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ORIGINAL RESEARCH PAPER

Numerical Simulation and Parametric Reduced Order Modeling of the Natural Convection of Water-Copper Nanofluid

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ABSTRACT: In this article, a coupled computational framework is presented for the numerical simulation of mass transfer under the effects of natural convection phenomena in a field contains water-copper Nano-fluid. This CFD model is build up based on accurate algorithms for spatial derivatives and time integration. The spatial derivatives have been calculated using first order upwind and second order central differencing approaches. Also, time integration is performed using the fourth order Runge-Kutta method. A parametric reduced order model is developed to compute the whole flow field under the effects of some important parameters. This model is constructed using POD-snapshots method based on Karhunen-Loeve decomposition. The POD modes have been calculated based on the solution of an eigenvalues problem. The obtained eigenfunctions are POD modes which are arranged using energy-based criteria based on total kinetic energy of the flow field. This approach leads to the model order reduction procedure, and the outcome model can be used as a surrogate model of CFD high order model. The results obtained from the reduced order model show close agreements to the benchmark DNS data and proving high accuracy of the proposed model.

KEYWORDS: *Computational Fluid Dynamics; Model Order Reduction; Nano-fluid; Natural Convection*

INTRODUCTION

Analysis, simulation and experimental investigation of natural convection in enclosures filled with Nanofluids have been studied extensively for various geometries and problem statements in the last few years. The heat transfer enhancement in a differentially heated enclosure based on variable thermal conductivity and variable viscosity of Al_2O_3–water and CuO–water Nanofluids are investigated by Abu-Nada et al.[1].

Numerical methods are the most favorable engineering approach for studying of the Nanofluid flows. Bahiraei reviewed and summarized the numerical investigations implemented on nanofluids including conventional and novel methods[2].

Yanwei Hu et al. studied the coefficient of thermal conductivity and viscosity of Al_2O_3–water Nanofluid, and its heat transfer using the experimental approach in a square enclosure. Also, they have been used a 2D two-phase Lattice Boltzmann model considering interaction forces between Nano-particles and base fluid for natural convection of Nanofluid[3]. Bouhalleb and Abbasi investigated heat transfer, and fluid flow of natural convection in an inclined cavity filled with CuO-water Nanofluid heated from one side and cooled from the ceiling[4].

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Bishwajit Sharma et al. studied laminar flow heat transfer of Cu-water Nanofluid inside a square cavity using the numerical approach. The cavity is heated by different length heaters with isothermal boundary condition placed symmetrically on two adjacent sides[5]. Riahi and his colleagues investigated the fluid flow structures and heat transfer rates in a rectangular enclosure of aspect ratio of two containing two heated cylindrical blocks and filled with various water-based Nanofluids [6].

The reduced order models (ROMs) have prepared new bases for fast computation of engineering and science problems. The ROMs are divided into two primary forms, one is based on estimation and approximation frameworks which are called parametric reduced order models. Another kind of the ROMs have been obtained from the conservation laws, and are called reduced order dynamical systems.

These have prepared an adequate base for coupling different dynamical systems and have helped the researchers and engineers to test and validate their new ideas and theories. The POD approximations contain two types of errors, one from the projection and the second due to the modeling and the integration.

The first type of error, refers to the projection procedure, for example, the snapshots resolution. The second type of error is due to some reduced order model construction assumption.

Nomenclature

a	Modal coefficient	β	Thermal expansion coefficient
g	gravitational acceleration	κ	fraction number
P	pressure	λ	eigenvalue
Pr	Prandtl number	μ	viscosity
Ra	Rayleigh number	φ	POD modes
Re	Reynolds number	Φ	coherent structures eigenfunction
Ri	Richardson number	ϕ	density ration
t	time	Ψ	streamfunction
T	temperature	Ω	vorticity
$\boldsymbol{u}$	velocity vector		**Subscripts**
u	x-velocity component	f	fluid
v	y-velocity component	n	time step
x	coordinate along horizontal axis	nf	Nano fluid
y	coordinate along vertical axis	p	particle
	Greek symbol	r	reduced number
α	Thermal diffusion coefficient		

The preliminary application of POD was proposed by Lumley for extracting large scale structures of turbulent flows [7]. Lucia was presented a historical review of POD [8].

Analysis of statistical data using POD was performed firstly by Karhunen and Loeve [8]. Smith developed a reduced order model for simulation of turbulent flow using POD [10].

Sirovich proposed the method of snapshots and this caused that the POD presented as a useful tool to develop reduced order models of complex dynamical systems having some data from experimental tests or direct numerical simulation [11]. One of the most important properties of POD is the ability of the method in extracting high-level energy modes.

Therefore this method can be used for fluid and structure interactions and flow control problems [12].

Ravindran used POD low order model for optimal control of fluid flow past a backward step. The ability of the low dimensional dynamical system in the flow control applications have been shown on a recirculation control problem using blowing on the channel boundaries [13]. Atwell proposed POD based reduced order model for control of Burgers' equation with periodic boundary conditions and Non-linear observers. This controller is designed using the MinMax approach [14].

