AGENT CODE – NEUTRON TRANSPORT BENCHMARK EXAMPLE AND EXTENSION TO 3D LATTICE GEOMETRY

by

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Received on May 9, 2005; accepted in revised form on July 13, 2005

The general methodology behind 2D arbitrary geometry neutron transport – AGENT code is the theory of R-functions, which allows for simple modeling of complex geometries, and the method of characteristics, which solves the integral transport equation along characteristic neutron trajectories. This paper focuses on the extension of the methodology to account for 3D lattice geometries. Since the direct application of method of characteristics to 3D non-homogenized core configuration may require a tremendous amount of memory and computing time, an alternative approximate solution based on coupling 2D method of characteristics and 1D diffusion solution is developed. The planar 2D method of characteristics and axial 1D diffusion solutions are coupled through the transverse leakage. The use of a lower order 1D solution in the axial direction is justified by the fact that more heterogeneity in current PWR and BWR reactor cores occurs in the radial direction than in the axial one. In order to demonstrate the versatility and accuracy of the AGENT code, a 2D heterogeneous lattice problem, C5G7 is described in details. A theoretical description of the coupling methodology for 3D method of characteristics solution is followed by preliminary validation in comparison to the DeCART code.

Key words: method of characteristics, heterogeneous reactors, reactor lattice, benchmark problems

INTRODUCTION

This paper focuses on the recent development of an advanced computational environment intending to provide researchers and educators with tools for an open-architecture neutronic analysis and configuration of University Research and Training Reactors (URTRs). This environment is to allow users to optimize the experiments, test fuel configurations and provide "virtual" demonstrations. The centerpiece of the environment is the method of characteristics based computer code, Arbitrary Geometry Neutron Transport (AGENT).

Scientific paper
UDC: 539.125.52:519.6
BIBLID: 1451-3994, *20* (2005), 2, pp. 10-16

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There are a few different methods available to solve the transport equation in 2D and 3D: Collision Probability Method (CPM), S_n Method or Spherical Harmonics being some of them. The Method of Characteristics (MOC) has been chosen to solve the transport equation to address the problems related to the treatment of multi-scale calculations in exact geometry. MOC and CPM allow the representation of local heterogeneities, but the CPMs yield full collision matrices that set a practical limit to the size of the problems that can be treated within reasonable computer resources.

MAIN ASPECTS OF THE AGENT METHODOLOGY

AGENT solves the integral transport equation using the MOC [1] in a user-defined number of energy groups in a geometry represented via the theory of R-functions [2].The combination of the R-function based solid modeler and MOC permits

accurate, efficient and fast particle transport analysis in complex and heterogeneous geometrical domains. The MOC allows a full treatment of highly heterogeneous systems with a large number of energy groups and detailed neutron traks map (satisfactory number of directions and fine spatial resolution).

Neutron tracking

A general and efficient way of representing complex 3D geometries is a problem that spans many disciplines, from CAD and computer graphics to pattern recognition and particle transport. The R-function modeler is used to represent complex domains through the combination of simple primitives into a single analytical equation (see fig. 1). This equation defines the domain function representing a given geometry. It evaluates positive as a point within the domain, negative as a point outside the domain and zero as a point on the domain boundary. Therefore, to test if a point is within a certain object, the code merely has to evaluate the function at that point. This method is as general as the typical Monte Carlo approach, but much simpler and significantly faster.

MOC, Monte Carlo, and CPMs, all use the neutron tracking through so called ray tracing. Thus, it is necessary to find an effective yet accurate method to simulate neutron trajectories through complex and heterogeneous domains. The R-function method provides an elegant solution to the ray tracing problem in AGENT. The method involves taking discrete steps along the ray, testing the domain functions of the objects of interest at each point. As mentioned above, if the point is outside the object, the function will evaluate negative; if the point is within the object, the function will evaluate positive. Therefore, if the signs of the function at two consecutive points are opposite, a boundary has been crossed. Then it is simply a matter of "homing in" on the boundary, *i. e.*, the point along the ray where the function evaluates within a certain tolerance of zero.

