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Analytical study of a moving boundary problem describing sublimation process of a humid porous body with convective heat and mass transfer

Vikas Chaurasiya[1] · Ankur Jain[2] · Jitendra Singh[1]

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Abstract

Sublimation of a humid porous body occurs commonly in food technology and thermal energy storage system . Especially, in accelerated freeze-drying, preservation of biological materials to be denatured is the prime interest. Despite the available literature on sublimation, there is a general lack of mathematical analysis of the effect of convection in the frozen and vapour regions, and rate of evaporation of water vapour in the vapour region. Therefore, it is essential to explore a mathematical model which accounts for these physical processes. This paper attempts to address these gaps in the modeling of sublimation of a humid porous body. For a specific form of the velocity profile, an exact solution of the current problem is obtained via similarity technique. Particularly, results from the current work are shown to be in strong agreement with the results of a previous work. The impact of various dimensionless problem parameters on the sublimation process is discussed extensively. Condition for sublimation limit is discussed. It is obtained that sublimation can take place only under limit of sublimation curve. It is found that, in the presence of convection, sublimation process becomes fast and the material requires less time than usual to sublimate. Furthermore, higher rate of evaporation of water vapour produces a lower temperature field and slower propagation rate of sublimation interface.

Keywords Sublimation · Heat and mass transfer · Sublimation interface · Porous medium · Convection

List of symbols

Thermophysical properties

α	Thermal diffusivity ($m^2 s^{-1}$)
c_p	Specific heat ($Jkg^{-1}K^{-1}$)
c_{pv}	Specific heat of water vapour ($Jkg^{-1}K^{-1}$)
k	Thermal conductivity ($Wm^{-1}K^{-1}$)
ρ	Material density (kg m^{-3})
L	Latent heat of sublimation (J kg^{-1})
u	Unidirectional molecular motion (m s^{-1})
C_m	Molar concentration of vapour moisture (mol m^{-3})
M_m	Molecular mass (kg mol^{-1})
p_v	Vapour pressure (kg m^{-1} s^{-2})
R_0	Universal gas constant (kg m^2 s^{-2} K^{-1} mol^{-1})
t	Time (s)
Exp(.)	Exponential function
Erf(.)	Error function

Temperature profile

F	Temperature (K)
F_v	Sublimation temperature (K)
F_s	Surface temperature (K)
T_1	Non-dimensional temperature profile $\left(T_1 = 1 + \frac{F_1 - F_v}{F_s - F_v}\right)$
T_2	Non-dimensional temperature profile $\left(T_2 = \frac{F_2 - F_0}{F_v - F_0}\right)$
Ç	Non-dimensional molar concentration $\left(Ç = \frac{C_m - C_{m,s}}{C_{m,0} - C_{m,s}}\right)$
θ	Non-dimensional temperature/concentration profile

✉ Jitendra Singh
jitendra.singh@bhu.ac.in

Vikas Chaurasiya
vikas.chaurasiya5@bhu.ac.in

Ankur Jain
jaina@uta.edu

[1] Department of Mathematics, Institute of Science, Banaras Hindu University, Varanasi, India

[2] Mechanical and Aerospace Engineering Department, The University of Texas at Arlington, Arlington, TX, USA

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Space variables

x Space coordinate (m)
ξ Non-dimensional space coordinate
$s(t)$ Moving sublimation front (m)

Non-dimensional quantities

α_{21} Non-dimensional thermal diffusivity $\left(\frac{\alpha_2}{\alpha_1}\right)$
C Non-dimensional molar limit concentration $\left(C = \frac{C_{m,0} - C_{m,max}}{C_{m,max} - C_{m,s}}\right)$
β Non-dimensional quantity $\left(\beta = \frac{c_{pv} M_m C_{m,0}}{c_p \rho_1}\right)$
γ Non-dimensional heat flux $\left(\gamma = \frac{k_1 (F_s - F_v)}{k_2 (F_v - F_0)}\right)$
l_0 Non-dimensional latent heat of sublimation $\left(l_0 = \frac{C_{m,0} M_m L}{k_2 (F_v - F_0)} \alpha_1\right)$
λ Unknown constant $\left(\lambda = \frac{s(t)}{2\sqrt{\alpha_1 t}}\right)$

Non-dimensional numbers

Pe Péclet number $\left(Pe = \frac{u}{\sqrt{\frac{\alpha}{t}}}\right)$
Lu Luikov number $\left(Lu = \frac{\alpha_m}{\alpha_1}\right)$

Subscripts

0 Initial
1 Vapour region
2 Frozen region
m Moisture
s Surface $x = 0$

Introduction and Literature review

Introduction

Heat and mass transfer processes, such as sublimation–desorption, evaporation, condensation, melting and solidification have a wide range of applications in food technology [1–3], separation processes [4–7], spray-freezing [8] migration of heat and moisture in soils and grounds [9–13]. In addition to the commonly studied freezing and melting processes, sublimation is also of much technological importance [14]. Porous medium offers an extensive contact surface with fluids, which can enhance the effect of heat and mass transfer [15–17]. Sublimation converts a solid directly into vapour form without the intermediate liquid phase. Sublimation is driven by addition of energy into the solid, in order to meet the internal energy required for change of state, i.e. the latent heat and work done by the molecules at constant pressure. Raising the temperature above the sublimation point, results in propagation of a sublimation interface, determining the location of which is usually of primary interest. Sublimation of solid carbon dioxide, also known as dry ice, which is used commonly for shipping very cold objects and sublimation of arsenic at 615 °C [18] are well known examples of sublimation. Moreover, sublimation of ice plays a key role in the earth's energy balance and global climate [19].

Literature review

Heat and mass transfer in phase change processes can be highly coupled and complicated, particularly when the solid phase is porous. While conduction is often the dominant heat transfer mechanism in solid [20, 21], in specific practical applications, heat transfer due to convection driven by fluid motion within porous frozen region and in the liquid region may also be important [22]. Similar to melting and solidification problems, the sublimation problem is, in general, nonlinear, and closed-form solutions are expected only for special cases. Many approximate analytical and numerical methods have been proposed to solve the problem numerically. Examples include, homotopy perturbation method [23], heat balance method [24, 25] and wavelet method [26–28]. A mathematical framework of heat and mass transfer problem in capillary-porous bodies was presented by Luikov [29]. Exact solutions for specific heat and mass transfer problems have been reported in previous literatures [30–33]. An exact treatment of the drying problem using similarity method is presented by Marcus and Tarzia [34], in which, coupled phase change in a porous medium with heat flux of the form $-\frac{q_0}{\sqrt{t}}$ has been accounted for. Hayashi et al. [35] presented an experimental and analytical study of self-freezing of a wet substance. A mathematical model describing sublimation of frozen moisture in a porous space is reported in [36]. The present mathematical formulation is inspired from the work [36], in which sublimation process is presented in the absence of convective. In this work, an exact solution of the governing heat and mass transfer model was obtained and effect of various parameters were discussed. The optimal condition for sublimation rate in a porous half-space and exact solution for the temperature, vapour and track of moving sublimation interface has been obtained in [37]. Douglas and Mellon [38] presented a study on the rate of ice sublimation, which is controlled by vapour transport away from the planet's outer surface, may have led to the formation of landforms on Mars. Approximate and experimental study of sublimation of water in porous medium has been presented by Zhang et al. [39]. An analytical model involving heat and moisture flow describing sublimation process in a porous half-space is seen in [40]. This work did not account the convection term in the porous frozen region and convective term of moisture transfer of the water vapour in the vapour region, which is being accounted in detail in the present work. In sublimation–dehydration process, porous materials are merely associated with some water crystals present there. Removing these water crystals from the vapour region is one of the key important process in sublimation to obtain a stable biological material. In connection with this, the convective term due to mass transfer of water vapour is more realistic in vapour region than in the frozen part [35]. The convective drying of biological materials is the most favourable approach to stabilize them for long time and avoid denaturation [41, 42]. Therefore, mathematical formulation of sublimation–dehydration of biological products such as fruits is a key relevant process in dryer design [43]. Recently, Chaurasiya and Singh [44] obtained an analytical solution of a freeze-drying problem which accounts sublimation as well as desorption and it was shown that sublimation and desorption can take place only under sublimation and desorption curve.

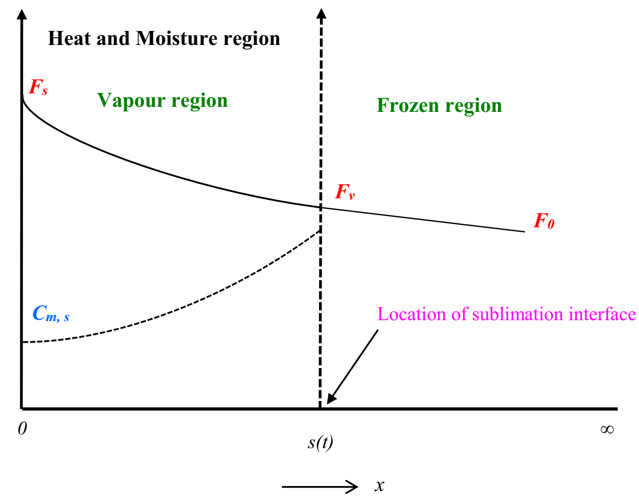


Fig. 1 Schematic diagram describing the one-dimensional sublimation process of a humid porous body

Present contribution

The study of heat and mass transfer problems is an important aspect of the field of moving boundary problems. Treatment of such type of problems becomes more challenging by the addition of convection term driven by fluid flow in the vapour, frozen porous and convective term due to mass transfer of the water vapour. Based on the literature cited above, a key shortcoming of available research on modelling of sublimation is related to insufficient modelling of the effect of convection in the frozen porous region and convective term of moisture transfer due to water vapour in the vapour region. Therefore, study of convective sublimation is necessary to meet the current technological demand of sublimation–dehydration. The major contribution of the present work are:

1. convective term due to moisture flow of water vapour is considered in vapour region.
2. presence of convection driven due to fluid flow is assumed within the porous frozen region, molar concentration of vapour moisture and in vapour region.
3. exact treatment for temperature and moisture profile as well as the location of the tracking of sublimation interface is presented for a particular velocity profile.