POD was also used in database generation of F16 aeroelasticity in various Mach numbers and angle of attacks[15].

Modeling the turbulent velocity structures of an open channel flow problem, reduce order modeling of the supersonic developed compressible and transonic flow around an airfoil for studying the small deformations of the airfoil is also part of the applications of this approach [15-21].

A finite volume based reduced order model has been reconstructed for two-dimensional viscoelastic equations. The model used a fully discrete finite volume element algorithm with fewer degrees of freedom and sufficiently high accuracy based on the POD method[22].

Chen used proper orthogonal decomposition (POD) to establish a reduced-order model of viscoelastic turbulent channel flow[23].

A coupled approach of the SVD method and POD technique has been used to establish a reduced order finite difference extrapolation algorithm for the solution of non-stationary Navier-Stokes equations[24]. A POD-based reduced order stabilized mixed finite volume element (SM-FVE) extrapolating model has been established with very few degrees of freedom for the non-stationary incompressible Boussinesq equations[25].

In the sequel, the mathematical formulation of the modified version of the Navier-Stokes equations for simulation of Nanofluid in vorticity-streamfunction form is presented.

In the next section, the computational approach for the spatial and temporal terms will be explained.

Also, the basic theory of the POD method and the reduced order framework for computation of fluid flow and thermal field is introduced. So, the order reduction manner and the outcomes of this research will be presented in the next sections.

GOVERNING EQUATIONS

The governing equations of fluid flow contain continuity and linear momentum equations with a term due to the effects of temperature gradients (Boussinesq approximation) as follow[1]:

$$\begin{aligned}
&\nabla.\mathbf{u} = 0\\
&\frac{\partial \mathrm{u}}{\partial t} + (\mathbf{u}.\nabla)\mathrm{u} = -\frac{1}{\rho_{\mathrm{nf}}}\frac{\partial \mathrm{p}}{\partial \mathrm{x}} + \frac{1}{\rho_{\mathrm{nf}}}(\mu_{\mathrm{nf}}\nabla^2\mathrm{u})\\
&\frac{\partial \mathrm{v}}{\partial t} + (\mathbf{u}.\nabla)\mathrm{v} = -\frac{1}{\rho_{\mathrm{nf}}}\frac{\partial \mathrm{p}}{\partial \mathrm{y}} + \frac{1}{\rho_{\mathrm{nf}}}(\mu_{\mathrm{nf}}\nabla^2\mathrm{v}) + \beta_{\mathrm{nf}} \times \\
&\mathrm{g}\left(\widetilde{\mathrm{T}} - \widetilde{\mathrm{T}}_{\mathrm{c}}\right)
\end{aligned} \tag{1}$$

The continuity and momentum equations can be expressed in vorticity-stream function form:

$$\nabla^2\Psi = -\Omega,$$
$$\frac{\partial\Omega}{\partial t} + (\mathbf{u}.\nabla)\Omega = \mathrm{Pr}\times\frac{\rho_f}{\rho_{nf}}\nabla^2\Omega + \mathrm{Pr} \times \mathrm{Ra}\left(\left(\frac{\beta_p}{\beta_f}\right)\phi + (1-\phi)\right)\times\left(\frac{\partial T}{\partial x}\right) \quad (2)$$

Where, Re is Reynolds number, Pr is Prandtl number, and Ra is Rayleigh number. Thermal expansion coefficient and density of Nanofluid is calculating by the following equation:

$$\beta_{nf} = (1-\phi)\beta_f + \phi\beta_p$$
$$\rho_{nf} = (1-\phi)\rho_f + \phi\rho_p \quad (3)$$

The energy transport equation of flow in non-dimensional form is as:

$$\frac{\partial T}{\partial t} + (\mathbf{u}.\nabla)T = \frac{\alpha_{nf}}{\alpha_f}\nabla^2 T \quad (4)$$

Reynolds number has a relationship with Rayleigh, Prandtl and Richardson numbers. The Reynolds number and the heat diffusivity coefficient of Nanofluid are calculated as follows:

$$Re = \sqrt{\frac{Ra}{Ri\times Pr}} \quad (5)$$

$$\alpha_{nf} = (1-\phi)\alpha_f + \phi\alpha_p \quad (6)$$

COMPUTATIONAL APPROACH

The governing equations are discretized in both time and space and then used a time-marching approach for the solution of them (except for the stream-function equation). For the stream-function equation used a conventional iterative solution method for elliptic equations (Such as SOR algorithm in explicit or implicit form).