Computational MOC

The AGENT code solves the neutron transport equation providing eigenvalue, volumetric scalar flux and reaction rates. The multigroup energy cross sections are obtained from the front-end code. Currently, the cross sections are generated by the lattice code HELIOS v-1.8 [3]. The spatial discretization allows for a flexible selection of neutron trajectories by specifying the number of azimuthal angles, number of polar angles and the distance between neutron tracks. Isotropic neutron propagation along neutron trajectories for each set of discrete angles starts at the most outer boundary and reflects back into the system following the user-selected boundary conditions (reflective, white or vacuum). The flux solution incorporates a power it-

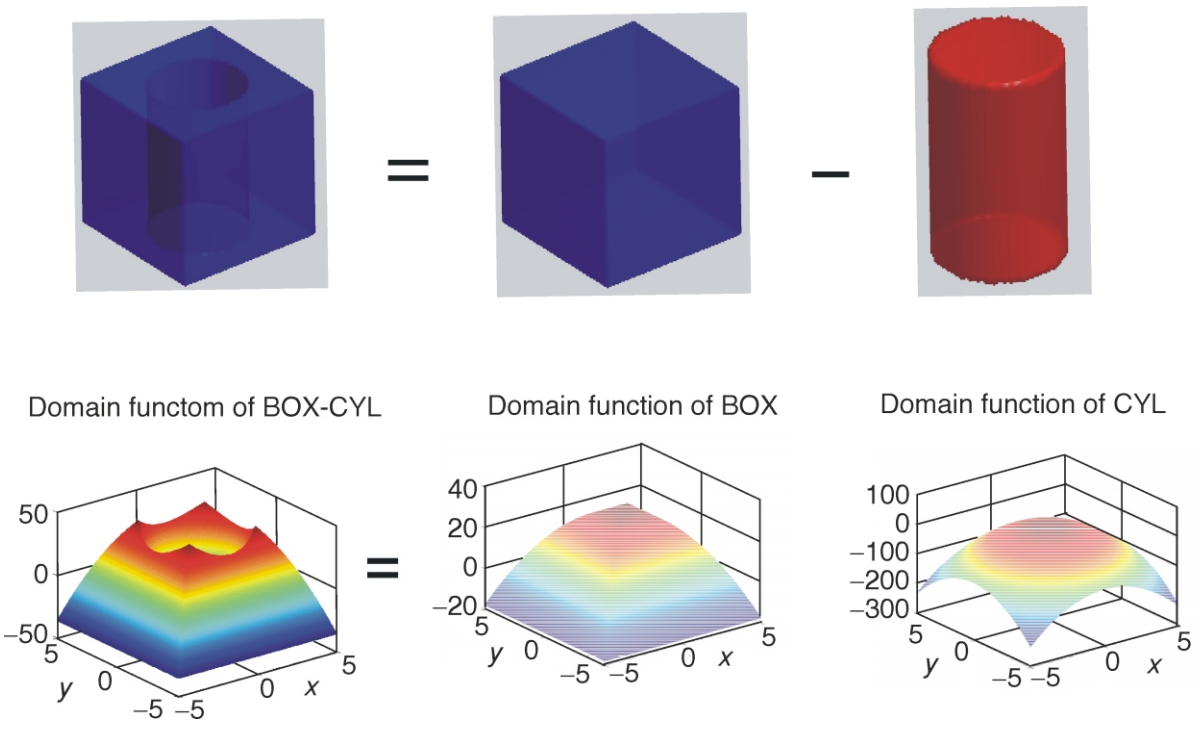

Figure 1. AGENT solid modeler based on R-function geometry

eration with two different acceleration techniques: Coarse Mesh Rebalancing (CMR) and Coarse Mesh Finite Difference (CMFD) [4-6].

2D NUMERICAL EXAMPLE

The C5G7 UO_2 benchmark lattice [7], as shown in fig. 2, is selected to demonstrate the accuracy and efficiency of the code. The results are compared to the DeCART code [8]. DeCART 3D methodology is used as a base to extend the current 2D AGENT to 3D capability. Therefore, since the DeCART code is used to validate the 3D methodology of the AGENT code, the agreement between the AGENT and DeCART codes in 2D is of crucial importance.

