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Numerical simulation for thermohaline multiple equilibrant system in non-rectangular domains*

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In this paper, incompressible, double-diffusive convection is simulated using finite-difference schemes. The Navier–Stokes equations are expressed in terms of stream function and vorticity. Because of the existence of large velocity, temperature and salinity gradients in boundary layers, a boundary-fitted coordinate system is used to concentrate the grid points near the wall and fit complex boundaries. The finite-difference methods used include the high-order accurate upwind difference scheme. It is shown that the scheme is a good candidate for direct simulations of double-diffusive convection flows. The proposed method is first applied to symmetry breaking and overturning states in thermohaline-driven flows in trapezoid basins. The basic phenomena agree well with those by Dijkstra and Molemaker (1997 *J. Fluid Mech.* **331** 169) and Quon and Ghil (1992 *J. Fluid Mech.* **245** 449), but symmetry breaking and overturning states can occur in an asymmetric geometrical region without perturbations. Then the method is applied to double-diffusive convections in a cavity with opposing horizontal temperature and concentration gradients at large thermal (Rt), solutal (Rs) Rayleigh numbers and Lewis number. There are three straight sides and a sine curve side in the cavity. Basically, numerical results are in agreement with those of Lee and Hyun (1990 *Int. J. Heat Mass Transfer* **33** 1619) qualitatively, but eddies mixing in the top left-hand corner near the curved wall affects the layered structure.

Keywords: double-diffusive convection, high-order accurate difference scheme, multiple equilibrant system

PACC: 4725Q

1. Introduction

Thermosolutal convection has been receiving much attention over the past three decades because of its occurrence in many transport processes in both nature and industrial flow systems, and in both terrestrial and astrophysical environments, such as crystal growth, solar collectors, atmospheric flows and thermohaline ocean circulation, etc.

A number of numerical studies on double-diffusive convection problems have been carried out. Thangam *et al*[1] studied this nonlinear phenomenon using a Galerkin method for both vertical and inclined geometries. Heinrich[2] used a finite element method and the results compared well with the experiments of Chen *et al.*[3] Lee and Hyun[4] used a finite-difference method to simulate the experiments of Chen *et al.*[3] The time-dependent double-diffusive convection in a rectangular enclosure was studied to clarify the mechanism of layer merging in a salt-stratified system by Nishimura and Kunitsugu[5] using the Chebyshev collocation method. The numerical modelling of double-diffusive convection problems with a boundary layer is difficult because of the existence of large velocity, temperature and salinity gradients. A lot of complicated phenomena are associated with a large velocity gradient.[6,7] The finite element method, with the flexibility of a variable mesh, is superior to the finite-difference method in solving these problems. However, the latter is much less complicated than the former at least in terms of computer programming. The boundary-fitted coordinate system, which has both the advantages of geometric flexibility in the finite element method and the simplicity of the finite-difference method, has gained popularity in solving boundary layer problems.

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Different dynamical behaviours result from the competition of the two diffusive species: solute and temperature which have opposite effects on the density field, leading to the formation of fronts and multiple equilibria because of the use of different initial and boundary conditions and different values of the Rayleigh number and other parameters. Ghorayeb and Mojtabi[8] studied the onset of convection in vertical enclosures with a constant temperature along the vertical sidewalls. Tsitverblit[9] studied the flow for several values of the salinity Rayleigh number around the borders of the double-diffusive region and reported that, when the thermal Rayleigh number is either very small or sufficiently large, the steady solution is unique, while for intermediate values of the thermal Rayleigh number, there exists a great variety of multiple steady flows. Zhan and Li[10] emphasized their work on the study of the flow characteristic of the two-dimensional (2D) thermosolutal equilibrant regime for different Lewis numbers and found that there exist several different states in this system, which could be the symmetric states, the periodic oscillations or non-periodic (random) states. Dijkstra and Molemaker[11] studied the bifurcation structure of thermohaline-driven flows under prescribed surface temperature and fresh-water flux.

In this paper, the boundary-fitted coordinate system[12−14] is introduced also for studying double-diffusive convection problems so that finer grids can be used to resolve the flow in the boundary layers without excessive computational effort. The finite-difference methods used include the high-order accurate upwind difference scheme.

