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(**Research Article)**

Numerical Solution of Advection-Diffusion Equation via Quartic B-Spline Least Squares Method

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Abstract: Numerical solutions are obtained for the time dependent one dimensional Advection-Diffusion equation (ADE) using the least squares method (LSM). After the time-integration of the ADE by use of the Crank-Nicolson technique, the combination of the quartic B-splines as a trial function is substituted in the time discretized ADE and for the LSM procedure, a weight function is obtained by taking derivative of the integrand of integral of squared ADE with respect to time parameters of the trial functions. Thus solution of obtained recursive system of the unknown parameters provides solutions of the ADE at discrete times. Achievement is displayed by studying three test problems.

(**Araştırma Makalesi**)

Adveksiyon Difüzyon Denkleminin Kuartik B-Spline En Küçük Kareler Metodu ile Sayısal Çözümü

Anahtar Kelimeler:
Advection-diffusion denklemi,
En küçük kareler metodu,
Kuartic B-spline

Özet: En küçük Kareler metodu (LSM**)** kullanılarak zamana bağlı bir boyutlu Advection-Diffusion denklemi (ADE) için yaklaşık çözümler elde edilmiştir. Crank-Nicolson yöntemi ile ADE'in zaman ayrıştırması yapıldıktan sonra, Kuadratik B-spline fonksiyonların kombinasyonundan oluşan deneme fonksiyonu zaman ayrışmış ADE'nin bilinmeyen fonksiyonuna yerleştirilmiştir. Böylece elde edilen cebirsel ifadenin karesi alınmış integralinin integrantının deneme fonksiyonun da tanımlı zaman parametresine göre türevi alınarak ağırlık fonksiyonu belirlenmiştir. Bulunan iterative sistemin çözümlerinden ADE'nin ayrık zamanlardaki çözümlerini elde edilir. Metodun başarısı üç test problem çalışılarak gösterilmiştir.

1. INTRODUCTION

The ADE is the time dependent one-dimensional partial differential equation which models many problems of physics, chemistry and biology. It describes advection-diffusion processes depending on the given parameters such as heat, energy, mass, etc. It indicates combination of both non-dissipative (hyperbolic) advective and a dissipative (parabolic) diffusive behaviors. The ADE, as an mathematical model, is used to designate water transfer in soils, heat transfer in draining film, spread of pollutants in rivers, dispersion of tracers in porous media, the Timoshenko beam problem, the Reissner-Mindlin plate, the arch problem and the axisymmetric shell problem. It is known that the numerical solution is obtained well when the diffusion is dominant whereas for the larger advection coefficient taken, numerical methods produce higher error solutions. The effort has been made on producing the efficient numerical methods. Various numerical techniques including B-splines have been set up for solving the one-dimensional ADE of constant

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coefficients with appropriate initial and boundary conditions [1].

The numerical solution of the advection-diffusion problem is provided by use of both quadratic and cubic B-spline finite element methods in which Taylor series expansion is used for the time discretization [2]. Cubic B-spline collocation methods are build up for solving convection diffusion equations in the studies [3,4]. The differential quadrature methods based on the cubic B-splines is constructed for the advection-diffusion equation [5]. ADE is solved by using the extended cubic B-spline collocation method [6] . Differential quadrature together with B-spline functions of degree four and five have been designed to compute advection-diffusion equation numerically [7]. ADE is integrated using the extended cubic B-spline Galerkin method to find its numerical solutions [8]. The fourth order single step methods for time integration and cubic B-spline Galerkin method for space integration is used to solve ADE in the work [9]. The cubic trigonometric B-spline for space discretization and finite difference scheme for time discretization is established to discretize the ADE fully [10]. ADE is also handled by means of the least squares method. A space time least-squares finite elements scheme is constructed for advection-diffusion equation [11], space-time Galerkin least squares method for the one-dimensional ADE is proposed in the works [12,13]. The space time least squares method was set up by way of both linear and quadratic B-spline shape functions for computing numerical solutions of the ADE [14]. A p-version based space-time least-squares finite-element method is applied to solve the unsteady convection-diffusion equation [15] . The linear and quadratic B-spline basis functions have been used in the space time least squares formulation for solving the ADE in the study [16]. The cubic B-spline leasts square finite element method is established for solving the ADE [17]. The Nonic B-splines are adapted to form the collocation method for solving ADE numerically [18]