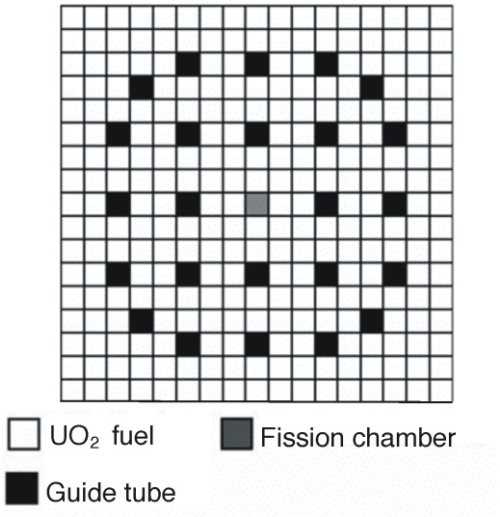

Figure 2. C5G7 UO_2 assembly geometry

The AGENT eigenvalue shown in tab. 1, obtained in less than two minutes computation time, is in good agreement with DeCART. This is to be expected, since both codes are based on the MOC and both codes use the same set of macroscopic cross sections and the same spatial discretization. The slight differences are caused by different ray tracing methods. DeCART uses a modular ray tracing technique, where the neutron tracking is the same for each pin cell and is repeated throughout the whole geometry, while in the AGENT code neutron tracking is carried out for the whole geometry, thus allowing arbitrary geometry to be easily modeled. The AGENT fine mesh spatial distribution of thermal neutron flux across the assembly is depicted in fig. 3.

Table 1. C5G7 UO_2 assembly: eigenvalue AGENT and DeCART comparison

C5G7 UO_2 assembly	AGENT	DeCART	Difference $[10^{-5}]$
K-effective	1.33336	1.33321	11.3

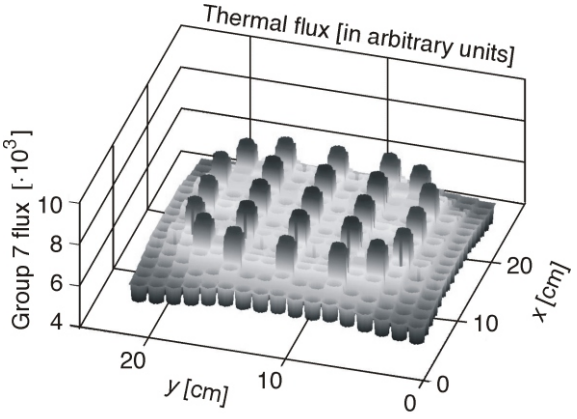

Figure 3. AGENT thermal scalar flux distribution across C5G7 UO_2 assembly

2D-1D COUPLING THEORY OF AGENT

The AGENT code system will be used for research and educational purposes with the capability of performing "virtual" experiments and demonstrations. Therefore, there is an obvious need for a 3D whole reactor core model.

Since the direct application of MOC to 3D non-homogenized core configurations may require, at present, a tremendous amount of memory and computing time, an alternative approximate 3D solution was developed based on the DeCART code. The 2D planar and 1D axial solutions are coupled through the transverse leakage. The use of a lower order 1D solution in the axial direction is justified by the fact that more heterogeneity in current LWR reactor cores occurs in the radial direction than in the axial one.

The 2D-1D coupling strategy starts by slicing the reactor core into a user-defined number of axial planes, as shown in fig. 4. A 2D planar solution based on the MOC is obtained for each plane. The 1D axial solution is based on the finite difference method (FDM) and is obtained for each pin region.

The derivation of the coupled 2D-1D equations is shown as follows. In 3D, the Boltzmann transport equation in steady state can be written as:

$$\Omega \quad \Psi(\vec{r},\Omega,E) \quad \Sigma_t(\vec{r},E)\Psi(\vec{r},\Omega,E) \quad Q(\vec{r},E) \quad (1)$$

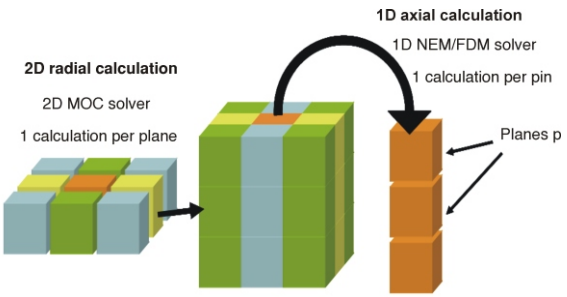

Figure 4. 2D-1D coupling methodology of AGENT code

The fission source, as well as the scattering term, are assumed to be isotropic (with plans to expand the scattering mode using the P1 approximation). By integrating the above equation over the axial direction on a computational plane whose thickness is h_z, the axially integrated equation is obtained as follows:

$$\sin\theta\cos\alpha\frac{\partial}{\partial x} \quad \sin\theta\sin\alpha\frac{\partial}{\partial y}\ \overline{\Psi}(r_r,\Omega,E)$$

$$\Sigma_t(r_r,E)\overline{\Psi}(r_r,\Omega,E)$$

$$\frac{1}{h_z}\ _{h_z} \quad Q(\vec{r},E) \quad \cos\theta\frac{\partial}{\partial z}\Psi(\vec{r},\Omega,E)\ \mathrm{d}z \qquad (2)$$

which can be also expressed as:

$$\sin\theta\cos\alpha\frac{\partial}{\partial x} \quad \sin\theta\sin\alpha\frac{\partial}{\partial y}\ \overline{\Psi}(r_r,\Omega,E)$$

$$\Sigma_t(r_r,E)\overline{\Psi}(r_r,\Omega,E) \quad \overline{Q}(r_r,E) \quad TL_{\mathrm{axial}} \qquad (3)$$

with

$$TL_{\mathrm{axial}} \quad \frac{\cos\theta}{h_z}(\Psi_{\mathrm{top}} \quad \Psi_{\mathrm{bottom}}) \qquad (4)$$

Here, $\overline{\Psi}(r_r,\Omega,E)$ is the integrated angular flux over the axial direction, r_r is the position vector in 2D space and α and θ are the azimuthal and polar angles of Ω. The cross sections are assumed to be constant over the node.

The term TL_{axial} represents the leakage of neutrons from one plane to another. The angular distribution of the axial leakage must be provided from the axial solver. However, as the diffusion equation is solved, access to the angular flux distribution becomes impossible. The DP0 approximation, *i. e.* an isotropic angular flux, is thus used to describe the angular flux. The axial leakage then only involves the incoming and outgoing partial currents obtained by solving the axial diffusion equation:

$$TL_{\mathrm{axial}} \quad \frac{\cos\theta}{h_z}(\Psi_{\mathrm{top}} \quad \Psi_{\mathrm{bottom}})$$

$$\frac{\cos\theta}{\pi h_z}(j_g^{\mathrm{top},} \quad j_g^{\mathrm{bottom},}) \ \text{for}\ \cos\theta \quad 0$$

$$\frac{\cos\theta}{\pi h_z}(j_g^{\mathrm{top},} \quad j_g^{\mathrm{bottom},}) \ \text{for}\ \cos\theta \quad 0 \qquad (5)$$

Concerning the axial diffusion solver, the 3D diffusion equation can be expressed as:

$$J(\vec{r},E) \quad \Sigma_t(\vec{r},E)\Phi(\vec{r},E) \quad Q(\vec{r},E) \qquad (6)$$

The multi-group constants are assumed to be available from the previous radial MOC solution and the conventional homogenization scheme. Integrated over the radial directions, the 3D diffusion equation leads to:

$$D_g\frac{\mathrm{d}^2}{\mathrm{d}z^2}\phi_{z,g} \quad \Sigma_{r,g}\phi_{z,g} \quad Q_g \quad TL_{\mathrm{radial}} \qquad (7)$$

where the term TL_{radial} is decribed by

$$TL_{\mathrm{radial}} \quad \frac{1}{h_z}\sum_{x,y}[J_{x,g}^{\mathrm{right}}(z) \quad J_{x,g}^{\mathrm{left}}(z)$$

$$J_{y,g}^{\mathrm{right}}(z) \quad J_{y,g}^{\mathrm{left}}(z)] \qquad (8)$$

The term TL_{radial} represents the leakage of neutrons from one pin to another. The net current at the boundary of the pins has to be provided. It is computed using the results of the radial MOC solver

$$J_{x,g}^{\mathrm{right}}(z) \quad \int_{\Omega}\Omega\psi(r_r,E,\Omega)d\Omega \qquad (9)$$

where $\Psi(r_r,E,\Omega)$ is the angular flux at the boundary of the pin.