2.Governing equations and boundary conditions

The governing equations are the 2D time-dependent Navier–Stokes equations with the Boussinesq assumptions incorporated. The stream function, vorticity, temperature and salinity in the boundary-fitted coordinate system,[12−14] expressed in the nondimensionalized form using a standard notation for the stream function ψ, vorticity ω, temperature T and salinity S, can be written as

$$-\frac{1}{J^2}(\alpha\psi_{\xi\xi}-2\beta\psi_{\xi\eta}+\gamma\psi_{\eta\eta}+\sigma\psi_\eta+\tau\psi_\xi)=\omega, \quad (1)$$

$$\frac{\partial\omega}{\partial t}+\frac{1}{J}\left(\frac{\partial\psi}{\partial\eta}\frac{\partial\omega}{\partial\xi}-\frac{\partial\psi}{\partial\xi}\frac{\partial\omega}{\partial\eta}\right)$$
$$=\frac{Pr}{J^2}(\alpha\omega_{\xi\xi}-2\beta\omega_{\xi\eta}+\gamma\omega_{\eta\eta}+\sigma\omega_\eta+\tau\omega_\xi)$$
$$+PrRt\left(y_\eta\frac{\partial(T-R_\rho S)}{\partial\xi}-y_\xi\frac{\partial(T-R_\rho S)}{\partial\eta}\right)/J, \quad (2)$$

$$\frac{\partial T}{\partial t}+\frac{1}{J}\left(\frac{\partial\psi}{\partial\eta}\frac{\partial T}{\partial\xi}-\frac{\partial\psi}{\partial\xi}\frac{\partial T}{\partial\eta}\right)$$
$$=\frac{1}{J^2}(\alpha T_{\xi\xi}-2\beta T_{\xi\eta}+\gamma T_{\eta\eta}+\sigma T_\eta+\tau T_\xi), \quad (3)$$

$$\frac{\partial S}{\partial t}+\frac{1}{J}\left(\frac{\partial\psi}{\partial\eta}\frac{\partial S}{\partial\xi}-\frac{\partial\psi}{\partial\xi}\frac{\partial S}{\partial\eta}\right)$$
$$=\frac{1}{LeJ^2}(\alpha S_{\xi\xi}-2\beta S_{\xi\eta}+\gamma S_{\eta\eta}+\sigma S_\eta+\tau S_\xi), \quad (4)$$

where

$$\alpha=x_\eta^2+y_\eta^2, \quad \beta=x_\xi x_\eta+y_\xi y_\eta,$$
$$\gamma=x_\xi^2+y_\xi^2, \quad J=x_\xi y_\eta-y_\xi x_\eta,$$
$$\sigma=J^2Q, \quad \tau=J^2P.$$

Here Pr is the Prandtl number, Rt is the thermal Rayleigh number, R_ρ is the buoyancy ratio, $Le=\kappa_T/\kappa_S$ is the Lewis number, t is time, and κ_T and κ_S are diffusivities of heat and salt, respectively. x and y are nondimensional coordinates. ξ and η are boundary-fitted coordinates. P and Q are the coordinate control functions, which may be chosen to concentrate the coordinate lines in certain parts of the domain where high variations of a given property are expected.

Boundary conditions are

$\psi=0$ on all solid boundaries,

$T=0.5$ on high-temperature wall,

$T=-0.5$ on low-temperature wall,

$S=0.5$ on high-salinity wall,

$S=-0.5$ on low-salinity wall,

$\dfrac{\partial T}{\partial n}=0$ on insulated wall,

$\dfrac{\partial S}{\partial n}=0$ on impervious wall.

If the upper boundary is the ocean surface, the usual mixed boundary conditions are given by (Ref.[11])

$$\psi = \omega = 0,\ T = T_s(x),\ \ \frac{\partial S}{\partial z} = \delta Q_s(x),$$

where function $T_s(x)$ is a prescribed temperature distribution along the ocean surface. The parameter δ measures the strength of the surface salt flux and $Q_s(x)$ represents the spatial structure of the flux.

3. High-order accurate finite-difference method

In this paper, Eq.(1) is solved using the over-relaxation method. Convergence is assumed to be achieved when the absolute values of the differences of ψ between successive time steps are less than 10^{-8}.

