Aspen Plus Preliminary Simulation of Nanofluids

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Abstract: A rising trend exists towards using nanofluids as heat transfer agent in process engineering. Hence there is a consequent justified need for process simulation softwares capable of treating nanofluids and recognizing their enhanced thermal properties and the resulting impact on the whole simulated process. Thus, this paper examines the capacity of one of the most known process simulation softwares, Aspen plus, to simulate nanofluids. Preliminary investigation indicates that process simulation software could have solid particles within default range down to microns- not nanoparticles, thus simulation of nanofluids potentially may give misleading results in terms of process energy consumption. This shortage can be omitted by the proposed approach, which paves the way for nanofluids broad applications in industrial plants to be examined easily and shortly via process simulation software packages. A two - step approach is proposed to introduce nanofluids and their altered thermophysical properties and consequent heat duty change into process simulation software: a proper mathematical model is chosen, and then introduced into Aspen plus Calculator block as FORTRAN code. A simulation example of a heat exchanger heats Water-Al_2O_3 nanofluid over a range of nanoparticles volumetric concentration via the proposed approach is executed. Simulation results prove the applicability and validity of the approach whereby the enhanced thermophysical properties and the energy conservation due to employing nanofluids have been recognized by the simulation software.

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1. Introduction

Recently, employing nanofluids as heat transfer agent becomes an upward trend and a considerable alternative to markedly enhance the heat transfer process (Das et al., 2008). Effective heat transfer during heating and cooling streams is an urgent demand in chemicals, petrochemicals, and pharmaceuticals industries (Tora and El-Halwagi, 2010). Obviously, industry relies on computer simulation as a quick and effective tool to test, monitor, analyze, and modify the individual units (e.g. heat exchangers) and the entire process performance as well.

Available process simulation software packages address in detail the conventional methods to enhance heat transfer like increasing the area of the heat exchangers, but that may not be the case considering nanofluids. These simulation software packages include their own build in modules library and components databanks. Furthermore, user defined components and equipments can be introduced into the simulation software packages (Aspen plus, 2012), but all rely on conventional thermophysical models which almost not applicable with nanofluids. Therefore, commercially available process simulation softwares may give misleading results when simulating energy systems employing nanofluids in terms of heat duty and pump power (Tora, 2012)!

Nanofluid refers to ' nanoparticles fluid suspension' according to Stephen Choi (Choi, 1995), who was the first to suspend nanoparticles (at least one of the main dimensions has length less than 100 nm) into a base fluid to get a suspension with heat transfer properties better than the original fluid (Abouali and Ahmadi, 2012). However, this concept dates back to Maxwell work (1873s), larger size solid particles had been used (Wong and Castillo, 2010). Both the conduction and convection heat transfer may be enhanced via using nanofluids. Nevertheless, the thermal conductivity enhancement is significant; more research is needed to investigate the augmentation of the convective heat transfer (Kim et al., 2004). Convection heat transfer depends on the flow type: laminar flow, turbulent flow, and pool boiling. Yet thermal conductivity is influenced by nanoparticles (material, shape, size, volumetric concentration), base fluid material, pH, additives, and the ratio (k_{np}/k_{bf}) between the nanoparticles and the base fluid. Dispersing 0.5 - 4 volume percentage of nanoparticles into a base fluid increases its thermal conductivity by 15 - 40 %. However, that enhancement is limited to certain volumetric concentration (Palm et al., 2006), and can be offset by other parameters.

Metals (Al, Cu, Au), metal oxides (Al_2O_3, CuO), and nonmetals (TiO_2, CNT, SiC, TiC) can act as appropriate nanoparticles [18]. Likewise, the base

fluid can be water, oil, and ethylene glycol (Pang and Kang, 2007). The thermal conductivities of some known nanoparticle solids and base fluids are given (Table 1) whereby the significant difference between the poor heat transfer properties of the base fluids and that of the nanoparticles is clear.

Table 1. Thermal conductivities of different solid nanoparticles and base fluids [Eastman et al., 1997; Kakaç and Pramuanjaroenkij, 2009; Linhard, 2005].

