METHODOLOGY

For the purpose of our study, we will assume that the fluid flow round the nanoparticles and the fluid flow along tube can be regarded as a continuum. To assess the plausibility of this assumption, we need to calculate the Knudsen number which is defined as the ratio of the water molecule mean free path to the nanoparticle diameter (Buongiorno, 2006):

$$Kn = \frac{\lambda}{d_p} \tag{23}$$

1. Knudsen number

1.1 Knudsen number (Particle)

This dimensionless number is used to indicate how far a system (including the particles) deviates from a continuous system. When this value is less than 0.1 (larger particles), the flow is in the continuum regime and one set of equations are used to obtain velocity. When the Knudsen number is between 0.1 and 1 (smaller particles), the flow is considered to be in the slip flow regime and a correction to the equations for the continuum regime is used when calculating velocity. With slip flow, the particle appears to "slip through" the molecules.

The water molecule's effective size and mean free path in liquid water are both of the order of 3 Å (0.3 nm). Therefore, for the nanoparticle range of interest 1-100 nm, the Knudsen number is relatively $Kn < 0.3$ and the continuum assumption is reasonable.

1.2 Knudsen number (Tube)

The Knudsen number for tube is defined as the ratio of the water molecule mean free path to the tube diameter (Kandlikar *et al*., 2006):

$$Kn = \frac{\lambda}{D} \tag{24}$$

For $Kn < 10^{-3}$, the flow is continuum flow and it is accurately modeled by the compressible flow Navier-Stokes equations with classical no-slip boundary condition.

For $10^{-3} < Kn < 10^{-1}$, the flow is a slip flow and the Navier-Stokes equations remain applicable, provided a velocity slip and a temperature jump are taken into account at the wall. These new boundary conditions indicate that rarefaction effects become sensitive at the wall first.

For $10^{-1} < Kn < 10$, the flow is a transition flow and the continuum approach of the Navier-Stokes equations is no longer valid. However, the intermolecular collisions are not yet negligible and should be taken into account.

For $Kn > 10$, the flow is a free molecular flow and the occurrence of intermolecular collisions is negligible compared with the collisions between the gas molecules and the wall.

In our tests, the water molecule effective size and mean free path in liquid water are both of the order of 3 Å (0.3 nm). Therefore, our tube interest has diameter 1 cm, the Knudsen number is relatively $Kn < 3 \times 10^{-8}$ and the continuum assumption is reasonable.

2. Modified thermal conductivity models for nanofluids

In this research, we modified 2 thermal conductivity models of nanofluids in order to find a suitable model. The 2 modifid models for nanofluids are a modified dynamic model and a modified stationary model including effect of the temperature-dependent interfacial layer (Present model).

2.1 The Leong et al.'s stationary model including effect of the interfacial layer

The interfacial layer has different thermo-physical properties from bulk liquid and solid particles. Hence, it is important to consider the interfacial layer as a separate component in the solid (particle)-liquid mixture in order to determine its effect on the mixture (nanofluids). A sketch of a single particle with an interfacial layer in a liquid medium is shown in Figure 1.