From this study it is found that convection plays a key important role during sublimation of a porous body. In the presence of convection, the rate of sublimation is enhanced and the material requires less time than usual to sublimate. It is also found that a large rate of evaporation of water vapour reduces the sublimation process. This result can be improved with offering lower rate of evaporation of water vapour. Results obtained from this study expected to contribute in food technology, especially in accelerated freeze-drying (AFD) technique. Similar to the sublimation, current study is also useful in desorption process, which is one of the important step in freeze-drying. The goal of the modern sublimation–dehydration process is designed to increase the temperature field of the desorption region to a high level under high vacuum (without loss of flavour of the biological products) after end of sublimation process. Thus, for future scope, the current study can have its direct application in freeze-drying involving sublimation and desorption, and evaporation of water crystals from vapour region.

Physical description and mathematical modelling of the problem

Analysis

To study the problem, consider a rigid, solid, porous half-space that contains evenly frozen moisture. The schematic diagram of the sublimation process described in the problem is depicted in Figs. 1 and 2 . The porous body resides in a low-pressure environment, therefore the main pressure acting on the frozen region is the moisture vapour pressure. Thus, we consider that during the sublimation, the environmental pressure (which remains unchanged) and vapour pressure (acting on the frozen region) are equal. Following these assumptions, the process of sublimation will occur at a constant sublimation temperature corresponding to the vapour pressure acting on the frozen region. The following additional assumptions are also made in order to formulate the sublimation process:

1. The vapour is treated to be an ideal gas due to the low vapour pressure.
2. Initial concentration profile within frozen phase is assumed to be uniform, denoted by $C_{m,0}$. For conveni-

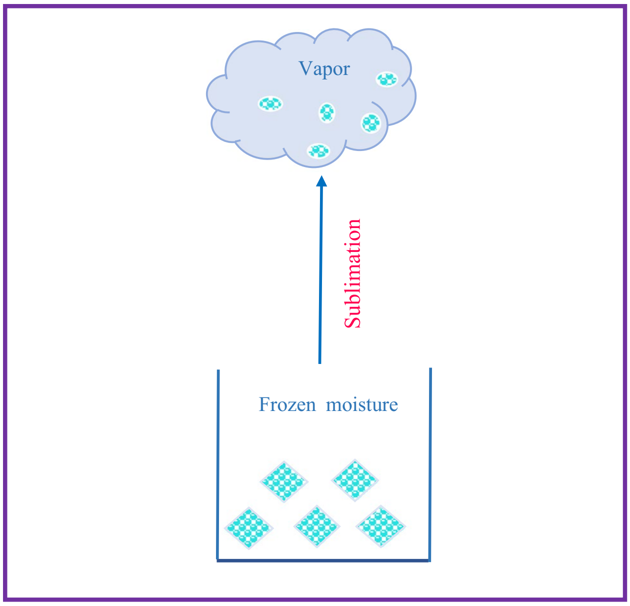


Fig. 2 Physical phenomena of the one-dimensional sublimation process of a frozen porous body in the presence of conduction as well as convection

ence, it is considered that at the sublimation state, p_v/F_vR_0, the value of $C_{m,0}$ is higher in compare to the value of the vapour molar concentration, where F_v and p_v denotes the sublimation temperature and vapour pressure acting on the frozen region, respectively, and R_0 represents the universal gas constant.
3. The frozen porous body is initially assumed to be at a fixed temperature $F_0(< F_v)$. Sublimation begins when the temperature of the frozen body reaches F_v.
4. At $x = 0$, a fixed molar concentration of the moisture, $C_{m,s}(< C_{m,0})$ and a fixed temperature $F_s(> F_v)$ is maintained to sublimate the frozen porous body.
5. The space $0 < x < s(t)$ represents the vapour region in which heat and mass transfer occurs, whereas the space $s(t) < x < \infty$ is the frozen region without moisture flow. $s(t)$ is the position of sublimation front.
6. The effect of the convective term due to moisture flow of the water vapour is accounted for in the vapour region.
7. Both conduction as well as convection heat transfer mechanism are considered in each region.
8. Constant thermophysical properties are assumed in each region.
9. Volumetric expansion during sublimation is neglected.

In the view of above assumptions, the mathematical description of sublimation process in heat and mass transfer is formulated as follows:

Mathematical modelling

The dynamics of one-dimensional heat-mass transfer in the sublimation process can be governed by below system of differential equations:

Vapour region for heat and mass transfer

$$\frac{\partial F_1}{\partial t} + u_1\frac{\partial F_1}{\partial x} = \alpha_1\frac{\partial^2 F_1}{\partial x^2} + \left(\frac{c_{pv}}{\rho_1 c_p}\frac{\mathrm{dw}}{\mathrm{dt}}\right)\frac{\partial F_1}{\partial x}, \quad 0 < x < s(t), \tag{1}$$

where F_1 represents the unknown temperature profile and ρ_1 is density, in the vapour region. The term on right side $\left(\frac{c_{pv}}{\rho_1 c_p}\frac{\mathrm{dw}}{\mathrm{dt}}\right)$ represents the convective term due to mass transfer of the water vapour, where w stands for rate of mass transfer [35].

$$\frac{\partial C_m}{\partial t} + u_m\frac{\partial C_m}{\partial x} = \alpha_m\frac{\partial^2 C_m}{\partial x^2}, \qquad 0 < x < s(t), \tag{2}$$

where C_m represents the unknown molar concentration of vapour moisture.

Frozen region

$$\frac{\partial F_2}{\partial t} + u_2\frac{\partial F_2}{\partial x} = \alpha_2\frac{\partial^2 F_2}{\partial x^2}, \qquad s(t) < x < \infty, \tag{3}$$

where F_2 is the unknown temperature distribution in the frozen porous region. α_1, α_m and α_2 are the thermal and mass diffusivity in the vapour and frozen regions, respectively. u_1, u_m and u_2 denote the unidirectional motion of phase change material in the vapour and frozen regions, respectively [45–48].

Initial condition

In the sublimation process, it is assumed that the frozen porous body is at a uniform initial temperature F_0, i.e.

$$F_2(x, t) = F_0, \qquad t = 0. \tag{4}$$

Boundary condition

At $x = 0$ the temperature and mass for vapour region is subjected to the following conditions,

$$F_1(x, t) = F_s, \qquad x = 0. \tag{5}$$

$$C_m(x, t) = C_{m,s}, \qquad x = 0. \tag{6}$$

Heat and mass balance condition

In order to determine the location of moving sublimation front as a function of time, an expression for energy balance may be written as follows:

$$k_2 \frac{\partial F_2}{\partial x} - k_1 \frac{\partial F_1}{\partial x} = C_{\mathrm{m},0} M_{\mathrm{m}} L \frac{\mathrm{d}s(t)}{\mathrm{d}t}, \qquad x = s(t), \tag{7}$$

and

$$\alpha_{\mathrm{m}} \frac{\partial C_{\mathrm{m}}}{\partial x} = \left(C_{\mathrm{m},0} - C_{\mathrm{m}}(x,t)\right) \frac{\mathrm{d}s(t)}{\mathrm{d}t}, \qquad x = s(t), \tag{8}$$

where latent heat of sublimation is denoted by L and M_{m} denotes molar mass of the moisture. In addition, at the sublimation interface, the temperature of the vapour and frozen regions is equal to the sublimation temperature, i.e.

$$F_1(x,t) = F_2(x,t) = F_{\mathrm{v}}, \qquad x = s(t). \tag{9}$$

It is assumed that as $x \to \infty$ the temperature of the frozen region approaches the initial temperature

$$F_2(x,t) = F_0, \qquad x \to \infty. \tag{10}$$

Dimensionless scaling parameters

The dimensional problem presented in Sect. 3.2 can be converted into non-dimensional form by introducing the following scaling parameters:

$$T_1 = 1 + \frac{F_1 - F_{\mathrm{v}}}{F_{\mathrm{s}} - F_{\mathrm{v}}}, \quad T_2 = \frac{F_2 - F_0}{F_{\mathrm{v}} - F_0}, \quad Ç = \frac{C_{\mathrm{m}} - C_{\mathrm{m,s}}}{C_{\mathrm{m},0} - C_{\mathrm{m,s}}}, \quad \alpha_{21} = \frac{\alpha_2}{\alpha_1}, \quad Lu = \frac{\alpha_{\mathrm{m}}}{\alpha_1},$$
$$\gamma = \frac{k_1(F_{\mathrm{s}} - F_{\mathrm{v}})}{k_2(F_{\mathrm{v}} - F_0)}, \quad l_0 = \frac{C_{\mathrm{m},0} M_{\mathrm{m}} L}{k_2(F_{\mathrm{v}} - F_0)} \alpha_1, \quad \beta = \frac{c_{\mathrm{pv}} M_{\mathrm{m}} C_{\mathrm{m},0}}{c_{\mathrm{p}} \rho_1}, \quad Pe = \frac{u_{\mathrm{i}}}{\sqrt{\frac{\alpha_{\mathrm{i}}}{t}}}, \; i = 1, 2, m. \tag{11}$$

Note that the definition of Pe presented above assumes that the velocity decays as $\frac{1}{\sqrt{t}}$. Under these transformations (11), the system of Eqs. (1)–(10) is converted into the following form,

Vapour region for heat and mass transfer

$$\frac{\partial T_1}{\partial t} + Pe\sqrt{\frac{\alpha_1}{t}} \frac{\partial T_1}{\partial x} = \alpha_1 \frac{\partial^2 T_1}{\partial x^2} + \left(\frac{c_{\mathrm{pv}}}{\rho_1 c_{\mathrm{p}}} \frac{\mathrm{d}w}{\mathrm{d}t}\right) \frac{\partial T_1}{\partial x}, \qquad 0 < x < s(t), \tag{12}$$

$$\frac{\partial Ç}{\partial t} + Pe\sqrt{\frac{\alpha_{\mathrm{m}}}{t}} \frac{\partial Ç}{\partial x} = \alpha_{\mathrm{m}} \frac{\partial^2 Ç}{\partial x^2}, \qquad 0 < x < s(t). \tag{13}$$

Frozen region

$$\frac{\partial T_2}{\partial t} + Pe\sqrt{\frac{\alpha_2}{t}} \frac{\partial T_2}{\partial x} = \alpha_2 \frac{\partial^2 T_2}{\partial x^2}, \qquad s(t) < x < \infty, \tag{14}$$

Initial condition

$$T_2(x,t) = 0, \qquad t = 0. \tag{15}$$

Boundary condition

$$T_1(x,t) = 2, \qquad x = 0. \tag{16}$$

$$Ç(x,t) = 0, \qquad x = 0. \tag{17}$$

Heat and mass balance condition

$$\frac{\partial T_2}{\partial x} - \gamma \frac{\partial T_1}{\partial x} = \frac{C_{\mathrm{m},0} M_{\mathrm{m}} L}{k_2(F_{\mathrm{v}} - F_0)} \frac{\mathrm{d}s(t)}{\mathrm{d}t}, \qquad x = s(t), \tag{18}$$

and

$$\frac{\partial Ç}{\partial x} = \frac{1}{\alpha_m} \left(\frac{C_{m,0} - C_m(x,t)}{C_{m,0} - C_{m,s}}\right) \frac{ds(t)}{dt}, \qquad x = s(t), \tag{19}$$

$$T_1(x,t) = T_2(x,t) = 1, \qquad x = s(t). \tag{20}$$

It is assumed that as $x \to \infty$ the temperature of the frozen region becomes approximately equal to the initial temperature, i.e.

$$T_2(x,t) = 0, \qquad x \to \infty. \tag{21}$$

Solution of the problem

The system of Eqs. (12, 14, 15, 16, 18, 20) and (21) that represent temperature distributions during the sublimation process in a half-porous space is similar to those that model temperature distribution during melting of a pure material in a similar geometry [36]. The solution of the current problem can be obtained by the use of similarity transformations to obtain ordinary differential equations as follows:

$$T \cong \theta_i, \qquad Ç \cong \theta_i, \qquad \xi = \frac{x}{2\sqrt{\alpha_1 t}}, \qquad s(t) = 2\lambda\sqrt{\alpha_1 t}, \tag{22}$$

where $i = 1, 2, m$ and λ is an unknown constant.