		Material	Thermal conductivity W/K m
Nanoparticles:			
(i)	Metal		
		Silver (Ag)	429
		Copper (Cu)	401
		Aluminum (Al)	237
(ii)	Nonmetal		
		Diamond	3300
		Carbon nanotubes	3000
		Silicone	148
(iii)	Oxides		
		Alumina (Al_2O_3)	40

Available process simulation software mostly has these pre-mentioned base fluids as conventional fluids in their build in databanks; hitherto those databanks lack the corresponding nanofluids. Therefore, this work tackles introducing an approach to overcome this shortage, and to pave the way in front of extending these software packages' capability to simulate thermal processes employing nanofluids. To accomplish this target, taking advantage of the developed models representing the heat - transfer enhancement due to replacing conventional fluids with corresponding nanofluids, treating them to be compiled into simulation software packages, and adopting simulation software to consider those nanofluids' models when performing energy calculations are the core steps of the proposed approach.

1. Heat transfer enhancement via using nanofluids

Employing nanofluids as heat transfer agents in thermal energy systems has high potential to enhance the systems' efficiency, since suspending nanoparticles with high thermal conductivity into a base fluid (bf) produces a nanofuid (nf) with higher thermal conductivity (k), density (ρ), and viscosity but lower specific heat. Thoose changes significantly impact the heat exchanger areas and the pump power which in turn influences on the capital cost and operating cost as well (Tora, 2012).

2.1. Modeling nanofluids thermophysical properties

The enhanced specific heat of the nanofluid can be anticipated via two mathematical models [Maré et al., 2012]. First is known as equation of Xuan and Roetzel (2000); workability of the ideal mixture theory ($\Psi = \sum_{i=1}^{n} \Psi_i \, \phi_i$) is assumed and is given by

$$C_{p,nf} = \phi C_{p,p} + (1-\phi) C_{p,bf}, \qquad 1$$

where Ψ is any thermo physical property of an ideal mixture, Ψ_i is the corresponding value of pure components ($i : n$) forming the mixture and ϕ_i is the fraction of the component in the mixture.

Other model is based on proposing a thermal equilibrium between the nanoparticles and the base fluid. That model (model II) has been selected for this work due to its justification; it can estimate the nanofluid specific heat as

$$C_{p,nf} = \frac{(1-\phi)\ \rho_{bf}\ C_{p,bf} + \phi\, \rho_p\, C_{p,p}}{\rho_{nf}}, \qquad 2$$

(ρ_{nf}) is the nanofluid enhanced density and given as

$$\rho_{nf} = (1-\phi)\,\rho_{bf} + \phi\,\rho_p \qquad 3$$

$$\phi = \frac{V_{np}}{V_{np} + V_{bf}} = \frac{m_{np}/\rho_{np}}{m_{np}/\rho_{np} + m_{bf}/\rho_{bf}} \qquad 4$$

Thermo physical properties of pure water as a base fluid and pure alumina as nanoparticles [Maiga et al., 2005; Kakaç and Pramuanjaroenkij, 2012] are listed (Table 2).

Both the resulting nanofluids' specific heat and density have been calculated considering different nanoparticles volumetric fraction (0 - 7) %. Using those models, the augmentation of nanofluid density and decrease in the specific heat are listed (Table 3).

Table 2. Comparison between properties of pure water as a base fluid and 30 nm alumina nanoparticles (Palm et al., 2012; Wong and Castillo, 2010].

Property	Base fluid (water)	Nanoparticles (Al_2O_3)
Specific heat, C_p, (kJ/kg K)	4.182	7.73
Density, ρ, (kg/m^3)	998.2	3880
Thermal conductivity, k, (W/m K)	0.6	36
Thermal diffusivity, α, m^2/s	1.465	1.19*10^{-9}

Table 3. Al_2O_3-Water nanofluid properties with different nanoparticles volumetric concentration

Nanoparticles volumetric concentration (ϕ)	Density, ρ, kg/m^3	Model II Specific heat, C_p, kJ/kg K
0	998.2	4.182
0.01	1027.0	4.053
0.02	1055.8	3.931
0.03	1084.7	3.816
0.04	1113.5	3.707
0.05	1142.3	3.603
0.06	1171.1	3.504
0.07	1199.9	3.410

2.2. Heat transfer rate

For constant volume system, heat transfer rate, Q, can be given as:

$$Q = \frac{dU}{dt} = m C_v \frac{dT}{dt} , \qquad 5$$

Likewise, rate of heat transfer in constant pressure system can be calculated as:

$$Q = \frac{dH}{dt} = \frac{d(U + PV)}{dt} = m C_p \frac{dT}{dt} , \qquad 6$$

Liquid and solid systems can be considered as incompressible materials (Linhard, 2005). Therefore, nanofluid is treated as incompressible fluid in this study, since nanofluid is a mixture of solid and liquid. Additively, for constant pressure and constant volume systems, the two specific heats are similar, thus C can be used generally to refer to the nanofluid specific heat. Therefore, heat flow can be written as

$$Q = m C \Delta T , \qquad 7$$

In the next section, simulation will be conducted on the basis of using equation 7 combined with the mentioned model of the specific heat.

