони, уран дікарбід, рівняння дифузії нейтронів, конструкція реактора, саможивильна хвиля поділу.

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