Spatial discretization

For spatial discretization of convective terms of vorticity transport, energy and mass transfer (contaminant concentration) equations used an upwind Riemann variable method based on the sign of velocity vector, as:

$$uu_x = a^+_{i,j}u^-_x + a^-_{i,j}u^+_x$$
$$u^+_x = \frac{u_{i+1,j}-u_{i,j}}{\Delta x}$$
$$a^+_{i,j} = \max(u_{i,j},0)$$
$$u^-_x = \frac{u_{i,j}-u_{i-1,j}}{\Delta x}$$
$$a^-_{i,j} = \min(u_{i,j},0) \quad (7)$$

The central difference formulation for interior nodes of computational domain is as follows:

$$\frac{\partial F}{\partial x} = \frac{F_{i+1,j}-F_{i-1,j}}{2\Delta x} \quad (8)$$

for the points on the boundaries a forward or backward second-order differential formula is used as follows:

$$\frac{\partial F}{\partial x} = \frac{-3F_{i,j}+4F_{i+1,j}-F_{i+2,j}}{2\Delta x}$$
$$\frac{\partial F}{\partial x} = \frac{3F_{i,j}-4F_{i-1,j}+F_{i-2,j}}{2\Delta x} \quad (9)$$

Diffusion terms have been discretized using second-order finite difference method, as:

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{i+1,j}-2u_{i,j}+u_{i-1,j}}{\Delta x^2} \quad (10)$$

Time integration

Time discretization of transport equations is performed using fourth order Explicit Runge-Kutta method. This method is a convenient and accurate way for time integration of governing equations of unsteady problems[26].

Proper orthogonal decomposition

The Reduced-order model based on POD builds up by calculation of the empirical eigenfunctions using the Karhunen-Loève decomposition. Then the flow variables are approximated using expansions of these eigenmodes. POD is a powerful method in the selection of basis functions which are not just appropriate but are optimal in the analysis section. POD was firstly introduced for calculation of the turbulence coherent structure by Lumley in 1967. Before that, this method was already used in statistics as the Karhunen-Loève expansion. Lumley suggested that some functions of the spatial variables are available that have maximum energy content and can be used to identify the coherent structures. These structures are defined as a linear combinations of Φ 's, which maximize the following expression:

$$\max\frac{\langle(\Phi,u)^2\rangle}{\langle\Phi,\Phi\rangle} \quad (11)$$

where, (Φ,u) is the inner product of the basis vector Φ with the field, u. Note $\langle\rangle$ is the time-averaging operation. It can be shown that the POD basis vectors are eigenfunctions of the Kernel k given by:

$$K = \langle(u,u')^2\rangle \quad (12)$$

where u'denotes the Hermitian of u.This equation is converted to the Fredholm's second kind integral equation,

and its discretization leads to an eigenvalue problem. In this work, the SVD method has been used to solve this eigenvalue problem [4]. If equation (11) was maximized, the projected field along with φ(x), has a larger amount average energy than any other reconstructions along with other basic functions. POD eigenfunctions are defined as eigenvectors of space correlation tensor. Approximation of this tensor is very difficult. But using the POD snapshot method which needs an ensemble of fluctuations, $u_n(x)$, with N members in different time or other variable steps, can be obtained from CFD simulations or experimental tests as follow:

$$u_n(x) = u(x, t^n) \tag{13}$$

t^n is a variable which can belong to parameters of time or any effective parameters. By using flow field modes, it can be reconstructed by the following expression:

$$u(x,t) = \rangle\ a^k(t)\varphi^k(x) \tag{14}$$

Combined POD-snapshot method with inter polation

Generally, on a POD solution, changes of the flow field, in the form of a matrix of numerical data in different some important parameters, separately, are considered as initial data. This process can also be used for other optional parameters. Assumed, this parameter can be arbitrary parameter δ such as Rayleigh number, density ratio, or etc. To predict the flow field for each value of δ, should precede a set of numerical data of the flow field for different values of δ, which is arranged, intentionally. Then an eigenvalue problem has to solve. φ^k, are eigenvalues of the flow field. For reconstructing of the flow field for the desired values of δ, the modal coefficients (a^k) have to interpolate. The flow field is reconstructed by equation14 [20]. Given a tabulated function $y_i = y(x_i)$, $i = 1...N$, focus attention on one particular interval, between x_j and x_{j+1}. Linear interpolation in that interval gives the interpolation formula:

$$\begin{aligned} y &= Ay_j + By_{j-1} \\ A &= \frac{x_{j+1} - x}{x_{j+1} - x_j} \\ B &= \frac{x_j - x}{x_{j+1} - x_j} \end{aligned} \tag{15}$$

Equation 15 is a special case of the general Lagrange interpolation formula since equation. Since it is (piecewise) linear, equation 15 has zero second derivative in the interior of each interval, and an undefined, or infinite, second derivative at the abscissas x_j.

The goal of cubic spline interpolation is to get an interpolation formula that is smooth in the first derivative, and continuous in the second derivative, both within an interval and at its boundaries.

Order reduction criterion

Normally, when the number of modes is increased, the reconstruction is performed with better accuracy. It is required to use the optimal number of modes for data reconstruction. This is equivalent to capturing the highest level of energy and the least number of modes for model construction (Fig. 5). In this manner, a fraction number is defined for automatic selection of modes as follow:

$$\kappa = \frac{\sum_{i=1}^{N_r} \lambda_i}{\sum_{i=1}^{N} \lambda_i} \tag{16}$$

where κ is about 99.9%, and N_r is the optimum number of modes for reduced order model construction [20].

