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A new SP_n theory formulation with self-consistent physical assumptions on angular flux

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ABSTRACT

The conventional SP_n theory cannot provide the explicit angular flux solution. Chao and Yamamoto (2012) proposed the explicit angular flux representation for the SP_n theory as cylindrically symmetric with respect to the net current direction at any point in space, such that the angular flux is an expansion in Legendre polynomials of the cosine of the polar angle with respect to the local net current. Such a model however cannot lead to the SP_n equations without further ad hoc assumptions because the multiple directions of the spatial gradients of the flux moments cannot be all parallel to the net current. In this paper we relax the assumption of the total angular flux being locally one-dimensional and generalize it to each of the flux moments being locally one-dimensional along the direction of the spatial gradient of each individual flux moment. The angular distribution of the nth order flux moment is the nth order Legendre polynomial of the cosine of the polar angle with respect to the direction of the spatial gradient of the nth order flux moment, $\nabla\phi_n(r)$. With this physical model one can rigorously derive the equations for the current and the boundary conditions. The SP_n equations can also be derived with the additional assumption of the total cross-section being locally constant, which is practically always valid when the spatial variation is discretized in numerical calculations. However the boundary conditions turn out to be different from the conventional ones, containing some non-linear factors. The internal interface boundary conditions are not affected by the non-linear factors as they cancel out on the interface. But the external boundary condition does get affected by the non-linear factors. The effect of non-linear factors is of higher order and if neglected, the external boundary condition also reduces to the conventional one. The non-linear external boundary condition can be iteratively updated to estimate the correction effect. A numerical calculation problem is suggested to test the new SP_n theory and to assess the non-linear effect.

1. Introduction

The SP_n equations were initially proposed without adequate mathematical derivation or justification (Gelbard, 1960). The one dimensional P_n equations are generalized to the three dimensional SP_n equations by directly replacing the 1D differentiation operator with 3D gradient operator. Later on mathematically more sophisticated formulations using either the asymptotic theory approximation or the variational method were introduced to provide a more rigorous mathematical justification, in particular for the SP_3 case (Pomraning, 1993; Brantley and Larsen, 2000). Although the SP_3 equations can be derived in these formulations, they do not provide a way to explicitly reconstruct the angular flux representation from the SP_3 solution. One does not have a "physical picture" for the angular flux for the SP_n solution. It is therefore not possible to compare the angular distribution of the correct transport solution to the approximate SP_n solution nor to extract from a given reference transport solution the corresponding SP_n solution. This makes it difficult to understand and visualize the physical meaning of the SP_n approximation. Moreover this causes a problem in practical engineering applications of SP_n, as one cannot introduce correction factors, such as the popular discontinuity factors, to compensate for the approximations in the SP_n solution. As a result, even if a reference transport solution is given, one still cannot reproduce the reference solution by using correction factors in the process of solving the SP_n equations. It has been demonstrated that SP_3 calculation per se without using any correction factor cannot compete in accuracy with the conventional diffusion calculation using discontinuity factors (Yu et al., 2014).

To resolve the above cited problem Chao and Yamamoto (2012) adopted the physical interpretation of the SP_n model as the neutron transport being locally one dimensional at any point in space (Pomraning, 1993). As Chao and Yamamoto (2012) pointed out,

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this necessarily implies that the angular flux distribution is always cylindrically symmetric with respect to the net current whose direction may change continuously thru space. In this picture the angular flux is an expansion in Legendre polynomials of the cosine of the polar angle with respect to the net current direction. Chao and Yamamoto showed how the SP_n equations can be derived by plugging this angular flux function into the transport equation and assuming certain specific approximations. This explicit angular flux representation was then used to calculate the SP_3 discontinuity factors to show that the SP_3 superiority over diffusion can be restored when discontinuity factors are applied to SP_3 calculation as well (Yu et al., 2014; Yu and Chao, 2015).

However the assumption of local 1D planar behavior of the angular flux is not consistent with the fact that in SP_n equations at any spatial point there may exist many vector directions given by the gradients of the flux moment functions, $\nabla\phi_n(r)$, which can all be different from the direction of the net current J. As a result, Chao and Yamamoto had to make additional ad hoc assumptions to derive the SP_n equations and for the generation of the correct expression of the net current in terms of the gradients of the 0th and 2nd order flux moments, $\nabla\phi_0(r)$ and $\nabla\phi_2(r)$. In this paper we recognize that a self-consistent physical model for SP_n is a combination of multiple locally planar functions along different directions instead of along the net current direction alone. Each order of the flux moments contributes to one of the superposed locally planar functions. The angular distribution of the nth order flux moment is the nth order Legendre polynomial of the cosine of the polar angle with respect to the direction of the spatial gradient, $\nabla\phi_n(r)$, of the nth order flux moment. With this physical model one can rigorously derive the equations for the current and the boundary conditions. The SP_n equations can also be derived with the additional assumption of the total cross-section being locally constant, which is practically always valid when the spatial variation is discretized in numerical calculations. However the boundary conditions turn out to be different from the conventional ones, containing some non-linear factors involving the cosine of the angle between the boundary surface normal vector and the spatial gradient vectors of the flux moments. The internal interface boundary conditions are not affected by the non-linear factors as they cancel out on the interface. But the external boundary condition does get affected by the non-linear factors. The effect of non-linear factors is of higher order, as the non-linear factors disappear when the spatial gradients are parallel to the surface normal vector. So if the non-linear factors are neglected, the external boundary condition also reduces to the conventional one. The non-linear external boundary condition can nevertheless be iteratively updated to estimate the correction effect.