Solution of the vapour region

For heat transfer

The rate of moisture flow of the water vapour dw/dt vaporizes from the sublimation surface into gaseous form and this can be related with speed of sublimation front ds/dt. In Eq. (12), the term in right hand side dw/dt can be expressed in the manner [35],

$$\frac{\mathrm{d}w}{\mathrm{d}t} \simeq C_{\mathrm{m},0} M_{\mathrm{m}} \frac{\mathrm{d}s}{\mathrm{d}t}. \tag{23}$$

Combining Eqs. (22) and (23), one may obtain

$$\frac{\mathrm{d}w}{\mathrm{d}t} \simeq C_{\mathrm{m},0} M_{\mathrm{m}} \lambda \sqrt{\frac{\alpha_1}{t}}. \tag{24}$$

Now, Eq. (12) along with respective boundary conditions may be written as,

$$\frac{\mathrm{d}^2\theta_1}{\mathrm{d}\xi^2} + 2(\xi - Pe + \beta\lambda)\frac{\mathrm{d}\theta_1}{\mathrm{d}\xi} = 0, \qquad 0 < \xi < \lambda. \tag{25}$$

with

$$\theta_1(\xi) = 2, \qquad \xi = 0 \tag{26}$$

and

$$\theta_1(\xi) = 1, \qquad \xi = \lambda. \tag{27}$$

The exact solution of Eqs. (25) and (26) satisfying the boundary conditions can be obtained as [29, 40]

$$\theta_1(\xi) = \frac{\mathrm{Erf}(Pe - \beta\lambda) + \mathrm{Erf}(Pe - \xi - \beta\lambda) - 2\,\mathrm{Erf}(Pe - (1+\beta)\lambda)}{\mathrm{Erf}(Pe - \beta\lambda) - \mathrm{Erf}(Pe - (1+\beta)\lambda)}, \tag{28}$$

where Erf(.) is the error function that occurs commonly in transport problems in semi-infinite bodies [49].

For mass transfer

With the help of Eq. (22), the moisture Eq. (13) with their associated boundary conditions can be reduce to

$$Lu\frac{\mathrm{d}^2\theta_{\mathrm{m}}}{\mathrm{d}\xi^2} + 2(\xi - Pe\sqrt{Lu})\frac{\mathrm{d}\theta_{\mathrm{m}}}{\mathrm{d}\xi} = 0, \qquad 0 < \xi < \lambda. \tag{29}$$

with

$$\theta_{\mathrm{m}}(0) = 0, \qquad \xi = 0 \tag{30}$$

and

$$\frac{\mathrm{d}\theta_{\mathrm{m}}(\lambda)}{\mathrm{d}\xi} = 2\frac{\lambda}{Lu}\big(1 - \theta_{\mathrm{m}}(\lambda)\big), \qquad \xi = \lambda \tag{31}$$

for which, the solution may be expressed as,

$$\theta_{\mathrm{m}}(\xi) = \frac{\lambda\sqrt{\pi}\left(\mathrm{Erf}(Pe) - \mathrm{Erf}\left(Pe - \frac{\xi}{\sqrt{Lu}}\right)\right)}{\left(\sqrt{Lu}\,\mathrm{Exp}\left(-\frac{(\lambda - Pe\sqrt{Lu})^2}{Lu}\right) + \sqrt{\pi}\,\lambda\left(\mathrm{Erf}(Pe) - \mathrm{Erf}\left(Pe - \frac{\lambda}{\sqrt{Lu}}\right)\right)\right)}. \tag{32}$$

Solution of the frozen region

In a similar fashion, Eq. (14) for the frozen region can be reduced to the following form

$$\alpha_{21}\frac{\mathrm{d}^2\theta_2}{\mathrm{d}\xi^2} + 2(\xi - Pe\sqrt{\alpha_{21}})\frac{\mathrm{d}\theta_2}{\mathrm{d}\xi} = 0, \qquad \lambda < \xi < \infty \tag{33}$$

with

$$\theta_2(\xi) = 1, \qquad \xi = \lambda \tag{34}$$

and

$$\theta_2(\infty) = 0, \qquad \xi = \infty \tag{35}$$

for which, the solution is given by

$$\theta_2(\xi) = \frac{1 + \mathrm{Erf}\left(Pe - \frac{\xi}{\sqrt{\alpha_{21}}}\right)}{1 + \mathrm{Erf}\left(Pe - \frac{\lambda}{\sqrt{\alpha_{21}}}\right)}. \tag{36}$$

With the help of Eq. (22), the heat and moisture balance condition given by Eq. (18) can be put in the form

$$\frac{\mathrm{d}\theta_2}{\mathrm{d}\xi} - \gamma\frac{\mathrm{d}\theta_1}{\mathrm{d}\xi} = 2\,\lambda\, l_0, \qquad \xi = \lambda. \tag{37}$$

Condition for sublimation limit

A key limitation of the solution of the molar concentration in the vapour region, (Eq. (30)) is that the molar concentration of the vapour at the sublimation front $x = s(t)$ must not exceed the value of p_v/F_vR_0 [36]. Equation (32) can be written as

$$\frac{C_m(x,t) - C_{m,s}}{C_{m,0} - C_{m,s}} = \frac{\lambda\sqrt{\pi}\left(\mathrm{Erf}(Pe) - \mathrm{Erf}\left(Pe - \frac{\xi}{\sqrt{Lu}}\right)\right)}{\left(\sqrt{Lu}\,\mathrm{Exp}\left(-\frac{(\lambda - Pe\sqrt{Lu})^2}{Lu}\right) + \sqrt{\pi}\,\lambda\left(\mathrm{Erf}(Pe) - \mathrm{Erf}\left(Pe - \frac{\lambda}{\sqrt{Lu}}\right)\right)\right)} \tag{38}$$

In order to determine this limiting condition, let

$$C_{m,max} = \frac{p_v}{F_vR_0} \quad \text{and} \quad C = \frac{C_{m,0} - C_{m,max}}{C_{m,max} - C_{m,s}}. \tag{39}$$

The condition for the sublimation limit with Luikov number and convection effect can be obtained from Eq. (38). Since, $C_m(s(t),t) \le C_{m,max}$, therefore

$$\frac{\lambda\sqrt{\pi}\left(\mathrm{Erf}(Pe) - \mathrm{Erf}\left(Pe - \frac{\xi}{\sqrt{Lu}}\right)\right)}{\left(\sqrt{Lu}\,\mathrm{Exp}\left(-\frac{(\lambda - Pe\sqrt{Lu})^2}{Lu}\right) + \sqrt{\pi}\,\lambda\left(\mathrm{Erf}(Pe) - \mathrm{Erf}\left(Pe - \frac{\lambda}{\sqrt{Lu}}\right)\right)\right)} \le \frac{C_{m,max} - C_{m,s}}{C_{m,0} - C_{m,max}} = \frac{1}{C}, \tag{40}$$

which can be rearranged as

$$C \le \frac{1}{\lambda\sqrt{\pi}\left(\mathrm{Erf}(Pe) - \mathrm{Erf}\left(Pe - \frac{x}{2\sqrt{Lu\,\alpha_1 t}}\right)\right)\left(\sqrt{Lu}\,\mathrm{Exp}\left(-\frac{(\lambda-Pe\sqrt{Lu})^2}{Lu}\right) + \sqrt{\pi}\,\lambda\left(\mathrm{Erf}(Pe) - \mathrm{Erf}\left(Pe - \frac{\lambda}{\sqrt{Lu}}\right)\right)\right)^{-1}}. \tag{41}$$

Finally, using Eq. (22), the following limiting condition may be derived

$$C \le \frac{1}{\lambda\sqrt{\pi}\left(\mathrm{Erf}(Pe) - \mathrm{Erf}\left(Pe - \frac{\lambda}{\sqrt{Lu}}\right)\right)\left(\sqrt{Lu}\,\mathrm{Exp}\left(-\frac{(\lambda-Pe\sqrt{Lu})^2}{Lu}\right) + \sqrt{\pi}\,\lambda\left(\mathrm{Erf}(Pe) - \mathrm{Erf}\left(Pe - \frac{\lambda}{\sqrt{Lu}}\right)\right)\right)^{-1}}. \tag{42}$$

Eq. (42) represents the limiting condition for the sublimation process to occur in the presence of convection. From Eq. (39), we observe that for a constant sublimation pressure, either a large value $C_{m,0}$ or a large value of $C_{m,s}$ gives a large value of C.

Some of these trade-offs between various factors in this problem are illustrated in sublimation curves shown in Figs. 3 and 4 . Sublimation may occur only in the region under these curves. From Fig. 3, it is evident that in the presence of convection, the sublimation limit increases more in compare to in the absence of convection. Moreover, positive value of the Luikov number Lu accelerates the sublimation limit as shown in Fig. 4. Consequently, high diffusivity of moisture through the vapour zone is required to keep the process under the sublimation limit.