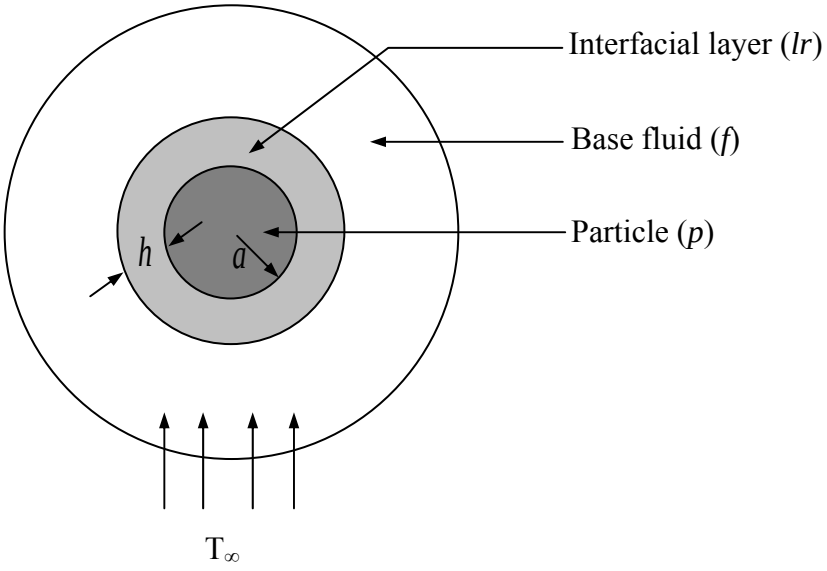


Figure 1 Single spherical particle with an interfacial layer in a liquid medium
Source: Leong *et al*. (2006)

The Leong et al.'s model for the effective thermal conductivity of nanofluids can be written as follows:

$$k_{eff} = k_{static} = \frac{\left(k_p - k_{lr}\right)\phi k_{lr}\left[2\beta_1^3 - \beta^3 + 1\right] + \left(k_p + 2k_{lr}\right)\beta_1^3\left[\phi\beta^3\left(k_{lr} - k_f\right) + k_f\right]}{\beta_1^3\left(k_p + 2k_{lr}\right) - \left(k_p - k_{lr}\right)\phi\left[\beta_1^3 + \beta^3 - 1\right]} \quad (25)$$

where $\beta = 1 + \gamma$, $\beta_1 = 1 + \frac{\gamma}{2}$ are the functions in the Leong et al.'s model. The thickness and the thermal conductivity of the interfacial layer in Leong et al.'s model are assumed to be 1 nm and 1-5 times the based fluid, respectively.

1.2 The modified dynamic model based on the Leong et al.'s stationary model

The effective thermal conductivity of the dynamic model for nanofluids can be generally written as

$$k_{eff} = k_{static} + k_V \quad (26)$$

where the static part k_{static} of the modified dynamic model is from Leong et al.'s stationary model (Eq.25) and the dynamic part k_V is modified from Khanafer et al.'s model (2003) and Koo and Kleinstreuer's model (2004) as follows:

$$k_v = C\left(\rho c\right)_{nf}\left|\bar{V}\right|\phi d_p \quad (27)$$

where $\left|\bar{V}\right| = \sqrt{\frac{18k_bT}{\pi\rho_p d_p^3}}$ for the non-flowing fluid (Koo and Kleinstreuer, 2004) and $\left|\bar{V}\right| = \sqrt{u^2 + v^2 + w^2}$ for the flowing fluid (Amiri and Vafai, 1994; Khanafer et al., 2003). The C is an unknown parameter which can be determined by calibrating with the experimental data (Das *et al*., 2003; Chon *et al*., 2005). Also, the parameter *C* combines the probability for a particle to travel along any direction with the function of temperature and volume fraction. The parameter *C* is given in this work as:

$$C = \frac{0.1}{(\phi + 0.04)}(T - 298) \qquad \text{For } Al_2O_3 \text{ / Water}$$

$$C = \frac{0.1}{(\phi + 0.001)}(T - 298) \qquad \text{For CuO / Water}$$

It should be noted that the experiments on thermal conductivity were mostly done at room temperature, assumed to be 298 K. The stationary model was originally developed using data collected at room temperature. Thus when combining the effect of Brownian motion of nanoparticles with the stationary model, 298 K is deleted from the function of temperature because the stationary model is able to predict the effective thermal conductivity satisfactory at room temperature.

The modified dynamic model can be written using Eqs. (25-27) as:

$$k_{eff} = \frac{(k_p - k_{lr})\phi k_{lr}\left[2\beta_1^3 - \beta^3 + 1\right] + (k_p + 2k_{lr})\beta_1^3\left[\phi\beta^3(k_{lr} - k_f) + k_f\right]}{\beta_1^3(k_p + 2k_{lr}) - (k_p - k_{lr})\phi\left[\beta_1^3 + \beta^3 - 1\right]} + C(\rho c)_{nf}\left|\bar{V}\right|\phi d_p \quad (28)$$

2.3 The present model including effect of the temperature dependent-interfacial layer

The value of the interfacial layer thickness is negligibly small on a macroscopic scale. However, on the scale of a nanoparticle, the interfacial layer thickness can play an important role in the thermal conductivity of nanofluids. Moreover, the value of the interfacial layer thickness depends on temperature (Eastman *et al*., 2004).