Problem statement and boundary conditions

The problem which has been studied in this research is a square cavity with heated and cooled walls at the left and right sides. At the upper and lower boundaries of this control volume used adiabatic wall boundary condition. At all sides of the cavity used no slip boundary condition for velocity. This field contains water-copper Nano-fluid and the developed computer code can be applied a different percentage of Nano particles to the primary fluid. Figure 1 shows the geometry configuration of the considered control volume and the appropriate boundary conditions. A structured form mesh is used as the required grid points for the numerical solution of the flow field. The grid points are refined near to the wall faces, and it tried to maintain the quality of the mesh at the domain interior.

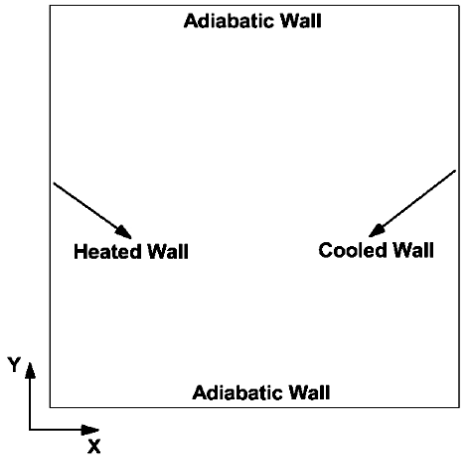


Fig. 1. Geometry of and related boundary conditions of the square cavity test case

RESULTS AND DISCUSSION

In this section, the results of the paper will be presented and discussed them. The selected problems are two test cases, in the first problem flow field simulation in the field contains Nano-fluid of Water Copper under the effects of natural convection without mass transfer has been

considered. The next section is about the outcomes of the reduced order model of this problem. The results of the surrogate model have been compared with the direct simulation data.

Direct numerical simulation

For verification of the accuracy of developed code, the obtained results compared with suitable benchmark data.

In Figure 2, distribution of normalized temperature along the horizontal line at the mid height of the cavity. It is clear that the obtained results of the present computer code have good accuracy compared to related benchmark experimental and other numerical results.

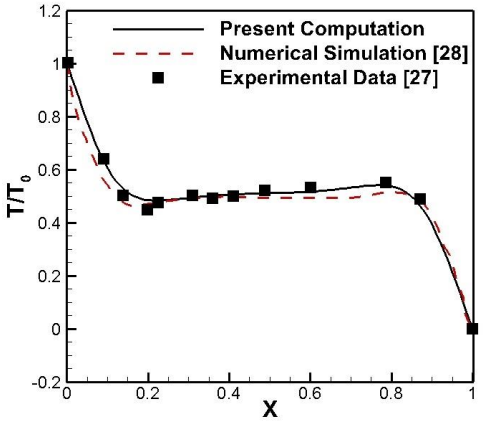
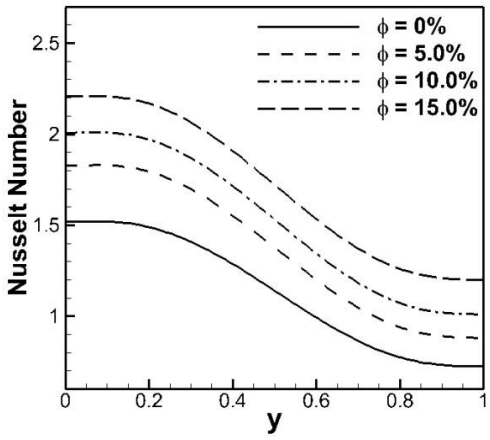
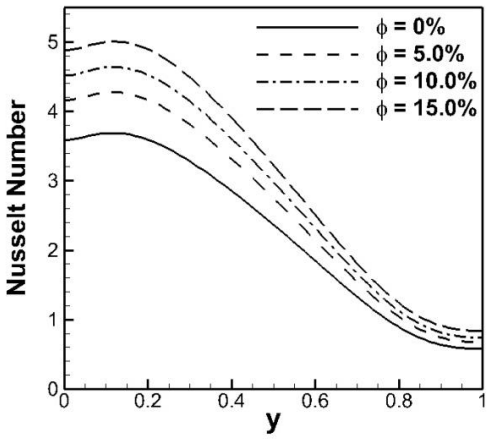


Fig. 2. Comparison of temperature distribution along horizontal line at vertical centerline of Cavity, $Ra=10^5$, Pr = 0.7

Figure 3 shows the distribution of local Nusselt number along the vertical centerline of the cavity at a fixed Reynolds number and for two different Rayleigh numbers. Both parts of this figure are illustrating the distribution of Nusselt number for different values of density ratio of Nano particles.



(a)



(b)

Fig. 3. Distribution of local Nusselt number along the vertical centerline of the Cavity at Pr = 7. 2 and $Ra=10^3$(Left) and $Ra=10^4$(Right) for different density rate of Nano Particles

It is concluded that by increasing the density ratio, the maximum value of the local Nusselt number is increased near to top wall which shows that the heat transfer is enhanced in different layers of the flow.