In the spatial discretization, the first- and second-order derivatives in Eqs. (1)–(4), except for convective terms, are discretized using central differencing which are fourth-order accurate. The convective terms are approximated using fourth-order accurate upwind-biased differences (Ref.[15]). In the time discretization, the second-order accurate Adams–Bashforth method is used. The philosophy of the numerical scheme used in this paper has been described in Ref.[10] in detail and is not repeated here.

4. Examples and discussions

4.1. Symmetry breaking and overturning states in thermohaline-driven flows

Figure 1 shows the boundary-fitted coordinate system and boundary conditions of a trapezoid cavity. The computational mesh consists of 81×51 grid points. The function $T_s(x)$ is given by

$$T_s(x) = \frac{1}{2}\left[\cos\left(2\pi\left(\frac{x}{A} - \frac{1}{2}\right)\right) + 1\right],$$

and the flux $Q_s(x)$ is the same as that in Ref.[11]. It is chosen such that the integral over the surface is zero, and this constraint is automatically satisfied when the parameters are varied, i.e.

$$Q_s(x) = 3\cos\left(p\pi\left(\frac{x}{A} - \frac{1}{2}\right)\right) - \frac{6}{p\pi}\sin\left(p\frac{\pi}{2}\right),$$

where A=5 and p=2.6.

In our computation, the parameters are $Rt = Rs = 4 \times 10^4$, Pr=2.25, R_ρ=1, Le=1 and the time step is $\Delta t = 10^{-5}$. To obtain the symmetry-breaking flow pattern, perturbations of salinity were introduced in Refs.[11] and [16]. When δ is small, the symmetry state cannot be broken. As δ increases, the asymmetry state and overturning state can be obtained. Can symmetry-breaking and overturning oscillations occur only from perturbations? The answer is negative. The phenomena can occur in a complicated geometrical region without the perturbation. Figure 1 shows the boundary-fitted coordinate system of a trapezoid cavity. The right-hand side length and the top side length are the same as those of a rectangular cavity used in Ref.[11] and the bottom side length is 5.2. The boundary conditions are shown in Fig.1. Figures 2(a)–2(e) shows the process of the symmetry breaking and the overturning oscillation. At an early time, the symmetry state has been broken and the overturning oscillation occurs. At large time, the overturning state becomes steady. The symmetry and asymmetry states can also repeat in the trapezoid cavity, because of the domination of symmetric conditions on the surface and the flow instability in the cavity. The irregular boundary mainly acts as a perturbation for the states.

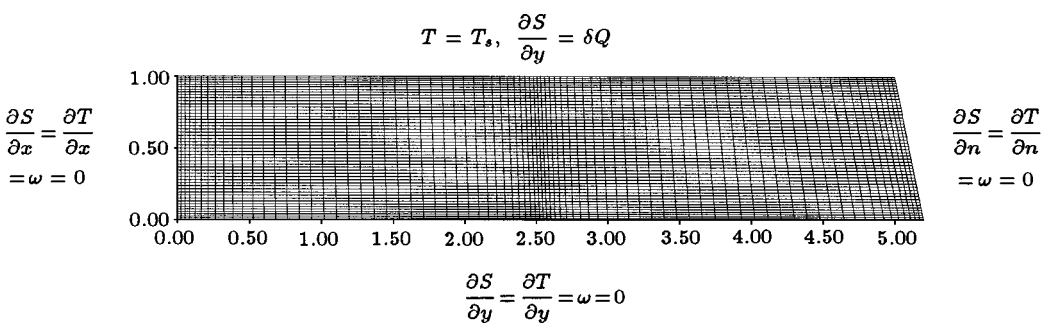


Fig.1. A boundary-fitted coordinate system of a trapezoid cavity.

