Numerical Simulation of a Vapor Flow with Evaporation and Condensation in the Presence of a Small Amount of a Noncondensable Gas

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Abstract. A steady flow of a vapor evaporating from a plane condensed phase and condensing onto a corrugated condensed phase of sinusoidal shape is considered in the case where another gas that neither evaporates nor condenses (noncondensable gas) is contained in the gap between the condensed phases. The flow is investigated numerically on the basis of kinetic theory for small Knudsen numbers, with special interest in the continuum limit (i.e., the limit where the Knudsen number vanishes), in the case where the average concentration of the noncondensable gas is small, more specifically, it is of the order of the Knudsen number. The direct simulation Monte Carlo method is employed as the solution technique. The obtained flow properties, such as the stream lines, at small Knudsen numbers demonstrate a decisive difference from the corresponding flow properties in the pure-vapor case where the noncondensable gas is absent, in spite of the fact that the average concentration of the noncondensable gas is as small as the Knudsen number. In the present parameter setting, the average concentration of the noncondensable gas vanishes in the continuum limit. The numerical result nevertheless indicates that the decisive difference is likely to remain even in this limit. This is consistent with the recent theoretical investigation by Aoki, Takata, and Taguchi.

INTRODUCTION

In a previous paper [1], a steady flow of a vapor in the gap between two parallel plane condensed phases at rest, caused by evaporation and condensation on the condensed phases, was investigated on the basis of kinetic theory in the case where a noncondensable gas (a gas that neither evaporates nor condenses on the condensed phases) is also contained in the gap. Special attention was paid to the near continuum regime, in which the Knudsen number Kn with respect to the vapor is small, in the case where the average concentration of the noncondensable gas is also small. To be more specific, the latter condition is such that $n_{av}^B/n_r = O(Kn)$, where $n_{av}^B$ is the average number density of the noncondensable-gas molecules over the gap, and $n_r$ is a reference number density of the vapor molecules. A systematic asymptotic analysis for small Kn guided by e.g., [2,3] as well as a numerical computation using the direct simulation Monte Carlo (DSMC) method was performed, and the process of approach to the continuum limit (Kn $\to$ 0) was clarified. As in the pure-vapor case [2], the vapor flow becomes uniform except in the thickless Knudsen layers on the condensed phases in the continuum limit. A striking feature in this limit is that, in spite of the fact that the average concentration of the noncondensable gas becomes infinitesimal ($n_{av}^B/n_r \to 0$), the noncondensable gas still gives a significant effect on the uniform vapor flow. The reason is as follows. The noncondensable gas with an infinitesimal average concentration accumulates in the vanishingly thin Knudsen layer on the condensing surface, so that its local concentration there becomes finite. This high local concentration impedes the condensation of the vapor and thus affects the global uniform flow of the vapor.

However, it was still unclear how the effect of the small amount of the noncondensable gas manifests itself in the general two and three-dimensional problems. In order to obtain information about this point, we started
the present study that contains a numerical simulation of a two-dimensional problem, described in the following section, by the DSMC method. In the mean time, the asymptotic analysis of the Boltzmann equation for small Kn in [1] was extended to the general geometry [4]. Actually, the asymptotic analysis in [4] has been carried out interactively with the present study. As a result, it turned out that the effect of an infinitesimal average concentration of the noncondensable gas in the continuum limit appears in a more conspicuous manner in the general geometry. In the present paper, we are going to present the result of the above-mentioned DSMC computation that demonstrates such an effect.

**PROBLEM**

Consider a vapor in a gap between two condensed phases at rest, one is of sinusoidal shape (temperature $T_I$) located at $X_1 = A \cos(\pi X_2/L)$ and the other is a plane (temperature $T_{II}$) located at $X_1 = L$, where $A$ and $L$ are constants, and $X_i$ is a rectangular coordinate system (Fig. 1). Evaporation and condensation of the vapor may take place on these condensed phases. Suppose that a noncondensable gas is also contained in the gap. Investigate the steady flow of the vapor caused by evaporation and condensation, together with the behavior of the noncondensable gas, on the basis of kinetic theory in the following situation: (i) the Knudsen number (Kn) with respect to the vapor is small (near continuum regime); (ii) the amount of the noncondensable gas is small, more specifically, its average concentration over the gap is of $O(Kn)$.