The Leong et al.'s model has already included the interfacial layer effect in their model. However, their model cannot predict the dependence of the thermal conductivity of nanofluids on temperature. In this section, the thermal conductivity model by Leong et al. is modified to include the effects of the temperature and the nanoparticle size variations on the thickness and consequently on the thermal

conductivity of the interfacial layer. The thickness and the thermal conductivity of the interfacial layer are assumed to be as $h = f(T, a)$ and $k_{lr} = f(h, a)$, respectively.

The expression for the interfacial layer thickness, h can be found using the available experimental data (Masuda et al., 1993; Eastman et al., 1997; Pak and Cho, 1998; Lee *et al*., 1999; Das et al., 2003; Chon *et al*., 2005; Li and Peterson, 2006) as follows:

$$h = 0.01(T - 273)a^{0.35} \tag{29}$$

Also, the expression for the thermal conductivity of the interfacial layer, k_{lr} is found using the same experimental data as for the expression for the interfacial layer thickness as follows:

$$k_{lr} = C\frac{h}{a}k_f \tag{30}$$

where the constants C = 30 and 110 for Al_2O_3 and CuO nanoparticles, respectively. Therefore, the present model can be written as Eqs. (25, 29, 30).

3. Convective transport in nanofluids

3.1 Properties of nanofluid

3.1.1 Density

In the absence of experimental data for nanofluid density, constant-value temperature independent densities based on nanoparticle volume fraction are used (Maiiga *et al*, 2004)

$$\rho_{nf} = (1-\phi)\rho_f + \phi\rho_p \tag{31}$$

3.1.2 Specific heat

The specific heat is proposed following two formulas. First, it has been suggested that the effective specific heat be calculated using the following equation (Maiiga *et al*, 2004)

$$cp_{nf} = (1-\phi)cp_f + \phi cp_p \tag{32}$$

The second, has used an alternate approach based on heat capacity concept (Xuan and Roetzel, 2000)

$$(\rho cp)_{nf} = (1-\phi)(\rho cp)_f + \phi(\rho cp)_p \tag{33}$$

However, no experimental data has been advanced regarding specific heat that would permit clear choice between these properties. Both of equations have been tested in our simulation case.

3.1.3 Viscosity

The effective dynamic viscosity of nanofluids can be approximated by many models (Maiiga *et al*, 2004; Brinkman, 1952). In the last few years, the effective dynamic viscosity was found by Putra *et al*. (2003) that is also dependent on temperature. It is given in a polynomial function as

$$\mu_{nf} = \left(2.9\times10^{-7}\right)T^2 - \left(2.0\times10^{-4}\right)T + 3.4\times10^{-2} \tag{34}$$

For Al_2O_3/water nanofluid with $\phi = 1\%$

$$\mu_{nf} = \left(3.4\times10^{-7}\right)T^2 - \left(2.3\times10^{-4}\right)T + 3.9\times10^{-2} \tag{35}$$

For Al_2O_3/water nanofluid with $\phi = 4\%$

However, there are still no functions of volume fraction and the sizes of nanoparticle in this polynomial function. In order to calibrate the heat transfer coefficient with the experiment by Pak and Cho (1998), general and accurate models for prediction of the viscosity of nanofluid are not available at this time. The viscosity measured by Pak and Cho (1998) can be correlated as

$$\mu_{nf} = \mu_f \left(1 + 39.11\phi + 533.9\phi^2\right) \tag{36}$$

For Al_2O_3 nanoparticles

3.2 Approaches to convective transport in nanofluids

The approaches used so far for the convective transport in nanofluids are homogeneous approach, dispersion approach and species transport approach. In homogeneous approach, the conventional transport equations for pure fluids are directly extended to nanofluids. This means that all traditional heat transfer correlations can be used also for nanofluids, provided that the nanofluid's thermophysical properties are used in calculations. Therefore, the enhancement in heat transfer is assumed to come only from the higher thermal conductivity of nanofluids. The approach was used by Maïga *et al*. (2004) and it was found by Buongiorno (2006) that the nanofluid heat transfer coefficient was under-predicted. This was because the thermal conductivity model used in Maïga et al. did not depend on temperature.