Analysis of existence of the analytical solution

Determination of location and speed of the sublimation front depending on time is usually important in moving boundary problems. In the current work, this can be obtained from Eq. (37) along with the use of Eqs. (28) and (36), i.e.

$$\frac{\gamma\,\mathrm{Exp}\left(-(Pe-(1+\beta)\lambda)^2\right)}{\mathrm{Erf}(Pe-\beta\lambda) - \mathrm{Erf}(Pe-(1+\beta)\lambda)} - \frac{\mathrm{Exp}\left(-(Pe - \frac{\lambda}{\sqrt{\alpha_{21}}})^2\right)}{\sqrt{\alpha_{21}}\left(1 + \mathrm{Erf}\left(Pe - \frac{\lambda}{\sqrt{\alpha_{21}}}\right)\right)} = \lambda\, l_0\sqrt{\pi}. \tag{43}$$

Now, we show the existence of the solution of the problem (25)-(37) by defining a function of the form [45, 46],

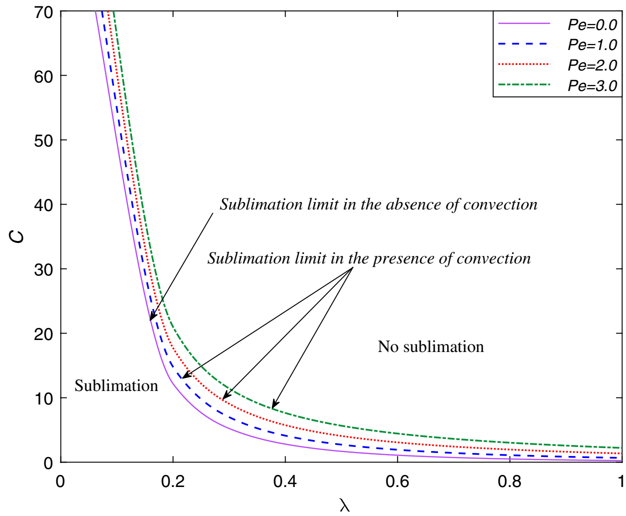


Fig. 3 Condition for the limitation of the sublimation process in absence of convection ($Pe = 0.0$) and in the presence of convection ($Pe = 1.0, 2.0, 3.0$)

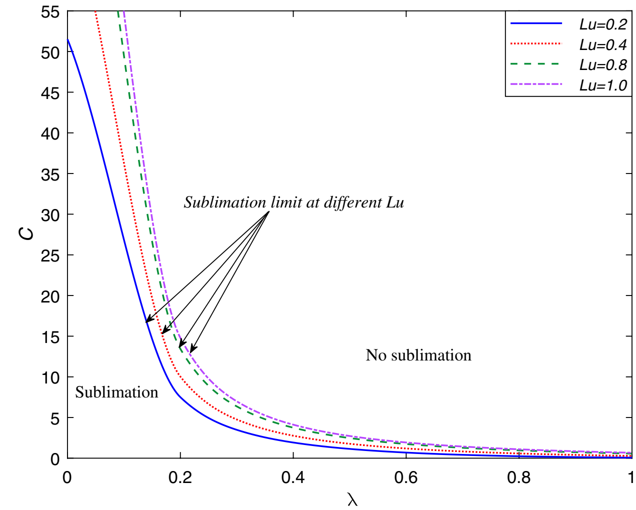


Fig. 4 Condition for the limitation of the sublimation process for different value of Luikov number Lu

$$f(\lambda) = \frac{\gamma \, \mathrm{Exp}\left(-(Pe - (1+\beta)\lambda)^2\right)}{\mathrm{Erf}(Pe - \beta\lambda) - \mathrm{Erf}(Pe - (1+\beta)\lambda)} - \frac{\mathrm{Exp}\left(-(Pe - \frac{\lambda}{\sqrt{\alpha_{21}}})^2\right)}{\sqrt{\alpha_{21}}\left(1 + \mathrm{Erf}\left(Pe - \frac{\lambda}{\sqrt{\alpha_{21}}}\right)\right)} - \lambda \, l_0 \sqrt{\pi}. \tag{44}$$

Eq. (43) represents a transcendental condition governing the sublimation front location, which can be solved to determine the value of λ, for example, using the Newton–Raphson method.

Note that, for positive real values of parameters Pe, β, γ and α_{21}, $\lim_{\lambda \to 0^+} f(\lambda)$ is negative while $\lim_{\lambda \to \infty} f(\lambda)$ gives positive. This, along with the continuous and differentiable nature of the function based on Eq. (44) confirms that there exists at least one root of $f(\lambda)$ over $(0, \infty)$. Moreover, under these conditions, the derivative of $f(\lambda)$ is always positive over $(0, \infty)$. Hence, $f(\lambda)$ has a unique root over $(0, \infty)$. The next section discusses the effect of various parameters of this problem on the sublimation process.

Results and discussion

This section discusses the heat transfer phenomena, molar concentration and heat and mass transfer with molar concentration in vapour region. In the last subpart, the effect of various parameters on sublimation process is also discussed. For the clear illustration of the results we have discussed each subpart separately. All computations and figures are performed in MATHEMATICA and MATLAB software.

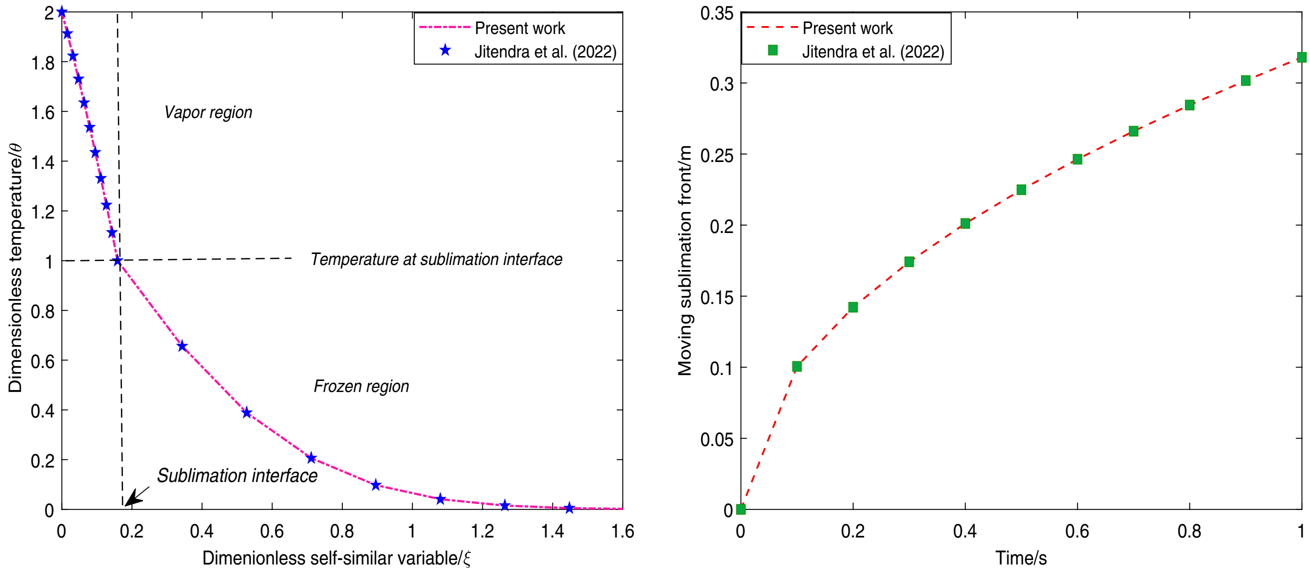
Validation of analytical work

It is much important and necessary to validate our analytical/numerical work with previous studies either in general or specific cases. To validate the current analytical work, we compare our study with the study presented by Jitendra et al. [40]. To proceed with comparison, we have removed convective term due to mass transfer of water vapour in vapour region and convection in frozen region in the current model. In the similar manner, we have removed convective term of mass transfer of the water vapour in the frozen region in the mathematical model presented by Jitendra et al. [40]. Range of value of parameters are taken as those given in [40]. Fig. 5a plots for temperature field at fixed parameter $\alpha_{21} = 0.5, Pe = 1.0, \gamma = 0.5, l_0 = 5$ and Fig. 5b plots for sublimation interface at fixed parameter $\alpha_{21} = 0.5, Pe = 1.0, \gamma = 0.5, l_0 = 5, \alpha_1 = 1.0$. Fig. 5a shows a strong agreement of our temperature field with temperature field of Jitendra et al. [40]. Fig. 5b also depicts that result for sublimation interface obtained in current work and those given in Jitendra et al. [40] are in strong acceptance. Therefore, current analytical work has an excellent agreement with the results presented by Jitendra et al. [40].

Heat transfer process

Effect of Péclet number (*Pe*)

In the present work, impact of convection is illustrated in the vapour and frozen region with variation of Péclet number Pe. Péclet number is the non-dimensional ratio of rate of advective transport of a material to the rate of moving molecules from high concentration to lower concentration of

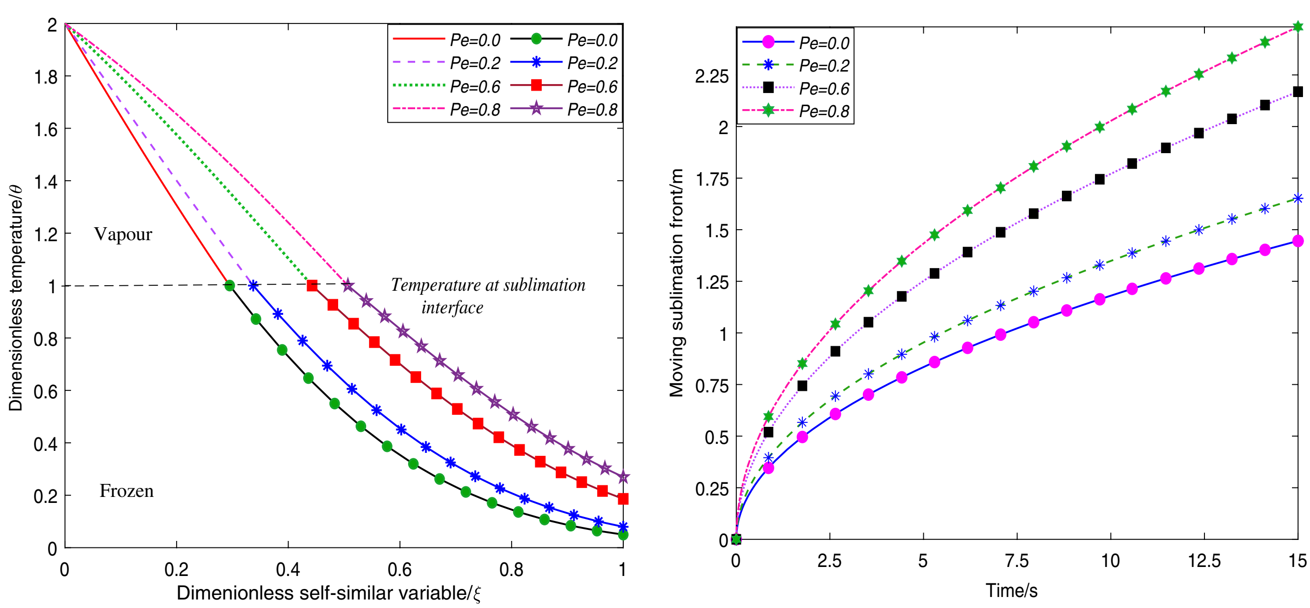


(a) Temperature profile in vapour and frozen region at $\alpha_{21} = 0.5, Pe = 1.0, \gamma = 0.5, l_0 = 5$

