Numerical Study of MXene Enhanced Therminol®VP-1 Nanofluid for Solar Photothermal Conversion

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Abstract. Effective and efficient utilization of solar energy is highly demanded in the energy industry. Herein, based on the excellent optical properties of MXene, an MXene enhanced therminol®VP-1 nanofluid is proposed for direct absorption solar collector to efficiently absorb solar radiation. The nanofluid is experimentally prepared and characterized. Subsequently, the influence of mass fraction of MXene, collector height, and working temperature on the collecting efficiency of the nanofluid in DASCs is numerically investigated. The results show that even with a low mass loading such as 50 ppm, MXene enhanced therminol®VP-1 nanofluid still can effectively absorb solar spectrum. The intercept efficiency of 50ppm nanofluid is 83.32%, which is higher by 20.48% than that of therminol®VP-1. The efficiency is strongly affected by collector height and MXene content and first increases and then decreases with increasing the mass loading of MXene. Moreover, the best content of MXene gradually decreases with the increase of the collector height. These findings suggest that MXene enhanced therminol®VP-1 nanofluid has promising prospects to achieve efficient solar photothermal conversion.

1. Introduction

With the depletion of fossil fuels and the increasing greenhouse effect, all kinds of new energy are being widely applied, especially solar energy. There are many ways to leverage solar energy, one of which is solar photothermal conversion [1]. Conventional surface solar collectors, which capture solar spectrum through a selective absorption surface, are extensively applied for solar photothermal conversion. However, due to the heat loss of the surface and thermal resistance from the surface to heat transfer fluid (HTF), the collecting performance of conventional collectors cannot be further elevated [2]. Different from conventional surface solar collectors, direct absorption solar collectors (DASCs) can directly assimilate solar energy through HTF and preserve it in the form of thermal energy of HTF as shown in Figure 1. The collecting performance of DASCs is directly affected by the absorption ability of HTFs for solar energy. Conventional fluids have high transmittance for solar spectrum and cannot effectively absorb solar energy [3]. Nevertheless, some nanoparticles can be used to enhance the optical properties of traditional liquids and thus greatly enhance the collecting efficiency of DASCs. Furthermore, the amounts of nanoparticles used to improve the optical properties of nanofluids are far less than the amounts used to enhance the thermal conductivity of nanofluids, which benefits to reduce settling of nanoparticles [4]. The photothermal conversion efficiency between conventional surface-based solar collectors and DASCs has been investigated comparatively [5]. Khullar et al. numerically investigated the photothermal performance of a concentrating parabolic solar collector with nanofluid to absorb solar radiation and revealed that the efficiency of the collector is about 5-10% higher than that of the conventional parabolic solar collector [6]. Lee et al. demonstrated that MWCNT nanofluid can achieve
higher efficiency (over 10%) than conventional surface-based solar collectors by means of theoretical and experimental methods [7]. It can be found that DASCs have great potential in achieving higher thermal performance than surface-based solar collectors.

The optical properties of nanofluids for DASCs can be strongly tuned by nanomaterials. MXene is a kind of layered two-dimensional nanomaterials and has the localized surface plasmon resonance (LSPR) effect, which significantly heightens the absorption of solar spectrum [8]. Based on its outstanding optical properties, MXene has broad applications in the scopes of solar thermal conversion [9, 10]. The collecting performance of MXene enhanced water nanofluid has been investigated in our previous work [11]. However, the nanofluid is not suitable for temperature higher than 100°C due to the thermophysical properties of water. MXene enhanced Therminol® VP-1 nanofluid can be applied under higher working temperature and have a broader application prospect in DASCs. Therefore, this research prepared, characterized MXene enhanced Therminol® VP-1 nanofluid, and the effects of mass fraction, collector height, and temperature on the collecting performance of the nanofluid are numerically studied.