Linear joining of $\frac{\partial U}{\partial t}$, advection $\frac{\partial U}{\partial x}$ and diffusion $\frac{\partial^2 U}{\partial x^2}$ terms constitute the ADE,

$$u_t + \varepsilon u_x - \lambda u_{xx} = 0, x \in [a,b], t > \quad (1)$$

where ε and λ are parameters, x and t are time and space coordinates respectively. The initial condition (IC) is given as,

$$u(x,0) = f(x). \quad (2)$$

Dirichlet boundary conditions (BCs) are,

$$u(a,t) = 0, \quad u(b,t) = 0. \quad (3)$$

The equation includes behaviors of both advection and diffusion processes depending upon value of ε (advection coefficient) and γ (diffusion coefficient). Numerical difficulties arise like exhibiting both spurious oscillations and excessive numerical diffusion when the advection becomes dominant. Thus, numerical methods have been constructed to overcome the adversity of advection domination for getting right solutions of the ADE.

In this paper, fully-integration of ADE is managed by help of the Crank-Nicolson method in time and quartic B-spline least squares method in space. Solution steps are illustrated in section 2. Three standard test problems are presented to show the performance of the suggested algorithm.

2. THE QUARTIC B-SPLİNE LEAST SQUARE METHOD

Let the interval $[a,b]$ be partitioned into subintervals $[x_i, x_{i-1}], i = 1, \dots N$ at a uniformly distributed mesh points $x_i = a + ih, i = 0, \dots, N$ with $x_0 = a$ and $x_N = b$. The quartic B-splines $P_i^4(x), i = -2, \dots, N+1$ are defined at the defined mesh points and fictitious points $x_{-4}, x_{-3}, x_{-2}, x_{-1}, x_{N+1}, x_{N+2}, x_{N+3}, x_{N+4}$ outside problem interval $[a,b]$ in the following form:

$$P_i^4(x) = \frac{1}{h^4}\begin{cases}(x-x_{i-2})^4 & , \quad [x_{i-2}, x_{i-1}] \\ (x-x_{i-2})^4 - 5(x-x_{i-1})^4 & , \quad [x_{i-1}, x_i] \\ (x-x_{i-2})^4 - 5(x-x_{i-1})^4 + 10(x-x_i)^4 & , \quad [x_i, x_{i+1}] \\ (x_{i+3}-x)^4 - 5(x_{i+2}-x)^4 & , \quad [x_{i+1}, x_{i+2}] \\ (x_{i+3}-x)^4 & , \quad [x_{i+2}, x_{i+3}] \\ 0 & , \quad \text{otherwise}\end{cases} \quad (4)$$

$P_i^4(x)$ are basis functions for the functions defined in the problem interval $[a,b]$ so that any function can be arranged as a linear combination of the quartic B-spline basis functions:

$$u(x,t) \approx U(x,t) = \sum_{i=-2}^{N+1} \psi_i(t) P_i^4(x). \quad (5)$$

Where $\psi_i(t)$ are time dependent parameters determined by application of the least squares method to the ADE. The B-spline approximation at the mesh points to the nodal value $u(x,t)$ can be expressed in terms of element parameters.

$$\begin{aligned} U(x_i,t) &= U_i = \psi_{i-2} + \psi_{i-1} + \psi_i + \psi_{i+1} \\ U_i' &= \frac{4}{h}(-\psi_{i-2} - 3\psi_{i-1} + 3\psi_i + \psi_{i+1}) \\ U_i'' &= \frac{12}{h^2}(\psi_{i-2} - \psi_{i-1} - \psi_i + \psi_{i+1}) \\ U_i''' &= \frac{24}{h^3}(-\psi_{i-2} + 3\psi_{i-1} - 3\psi_i + \psi_{i+1}) \end{aligned} \quad (6)$$

To start the integration of the ADE (1), first, time integration is managed via the Crank-Nicolson technique to obtain time-integrated ADE

$$\frac{U^{n+1} - U^n}{\Delta t} + \varepsilon\left(\frac{U_x^{n+1} + U_x^n}{2}\right) - \lambda\left(\frac{U_{xx}^{n+1} + U_{xx}^n}{2}\right) = 0 \quad (7)$$

and organize (7) to have the form:

$$2U^{n+1} - 2U^{n} + (\varepsilon\Delta t)(U_x^{n+1} + U_x^{n}) - (\lambda\Delta t)(U_{xx}^{n+1} + U_{xx}^{n}) = 0 \quad (8)$$