(b) Moving sublimation front at $\alpha_{21} = 0.5, Pe = 1.0, \gamma = 0.5, l_0 = 5, \alpha_1 = 1.0$

Fig. 5 Comparison of analytical results with the results of Jitendra et al. [40] for temperature field as well as sublimation interface

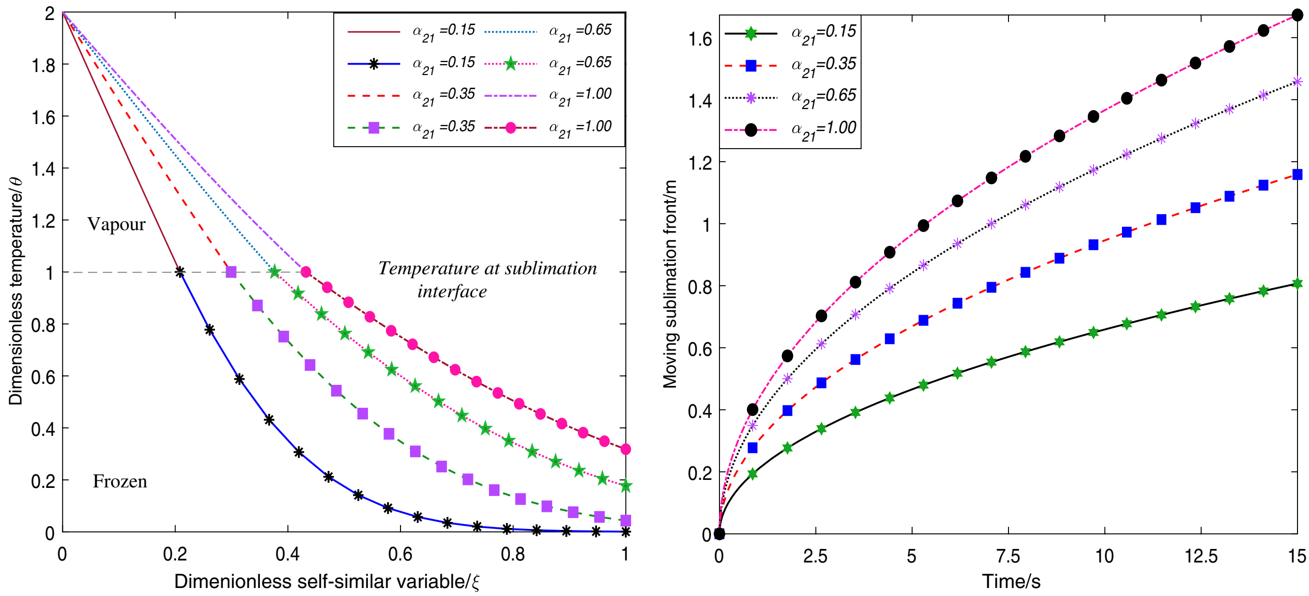
the same physical substance. Fig. 6a and b depicts the temperature profile in the vapour and frozen region and corresponding propagation rate of sublimation front for different Péclet numbers ($Pe = 0.0, 0.2, 0.6, 0.8$) at the fixed value of parameters $\alpha_{21} = 0.4, \beta = 0.3, \gamma = 1.0, l_0 = 0.5$. From Fig. 6a and b, we found that temperature profile in the vapour and frozen region rises with increasing the value of Pe. Further, the rate of propagation of the sublimation interface grows as well. For higher rate of convection, the energized particles vibrates faster and faster than usual at a certain temperature, as a result, temperature field increased and material sublimate faster. This observation is similar to the observation obtained by Jitendra et al. [40] and Chaurasiya and Singh [44].



(a) Temperature profile in vapour and frozen region at $\alpha_{21} = 0.4, \beta = 0.3, \gamma = 1.0, l_0 = 0.5$

(b) Moving sublimation front at $\alpha_{21} = 0.4, \beta = 0.3, \gamma = 1.0, l_0 = 0.5, \alpha_1 = 1.0$

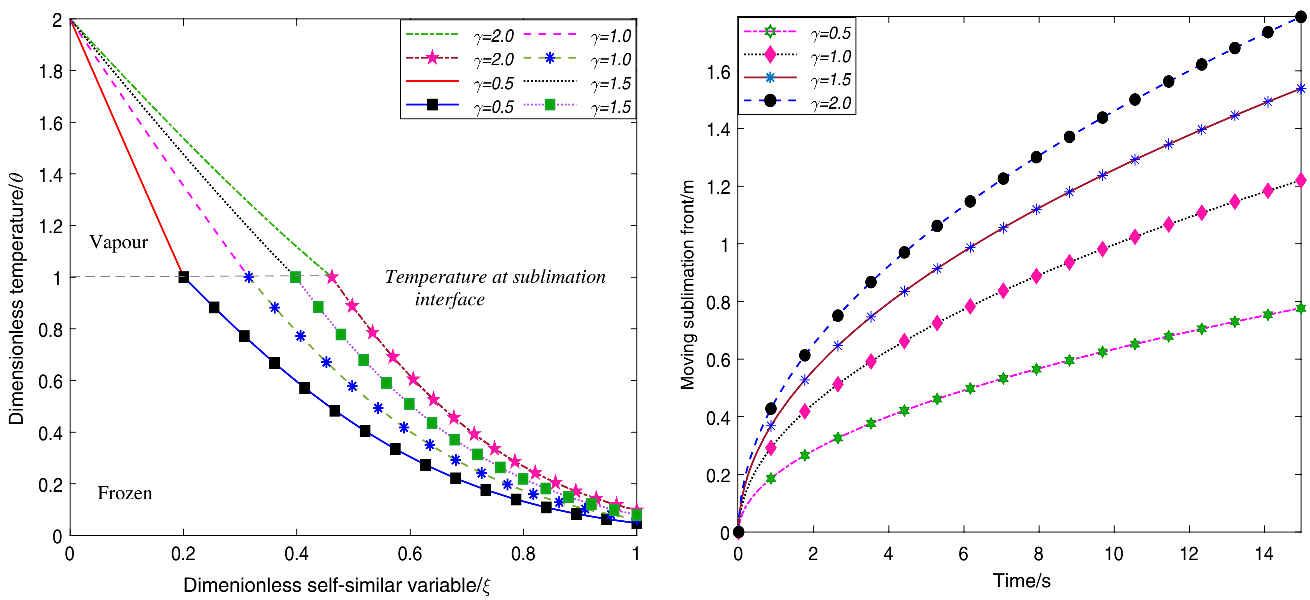
Fig. 6 Effect of Péclet number on temperature and moving sublimation front



(a) Temperature profile in vapour and frozen region at $Pe = 0.1, \beta = 0.3, \gamma = 1.0, l_0 = 0.5$

(b) Moving sublimation front at $Pe = 0.1, \beta = 0.3, \gamma = 1.0, l_0 = 0.5, \alpha_1 = 1.0$

Fig. 7 Effect of thermal diffusivity on temperature and moving sublimation front



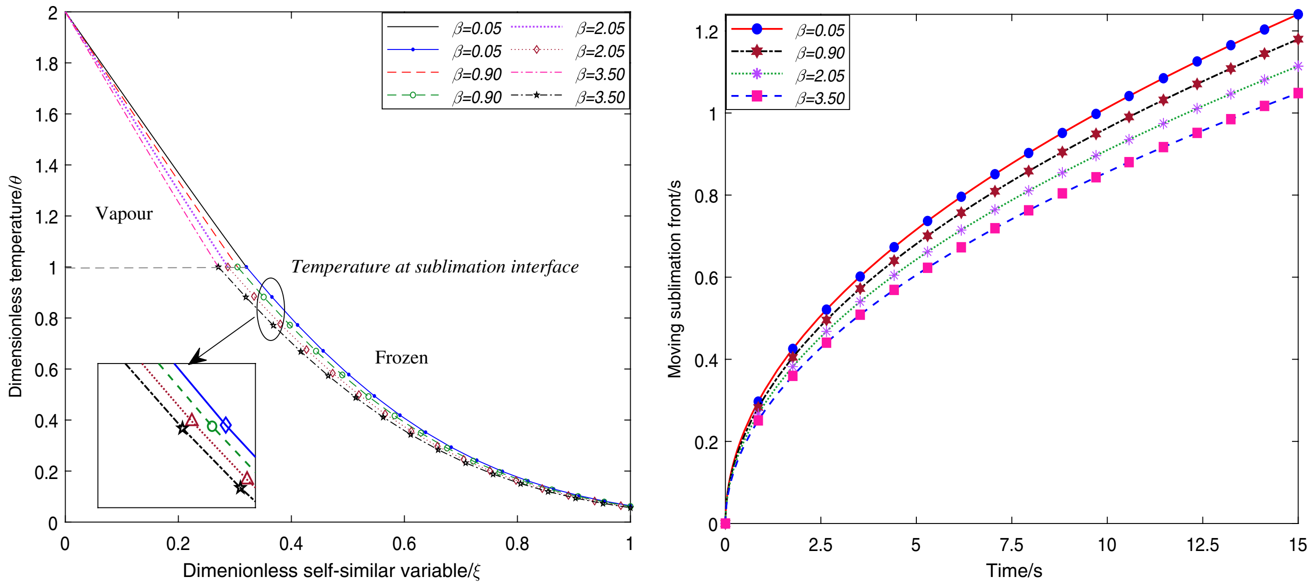
(a) Temperature profile in vapour and frozen region at $Pe = 0.1, \alpha_{21} = 0.4, \beta = 0.3, l_0 = 0.5$