The dispersion approach is based on the assumption that the convective heat transfer enhancement in nanofluids comes from two factors, the higher thermal conductivity and the dispersion of the nanoparticles. This approach was firstly proposed for nanofluids by Xuan and Roetzel (2000). The effect of the nanoparticle/base fluid relative velocity is treated as a perturbation of the energy equation and an empirical dispersion coefficient is introduced to describe the heat transfer enhancement. Nevertheless, Buongiorno's work (2006) on the energy equation using dimensional analysis showed that the heat transfer enhancement from the nanoparticle dispersion can be negligible in nanofluids.

Buongiorno also suggested that the species transport equation of nanoparticles should be solved for convective transport in nanofluids. However, it is still not clear which approach should be used. In this work, the homogenous approach and the species transport approach are employed in order to find the suitable approach to describe the convective transport in nanofluids.

3.2.1 Homogeneous approach

The conventional transport equations for pure fluids are directly extended to the nanofluids. This approach was initially adopted by Choi (1995) and Xuan and Roetzel (2000). The energy equation for the incompressible pure fluid can be applied to to the nanofluid directly. It can be expressed as

$$\frac{\partial T}{\partial t} + \nabla \cdot uT = \nabla \cdot \left(\alpha_f \nabla T \right) \tag{37}$$

Maïga *et al*. (2004) presented a mathematical formulation and numerical method to determine the force convective heat transfer. The governing equations follow:

The continuity equation of nanofluids

$$\nabla \cdot \left(\rho u \right) = 0 \tag{38}$$

The momentum equation of nanofluids

$$\nabla \cdot \left(\rho u u_i \right) = -\frac{\partial P}{\partial X_i} + \nabla \cdot \left(\mu \nabla u_i \right) + S_i \tag{39}$$

The energy equation of nanofluids

$$\nabla \cdot \left(\rho u c T \right) = \nabla \cdot \left(k \nabla T \right) \tag{40}$$

Roy *et al*. (2004) also proposed a numerical simulation for radial laminar flow in a cooling system. All assumptions used in this study are similar those of Maïga et al. (2004)

3.2.2 Dispersion approach

This approach is based on the assumption that the convective heat transfer enhancement in nanofluids comes from two factors: the higher thermal conductivity and the dispersion of the nanoparticles. The effect of nanoparticles is treated as a perturbation of energy equation, and empirical dispersion coefficient is introduced to describe the heat transfer enhancement. This approach was proposed for nanofluids by Xuan and Roetzel (2000).

The energy equation of nanofluids with taking the axial direction can be given as

$$\frac{\partial T}{\partial t}+u\frac{\partial T}{\partial x}=\frac{1}{r}\frac{\partial}{\partial r}\left[\left(\alpha_{nf}+\frac{k_{D,r}}{\left(\rho c_p\right)_{nf}}\right)r\frac{\partial T}{\partial r}\right]+\frac{\partial}{\partial x}\left[\left(\alpha_{nf}+\frac{k_{D,x}}{\left(\rho c_p\right)_{nf}}\right)\frac{\partial T}{\partial x}\right] \qquad (41)$$

However, the dimensional analysis the energy equation (Buongiorno, 2006) shows that the heat transfer enhancement from nanoparticle dispersion is completely negligible in nanofluids

3.2.3 Species approach

This model eliminates the shortcoming of the homogenous and dispersion approach. The transport equation of nanoparticles is supposed to enhance the convective heat transfer. This approach was proposed for nanofluids by Buongiorno (2006).