At the second step, the least squares scheme is going to be performed to the Eq. (8) to reach the integral equation:

$$\int_a^b (2\mathrm{U}^{n+1} - 2\mathrm{U}^{n} + (\varepsilon\Delta t)(U_x^{n+1} + U_x^{n}) - (\lambda\Delta t)(U_{xx}^{n+1} + U_{xx}^{n}))^2 dx = 0 \quad (9)$$

For the purpose of suitability, the B-splines (4) and integral Equations (9) are transformed by using local coordinate system

$$\zeta\Delta x = x - x_i, 0 \le \zeta \le 1 \quad (10)$$

mapping the sample interval $[x_i, x_{i+1}]$ to interval [0,1]. Thus the quartic B-splines within interval $[x_i, x_{i+1}]$ have expression with respect to ζ on the interval [0,1]

$$\begin{aligned} P_{i-2}^4 &= 1 - 4\zeta + 6\zeta^2 - 4\zeta^{23} + \zeta^4 \\ P_{i-1}^4 &= 11 - 12\zeta - 6\zeta^2 + 12\zeta^{23} - \zeta^4 \\ P_i^4 &= 11 + 12\zeta - 6\zeta^2 - 12\zeta^{23} + \zeta^4 \\ P_{i-2}^4 &= 1 + 4\zeta + 6\zeta^2 + 4\zeta^{23} - \zeta^4 \\ P_{i-2}^4 &= \zeta^4 \end{aligned} \quad (11)$$

and using transformation (10) for derivative in ζ coordinates, the first and second derivatives becomes

$$U_x = \frac{\partial U}{\partial \zeta}\frac{\partial \zeta}{\partial x} = U_\zeta \frac{1}{\Delta x},$$

$$U_{xx} = \frac{\partial}{\partial x}(U_x) = \frac{1}{\Delta x}\frac{\partial}{\partial x}(U_\zeta)$$

$$= \frac{1}{\Delta x}\frac{\partial U_\zeta}{\partial \zeta}\frac{\partial \zeta}{\partial x} = \frac{1}{\Delta x^2}U_{\zeta\zeta},$$

an approximation

$$u^e(x,t) \approx U^e(x,t) = \sum_{i=m-2}^{m+1} \psi_i(t) P_i^4(\zeta) \quad (12)$$

in the interval [0,1], integral equation (9) yields

$$\int_0^1 (2(U^e)^{n+1} - 2(U^e)^{n} + \beta(U^e)_\zeta^{n+1} + \beta(U^e)_\zeta^{n} - \theta(U^e)_{\zeta\zeta}^{n+1} - \theta(U^e)_{\zeta\zeta}^{n}) d\zeta = 0 \quad (13)$$

Taking the derivative of the integral Equation (13) with respect to time parameter ψ^{n+1} yield

$$\frac{d}{d\psi^{n+1}}\int_0^1 (2U^{n+1} - 2U^{n} + \beta U_\zeta^{n+1} + \beta U_\zeta^{n} - \theta U_{\zeta\zeta}^{n+1} - \theta U_{\zeta\zeta}^{n})^2 d\zeta = 0 \quad (14)$$

so that the least squares weak formulation is obtained in the form of Galerkin with weight function

$$\frac{d}{d\psi_i^{n+1}}\left(2U^{n+1} - 2U^{n} + \beta U_\zeta^{n+1} + \beta U_\zeta^{n} - \theta U_{\zeta\zeta}^{n+1} - \theta U_{\zeta\zeta}^{n}\right). \quad (15)$$