(b) Moving sublimation front at $Pe = 0.1, \alpha_{21} = 0.4, \beta = 0.3, l_0 = 0.5, \alpha_1 = 1.0$

Fig. 8 Effect of heat flux on temperature and moving sublimation front

Effect of thermal diffusivity (α_{21})

Thermal diffusivity α_{21} is the ratio of the thermal diffusivities of the frozen and vapour regions. Fig. 7a and b shows the effect of α_{21} on temperature profile in the vapour and frozen regions and tracking of sublimation front at fixed value of parameters $Pe = 0.1, \beta = 0.3, \gamma = 1.0, l_0 = 0.5$. Fig. 7a and b shows that the temperature distribution in the vapour and frozen region increases with increasing value of α_{21}. Moreover, the growth rate of the sublimation front increases for



(a) Temperature profile in vapour and frozen region at $Pe = 0.1, \alpha_{21} = 0.4, \gamma = 1.0, l_0 = 0.5$

(b) Moving sublimation front at $Pe = 0.1, \alpha_{21} = 0.4, \gamma = 1.0, l_0 = 0.5, \alpha_1 = 1.0$

Fig. 9 Effect of coefficient of convective term on temperature and moving sublimation front

large value of α_{21}. The physical reasoning behind this observation is that large α_{21} implies large value of α_2 relative to α_1, which implies the faster heat flow in the frozen region or less water vapour will be absorbed by the sublimated region. This result is similar to the result those obtained by Lin [36].

Effect of heat flux (γ)

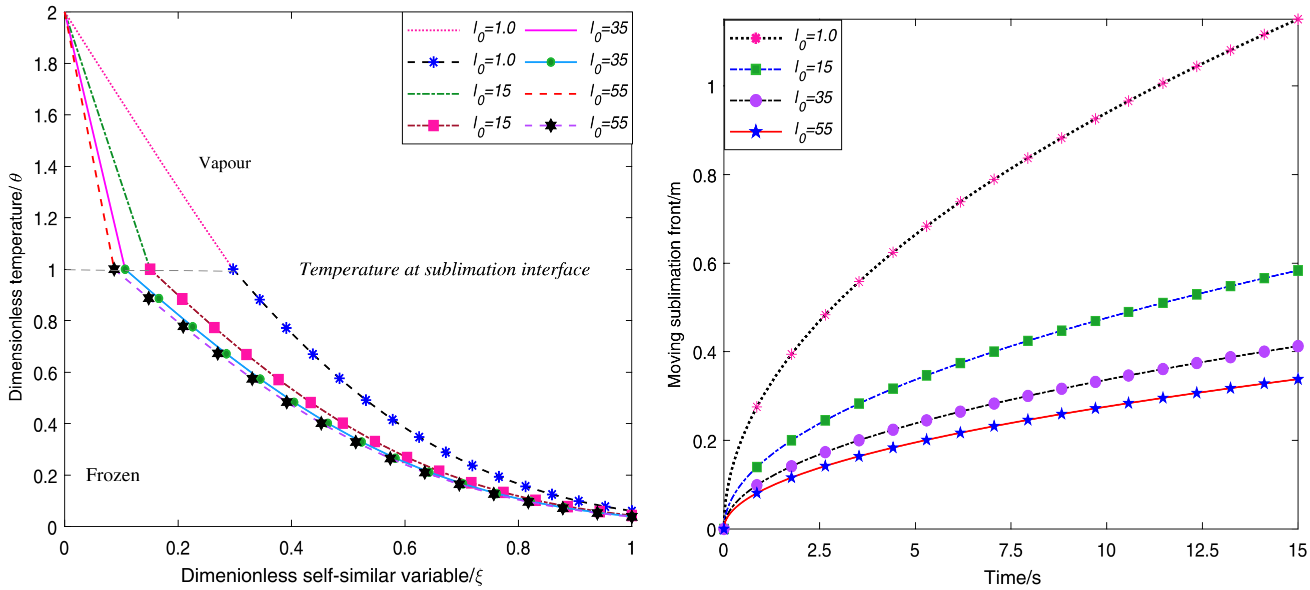
Heat flux γ is the ratio of steady thermal flux within vapour region to that in the frozen region with the same thermal conduction space. The effect of γ on the temperature profile and moving sublimation front at fixed value of parameters $Pe = 0.1, \alpha_{21} = 0.4, \beta = 0.3, l_0 = 0.5$ is shown in Fig. 8a and b. From Fig. 8a, it is evident that with increasing the value of heat flux, temperature in the vapour and frozen region increases. Furthermore, the transition process speed up with increasing γ and thus, the material sublimates faster, as shown in Fig. 8b. The lower heat flux within frozen region produces higher heat flux, as a result faster sublimation rate is obtained. This situation is similar to the result presented by Lin [36].

Effect of coefficient of convective term (β)

The coefficient of convective term β models vapour flow in the vapour region. Fig. 9a presents the effect of changing β on the temperature distribution in the vapour and frozen regions. Fig. 9b plots the evolution of the sublimation interface. Parameter values are $Pe = 0.1, \alpha_{21} = 0.4, \gamma = 1.0, l_0 = 0.5$. Fig. 9a shows that increasing the value of β results in steeper temperature profile and corresponding rate of propagation of the sublimation interface deterred. Hence, the sublimation process slows down for higher value of β. For higher rate of evaporation of water vapour, molecules require much energy at the sublimation interface to sublimate the material which causes a lower temperature response is recorded within vapour region. Therefore, sublimation deterred for large rate of water evaporation from sublimation surface. This finding is similar to the finding of the experimental work presented by Hayashi and Komori [35] and Chaurasiya and Singh [44].

Effect of latent heat of sublimation (l_0)

The impact of phase change heat of sublimation on temperature distribution in the vapour and frozen region and moving sublimation interface at fixed value of parameters $Pe = 0.1, \alpha_{21} = 0.4, \beta = 0.3, \gamma = 1.0$ as shown in Fig. 10a and b. Fig. 10a shows that for higher value of the latent heat of sublimation, there is lower temperature rise within the vapour and frozen region. Consequently, the sublimation process gets deterred with increasing the value of l_0 as illustrated in Fig. 10b. Due to higher rate of thermal transition within vapour region, the particle required more energy to sublimate material. As a result, material requires more time than usual to sublimate. This observation is similar to the observation obtained by Lin [36].



(a) Temperature profile in vapour and frozen region at $Pe = 0.1, \alpha_{21} = 0.4, \beta = 0.3, \gamma = 1.0$

(b) Moving sublimation front at $Pe = 0.1, \alpha_{21} = 0.4, \beta = 0.3, \gamma = 1.0, \alpha_1 = 1.0$

Fig. 10 Effect of latent heat of sublimation on temperature and moving sublimation front

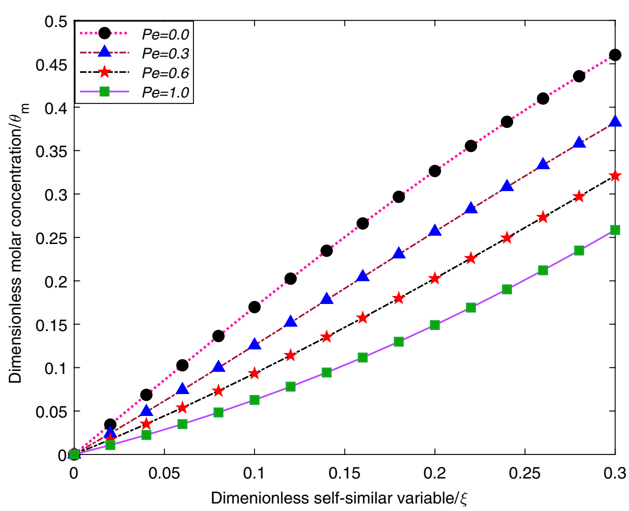


Fig. 11 Effect of Péclet number on molar concentration of vapour moisture

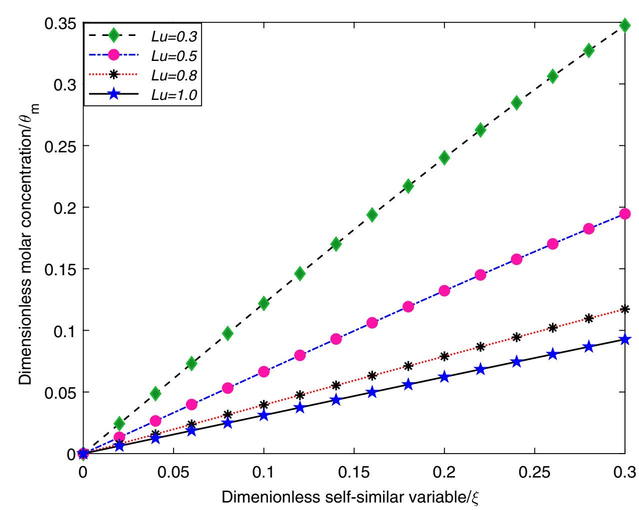


Fig. 12 Effect of Luikov number on molar concentration of vapour moisture

Moisture transfer process

At the sublimation interface $\xi = \lambda$,

$$\left.\begin{aligned} & C_{\mathrm{m}}(\lambda) > C_{\mathrm{m,s}} \\ \text{or} \quad & C_{\mathrm{m},0} - C_{\mathrm{m}}(\lambda) < C_{\mathrm{m},0} - C_{\mathrm{m,s}}, \\ \text{or} \quad & \frac{C_{\mathrm{m},0} - C_{\mathrm{m}}(\lambda)}{C_{\mathrm{m},0} - C_{\mathrm{m,s}}} < 1, \\ \text{or} \quad & \delta < 1, \end{aligned}\right\} \tag{45}$$

where $\delta = \frac{C_{\mathrm{m},0} - C_{\mathrm{m}}(\lambda)}{C_{\mathrm{m},0} - C_{\mathrm{m,s}}}$.