We further assume that both components consist of hard-sphere molecules and also assume the conventional condition for the vapor (i.e., the vapor molecules leaving each condensed phase obey the Maxwellian distribution corresponding to the saturated vapor at rest with the temperature of the condensed phase) and the diffuse reflection for the noncondensable gas on the condensed phases. If we assume that the flow field is periodic in $X_2$ and is symmetric with respect to $X_2 = 0$, we may consider the problem in the closed domain $A \cos(\pi X_2/L) \leq X_1 \leq L$, $0 \leq X_2 \leq L$, imposing the specular reflection condition on $X_2 = 0$ and $L$.

**RESULTS OF COMPUTATION**

We analyze the above problem numerically by means of the DSMC method [5,6]. Since the scheme used here is a straightforward extension of the method explained in [7] to a binary mixture, we omit it for shortness and give only the results. The additional notation used in this paper is as follows: $n_I$ and $n_{II}$ are the saturation molecular number densities of the vapor at temperatures $T_I$ and $T_{II}$, respectively; $n_{av}^B$ is the average number density of the noncondensable gas; $m^A$ and $d^A$ are the mass and diameter of a molecule of the vapor; $m^B$ and $d^B$ those of the noncondensable gas; $k$ is the Boltzmann constant; $l$ is the mean free path of the vapor molecules in the equilibrium state at rest with number density $n_I$ [$l = 1/\sqrt{2\pi (d^A)^2 n_I}$]; Kn = $l/L$ is the Knudsen number of the vapor; $n^A$ and $n^B$ are, respectively, the molecular number density of the vapor and that of the noncondensable gas; $(v_1^A, v_2^A, 0)$ is the flow velocity of the vapor; and $T$ is the temperature of the total mixture. To be consistent with the situation (ii) in PROBLEM, we put

$$n_{ave}^B/n_I = \Delta\text{Kn},$$

FIGURE 1. Vapor and noncondensable gas between plane and sinusoidal condensed phases.
where $\Delta$ is a constant to be specified. Therefore, \( \frac{n^B}{n_I} \) vanishes in the continuum limit \( \text{Kn} \to 0 \). Then, introducing appropriate dimensionless variables, we find that the present problem is characterized by the following dimensionless parameters: \( \frac{m^B}{m^A}, \frac{d^B}{d^A}, \frac{A}{L}, \frac{T_{II}}{T_I}, \frac{n_{II}}{n_I}, \text{Kn}, \text{and} \ \Delta \). In this paper, we show the results for \( \frac{m^B}{m^A} = 1 \), \( \frac{d^B}{d^A} = 1 \), \( A/L = 0.2 \), \( \frac{T_{II}}{T_I} = 1 \), and mainly for \( \frac{n_{II}}{n_I} = 2 \) and \( \Delta = 1 \), together with the corresponding results without the noncondensable gas (\( \Delta = 0 \)). In our parameter setting, evaporation takes place on the plane condensed phase, and condensation on the sinusoidal one.

**Flow properties**

Figure 2(a) shows the change of the stream lines of the vapor flow as Kn decreases from 0.1 to 0.005 in the presence of the noncondensable gas (\( \Delta = 1 \)) for \( \frac{n_{II}}{n_I} = 2 \), and Fig. 2(b) the corresponding stream lines in the absence of the noncondensable gas (pure-vapor case; \( \Delta = 0 \)). In Fig. 2(b), the stream lines for Kn ≤ 0.02 seem to have converged to those in the continuum limit (Kn → 0). In contrast, in Fig. 2(a), there is still a visible difference between the stream lines at Kn = 0.01 and those at Kn = 0.005. But, we may consider that the latter stream lines are sufficiently close to those in the continuum limit. Then, the limiting stream lines in the case of Fig. 2(a) are likely to be completely different from those in the case of Fig. 2(b), in spite of the fact that the average concentration of the noncondensable gas in the former case becomes infinitesimal in the limit \( \frac{n^B_{av}}{n_I} \to 0; \text{see Eq. (1)} \). The difference can clearly be seen in Fig. 2(c), where the stream lines for both cases at the smallest Kn in the present computation (Kn = 0.005) are compared. The features of the flow field will be discussed further in the section of DISCUSSIONS.