Replacing approximation (12) in Eq. (14) leads to a system of equations:

$$\int_0^1 \begin{aligned} &(4P_iP_i\psi_i^{n+1} - 4P_iP_i\psi_i^{n} + 2\beta P_iP_i'\psi_i^{n+1} \\ &+2\beta P_iP_i'\psi_i^{n} - 2\theta P_iP_i''\psi_i^{n+1} - 2\theta P_iP_i''\psi_i^{n} \\ &+2\beta P_i'P_i\psi_i^{n+1} - 2\beta P_i'P_i\psi_i^{n} + \beta^2P_i'P_i'\psi_i^{n+1} \\ &+\beta^2P_i'P_i'\psi_i^{n} - \beta\theta P_i'P_i''\psi_i^{n+1} \\ &-\beta\theta P_i'P_i''\psi_i^{n} - 2\theta P_i''P_i\psi_i^{n+1} \\ &+2\theta P_i''P_i\psi_i^{n} - \theta\beta P_i''P_i'\psi_i^{n+1} \\ &-\theta\beta P_i''P_i'\psi_i^{n} + \theta^2P_i''P_i''\psi_i^{n+1} \\ &+\theta^2P_i''P_i''\psi_i^{n})d\zeta = 0 \end{aligned} \quad (16)$$

In this system, we use the integral for brevity

$A_{ij}^e = \int_0^1 P_i P_j d\zeta,$	$B_{ij}^e = \int_0^1 P_i P_j' d\zeta,$
$(B_{ij}^e)^T = \int_0^1 P_i' P_j d\zeta$	$C_{ij}^e = \int_0^1 P_i P_j'' d\zeta,$
$(C_{ij}^e)^T = \int_0^1 P_i'' P_j d\zeta,$	$D_{ij}^e = \int_0^1 P_i' P_j' d\zeta,$
$E_{ij}^e = \int_0^1 P_i' P_j'' d\zeta$	$(E_{ij}^e)^T = \int_0^1 P_i'' P_j' d\zeta$
$F_{ij} = \int_0^1 P_i'' P_j'' d\zeta$	

(17)

to have the iterative matrix equation having the unknown ψ_i^{n+1} on each sample intervals $[x_i, x_{i+1}]$

$$[4A^e + 2\beta((B^e)^T + B^e) - 2\theta((C^e)^T + C^e) + \beta^2D^e - \beta\theta((E^e)^T + E^e) + \theta^2F^e](\psi^e)^{n+1} = [4A^e + 2\beta((B^e)^T + B^e) - 2\theta((C^e)^T + C^e) + \beta^2D^e - \beta\theta((E^e)^T + E^e) - \theta^2F^e](\psi^e)^{n}. \quad (18)$$

Putting together all the system of equations (18) to have the global matrix equation:

$$[4A + 2\beta(B^T + B) - 2\theta(C^T + C) + \beta^2 D - \beta\theta(E^T + E) + \theta^2F](\psi)^{n+1}] = [4A + 2\beta(B^T + B) - 2\theta(C^T + C) + \beta^2 D - \beta\theta(E^T + E) - \theta^2F](\psi)^{n}. \quad (19)$$

$A, B, B^T, C, C^TD, E, E^T, F$ are obtained by combining the element matrices $A^e, B^e, (B^e)^T, C^e, (C^e)^T, D^e, E^e, (E^e)^T$. The time-space discrete solutions can be found by implementing the system of equations(19) once the initial solution parameters are determined by way of the following equations

$$U(x_m,0) = \psi_{m-2}^0 + 11\psi_{m-1}^0 + 11\psi_m^0 + \psi_{m+1}^0$$

$$U'(x_0,0) = 4/h(-\psi_{-2}^0 - 3\psi_{-1}^0 + 3\psi_0^0 + \psi_1^0)$$

$$U''(x_0,0) = 12/h^2(\psi_{-2}^0 - \psi_{-1}^0 - \psi_0^0 + \psi_1^0)$$

$$U'(x_N,0) = 4/h(-\psi_{N-2}^0 - 3\psi_{N-1}^0 + 3\psi_N^0 + \psi_{N+1}^0)$$

3. NUMERICAL RESULTS

3.1. Pure advection in long channel

The effect of pure advection is going to be studied in an infinitely long channel of long constant cross-section when $\gamma = 0$. Peak of the initial wave is going to be positioned at $x = x_0$ in the channel whose length is taken L and then movement of the initial wave to the right side of the channel is going to be observed. Analytical solution of the ADE is

$$u(x,t) = 10exp\left(-\frac{1}{2\rho}(x - x_0 - \varepsilon t)^2\right), \quad 0 < x < L \qquad (20)$$

from which the initial condition is taken with $t = 0$:

$$u(x,0) = 10exp(-\frac{1}{2\rho}(x - x_0))^2. \qquad (21)$$

Boundary condition

$$u(0,t) = u(L,t) = \alpha, t > 0$$

are chosen.