Effect of Péclet number (*Pe*)

The variation of Péclet number on the molar concentration of the vapour moisture at the fixed value of parameters $Lu = 0.25$, $\delta = 0.5$ and $\lambda = 0.3$ is illustrated in Fig. 11. This plot shows that with positive value of Péclet number, the

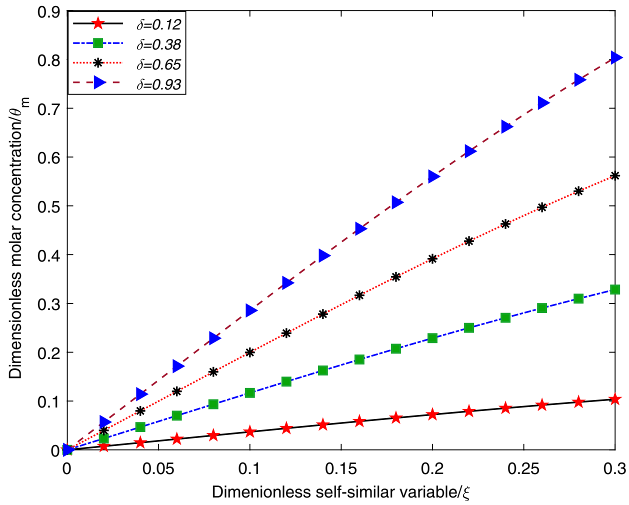


Fig. 13 Effect of δ on molar concentration of vapour moisture

molar concentration of the vapour moisture decreases. Furthermore, in the presence of the convection the rate of the molar concentration of the vapour moisture is lower than in the absence of convection as shown in Fig. 11. Similar situation is obtained in the work presented by Jitendra et al. [40].

Effect of Luikov number (Lu)

Luikov number Lu is defined as the dimensionless ratio of mass diffusivity to the diffusivity in vapour region. Fig. 12 presents the effect of Luikov number on the molar concentration of the vapour moisture at the fixed value of parameters $Pe = 0.1, \delta = 0.5$ and $\lambda = 0.3$. Fig. 12 shows that the molar concentration curve becomes steeper with higher value of Lu. Since, the diffusion of molecules within the frozen region deterred, therefore, the sublimation process becomes slow. This result is similar to the result of Jitendra et al. [40] and Chaurasiya and Singh [44].

Effect of δ

As defined in Eq. (45), the effect of δ for values less than unity on the molar concentration of the vapour moisture at the fixed value of parameters $Pe = 0.1, Lu = 0.25$ and $\lambda = 0.3$ is shown in Fig. 13. From this figure, we find that increasing the value of δ, then it increases the molar concentration of the vapour moisture. The larger value of difference between initial concentration and concentration at sublimation interface increases the value of δ.

Heat and moisture transfer process with molar concentration

Effect of thermal diffusivity (α_{21})

The effect of heat diffusivity (α_{21}) on temperature distribution is presented in Fig. 14. This plot shows that for higher value of α_{21} there is greater temperature rise in the vapour and frozen region and the molar concentration of the vapour moisture is also increased. This phenomenon confirms that the sublimation process gets accelerated with increasing the value of (α_{21}). During sublimation process, material absorbs little amount of heat and transfer maximum amount of heat so that material sublimate fast. This result is similar to the result of Lin [36].

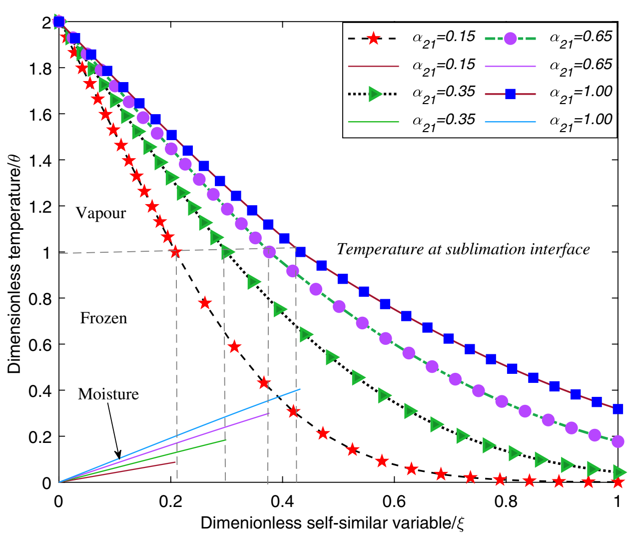


Fig. 14 Temperature profile in heat and mass transfer with molar concentration for different value of thermal diffusivity α_{21}

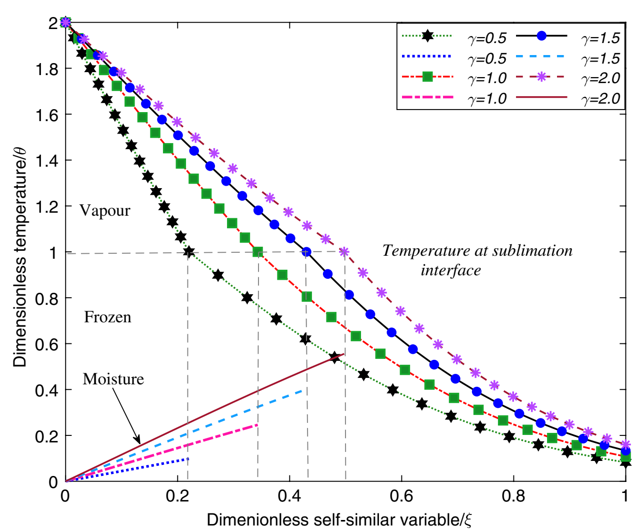


Fig. 15 Temperature profile in heat and mass transfer with molar concentration for different value of heat flux γ

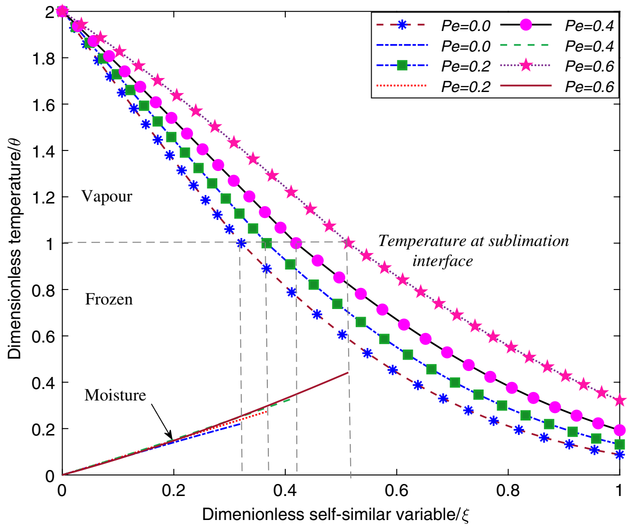


Fig. 16 Temperature profile in heat and mass transfer with molar concentration for different value of Péclet number *Pe*

Effect of heat flux (γ)

The variation of steady heat flux in the heat and mass transfer with molar concentration of the vapour moisture is shown in Fig. 15. From this figure, it is estimated that the temperature grows in the vapour and frozen region with corresponding increment in the value of heat flux. Further, the molar concentration of the vapour moisture get accelerated for positive value of γ. Consequently, the material sublimate fast for higher value of the heat flux. This conclusion is similar to the conclusion made by Lin [36].

Effect of Péclet number (*Pe*)

The impact of convection in the heat and mass transfer with molar concentration of the vapour moisture is shown with variation of Péclet number *Pe*. The temperature configuration in the vapour and moisture region increases with increasing the value of Pe as illustrated in Fig. 16. With positive value of *Pe*, the rate of the concentration of the vapour moisture also increases. Moreover, the sublimation process enhanced more with convection while it becomes slower without convection, see Fig. 16. Hence, less time will be required to complete the sublimation process. This result is similar to the result those obtained by Jitendra et al. [40] and Chaurasiya and Singh [44].

Effect of coefficient of convective term (β)

The effect of coefficient of convective term (β) due to moisture flow of the water vapour on temperature profile is given in Fig. 17. From this figure, it is observed that with increasing the value of β there is steeper in the temperature profile within the vapour and frozen region and the molar concentration of the vapour moisture is also deterred. This shows that the process of sublimation becomes slowed down for higher value of the coefficient of convective term (β). This result is similar to the result obtained by Chaurasiya and Singh [44].

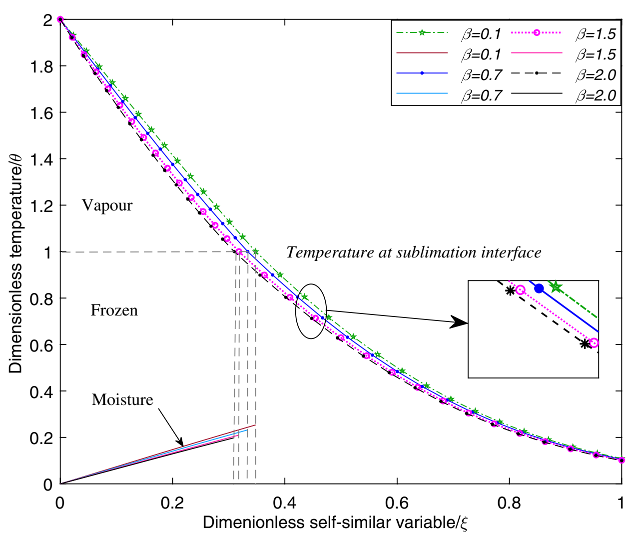


Fig. 17 Temperature profile in heat and mass transfer with molar concentration for different value of coefficient of convective term β