Also by increasing Rayleigh number the value of local Nusselt number is increased and by reducing the height and near to bottom wall the gradient of Nusselt number is reduced in contrast to the similar values near to the top wall.

Reduced order modelling of flow and thermal fields

In this section, the results obtained from the reduced order model are presented. The ROM is reconstructed using three modes.

In this section flow field and mass transfer in a domain contains Nano-fluid of Water Copper and a heated horizontal surface will be discussed.

In Table 1, the level (percentage) of the kinetic energy (in the dimensionless form) of the first four strongest modes of the x-velocity component and total energy for adding each new mode are shown.

Table 1
Relative Energy Level of the x-velocity Component at Rayleigh Number of 103.

Mode Number	1	2	3	4
Energy Value	99.11%	0.68%	0.17%	0.02%
Total Energy	99.11%	99.79%	99.96%	99.98%

As it is clear, only the first two modes capture more than 99% of the kinetic energy of the entire energy of the system, while the remaining two modes only change about 1% of the total energy.

Figure 4 shows the first three highest energy level modes of x-velocity, y-velocity, and temperature for the natural convection of water-copper Nanofluid field at Rayleigh number of 1000.

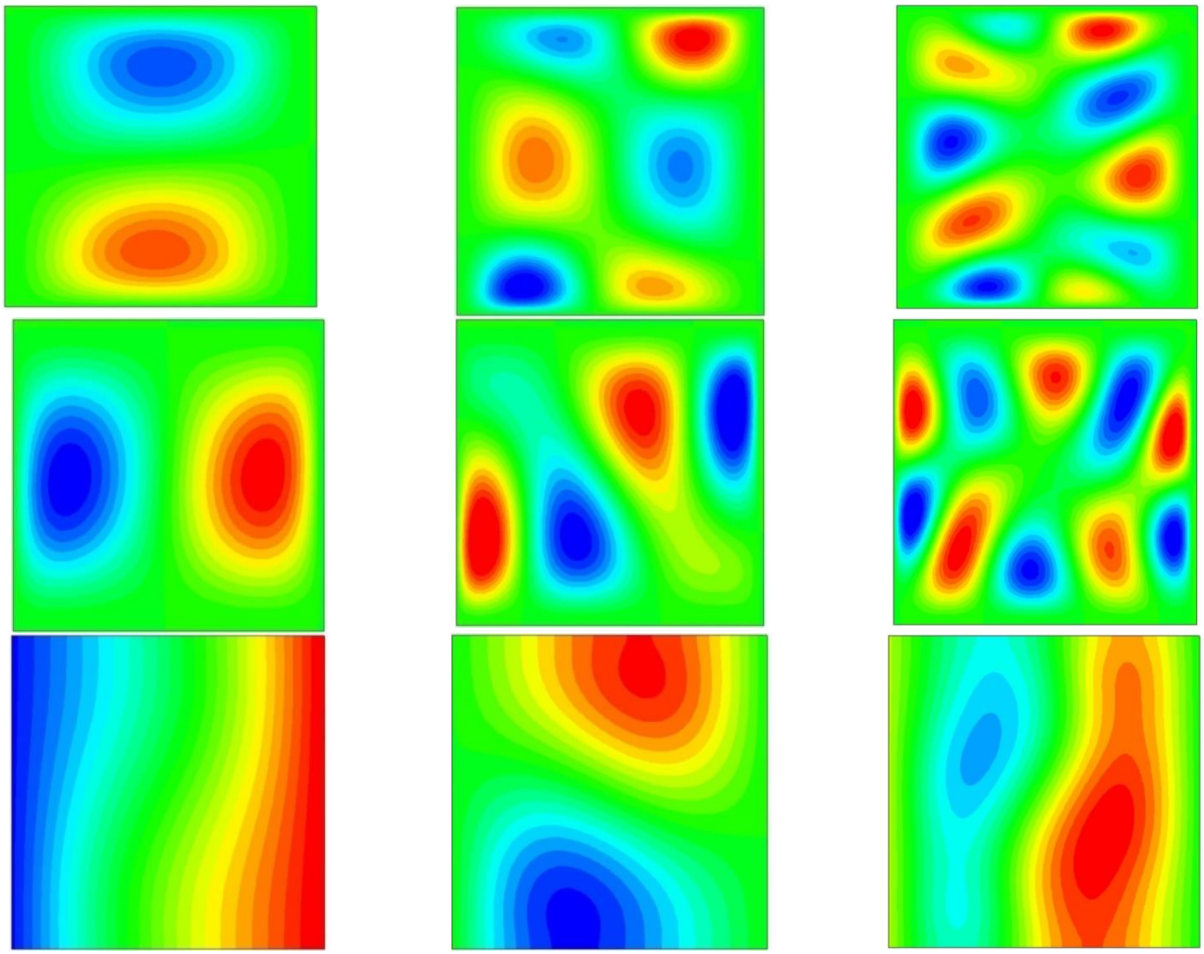


Fig. 4. Distribution of first three strongest modes of x-component velocity (top), y-component velocity (middle) and temperature (bottom) for natural convection of water-copper Nanofluid field at Rayleigh number of 10^3

Figure 5 shows the distribution of eigenvalues and relative energy of POD modes versus their number for the natural convection Nanofluid flow at Rayleigh Number of 10^3.