The profiles of the macroscopic quantities along the three lines \( \frac{X_2}{L} = 0.1, 0.5, \text{and} 0.9, \text{parallel to the} \ X_1 \text{axis, for various Kn are shown in Figs. 3–5 for} \ \Delta = 1 \text{and for} \ \frac{n_{II}}{n_I} = 2; \text{Fig. 3 is for the molecular number densities} \ n^A, n^B, \text{Fig. 4 for the temperature} T \text{of the total mixture, and Fig. 5 for the} X_1 \text{component} v^A_1 \text{of the vapor flow velocity. The corresponding profiles in the pure-vapor case (} \Delta = 0 \text{)} \text{are shown in Figs. 6–8; Fig. 6 is for} n^A, \text{Fig. 7 for} T \text{of the vapor), and Fig. 8 for} v^A_1. \text{In Figs. 5 and 8,} c_I \text{defined by} c_I = (2kT_I/m^A)^{1/2} \text{is used.} \text{As Kn decreases, the amount of the noncondensable gas relative to the vapor decreases because of Eq. (1). The noncondensable gas tends to accumulate in a layer, the thickness of which decreases with the decrease of Kn, on the sinusoidal condensed phase where condensation is taking place (Fig. 3). Except in the layer and another thin layer on the plane condensed phase where evaporation is taking place, the number density} n^A \text{and temperature} T \text{become almost uniform (Figs. 3 and 4). The two layers are the so-called Knudsen layers. The fact that a nearly uniform region develops in} n^A \text{and} T \text{in the bulk of the vapor is also true in the pure-vapor case (Figs. 6 and 7). However, the values of} n^A \text{and} T \text{in the region are different in both cases. The profile of} v^A_1 \text{is relatively uniform for all Kn in the pure-vapor case (Fig. 8), whereas that tends to approach a nonuniform distribution in Figs. 5(a) and 5(c).} \)
FIGURE 3. Profiles of the number densities $n^A$ and $n^B$ along the three lines parallel to the $X_1$ axis for $\Delta = 1$ in the case of $n_{II}/n_I = 2$ and Eq. (2). (a) $X_2/L = 0.1$, (b) $X_2/L = 0.5$, (c) $X_2/L = 0.9$. The scales are shown in (a), where the scale for $n^A$ is shown on the left-hand side and that for $n^B$ on the right-hand side.

FIGURE 4. Profiles of the temperature $T$ of the total mixture along the lines parallel to the $X_1$ axis for $\Delta = 1$ in the case of $n_{II}/n_I = 2$ and Eq. (2). (a) $X_2/L = 0.1$, (b) $X_2/L = 0.5$, (c) $X_2/L = 0.9$. The scale is shown in (a).

FIGURE 5. Profiles of the $X_1$ component $v^A_1$ of the vapor flow velocity along the lines parallel to the $X_1$ axis for $\Delta = 1$ in the case of $n_{II}/n_I = 2$ and Eq. (2). (a) $X_2/L = 0.1$, (b) $X_2/L = 0.5$, (c) $X_2/L = 0.9$. The scale is shown in (a). Here, $c_I = (2kT_I/m^A)^{1/2}$. 
FIGURE 6. Profiles of the number density $n^A$ along the lines parallel to the $X_1$ axis for the pure vapor ($\Delta = 0$) in the case of $n_{II}/n_I = 2$ and $T_{II}/T_I = 1$. (a) $X_2/L = 0.1$, (b) $X_2/L = 0.5$, (c) $X_2/L = 0.9$. The scale is shown in (a).

FIGURE 7. Profiles of the temperature $T$ of the vapor along the lines parallel to the $X_1$ axis for the pure vapor ($\Delta = 0$) in the case of $n_{II}/n_I = 2$ and $T_{II}/T_I = 1$. (a) $X_2/L = 0.1$, (b) $X_2/L = 0.5$, (c) $X_2/L = 0.9$. The scale is shown in (a).