The continuity equation of nanofluids is given as

$$\nabla \cdot v = 0 \tag{42}$$

The continuity equation of nanoparticles (species transport equation)

$$\frac{\partial \phi}{\partial t} + v \cdot \nabla \phi = -\frac{1}{\rho_p} \nabla \cdot j_p \tag{43}$$

The momentum equation of nanofluids

$$\rho \left[\frac{\partial v}{\partial t} + v \cdot \nabla v \right] = -\nabla P - \nabla \cdot \tau \tag{44}$$

The energy equation of nanofluids

$$\rho c \left[\frac{\partial T}{\partial t} + v \cdot \nabla T \right] = -\nabla \cdot q + h_p \nabla \cdot j_p \tag{45}$$

where

$$j_p = j_{p,B} + j_{p,T} = -\rho_p D_B \nabla \phi - \rho_p D_T \frac{\nabla T}{T}$$

j_p is the sum of Brownian diffusion and thermophoresis terms which possibly enhance the heat transfer coefficient (Buongiorno, 2006).

4. Numerical method

The computational fluid dynamics software FLUENT (version 6.2) is used to solve the transport equations for the turbulent flow in a uniformly heated tube of 1 m in length and 1 cm in diameter with the constant heat flux of 500,000 W/m^2 and Re = 50,000. The continuity, momentum, energy and species transport equations with the

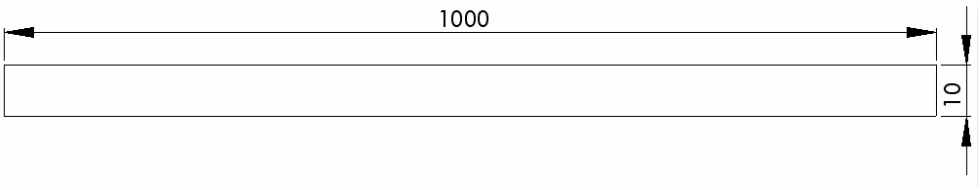
standard $k-\varepsilon$ turbulence model are solved using the finite volume method with the QUICK scheme. The grid-independent study is made. The thermal conductivity models for nanofluids are implemented separately in FLUENT using the user-defined functions.

4.1 Geometry domain

In this work, there are 2 geometry domains with 3-D models. First, a uniformly heated tube 1 m long and 1 cm diameter (Figure 2) follows the experimental test of convective heat transfer by Pak and Cho (1998) and the recent simulation by Maiiga *et al*., 2004. Second, is the U-tube dimensions are shown in of which in Figure 3. Also, the grids of the simulation in the Geometry domain are independent (Figure 4).

4.2 Boundary conditions

The boundary conditions are: a uniform axial velocity and temperature at the inlet section, a uniform heat flux and the usual non-slip condition on the tube wall, and the pressure condition prevails where a known pressure is specified at the outlet section (Figure 2 and 3). See also the definition of each boundary condition in Appendix D.