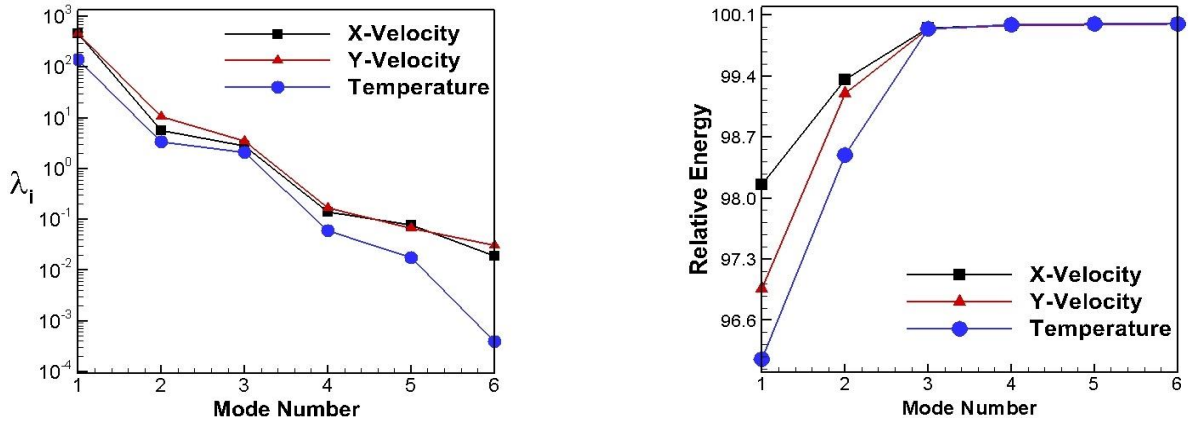


Fig. 5. Distribution of eigenvalues (left) and relative energy (right) versus mode number for natural convection Nanofluid flow at Rayleigh Number of 10^3

From these Figures, a similar trend related to Table 1 which is explained about the impact level of each mode of velocity components and temperature, can be found. Similar to the previous table, in Table 2, the level (percentage) of the kinetic energy of the first four strongest modes of the temperature and total energy for adding each new mode are demonstrated. It is clear, only the first two modes capture more than 98% of the total kinetic energy of the system, while the other two modes only contain approximately 2% of the total energy.

Table2
Percentage of Relative Energy Level of Temperature at Rayleigh Number of 10^4.

Mode Number	1	2	3	4
Energy Value	79.2%	18.6%	1.91%	0.23%
Total Energy	79.2%	97.8%	99.71%	99.94%

In Figure 6 distribution of local Nusselt number along the heated wall, which is reconstructed using CFD model and reduced order POD model, for different values of density ratio of Nanoparticles is illustrated. It is evident from this figure that the reduced order model predicts relatively accurate results.

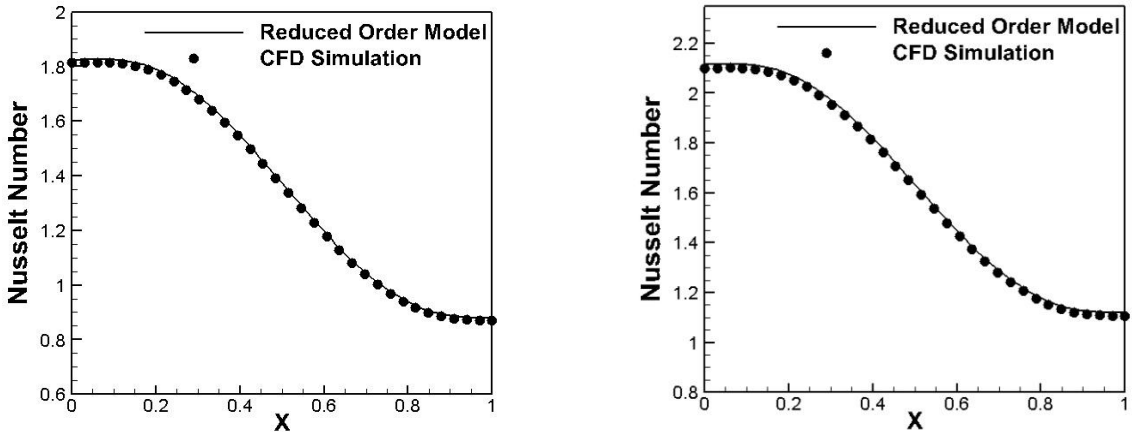


Fig. 6. Comparison between the distribution of local Nusselt number along the heated wall(left face) for density ratio of 0.065(left) and 1.35(right) at Rayleigh number of 10^3, POD reduced order model(solid Line) and CFD data (Points)

In Table 3, a comparison between the total computational time of CFD simulation and the reduced-order model, which is presented in this study, has been shown. These data show that the cost of computation using reduced-order model is very less than the CFD simulation method. But the accuracy of the results obtained from ROM is very good compared to the CFD data.