The velocity of $\varepsilon = 0.5m/s$, position of peak wave of $x_0 = 2000m$ and standard deviation $\rho = 264$ are used for purpose of comparison with earlier results. The program is run over the problem domain [0,9000] until time $t = 9600s$ at which time error norms are given at time $t = 9600$ in Table 1 for equal time/space increments.

When $h = \Delta t = 50$ are used, wave behavior is given at times $t = 1000, 2000, \ldots, 9000$ in Fig. 1a and absolute difference between exact and numerical solutions is displayed at time $t = 9600$ in Fig. 1b from which errors happen at most near peak position of wave. From Fig. 1a, wave magnitude remain almost same and move $4800m$ during the running of the algorithm as expected.

Table 1. Error norms at *t=9600*

$h = \Delta t$	$L_2(t = 9600)$	$L_\infty(t = 9600)$
200	54.39436	2.305734
100	15.65584	0.733745
50	4.00316	0.189633
25	1.00492	0.047043
10	0.16095	0.007502

3.2. Combined effect of advection-diffusion

Disappearance of the initial bell-shaped Gauss concentration can be illustrated by way of the analytical solution of ADE:

$$u(x,t) = \frac{1}{\sqrt{4t+1}} exp\left(-\frac{(x - x_0 - \varepsilon t)^2}{\lambda\sqrt{4t+1}}\right) \qquad (22)$$

Initial concentration is derived from the analytical solution (22) for $t = 0$:

$$u(x,t) = exp\left(-\frac{(x - x_0)^2}{\lambda}\right) \qquad (23)$$

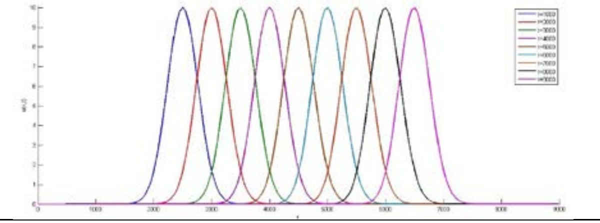

Figure 1.a. Solutions at some times.

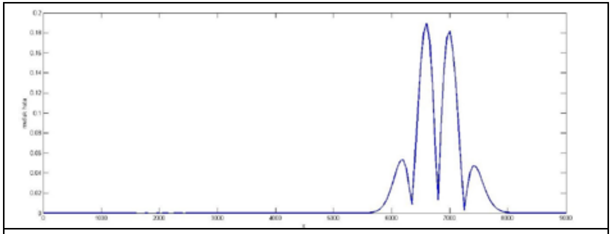

Figure1. b. |Exact − numerical| solution at t=9600.

The velocity $\varepsilon = 0.8m/s$, diffusion coefficient $\lambda = 0.005\ m^2/s$ and peak position of initial concentration $x_0 = 1m$ and time-space increments $h = \Delta t$ combinations are selected to run the algorithm over the integral [0,9] with boundary conditions $u(0,t) = u(9000,t) = 0$. Results of L_2 and L_∞ norms are documented at time $t = 5$ in Table 2.

Table 2. Error norms at *t=5*

$h = \Delta t$	$L_2(t = 5)$	$L_\infty(t = 5)$
0.1	0.033049	0.053645
0.05	0.008523	0.014100
0.02	0.001359	0.002173
0.01	0.000340	0.000538
0.005	0.000085	0.000134

Smaller increments cause smaller errors seen in Table 2. Initial concentration can be observed to vanish drawn in Fig. 2a as time increase and error distribution at time $t = 5$ is depicted in Fig. 2b.