2. Simulation

Process simulation softwares like ASPEN PLUS and HYSYS, etc. are widely used in industrial facilities and energy plants as quick and efficient tool to monitor and evaluate the system performance. Thus incorporating nanofluids into process simulation softwares - particularly Aspen plus - is tackled herein aiming to enable the simulation software to recognize the occurring difference due to nanofluids usage in the simulated process. That may facilitate investigating the impact of employing nanofluids into industrial processes considering thermal energy systems and applications, and furthermore pave the way to wide and large scale applications of nanofluids.

Simulation programs mostly have built in databanks containing conventional solids such as metals and conventional fluids like water. They may have particles size distribution but in the ranges of microns (Aspen plus, 2012); they lack the corresponding nanoparticles. Therefore, simulation of energy systems or processes employing nanofluids may be unworkable or even gives misleading results.

Nanoparticles can be Al_2O_3, TiO_2, and Cu, however, the base fluid can be water, oil, and lubricant which are just a few to name. Available process simulation softwares mostly have them as conventional solids and fluids in their build in databanks (Palm et al., 2006), but so far those databanks lack the corresponding nanofluids (Tora, 2012). The feasibility of simulating nanofluids using Aspen plus needs to be investigated seeking to treat with its default capacity to cope with the rising applied research in the field of nanofluids applications in processes and energy systems.

3.1. Process simulation software: Aspen plus

One of the process simulation softwares, Aspen plus, is used to investigate the feasibility of simulation of nanofluids – with assuming that the nanofluids are well prepared and have a stable properties during the entire process, with considering nanofluid a single phase [Maiga et al., 2005; Pang and Kang, 2012). A simple flow sheet given in Fig. 1 was built using Aspen plus; it consists of a heat exchanger (HX-BF) used to heat conventional fluid which is water in this case; another heat exchanger (HX-NF) used to heat nanofluid that is Al_2O_3- water nanofluid. The heat exchangers task is to raise the temperature of the working fluid by 50 degrees Celsius. The target is to

check the default capacity of the software to simulate nanofluid, and to accurately recognize the difference between nanofluid and conventional fluid.

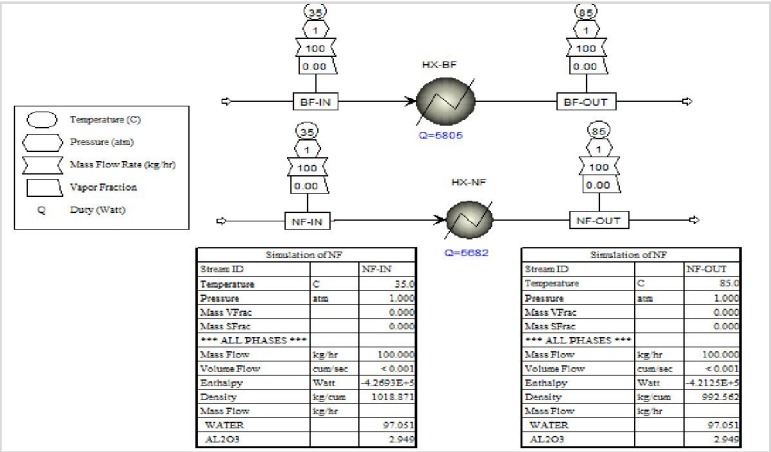


Figure 1. Aspen plus simulation of base fluid and corresponding nanofluid (1vol.% Al_2O_3) in thermal energy system.

The simulation run results show that the base fluid heat exchanger heat rate is 58095 W, while the nanofluid heat exchanger heat rate is 5664 W. Thus according to equation 7, specific heat of the base fluid (water) is 4179.6 J/kg K and that of the nanofluid, Al_2O_3-water, is 4091 J/ kg K. Therefore, the results are accurate with the base fluid, but inaccurate with the nanofluid according to eq. 2 and Table 3 that represent the predicted values of nanofluids properties.