FIGURE 8. Profiles of the $X_1$ component $v_i^A$ of the vapor flow velocity along the lines parallel to the $X_1$ axis for the pure vapor ($\Delta = 0$) in the case of $n_{II}/n_I = 2$ and $T_{II}/T_I = 1$. (a) $X_2/L = 0.1$, (b) $X_2/L = 0.5$, (c) $X_2/L = 0.9$. The scale is shown in (a). Here, $c_I = (2kT_I/m^A)^{1/2}$. 
Now let us investigate the behavior of the noncondensable gas more closely. Figure 9(a) shows the distribution of $n^B$ along the sinusoidal condensed phase for $\Delta = 1$ and for various Kn in the case of $n_{II}/n_I = 2$. This figure, together with Fig. 3, demonstrates that more molecules are present in the hollow (near $X_2/L = 1$) than on the crest (near $X_2/L = 0$) of the condensed phase. As seen from Fig. 9(a), $n^B/n_I$ on the condensed phase decreases as Kn decreases. More precisely, in the part of the hollow ($X_2/L \geq 0.5$), it tends to converge to a finite value that depends on the position ($X_2/L$) on the condensed phase; however, in the part near the crest (near $X_2/L = 0$), it tends to decrease to zero. From this, together with the profiles in Fig. 3, we may conclude that the amount of the noncondensable gas, relative to that of the vapor, vanishes in the continuum limit in the following manner: in the part of the hollow, the thickness of the Knudsen layer, in which the noncondensable gas is present, vanishes in such a way that the value of $n^B/n_I$ on the condensed phase remains finite; in the part near the crest, the noncondensable gas disappears completely from the Knudsen layer. The situation in the former part is similar to that in the case of the flow between two parallel plane condensed phases [1]. For further confirmation of the above conclusion, it is desirable to obtain results for smaller Kn. However, such a computation is extremely hard, as will be mentioned in the next subsection. The above conclusion about the distribution of $n^B$ will be reviewed in the next section (DISCUSSIONS).

Figure 9(b), which is prepared for the section of DISCUSSIONS but placed here because of the limited space, shows the distribution of the ratio $v_2^A/v_1^A$ of the vapor flow velocity, i.e., the gradient of the tangent of a stream line, on the sinusoidal condensed phase for $\Delta = 1$ and for various Kn in the case of $n_{II}/n_I = 2$. If the flow is strictly perpendicular to the condensed phase, the $v_2^A/v_1^A$ takes the form $v_2^A/v_1^A = \pi(A/L) \sin(\pi X_2/L)$, which is shown by the solid curve in the figure.

The rate of evaporation of the vapor from the plane condensed phase (or that of condensation onto the sinusoidal condensed phase) for various $\Delta$ including the pure-vapor case ($\Delta = 0$) in the case of $n_{II}/n_I = 2$ and for $\Delta = 1$ in the case of $n_{II}/n_I = 4$ is shown in Table 1, where $N$ is the number of the vapor molecules evaporating from the plane condensed phase (or condensing onto the sinusoidal condensed phase) in the range $0 < X_2/L < 1$ per unit time and per unit thickness in $X_2$. The evaporation rate tends to converge as Kn approaches zero. Although the average concentration of the noncondensable gas vanishes with Kn according to Eq. (1), the limiting evaporation rate is likely to be different depending on $\Delta$, i.e., depending on the way of approach in the limiting process.

Data on simulation systems and accuracy

Some data on the simulation systems used in the computation for $n_{II}/n_I = 2$ and $\Delta = 1$ and 0 are summarized in Table 2. The basic cell is a square cell with side length $L/N_c$, and cells with rectangular and trapezoidal shape are used in the vicinity of the sinusoidal condensed phase; the number of the cells in the computational domain is approximately $N^2$. The $N_p$ is the number of simulation particles for the vapor that corresponds to the number $L^2 n_I$ of the real molecules; therefore, according to Figs. 3 and 6, the total number of the simulation particles for the vapor in the solution is $1.5 \sim 1.6$ times $N_p$. Correspondingly, the number
with less particles and cells were also carried out for many cases, from the results of which the accuracy was estimated. For example, for $\Delta = 0$ and 1, the values at $Kn = 0$ are fine enough. Equation (1) indicates that the total amount of the noncondensable gas thickness of the layer decreases and the change of $\Delta$ can be compared with the dimensionless molecular flux in the free time corresponding to it. The $M$ is the number of the time steps over which the average was taken after the steady state had been reached.