Table3
Comparison between Computational Time of CFD Simulation and Reduced Order Model.

Model	**Time(Second)**	**Total Time(Second)**
CFD	200	450
POD Modes Computation	15	35
POD Modes Selection	5	
Estimation of Flow Field in New Statement	15	

In Figure **7** distribution of the first three highest energy level modes of x-velocity, y-velocity and temperature for the natural convection of water-copper Nanofluid field at Rayleigh number of 10^4, is illustrated.

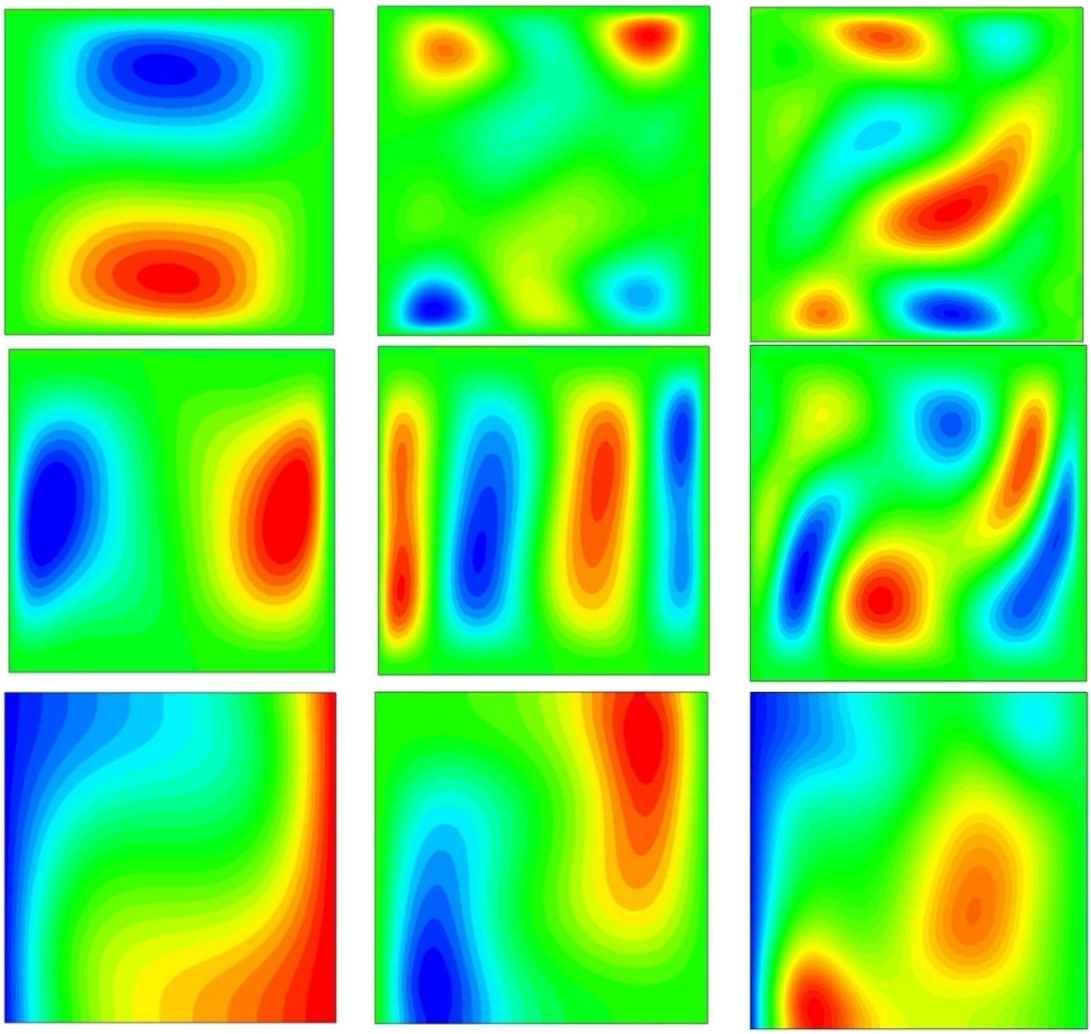


Fig. 7. Distribution of first three strongest modes of x-component velocity (top), y-component velocity (middle) and temperature (bottom) for natural convection of water-copper Nanofluid field at Rayleigh number of 10^4

Figure 8 shows the distribution of eigenvalues and relative energy of POD modes versus their number for the natural convection Nanofluid flow at Rayleigh Number of 10^4.