Simulation is executed using different nanoparticle volume fraction; the runs results are compared with the model values, whereby the simulation results indicate that:

(i) The accuracy of the simulation software decreases linearly with increasing the suspended nanoparticles volumetric concentration.

(ii) The difference between the simulation and the model results increases linearly with increasing the nanoparticles volumetric fraction, which can be described as $\rho_{Aspen} = \rho_{NF} - (0.24\phi + 0.685)$ and $C_{p\_Aspen} = C_{p\_NF} + (0.895\phi + 0.09)$ for the density and the specific heat.

(iii) The simulation predicts that the density decreases and the specific heat increases with the increase of the nanoparticles volumtric fraction, which is in contrast to the real case.

To get Aspen plus fully adopted for nanofluids' models, a Calculator block is proposed herein.

3.2. Incorporating nanofluids into process simulation software

A proposed method, Aspen plus Calculator block, to incorporate nanofluids into process simulation software is proposed here. 'Calculator block' is a tool in Aspen plus empowers the user to introduce mathematical models written in Fortran language using build in Fortran inside Aspen plus or via linking Aspen plus with Excel sheets, then the simulation calculations are performed based on those entered model, and overwrite the program default models. Fortran code is selected as its capacity to enter models into Aspen directly is significant. As given in Fig.2 first the flow sheet variables included in the nanofluids model (nanofluid specific heat, nanofluid density, etc.) are identified with setting values for the parameters (e.g. nanoparticle volumetric fraction) and the operating conditions (temperature, mass flow rate). Then, Fortran code of the model predicting nanofluids properties is written in the Calculator block, and finally the Calculator is executed.

In the Calculator block Fortran code, CPBF is the specific heat of the base fluid, CPP is the specific heat of the nanoparticles, DBF is the density of the base fluid, DP is the density of the nanoparticle, TIN is the temperature of the stream entering the heater, TOUT the temperature of the stream exiting the heater, VCNP is the volumetric concentration of the nanoparticles, DNF is the density of the nanofluid, CPNF is the specific heat of the nanofluid, and QNF is the heat duty of the heat exchanger needed to heat the nanofluid.

Results show that Aspen plus calculator blcok successfully calculate nanofluid specific heat and the consequently the heat duty. Different nanoparticle volumtric fractions have been used as given in Fig.3. Therefore, process simulator software can be used to accuratly handle nanofluids processes under different conditions.

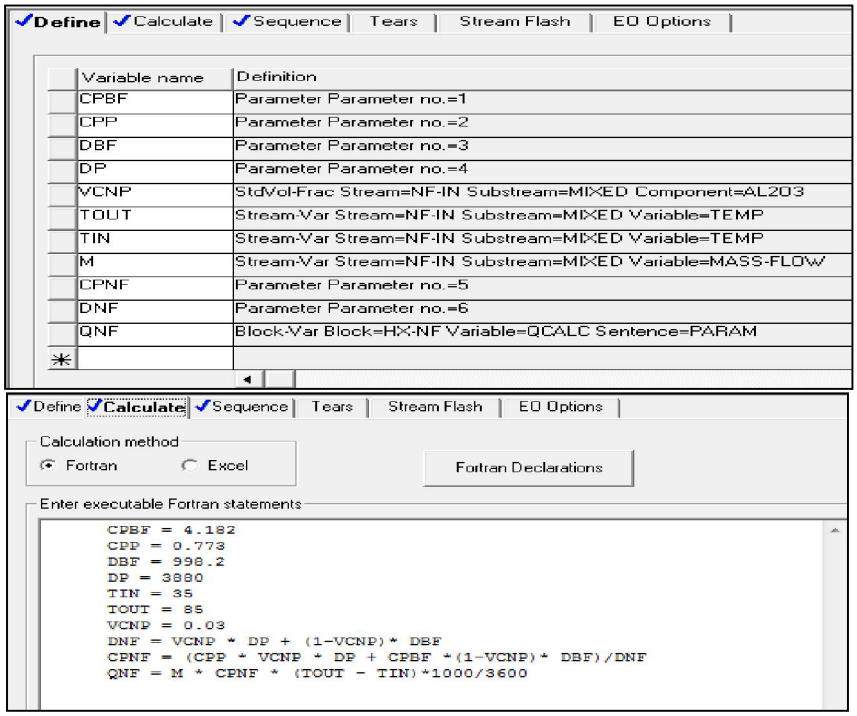
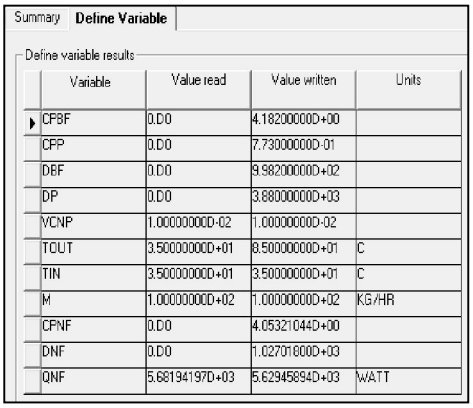
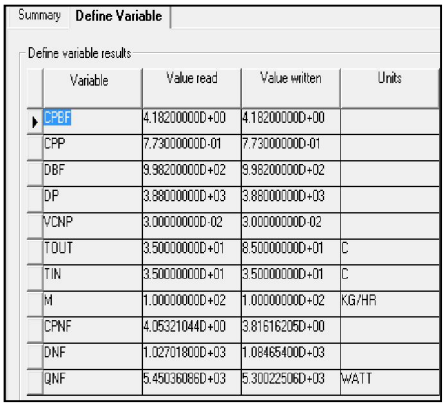