The accuracy of the computation was checked in various ways. First, the computations using coarser systems with less particles and cells were also carried out for many cases, from the results of which the accuracy was estimated. For example, for $\Delta = 0$ and 1, the values at $Kn = 0.005$ in Table 1 become 0.24873 (no change) and 0.20127 (no change) if the systems with $(N_c, N_p) = (120, 1.44 \times 10^6)$ and $(200, 4.00 \times 10^6)$ are used, respectively. The next check is to observe how accurately the conservation laws are satisfied. For example, the molecular-flow rate across a line $X_1/L = \text{const} \geq A/L = (0.2)$ in the range $0 \leq X_1/L \leq 1$ is constant theoretically, but its numerical value shows a slight variation with $X_1/L$. The values in Table 1 are the results of this quantity evaluated on the plane condensed phase, $X_1/L = 1$ (more precisely, in the cells in contact with the condensed phase). If the molecular-flow rate evaluated at four different positions around $X_1 = 0.3, 0.5, 0.6, 0.8$ is compared with that evaluated at $X_1 = 1$ (cf. Table 1), the relative variation is less than $5.8 \times 10^{-3}$% ($\Delta = 0$); $2.9 \times 10^{-3}$% for $Kn \leq 0.02$ and $8.2 \times 10^{-3}$% for $Kn \geq 0.05$ ($\Delta = 1, n_{II}/n_I = 2$); $1.2 \times 10^{-2}$% for $Kn \leq 0.02$ and $1.5 \times 10^{-2}$% for $Kn \geq 0.05$ ($\Delta = 2$); $8.4 \times 10^{-2}$% for $Kn \leq 0.02$ and $2.7 \times 10^{-1}$% for $Kn \geq 0.05$ ($\Delta = 5$); $7.6 \times 10^{-3}$% for $Kn \leq 0.05$ and $5.8 \times 10^{-2}$% for $Kn = 0.1$ ($\Delta = 1, n_{II}/n_I = 4$). The numerical result of the $X_3$ component of the vapor flow velocity $v_3^A$ (or the molecular flux $n^A v_3^A$), which is theoretically zero, does not vanish because of the numerical error. This also gives a good measure of accuracy. In the case of $n_{II}/n_I = 2$, the maximum of the dimensionless molecular flux $n^A v_3^A / n_I (2kT_I/m^A)^{1/2}$ is less than $5.0 \times 10^{-3}$ and the flux is less than $1.6 \times 10^{-3}$ in the $80\%$ of the cells for $\Delta = 0$ and 1. These values should be compared with the dimensionless molecular flux in the $X_1X_2$ plane $n^A [(v_3^A)^2 + (v_3^A)^2]^{1/2} / n_I (2kT_I/m^A)^{1/2}$, whose maximum is around 0.26 for $\Delta = 0$ and 0.21 $\sim$ 0.27 for $\Delta = 1$.

One of the important aims of the present study is to clarify the change of the profile of the noncondensable gas in the Knudsen layer on the condensing surface with the decrease of $Kn$ under the condition (1). Since the thickness of the layer decreases and the change of $n^B$ there becomes steeper as $Kn$ decreases (see Fig. 3), one needs smaller cells in order to describe the profile of $n^B$ in the layer precisely. Incidentally, the distributions of $n^B$ and $v_3^A / v_1^A$ on the sinusoidal condensed phase in Fig. 9 are those evaluated by using the cells in contact with the condensed phase. In order that the latter distributions are good approximations of the former, the cells should also be fine enough. Equation (1) indicates that the total amount of the noncondensable gas relative to that of the vapor decreases with decreasing $Kn$. On the other hand, to obtain a smooth profile of

<table>
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<th>$Kn$</th>
<th>$\Delta = 0$</th>
<th>$n_{II}/n_I = 2$</th>
<th>$\Delta = 1$</th>
<th>$n_{II}/n_I = 4$</th>
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<td>0.58927</td>
</tr>
<tr>
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<td>0.15649</td>
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<td>0.60857</td>
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<td>0.16129</td>
<td>0.10194</td>
<td>0.61490</td>
</tr>
<tr>
<td>0.005</td>
<td>0.24873</td>
<td>0.20154</td>
<td>0.16479</td>
<td>–</td>
<td>–</td>
</tr>
</tbody>
</table>

TABLE 2. Data on the simulation systems for $\Delta = 1$ and 0 in the case of $n_{II}/n_I = 2$ and Eq. (2).