The basic theory and the derivation of the equation for the current and the SP_n equations are presented and discussed in Section 2. Section 3 derives and discusses the boundary conditions, including the suggestion of a numerical test problem to assess the new SP_n theory with non-linear external boundary conditions. The relation of the boundary condition to the calculation of the SP_n discontinuity factor is also discussed in this section. Section 4 provides additional commentary discussion on the theoretical foundation of SP_n. Section 5 concludes the paper.

2. The theory and the SP_n equation derivation

2.1. The physical model and the angular flux representation

For simplicity we will consider the case of mono-energetic isotropic scattering, with the neutron transport equation given as,

$$\Omega\cdot\nabla\psi(\Omega,r)+\Sigma_t\psi(\Omega,r)=\frac{Q(r)}{4\pi} \tag{2.1}$$

In terms of the even and odd parity angular fluxes, Eq. (2.1) can be written as,

$$\psi(\Omega,r)=\psi_E(\Omega,r)+\psi_O(\Omega,r) \tag{2.2}$$

$$-\Omega\cdot\nabla\left[\frac{1}{\Sigma_t}\Omega\cdot\nabla\psi_E(\Omega,r)\right]+\Sigma_t\psi_E(\Omega,r)=\frac{Q(r)}{4\pi} \tag{2.3}$$

$$\psi_O(\Omega,r)=-\frac{1}{\Sigma_t}\Omega\cdot\nabla\psi_E(\Omega,r) \tag{2.4}$$

In the P_n method of solving the transport equation, the angular flux is expanded in orthogonal spherical harmonics. The nth order moment term in the expansion contains $(2n+1)$ components, each of which is a product of an angular part $Y_{n,m}(\Omega)$ and a spatial part $\phi_{n,m}(r)$ with m going from $-n$ to n. For the even parity angular flux we have,

$$\psi_E(\Omega,r)=\sum_{n=even}\sum_{m=-n}^{n}Y_{n,m}(\Omega)\phi_{n,m}(r) \tag{2.5}$$

Plugging Eq. (2.5) into Eq. (2.4) gives,

$$\psi_O(\Omega,r)=-\frac{1}{\Sigma_t}\sum_{n=even}\sum_{m=-n}^{n}Y_{n,m}(\Omega)\Omega\cdot\nabla\phi_{n,m}(r) \tag{2.6}$$

The additional $\Omega\cdot\nabla\phi_{n,m}(r)$ factor in Eq. (2.6) makes each term odd in parity and its product with $Y_{n,m}$ can be recast into combinations of orthogonal odd parity spherical harmonics. The fundamental problem in SP_n is that instead of $(2n+1)$ components it has only one component, $\phi_n(r)$, for the nth moment. The question is then how to replace the $(2n+1)$ components with a single "effective" one and how the corresponding angular distribution looks like for the nth flux moment. Noting that the only information to be provided by the solution of SP_n equations for the nth flux moment are $\phi_n(r)$ and $\nabla\phi_n(r)$, one can argue that in absence of other information a self-consistent physical picture for the angular distribution of the nth flux moment is cylindrically symmetric with respect to $\nabla\phi_n(r)$, which is the only direction vector available in the SP_n solution. The nth order spherical harmonics of cylindrical symmetry is the nth order Legendre polynomial of the cosine of the polar angle with respect to the symmetry axis. Therefore we propose the following explicit angular flux representation for the even parity angular flux in the SP_n theory, where Ω_n is defined as the unit vector along the direction of the gradient $\nabla\phi_n(r)$,

$$\psi_E(\Omega,r)=\sum_{n=even}\frac{2n+1}{4\pi}P_n(\Omega\cdot\Omega_n)\phi_n(r) \tag{2.7}$$

$$\psi_O(\Omega,r)=-\frac{1}{\Sigma_t}\sum_{n=even}\frac{2n+1}{4\pi}P_n(\Omega\cdot\Omega_n)[\Omega\cdot\nabla\phi_n(r)] \tag{2.8}$$

$$\Omega_n\equiv\frac{\nabla\phi_n(r)}{|\nabla\phi_n(r)|} \tag{2.9}$$

$$\nabla\phi_n(r)\equiv\Omega_n[\Omega_n\cdot\nabla\phi_n(r)] \tag{2.10}$$

Note that via using Eq. (2.10), Eq. (2.8) can be rewritten in the following form, with the angular variable Ω and spatial variable r decoupled in each term of the summation,

$$\psi_O(\Omega,r)=-\frac{1}{\Sigma_t}\sum_{n=even}\frac{2n+1}{4\pi}[P_n(\Omega\cdot\Omega_n)\Omega\cdot\Omega_n][\Omega_n\cdot\nabla\phi_n(r)] \tag{2.11}$$

Eq. (2.7) and Eq. (2.11) have consistent angular distributions for each flux moment term. They together provide a consistent trial function for the angular flux. The odd parity transport Eq. (2.4) has already been used to derive Eq. (2.8). The even parity transport Eq. (2.3) will then be used to determine the spatial expansion