The derivation of the 3D Boltzmann transport equation and the 3D diffusion equation, using the above approximations, leads to the following two coupled equations:

– a 2D MOC equation coupled with axial leakage:

$$\frac{\mathrm{d}\Psi_{g,m,i,k}^{(n)}}{\mathrm{d}s_{g,m,i,k}} \quad \Sigma_{g,i}\Psi_{g,m,i,k}^{(n)} \quad Q_{g,i} \quad TL_{\mathrm{axial}}^{(n)} \qquad (10)$$

– a 1D diffusion equation coupled with radial leakage:

$$D_p\frac{\mathrm{d}^2}{\mathrm{d}z^2}\phi_{z,p}^{(n)} \quad \Sigma_{r,p}\phi_{z,p}^{(n)} \quad Q_p \quad TL_{\mathrm{radial}}^{(n\ 1)} \qquad (11)$$

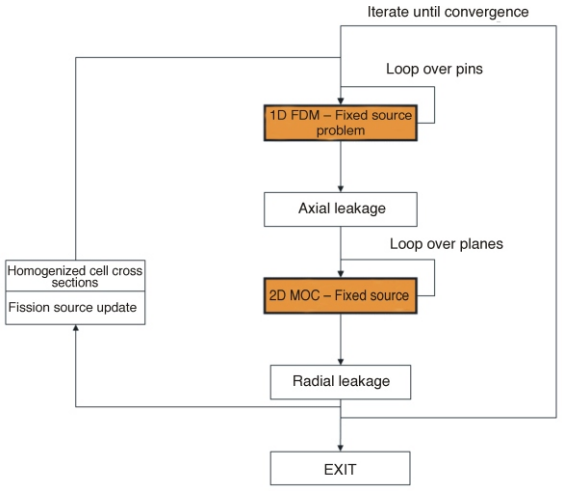

Figure 5. Flow chart for the AGENT 2D–1D flux solver

The flow chart of a 2D-1D solver is described in more detail in fig. 5.

Both MOC and FD equations are solved as a fixed source problem with only the transverse leakage varying from one iteration to the other. A converged solution, in terms of angular flux and leakages, leads to the computation of a new eigenvalue. The fission source for both equation is then updated.

PRELIMINARY 3D METHODOLOGY VALIDATION

In order to test the 2D-1D solver implemented in AGENT, two simple test cases have been developed from the L336 benchmark problem [9]. Both test cases are 3 3 assemblies with the z-direction split into three planes:

Test 1: MOX pin surrounded by eight UO_2 pins, and

Test 2: plane of MOX fuel surrounded by two planes of UO_2.

The results of these two tests, graphically shown in fig. 6, are summarized in tab. 2. DeCART and AGENT are giving close results in terms of eigenvalue for both test cases. However, the results for DeCART

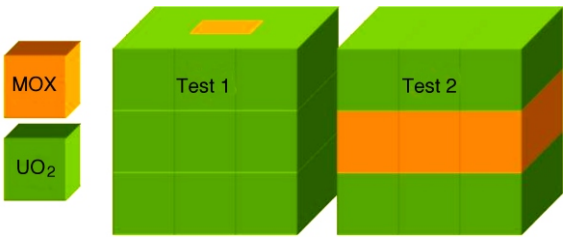

Figure 6. 3D test cases

Table 2. 3D results: *k*-infinity AGENT and DeCART comparison

Test	DeCART	AGENT	Difference [10^{-5}]
1	1.01654	1.01661	–7
2	1.03261	1.03064	190

and AGENT in test 1 are much closer than those obtained in test 2. This is due to the fact that in test 1 the geometry in the z-direction is homogenous, whereas in test 2, there is a large heterogeneity in the axial direction introduced by the plane of MOX.

In test 1 the axial leakage is negligible, since the three plans are identical. Consequently, the difference between AGENT and DeCART comes from the difference introduced by the MOC solver. The difference in terms of eigenvalue is equal to only 7 . However, in test 2, the radial leakage is negligible: all fuel pins are identical. The difference between AGENT and DeCART is then influenced by the 1D axial solver. DeCART uses a high order Nodal Expansion Method to treat the 1D problem, while AGENT uses a simple first order FDM. The difference in the 1D solver explains the 190 10^{-5} difference between AGENT and DeCART.