![Figure 1. Comparison of conventional solar collector and direct absorption solar collector.](image)

**Figure 1.** Comparison of conventional solar collector and direct absorption solar collector.

### 2. Preparation and characterization of MXene enhanced therminol® VP-1 nanofluids

Firstly, MXene was synthesized by etching Ti₃AlC₂ with synthetic HF. The specific preparation process is shown in our published literature [11]. Then, the Ti₃AlC₂ and prepared MXene were characterized with Scanning electron microscopy (SEM) to observe the morphology. Compared with the SEM of Ti₃AlC₂ in Figure 2(a), the obtained MXene has a typical accordion morphology in Figure 2(b). Finally, MXene enhanced therminol® VP-1 nanofluid was obtained with the two-step method [12]. 0.05 g MXene powder was dissolved in 100 g therminol® VP-1, and Triton X-100 was used to improve the dispersion of MXene. MXene enhanced therminol® VP-1 nanofluids with a mass loading from 25 ppm to 200 ppm were obtained by dilution and ultrasonic treatment. It can be observed from Figure 2(c) that with the increase of MXene loading, the therminol® VP-1 nanofluids gradually become opaque.

The transmittance spectra of therminol® VP-1 nanofluids were measured with a UV-visible spectrophotometer. It can be observed from Figure 3(a) that therminol® VP-1 has the highest transmittance in the visible spectrum (400 ~ 750 nm), which has nearly 50% solar radiation energy. With the increase of MXene content, the transmittance of therminol® VP-1 nanofluid to solar radiation rapidly declines. Furthermore, due to the LSPR effect of MXene, the therminol® VP-1 nanofluids can strengthen the absorption of solar radiation with waveband from 700 nm to 1000 nm, which benefits to lower the mass loading of MXene. The nanofluid achieves a relatively low transmittance to solar radiation with the content of MXene of 200 ppm. Next, the extinction coefficient of the nanofluids can be obtained from the Beer-Lambert law:

\[
K_{e\lambda}(\lambda) = \frac{-\ln(T(\lambda))}{L}
\]  

(1)
where $T$ is the transmittance of the therminol®VP-1 nanofluids with wavelength $\lambda$; $L$ is the optical path length; $K_{e \lambda}$ is the extinction coefficient. Finally, to assess the absorption of therminol®VP-1 nanofluids for solar spectrum, the fraction of absorbed energy is calculated [13].

$$F(x) = 1 - \frac{\int_{\lambda_{\text{min}}}^{\lambda_{\text{max}}} I(\lambda) \exp(-k_{e \lambda}(\lambda)x) d\lambda}{\int_{\lambda_{\text{min}}}^{\lambda_{\text{max}}} I(\lambda) d\lambda}$$  \hspace{1cm} (2)

where $I(\lambda)$ is the solar blackbody radiation distribution from the Planck’s law. The relationship among the fraction of absorbed energy ($F$), optical length ($x$) and mass fraction of MXene is presented in Figure 3(b). Both the content of MXene and optical length have a significant effect on the fraction of absorbed energy. When the optical length is fixed, the higher the concentration of MXene, the higher the fraction of absorbed energy. This conduces to determine the correspondence between collector height and content of MXene for the design of DASCs. However, heat loss is not considered in the above analysis. Further study on therminol®VP-1 nanofluid in DASC was conducted.

![Characterization of MXene](image1.png)

**Figure 2.** Characterization of MXene. (a) SEM of Ti$_3$AlC$_2$, (b) SEM of MXene, and (c) photograph of MXene enhanced therminol®VP-1 nanofluids

![Optical properties analysis](image2.png)

**Figure 3.** Optical properties analysis of MXene enhanced therminol®VP-1 nanofluid
3. Numerical analysis of MXene enhanced therminol®VP-1 nanofluid

The solar photothermal conversion performance of a DASC with MXene enhanced therminol®VP-1 nanofluid was numerically investigated and the schematic of the DASC is shown in Figure 4. A numerical model has been established in Fluent package to investigate the photothermal conversion performance of nanofluids in our previous work [11]. As the small concentration of MXene (<=200ppm, 0.007vol%) has a negligible effect on thermophysical properties according to theoretical calculation [14], the thermophysical properties of therminol®VP-1 are used for the nanofluid [15]. The absorption of the therminol®VP-1 nanofluid for solar energy is appraised by the solar weighted absorption coefficient. The solar weighted absorption coefficient in each waveband between \( \lambda_i \) and \( \lambda_{i+1} \) is:

\[
k_{\varepsilon\lambda_i} = \frac{\int_{\lambda_i}^{\lambda_{i+1}} k_{\varepsilon\lambda}(\lambda) d\lambda}{\int_{\lambda_i}^{\lambda_{i+1}} I(\lambda) d\lambda}
\]  