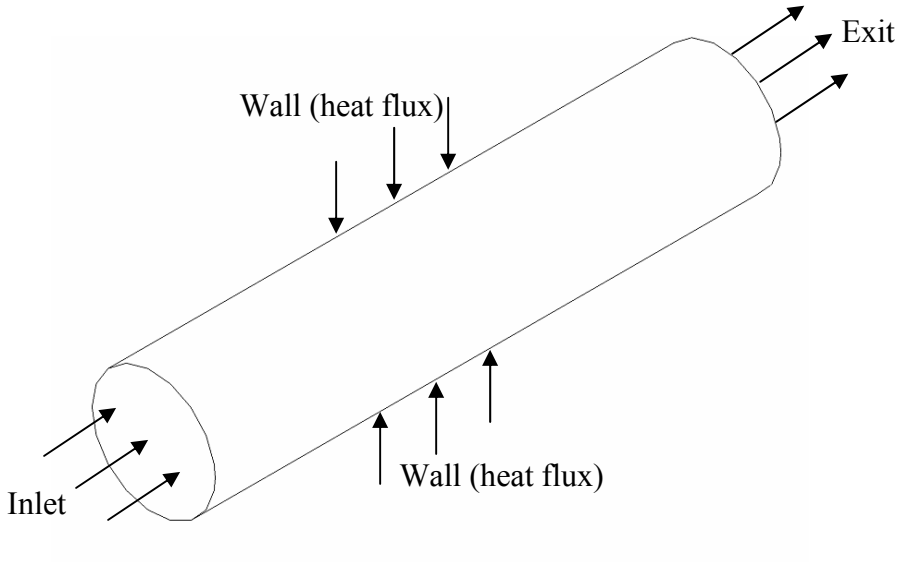


Figure 2 Geometry and boundary condition of a uniformly heated tube (Units in mm)