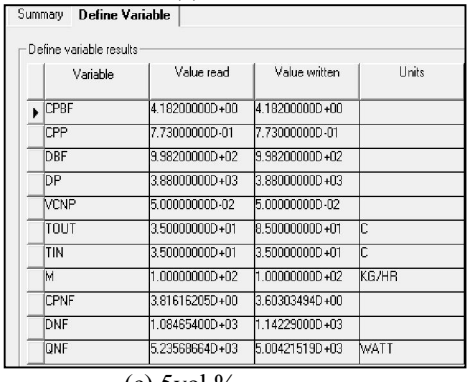
Figure 2. Aspen plus Calculator block to introduce nanofluids enhanced properties and perform resultant heating duty.



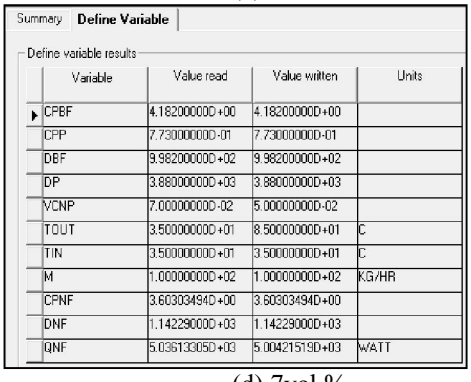
(a) 1vol.%



(b) 3vol.%



(c) 5vol.%



(d) 7vol.%

Figure 3. Calculator block results at different nanoparticles volume fractions (1 - 3 - 5 -7) %

4. Conclusion

Simulation of nanofluids as heat transfer agents via existing process simulation software (Aspen plus) is investigated. The simulation default models predict the thermophysical properties inaccurately especially with increasing the nanoparticles volumetric concentration. The simulation predicts increasing the specific heat and decreasing the density of the nanofluids with increasing the nanoparticles volumetric concentration, which is the opposite to what practically takes place.

To adopt the simulation software to fully recognize the existence of nanofluid, instead of the conventional fluid, a calculator block with a mathematical model predicting the considered nanofluids altered properties and consequent changes is incorporated into the software. This approach succeeds to empower the widely used process simulation software to treat with nanofluids perfectly. This paves the way for industrial plants as well as academies to easily and shortly investigate the impact of using nanofluids as working fluid on the entire process. However the given example considers only the specific heat and the density, that sounds enough to adequately illustrate the assumed approach to simulate nanofluids via process simulation software (Aspen plus), extra mathematical expressions of other thermophysical properties can be similarly added to the Calculator block. The proposed approach sounds applicable particularly with the investigated simulation software, yet further work is required to develop a global method.

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Nomenclature

k_{np}	thermal conductivity (W/m K)
C_p	specific heat of nanoparticles (kJ/kg K)
$C_{p,nf}$	specific heat of nanofluid (kJ/kg K)
V_p	volume of the nanoparticles (m^3)
Q	heat transfer rate (W)
C	specific heat (kJ/kg K)
Greet letters	
ρ	density (Kg/m3)
ϕ	volumetric fraction of nanoparticles
Subscripts	
np	nanofluid
bf	base fluid
np	nanoparticle

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