(3)

The ability of therminol®VP-1 nanofluid to absorb solar energy was analysed by the model [11]. The efficiency of photothermal conversion is defined as:

\[
\eta = \frac{\dot{V} \rho C_p (T_{\text{out}} - T_{\text{in}})}{A I}
\]  

(4)

where \( \dot{V} \) is volume flow, m³/s, \( C_p \) is specific heat of therminol®VP-1, J/ (kg K), \( I \) is the solar intensity, W/m², \( A \) is the area receiving solar radiation, m², \( T_{\text{out}} \) and \( T_{\text{in}} \) is the outlet and inlet temperature, K.

According to the above analysis about the fraction of absorbed energy, the collector height and mass fraction are the key parameters affecting the photothermal conversion of nanofluid. Therefore, the relationships among collector height, mass fraction, and efficiency are investigated and shown in Figure 5. Under the same collector height, the efficiency of therminol®VP-1 nanofluid first rises and then drops.
with increasing the content of MXene. The trend is different with the fraction of absorbed energy (F). Combined with the temperature contours from Figure 6, this can be understood in the following way: when the content of MXene is relatively low, although MXene can boost the absorption of therminol®VP-1 for solar energy, solar spectrum still can get to the bottom of nanofluid and heat the nanofluid, which thus improves the efficiency. However, excessive MXene makes the solar radiation almost utilized by the supernatant fluid, which leads to the higher temperature of the supernatant fluid and more heat loss to the ambient environment over the nanofluid of low MXene loading. Besides, for the collector height 5 mm and 25 mm, the optimal content of MXene is 150 ppm and 25 ppm for the therminol®VP-1, respectively. It can be found that the optimal content for MXene to achieve the highest efficiency gradually decreases with the increase of the collector height.

Figure 6 shows the efficiency of therminol®VP-1 nanofluids change with working temperature. The efficiency of the nanofluids decreases with the rise of working temperature. The addition of MXene can significantly change the intercept efficiency, which is the maximum theoretical efficiency that can be achieved. The intercept efficiency of 50ppm is 83.32%, which is higher by 20.48% than 0ppm due to the absorption of MXene for solar radiation. Besides, compared with the conventional surface solar collector, the thermal performance of the direct absorption solar collector is more affected by the thermal insulation performance of a cover. Silica aerogel has high transmittance and excellent thermal insulation performance, which can be used for the cover of DASCs [16]. When the thermal conductivity of the cover changes from 1.2 W/ (m K) to 0.02 W/ (m K), the efficiency of the DASC is obviously increased.

Figure 7. Temperature contours of MXene enhanced therminol®VP-1 nanofluid at collector height of 15mm

Figure 7. The effect of temperature on the efficiency of MXene enhanced therminol®VP-1 nanofluids for collector height of 10 mm
under elevated operating temperature. Therefore, to further improve the thermal performance of DASCs, the use of aerogel glass as a cover will be a good choice for DASCs.

4. Conclusions
An MXene enhanced therminol®VP-1 nanofluid is prepared and characterized and the collecting performance of the nanofluid in DASCs is numerically investigated. The results indicate that MXene can significantly improve the absorption of therminol®VP-1 for solar radiation even with a low content of MXene. For the collector height of 10 mm, the intercept efficiency of 50ppm nanofluid is 83.32%, which is higher by 20.48% than that of therminol®VP-1. The efficiency of MXene enhanced therminol®VP-1 nanofluid first rises and then drops with increasing mass loading of MXene. There is an optimal content for MXene to maximize the collecting performance. Moreover, the optimal loading of MXene gradually decreases with increasing the collector height. This research suggests that MXene enhanced therminol®VP-1 nanofluid has promising prospects to achieve efficient solar photothermal conversion.

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