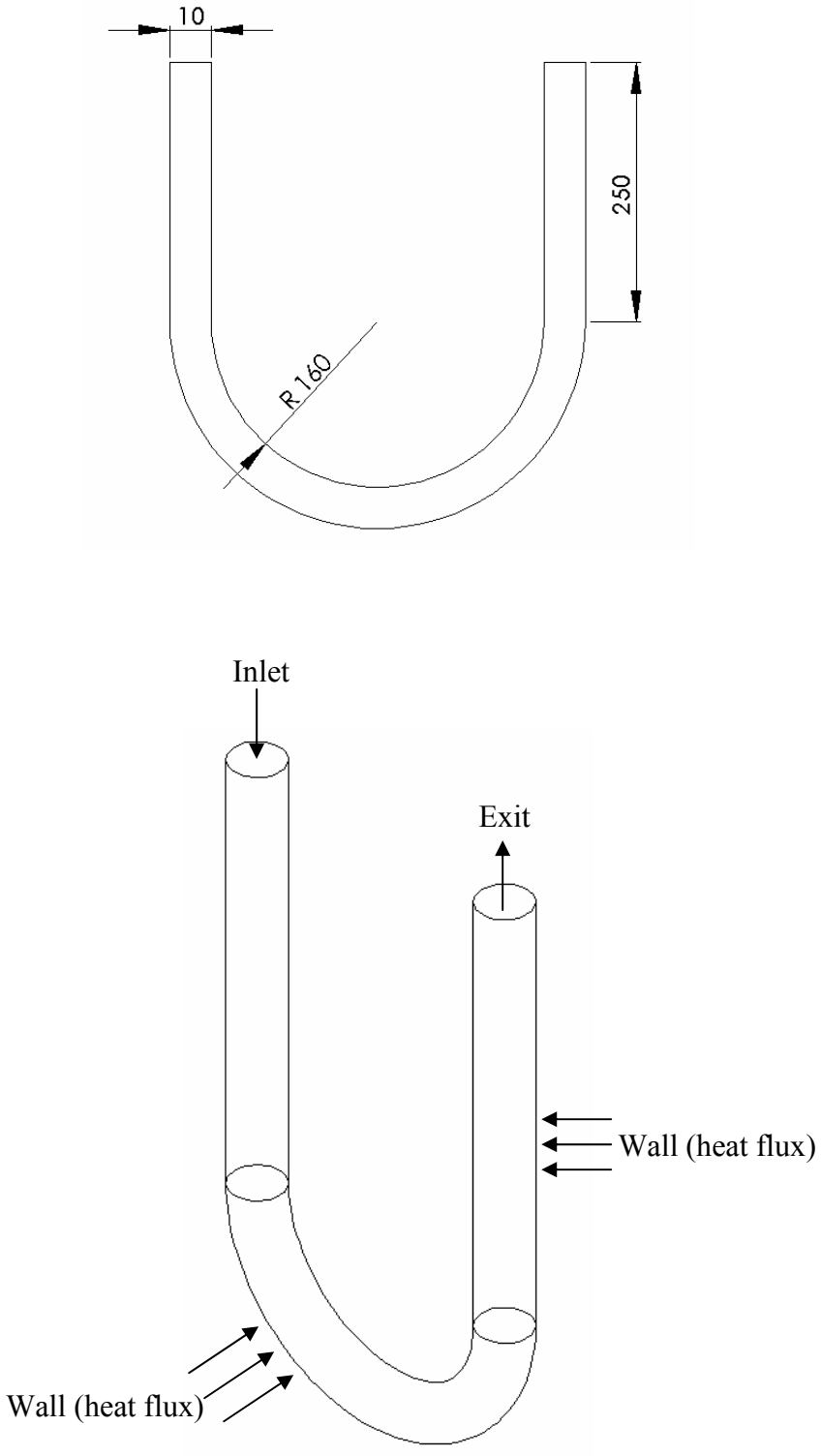


Figure 3 Geometry and boundary condition of U-tube (Units in mm)

4.3 Settings for convective transport in nanofluids

4.3.1 Homogeneous approach

The numerical simulation settings for convective transport in nanofluids for homogeneous approach are shown in Table 1-9

Table 1 Model settings for homogeneous approach

Model	Settings
Space	3D
Time	Steady
Viscous	Standard k-epsilon turbulence model
Wall Treatment	Standard Wall Functions
Heat Transfer	Enabled

Table 2 Types of the boundary conditions in each zone for homogeneous approach

Name	Types
Fluid	Fluid
Wall	Wall
Exit	Pressure-outlet
Inlet	Velocity-inlet
Default-interior	Interior

Table 3 Values of the initial condition at boundary conditions in each zone for homogeneous approach

Zones	Conditions	Values
Wall	Material Name	Aluminum
	Temperature	300
	Heat Flux	500000
Exit	Gauge Pressure	0
	Backflow Total Temperature	300
	Backflow Direction Specification Method	1
Inlet ($\phi = 1\%$)	Velocity Specification Method	2
	Velocity Magnitude	5.2949548
	Temperature	300

Table 4 Solver controls for homogeneous approach

Equation	Solved
Flow	Yes
Turbulence	Yes
Energy	Yes

Table 5 Relaxation in homogeneous approach

Variable	Relaxation Factor
Pressure	0.30000001
Density	1
Body Forces	1
Momentum	0.69999999
Turbulence Kinetic Energy	0.80000001
Turbulence Dissipation Rate	0.80000001
Turbulent Viscosity	1
Energy	1

Table 6 Linear solver in homogeneous approach

Variable	Solver type	Termination criterion	Residual reduction tolerance
Pressure	V-Cycle	0.1	-
X-Momentum	Flexible	0.1	0.7
Y-Momentum	Flexible	0.1	0.7
Z-Momentum	Flexible	0.1	0.7
Turbulence Kinetic Energy	Flexible	0.1	0.7
Turbulence Dissipation Rate	Flexible	0.1	0.7
Energy	Flexible	0.1	0.7

Table 7 Discretization scheme in homogeneous approach

Variable	Scheme
Pressure	Standard
Momentum	QUICK
Turbulence Kinetic Energy	QUICK
Turbulence Dissipation Rate	QUICK
Energy	QUICK

Table 8 Solution limits in homogeneous approach

Quantity	Limit
Minimum Absolute Pressure	1
Maximum Absolute Pressure	5e+10
Minimum Temperature	1
Maximum Temperature	5000
Minimum Turb. Kinetic Energy	1e-14
Minimum Turb. Dissipation Rate	1e-20
Maximum Turb. Viscosity Ratio	100000

Table 9 Material properties : water-alumina ($\phi = 1\%$) for homogeneous approach

Property	Units	Method	Value(s)
Density	kg/m^3	Constant	1027.918
Cp (Specific Heat)	J/kg.k	Constant	4148.98
Thermal conductivity	W/m.k	User-defined	(Keff_Al2O3::Keff)
Viscosity	kg/m.s	User-defined	(Veff_Al2O3::Veff)

4.3.2 Species transport approach

The numerical simulation settings for convective transport in nanofluids for species transport approach are shown in Table 10-20