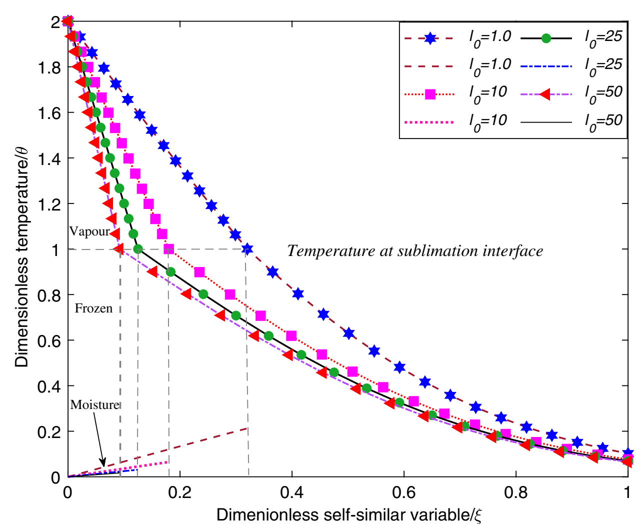
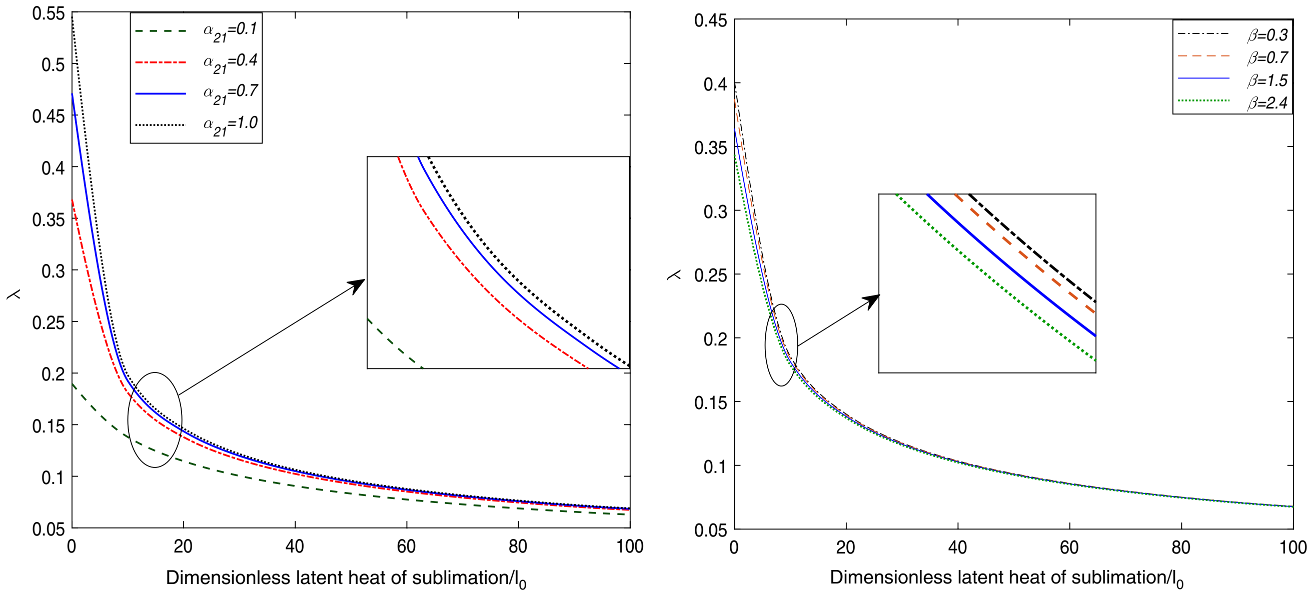
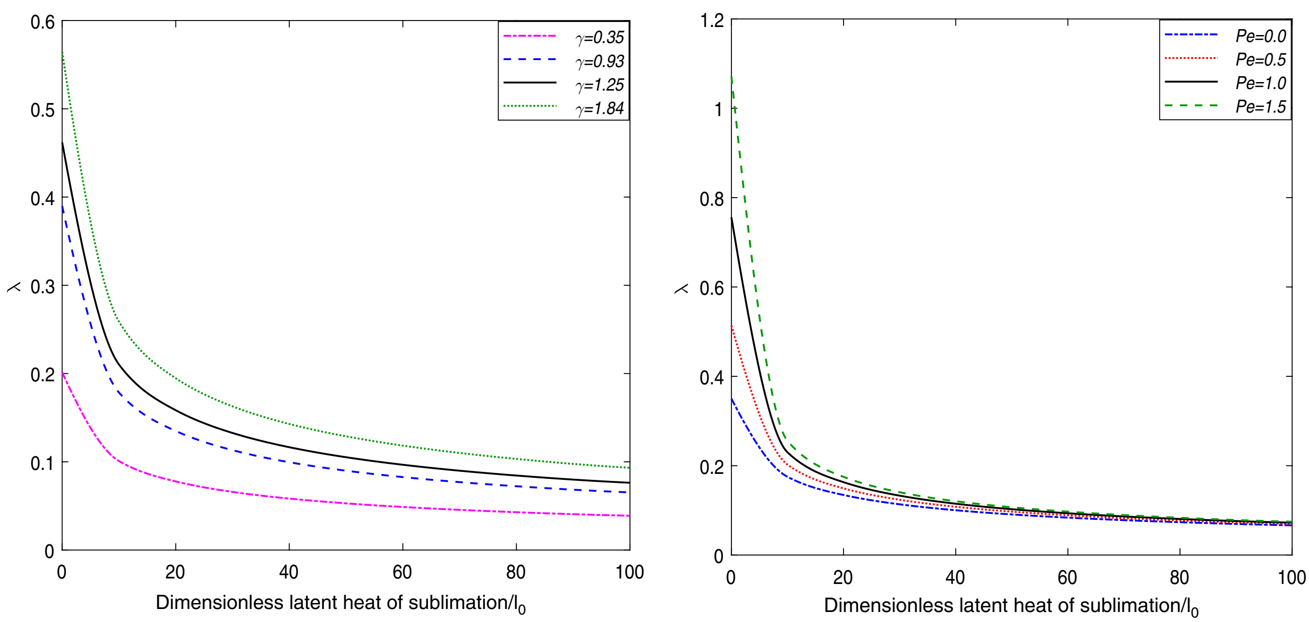


Fig. 18 Temperature profile in heat and mass transfer with molar concentration for different value of latent heat of sublimation l_0



(a) Variation of α_{21} at $Pe = 0.2, \beta = 0.15, \gamma = 1.0$ **(b)** Variation of β at $Pe = 0.2, \alpha_{21} = 0.5, \gamma = 1.0$

Fig. 19 Effect of thermal diffusivity α_{21} and β on growth rate parameter λ



(a) Variation of γ at $Pe = 0.2, \alpha_{21} = 0.5, \beta = 0.15$ **(b)** Variation of Pe at $\alpha_{21} = 0.5, \beta = 0.15, \gamma = 1.0$

Fig. 20 Effect of heat flux γ and Pe on growth rate parameter λ

Effect of latent heat of sublimation (l_0)

The phase change heat of sublimation at a fixed temperature is the amount of heat required to change a unit mass of frozen material into vapour. The latent heat of sublimation affects the temperature profile within the vapour and frozen region and also the molar concentration as shown in Fig. 18. This figure illustrated that with increasing the value of l_0 there is a decay in the temperature within the vapour and frozen region. For large value of the latent heat of sublimation,

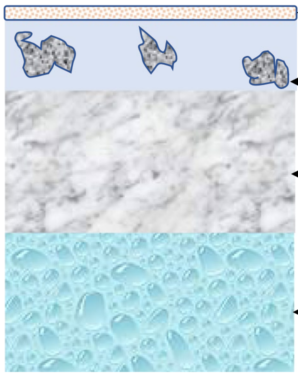


Fig. 21 Chemical reaction describing separation process of NH_4Cl and $NaCl$ [40]

the molar concentration of the vapour moisture decreases. Consequently, the sublimation process becomes slow. This observation is similar to the result of Lin [36].

Effect of latent heat of sublimation on λ

Figures 19a and 20b illustrate the effect of thermal diffusivity and latent heat of sublimation l_0 on the growth rate parameter λ. In Fig. 19a, we show the effect of thermal diffusivity on λ at $Pe = 0.2, \beta = 0.15$ and $\gamma = 1.0$. From this figure, it is evident that higher value of l_0 yields smaller λ and thus, sublimation process becomes slow. Further, with increasing the value of α_{21}, the corresponding value of λ increases for smaller value of l_0. Therefore, the sublimation process increases gradually. In the similar fashion, if we increase the value of β, then there is a small decrease in the value of λ. Consequently, sublimation process becomes slow, see Fig. 19b. Now, we discuss the effect of the heat flux on λ, as shown in Fig. 20a. This figure depicts that for a higher value of heat flux result in faster sublimation process. From Fig. 20b, it is seen that sublimation becomes fast with convection while there is delay in the absence of convection.

Applications and further extensions

Separation process

Sublimation is commonly used for separation processes involving a sublimate with volatile component and a non-sublimate impurity. Consider a compound of ammonium chloride (NH_4Cl) and sodium chloride ($NaCl$) in a disc. A cotton plug is placed over the funnel as shown in Fig. 21. When applying heat to the surface of the disc then the ammonium chloride (NH_4Cl) turns in the vapour form without passing through the liquid. Clearly, from the mixture both sodium chloride ($NaCl$) and ammonium chloride (NH_4Cl) separated via sublimation process.

Drying of foods

In the food drying process, sublimation allows frozen foods to be dried while avoiding a breakdown of the cellular structure of the food. The current work may provide the theoretical basis for understanding and optimizing microwave food drying process [2]. Microwave drying is used in food drying where microwaves penetrate the material and are converted into heat so that it can remove moisture.

Conclusions

The mathematical modelling of moving boundary problems in heat and mass transfer process is important for several practical engineering systems. Such models are useful in heat and mass transfer problem that include an unknown interface, such as vaporization and drying of food. In this paper, we investigated a one-dimensional moving boundary problem in heat and mass transfer describing sublimation process in a half-porous space. Convective term due to moisture flow of the water vapour in the vapour region is considered. Convection is considered in the vapour and frozen region and also in the molar concentration of the vapour moisture. For a specific velocity profile, an exact solution of the current problem is determined via similarity transformation. Existence of the solution of the problem is also discussed. Further, the impact of variation of different parameters of this problem is studied in detail. A few key learnings from this analysis are summarized below:

- It is found that sublimation limit is enhanced by increasing the Péclet number *Pe*. In a similar fashion, the sublimation limit also increases with increasing Luikov number *Lu*.
- We observed that for a large value of Péclet number, the temperature profile within the medium becomes high and hence, the sublimation front moves rapidly. It is therefore, concluded that the sublimation process becomes fast for larger convection rate.
- With higher value of thermal diffusivity α_{21}, the temperature distribution within the medium rises and thus, fast propagation of the sublimation front with respect to the time is achieved.
- Temperature profile within the medium rises with increasing the value of heat flux γ. In addition, the evolution of the sublimation interface increases rapidly.

- Higher the value of β, the steeper is the temperature profile within the medium. The sublimation front correspondingly grows at a slower rate.
- Increasing the value of latent heat of sublimation l_0 results in steeper temperature profile within the medium, resulting in a reduced rate of propagation of the sublimation front.

In addition, it is expected that the mathematical model proposed in the current study may also aid in chemical process, thermal management and energy storage.

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Author's contribution JS: Supervision, formulation of model, reviewing, planning and writing article.VC: Formulation of model, analytical solution of mathematical model, figure plotting, writing, analysis and data curation and original draft preparation.AJ: Supervision, reviewing, planning and writing article.

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Declarations

Conflict of interest The authors have no conflict of interest.

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