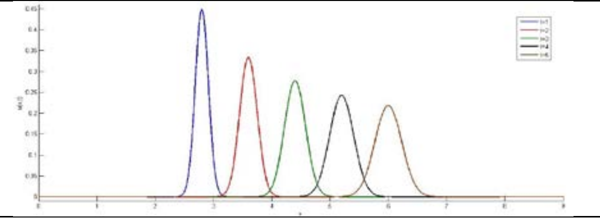

Figure 2.a. Solution behavior

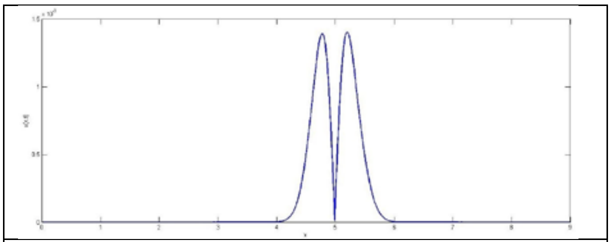

Figure 2. b. |Exact − numerical| solution

3.3. Convection-diffusion of continuous flow of pollutants

This test problem examines the effect of both advection and diffusion while flowing. During the simulation process, the velocity $\varepsilon = 0.01$, the diffusion constant $\lambda = 0.002$, the length of the channel $L = 200m$, boundary conditions $u(0,t) = 1$ and $u(200,t) = 0$, initial condition $u(x,0) = 0, x \geq 0$ are chosen. Analytical solution is

$$u(x,t) = \frac{1}{2} erfc(\frac{x-\varepsilon t}{\sqrt{4\lambda t}}) + \frac{1}{2}\exp(\frac{\varepsilon x}{\lambda})\frac{1}{2} erfc(\frac{x+\varepsilon t}{\sqrt{4\lambda t}}) \quad (24)$$

The program is run and error norm L_∞ at times 3000 and 6000 is documented for time/space combinations in Table 3.

Numerical solutions at times $t = 3000$ and $t = 6000$ and their absolute errors are given in Figs. 3a-b-c, from which the maximum errors at times $t = 3000$ and 6000 happens at about positions $30m$ and $60m$ respectively.

Table 3. Error norms L_∞ at various time

Δt	h	$L_\infty(= 3000)$	$L_\infty(= 6000)$
60	1	0.035207	0.024590
30		0.010528	0.00718
10		0.005212	0.003489
5		0.008159	0.00568
60	0.5	0.0336759	0.023552
30		0.0094947	0.006512
10		0.005397	0.003696
5		0.008398	0.005906

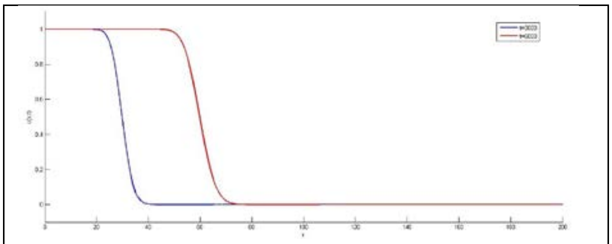

Figure 3.a. Solutions

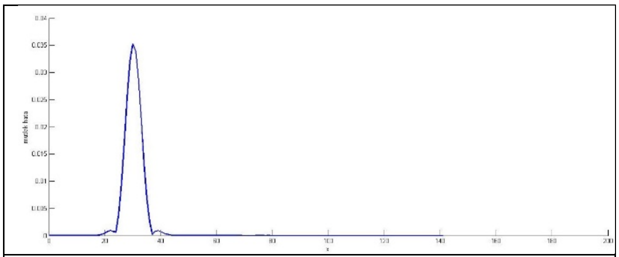

Figure 3. b. errors at time t = 3000

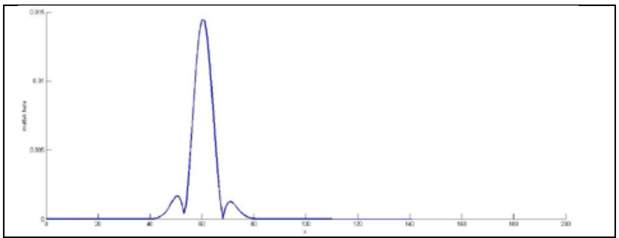

Figure 3. c. errors at time6000

An effective algorithm has been suggested for getting numerical solution of the ADE. Error for the diffusion dominant form of the ADE is obtained to be smaller than the pure advection form of it numerically as expected, seen the results of the example test problems 2 and 3. The quartic B-spline based least square method can be used as alternative numerical method for solving advection-diffusion systems fairly.

Ethical Considerations
Compliance with ethical guidelines

The study does not require ethical permission.

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Conflict of interest
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