Table 10 Model settings for species transport approach

Model	Settings
Space	3D
Time	Steady
Viscous	Standard k-epsilon turbulence model
Wall Treatment	Standard Wall Functions
Heat Transfer	Enabled
Species Transport	Non-Reacting (2 species)

Table 11 Types of the boundary conditions in each zone for species transport approach

Name	Types
Fluid	Fluid
Wall	Wall
Exit	Pressure-outlet
Inlet	Velocity-inlet
Default-interior	Interior

Table 12 Values of the initial condition at boundary conditions in each zone species transport approach

Zones	Conditions	Values
Wall	Material Name	Aluminum
	Temperature	300
	Heat Flux	500000
Exit	Gauge Pressure	0
	Backflow Total Temperature	300
	Backflow Direction Specification Method	1
Inlet ($\phi = 1\%$)	Velocity Specification Method	2
	Velocity Magnitude	5.2949548
	Temperature	300

Table 13 Solver controls for species transport approach

Equation	Solved
Flow	Yes
Turbulence	Yes
Al_2O_3	Yes
Energy	Yes

Table 14 Relaxation in species transport approach

Variable	Relaxation Factor
Pressure	0.30000001
Density	1
Body Forces	1
Momentum	0.69999999
Turbulence Kinetic Energy	0.80000001
Turbulence Dissipation Rate	0.80000001
Turbulent Viscosity	1
Energy	1

Table 15 Linear solver in species transport approach

Variable	Solver type	Termination criterion	Residual reduction tolerance
Pressure	V-Cycle	0.1	-
X-Momentum	Flexible	0.1	0.7
Y-Momentum	Flexible	0.1	0.7
Z-Momentum	Flexible	0.1	0.7
Turbulence Kinetic Energy	Flexible	0.1	0.7
Turbulence Dissipation Rate	Flexible	0.1	0.7
Al_2O_3	Flexible	0.1	0.7
Energy	Flexible	0.1	0.7

Table 16 Discretization scheme in species transport approach

Variable	Scheme
Pressure	Standard
Momentum	QUICK
Turbulence Kinetic Energy	QUICK
Turbulence Dissipation Rate	QUICK
Al_2O_3	QUICK
Energy	QUICK

Table 17 Solution limits in species transport approach

Quantity	Limit
Minimum Absolute Pressure	1
Maximum Absolute Pressure	5e+10
Minimum Temperature	1
Maximum Temperature	5000
Minimum Turb. Kinetic Energy	1e-14
Minimum Turb. Dissipation Rate	1e-20
Maximum Turb. Viscosity Ratio	100000

Table 18 Material properties: water-alumina ($\phi = 1\%$) (mixture) for species transport approach

Property	Units	Method	Value(s)
Mixture Species		Names	$Al_2O_3/H_2O(l)$
Density	kg/m^3	Volume-weighted-mixing-law	#f
Cp (Specific Heat)	J/kg.k	Constant	4148.98
Thermal conductivity	W/m.k	User-defined	Keff_Al2O3::Keffspecies1
Viscosity	kg/m.s	User-defined	Veff_Al2O3::Veffspecies1
Mass diffusivity	m^2/s	Constant-dilute-approximate	4e-11
Thermal diffusion coefficient	kg/m.s	Specified	Al_2O_3 (4.2083602e-06)

Table 19 Material properties: water (liquid) for species transport approach

Property	Units	Method	Value(s)
Density	kg/m^3	Constant	3970
Cp (Specific Heat)	J/kg.k	Constant	880
Thermal conductivity	W/m.k	Constant	40

Table 20 Material properties: alumina for species transport approach

Property	Units	Method	Value(s)
Density	kg/m^3	Constant	998.2
Cp (Specific Heat)	J/kg.k	Constant	4182
Thermal conductivity	W/m.k	Constant	0.613
Viscosity	kg/m.s	Constant	0.001003
Molecular Weight	kg/kgmol	Constant	18.0152

The material is also shown in Appendix D for different volume fractions and sizes of nanoparticles which are defined in text files (User-defined database)