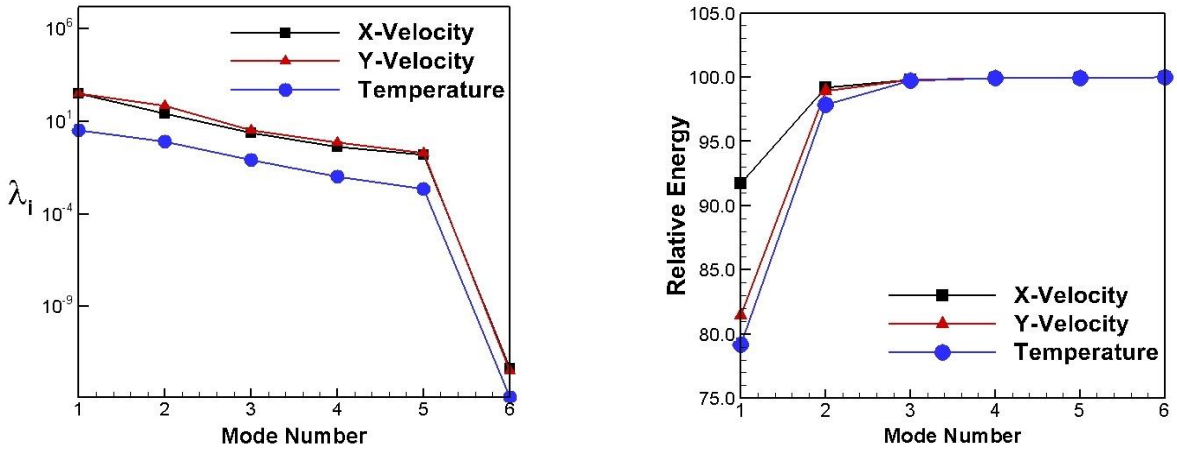


Fig. 8. Distribution of eigenvalues (left) and relative energy (right) versus mode number for natural convection Nanofluid flow at Rayleigh Number of 10^4

It is obvious that the first mode of both velocity components and temperature are very similar to the related field. This is related to the main concept which is shown in Figure 8, that the first mode of these variables is the most energetic and important feature. Therefore it can be formed as the original related flow field.

Figure 9 shows the distribution of local Nusselt number along heated wall computed using CFD model compared to the similar results from the reduced order POD model. The left Figure is for density ratio of Nanoparticles equal to 0.035 while the right figure plot for density ration of 1.35. Both values mentioned in these results are not available in the primary snapshots of the flow field. It is obvious from these Figures that the reduced order model predicts relatively accurate results.

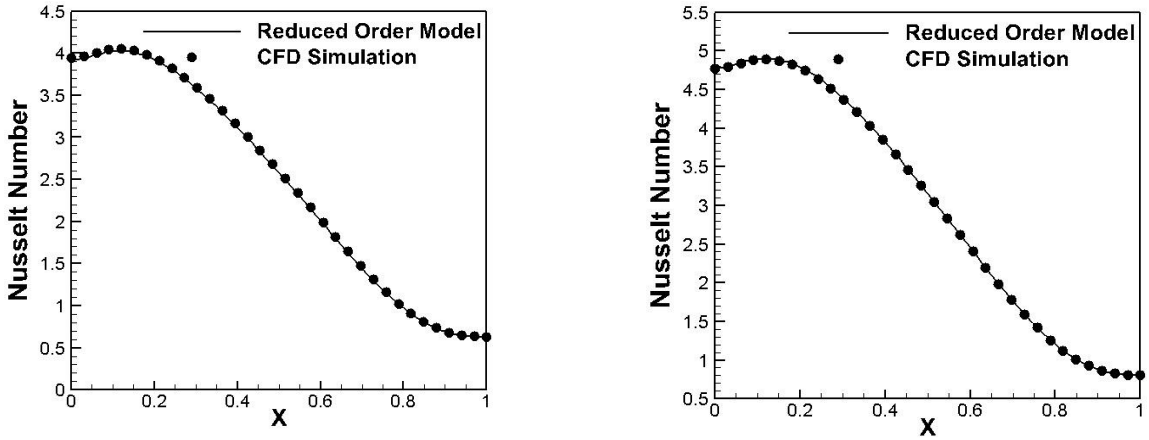


Fig. 9. Comparison between the distribution of local Nusselt number along the heated wall(left face) for density ratio of 0.035(left) and 1.35(right) at Rayleigh number of 10^4, POD reduced order model(solid Line) and CFD data (Points)

CONCLUSIONS

In recent years, considerable improvement has been made in advancing the state-of-the-art numerical simulation of Nano-fluid flow. Some of these researches for simulation and parametric studying of Nanofluid flow especially contains natural convection are discussed in the literature. To this effect, in this paper, the direct numerical simulation framework for the solution of the fluid flow and thermal field contains cu-water Nanofluid has been developed. On the other hand, this paper contributes a new extension of POD-based reduced order model for prediction of the mentioned flow field and demonstrates its suitability due to the variations of some effective parameters. In this work, a POD snapshots method was used for calculation of the POD modes. An order-reduction manner was used to choose the minimum number of modes for the reconstruction of the reduced order framework which is used for the fast prediction of the flow field. The outcomes show that the parametric reduced order model has relatively good accuracy compared to the results obtained from the direct numerical simulation.

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