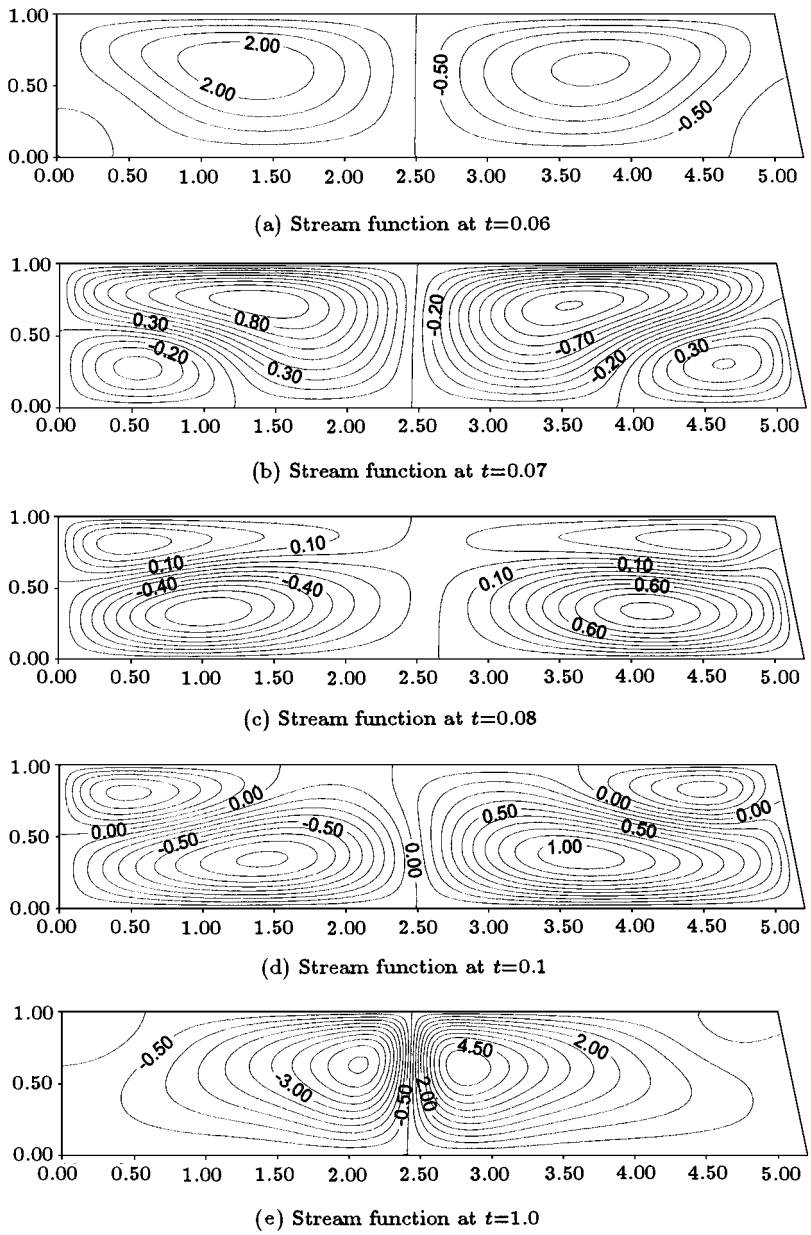


Fig.2. Overturning state in a trapezoid at δ=1.0.

4.2. Double-diffusive convection in a non-rectangular cavity with opposing horizontal temperature and concentration gradients

The geometrical configuration for the problem with a boundary-fitted coordinate system is shown in Fig.3. There are three straight sides and a sine-curved side in the cavity. The computational mesh consists of 81×101 grid points. The number of grid points would be increased by 100% if a uniform grid with a grid size equal to that near the walls is used. At the initial instant, the fluid is motionless and the temperature and concentration at the vertical side walls are abruptly altered. The parameters are Rs=6×10^7, Pr=7.0, R_ρ=9.0, Le=100 and the time step is Δt=5×10^{-7}. Obviously, for the double-diffusive flows at large values of Lewis number, the solutal boundary layer is much thinner than the thermal boundary layer. Resolving the thin boundary layer requires excessive computing resources. The present method can be used to solve this problem by arranging a finer mesh in the layer.

The computed results are shown in Fig.4. In a short time, the flow pattern is mainly of a coun-

terclockwise circulation because the thermal effect is dominant. The isohalines are highly concentrated in extremely thin regions near the vertical sidewalls. In the thin localized solutal layers by the vertical walls, the salinity gradients are relatively higher, resulting in a weak clockwise circulation and small secondary cells are visible. Because the buoyant convections driven by thermal gradients and solutal gradients counteract, the secondary cells are generated near the top right corner and the bottom left corner. They disappear near the bottom right and the top left corners. They become weaker at large time (see Fig.4(d)). At this moment, the flow becomes steady and the layered structure can be seen very clearly. The solutal field is of a step-like profile and the temperature field becomes S-shaped. In each step-like layer, the concentration is nearly uniform. Similar features can also be observed in the experiments of Thorpe *et al*[17] and the computed results of Lee and Hyun.[18] However, it can be seen that the layered process in the upper domain of the cavity is faster than in the lower domain. This is due to the faster eddy mixing in the top left corner near the curved side.