The second parameter which has to be compared in order to understand the accuracy of the model is the agreement in scalar fluxes. The energy integrated scalar flux for each region has been compared for both test cases. For test 1, as every plan is identical, the flux map is presented only for the first

DeCART flux
AGENT flux
Difference in %

MOX Node

Table 3. Test 1: 3D flux map comparison

0.4763 0.4774 –0.11	0.4718 0.4728 –0.10	0.4763 0.4774 –0.11
0.4718 0.4728 –0.10	1.0000 1.0000 0.00	0.4718 0.4728 –0.10
0.4763 0.4774 –0.11	0.4718 0.4728 –0.10	0.4763 0.4774 –0.11

Table 4. Test 2: 3D flux map comparison

0.4435 0.4744 –3.08
1.0000 1.0000 0.0
0.4435 0.4744 –3.08

plan. The results are shown in tab. 3. For test 2, as every fuel pin is the same, only the flux in the central fuel pin is presented. The results are summarized in tab. 4. Each box contains the AGENT scalar flux first, followed by the DeCART value and, finally, the difference in percentages between them. The scalar flux is normalized to 1.0 for both DeCART and AGENT in the MOX nodes of the geometry: central pin cell for test 1 and middle plan for test 2.

The comparison of the flux maps leads to the following conclusion: for test 1, the difference is less than 0.2% which represents a good agreement between AGENT and DeCART. For test 2, however, as the axial solver is involved, the maximum difference is increased to around 3%. This, again, is explained by the different methods used to solve the 1D problem in AGENT and DeCART.

CONCLUSION

The current state of computer codes that address the flexible neutron transport modeling in research reactor geometries is limited. The common method for accurate prediction of neutron behavior is the Monte Carlo method. It provides great 3D geometrical flexibility and high calculation accuracy, but long computation times. Highly accurate 2D modeling of neutron histories within heterogeneous domains in short computation runtimes has been documented using AGENT.

The AGENT code system will be used for research and educational purposes with the capability of performing "virtual" experiments. There is, therefore, an obvious need for a 3D whole reactor core model. The development of the 3D capability using a 2D-1D coupling strategy has been implemented into the AGENT showing good agreement with the DeCART methodology. Further improvement and the development of a more accurate 1D model are currently in progress.

ACKNOWLEDGEMENTS

Research supported through Grant Number 2402-PU-DOE-4423 under the *Innovations in Nuclear Infrastructure and Education* (INIE) Program of the US Department of Energy.

Authors wish to thank Prof. Thomas Downar and Dr. Deokjung Lee for their help in developing the 2D/1D coupling methodology for the AGENT code system.

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Метју ХУРСИН, Татјана ЈЕВРЕМОВИЋ

НУМЕРИЧКИ ПРОГРАМ AGENT ЗА СИМУЛАЦИЈУ ТРАНСПОРТА НЕУТРОНА – БЕНЧМАРК ПРОБЛЕМ И ОПИС АЛГОРИТМА ЗА ТРОДИМЕНЗИОНАЛНО МОДЕЛОВАЊЕ ГОРИВИХ СКЛОПОВА РЕАКТОРА

Нумерички програм AGENT развијен је за моделовање транспорта неутрона у генералним геометријама. Дводимензионална неутронска транспортна једначина решена је методом карактеристика, а генерална геометрија се описује помоћу теорије R–функција. У овом раду приказан је алгоритам који су аутори развили за тродимензионално решење транспортне једначине у комплексним геометријама нуклеарних реактора. С обзиром да директно проширење дводимензионалног у тродимензионално решење помоћу методе карактеристика захтева огромно рачунарско време као и велико заузеће меморијског простора, развијена је алтернативна метода. Метода се базира на комбинацији дводимензионалног решења методом карактеристика и једнодимензионалног решења помоћу дифузионе методе. Планарно решење методом карактеристика и аксијално решење дифузионом методом је повезано кроз трансверзално отицање неутрона. Ова алтернативна метода је валидна код прорачуна PWR и BWR с обзиром да је хетерогеност у погледу геометријске структуре и типа горива далеко мања у аксијалном правцу него што је то у планарним равнима реакторског језгра.

Карактеристике и тачност нумеричког програма AGENT приказани су за случај познатог бенчмарк проблема, C5G7. Дводимензионално решење је анализирано у поређењу са познатим нумеричким програмом DeCART. Алгоритам који је развијен за урачунавање и треће димензије детаљно је описан. Прелиминарни резултати су показани на примеру хетерогене комбинације различитих горивих ћелија.

Кључне речи: метода карактеристика, хетерогени реактори, реакторски гориви склоп, бенчмарк проблеми