<table>
<thead>
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<th>$Kn$</th>
<th>$N_c$</th>
<th>$N_p$</th>
<th>$M$</th>
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<td>$6.40 \times 10^4$</td>
<td>1.5 $\times 10^5$</td>
</tr>
<tr>
<td>0.05</td>
<td>80</td>
<td>$6.40 \times 10^5$</td>
<td>4.4 $\times 10^5$</td>
</tr>
<tr>
<td>0.02</td>
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<tr>
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<td>160</td>
<td>$2.56 \times 10^6$</td>
<td>4.5 $\times 10^5$</td>
</tr>
<tr>
<td>0.005</td>
<td>300</td>
<td>$9.00 \times 10^6$</td>
<td>6.8 $\times 10^5$</td>
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</table>
in the Knudsen layer, one needs a sufficient number of simulation particles for the noncondensable gas. In consequence, we are obliged to use a large number of particles for the vapor. These factors, in addition to the usual difficulty in the DSMC computation for small Kn, make the computation very hard. The present computation was carried out on CRAY Origin 2000 computer in the Institute for Chemical Research, Kyoto University as well as some VT-Alpha workstations in the authors' laboratory. A parallel computation with 12 CPU's was performed on the former computer in the case of Kn = 0.005, ∆ = 1, and nII/nI = 2, which took full seven months.

DISCUSSIONS

As mentioned in INTRODUCTION, the behavior of the vapor flows in the continuum limit in the presence of a small amount of the noncondensable gas is investigated for the general geometry in [4] by means of a systematic asymptotic analysis for small Knudsen numbers. According to [4], the vapor flows in the continuum limit are described by the compressible Euler set of equations with appropriate boundary conditions. The boundary condition on the evaporating surface is the same as that in the pure-vapor case [2,3], which has been derived by solving the half-space problem of strong evaporation of a pure vapor [8]. The effect of the noncondensable gas [of an infinitesimal average concentration; cf. Eq. (1)] appears only in the boundary condition on the condensing surface, which has been derived by solving the half-space problem of strong condensation of a vapor in the presence of a noncondensable gas [9,10]. The latter condition, applied to the present problem, tells that the vapor must condense onto the sinusoidal condensed phase perpendicularly if the noncondensable gas is contained in the (thickless) Knudsen layer, whereas it can condense at incidence if the noncondensable gas is absent there. Thus, in the pure-vapor case, the vapor can condense at incidence on all part of the sinusoidal condensed phase.

This difference in the continuum limit explains the difference in the stream lines at Kn = 0.005 shown in Fig. 2(c). That is, the stream lines enter the sinusoidal condensed phase almost perpendicularly for ∆ = 1, whereas they enter it at incidence in the pure-vapor case. The former fact is shown more clearly by Fig. 9(b) [see the fourth paragraph in the subsection “Flow properties” for Fig. 9(b) and recall that the solid curve indicates the case where the vapor flow enters the sinusoidal condensed phase perpendicularly]. But if we look at the figure more carefully, we notice the following: as Kn decreases, va/v1 tends to converge to the solid curve in the part of the hollow (X2/L ≈ 0.5), whereas it seems to approach another curve that is slightly lower than the solid curve in the part near the crest (near X2/L = 0). That is, the stream lines in the latter part would not strictly be perpendicular to the condensed phase in the continuum limit. This means, from the theoretical result mentioned above, that the noncondensable gas disappears from the Knudsen layer in the part near the crest in the limit. This agrees with the observation associated with Fig. 9(a) in the subsection “Flow properties”. In this way, the result of the present computation for small Kn is seen to be consistent with the theoretical investigation of the continuum limit in [4].

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