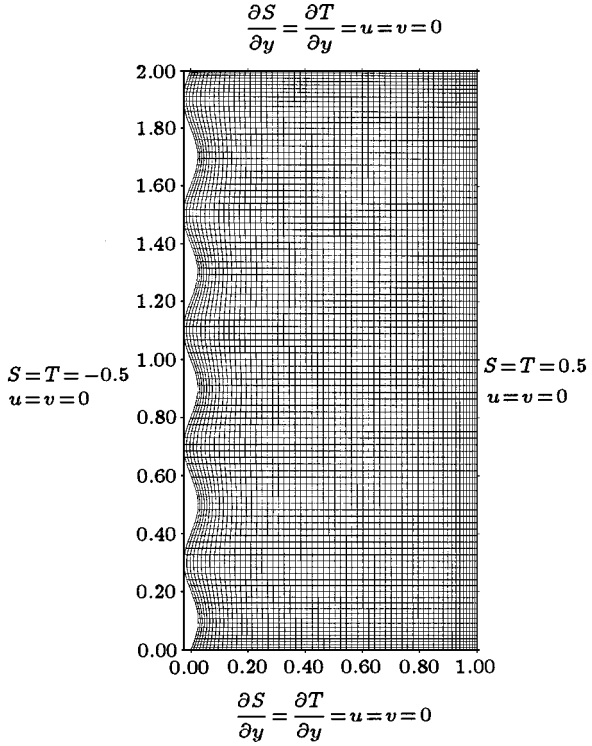
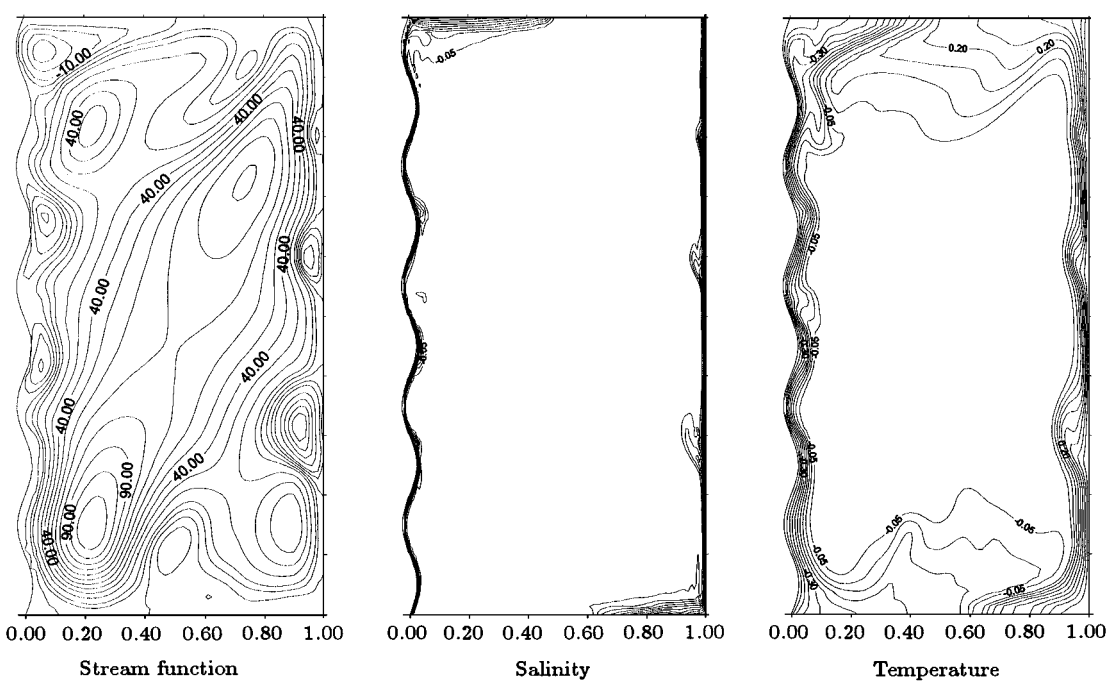
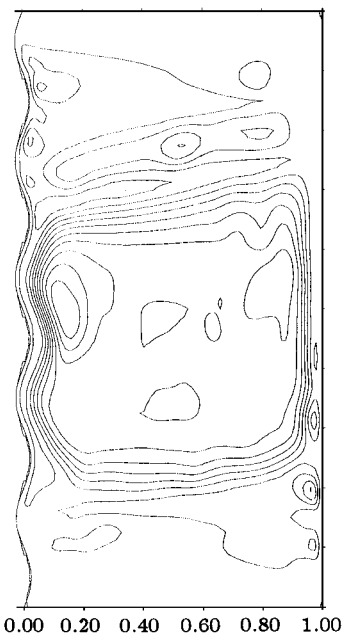


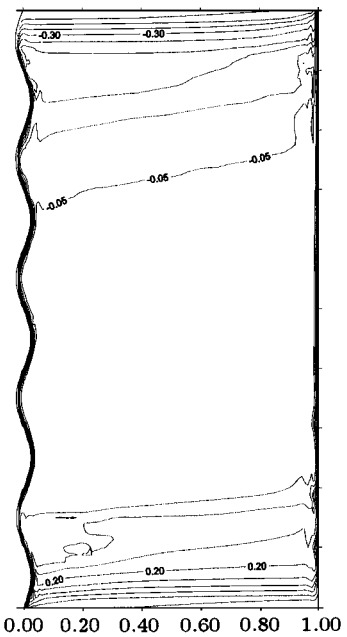
Fig.3. A boundary-fitted coordinate system of a cavity with a sine-curve side.



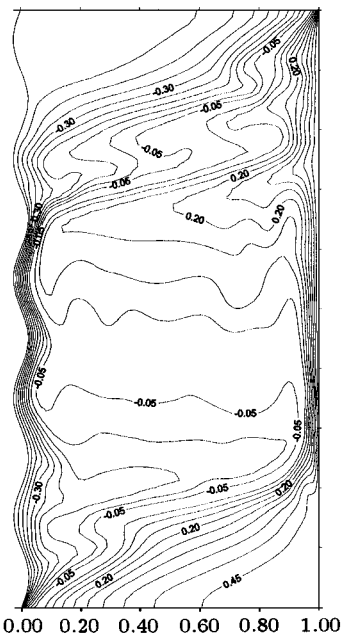
(a) t=0.004



Stream function

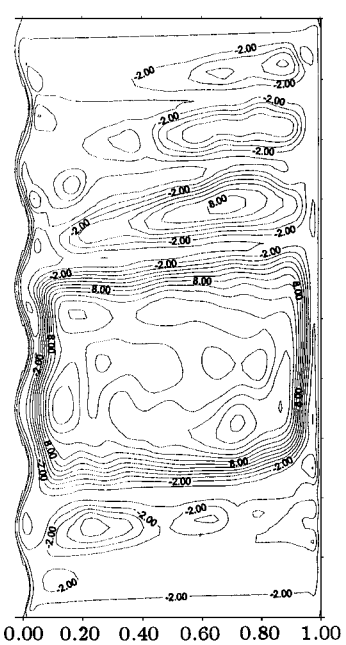


Salinity

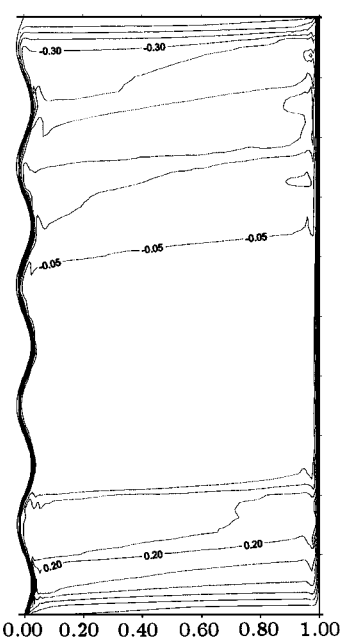


Temperature

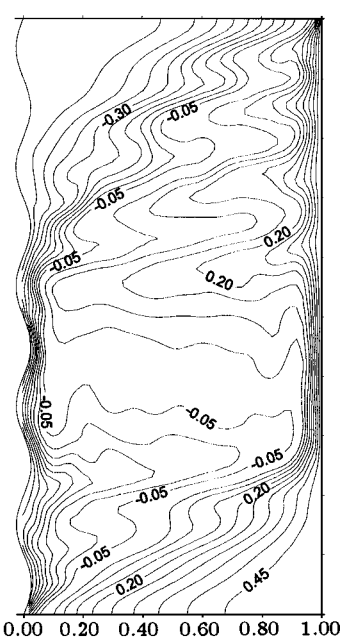
(b) t=0.05



Stream function



Salinity



Temperature

(c) t=0.1

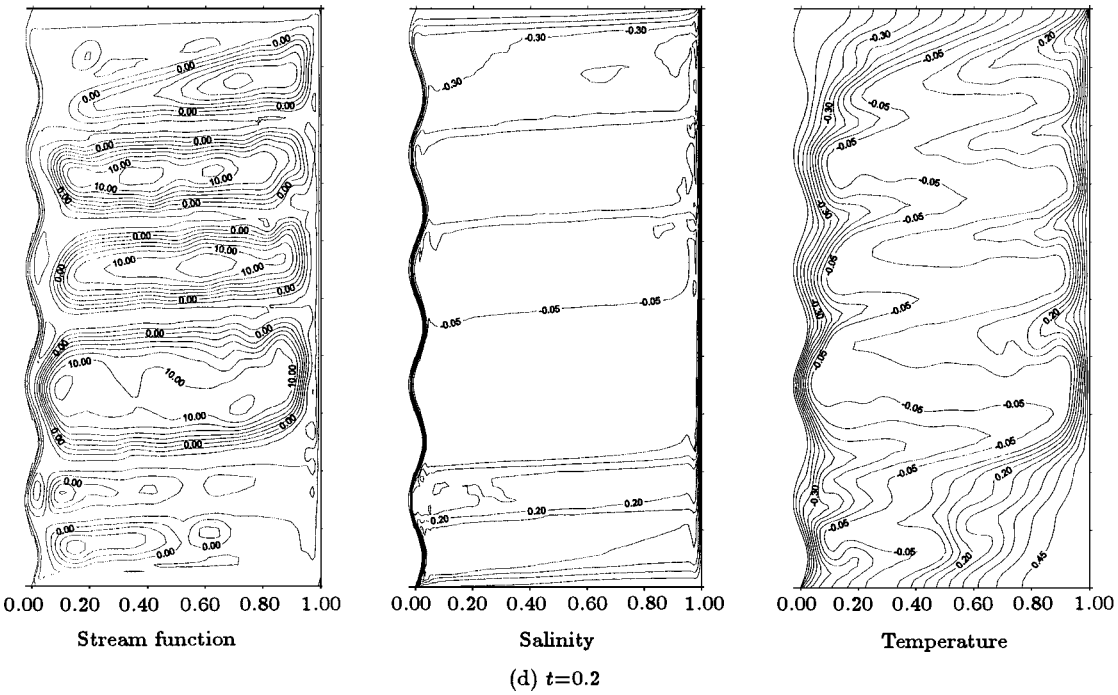


Fig.4. Time evolving plots of stream function, isotherms and isohalines.

5. Conclusions

A high-order accurate difference scheme coupled with boundary-fitted coordinates for solving double-diffusive convection problems is proposed in this paper. The method is shown to be a good candidate for direct simulations of double-diffusive convection flows. The proposed method has been verified by applying it to two test cases. Numerical results for the symmetry breaking and overturning states in the thermohaline-driven flows in a 2D trapezoid basin are qualitatively in agreement with those obtained in Refs.[11] and [16]. Double-diffusive convection in a non-rectangular cavity with opposing horizontal temperature and concentration gradients at large values of the thermal, solutal Rayleigh numbers and Lewis number are also in qualitative agreement with those in Ref.[18] in a rectangular cavity, but more detailed information is obtained near the wall. Because of the use of boundary-fitted coordinates, the method can also be applied to flow problems involving complex geometries.

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