

An improved BGK-type collision-term model for Direct Simulation Monte Carlo (DSMC) methods

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ABSTRACT

The BGK and BGKC (Bhatnagar, Gross, Krook, and Cercignani) collision-term models for the Boltzmann equation are compared to the more rigorous variable-hard-sphere (VHS) collision-term model of Bird. The BGKC model is based on the well-known BGK model but uses an ellipsoidal statistical (ES) distribution instead of a Maxwellian distribution so as to incorporate both viscous effects and heat conduction accurately. The Direct Simulation Monte Carlo (DSMC) method of Bird is used with the BGK, BGKC, and VHS collision terms to simulate supersonic flow of a monatomic gas over a wedge. The BGKC results are consistently in good agreement with the VHS results, whereas the BGK results show systematic differences.

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I. INTRODUCTION

The issue of modeling collisional processes in a gas extends back to the earliest attempts to solve the Boltzmann equation. One early approach involved replacing the integral collision term of the Boltzmann equation for a monatomic gas with simpler forms that maintain most of the fundamental properties of the original collision term. The rationale behind this type of simplification is that most of the details of the collision term are not important for reproducing macroscopic flow behavior. As well as enabling analytical results to be obtained under certain circumstances, such simplifications can reduce the effort to compute collisions in numerical simulations compared to the effort required by more rigorous approaches like the variable-hard-sphere (VHS) model of Bird¹. However, the accuracy of such simplifications remains an issue.

One of the most popular simplifications of this type is the BGK² model (Bhatnagar, Gross, and Krook). Cercignani³ has used the BGK model extensively to produce analytical results and has also proposed an extension (herein termed the BGKC model) that uses an ellipsoidal statistical (ES) distribution instead of a Maxwellian distribution to incorporate heat conduction accurately. Liepmann, Narasimha, and Chahine⁴ conducted an extensive study of the BGK model applied to the shock-structure problem and found reasonable agreement with Navier-Stokes results. More recently, Montanero *et al.*⁵ implemented the BGK model using a Direct Simulation Monte Carlo (DSMC) method and found good agreement with analytical solutions of the Boltzmann equation for near-equilibrium cases.

In this paper, the BGK, BGKC, and VHS collision-term models are compared. A DSMC technique developed by Bird¹ and implemented by Bartel *et al.*⁶ is used with the BGK, BGKC, and VHS models to simulate supersonic flow of a monatomic gas over a wedge. The BGKC results agree closely with the VHS results, but the BGK results show systematic differences.

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II. THEORETICAL CONSIDERATIONS

A. The Boltzmann equation

The velocity distribution function f provides a complete description of a dilute monatomic gas at the molecular level.⁷ The relationship between the velocity distribution function and the variables it depends on is given by the Boltzmann equation:

$$\frac{\partial}{\partial t}(nf) + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{x}}(nf) + \mathbf{F} \cdot \frac{\partial}{\partial \mathbf{v}}(nf) = \left[\frac{\partial}{\partial t}(nf) \right]_{\text{collision}}, \quad (1)$$

where t is time, \mathbf{x} is the position in physical space, \mathbf{v} is the molecular velocity, \mathbf{F} is any external force (here, velocity-independent), n is the number density, and the right-hand side is the integral collision term:

$$\left[\frac{\partial}{\partial t}(nf) \right]_{\text{collision}} = \int_{-\infty}^{\infty} \int_0^{4\pi} n^2 (f^* f_1^* - ff_1) c_r \sigma d\Omega d\mathbf{v}_1. \quad (2)$$

In the integral collision term, the distribution functions f and f^* are evaluated at the molecule's pre-collision velocity \mathbf{v} and post-collision velocity \mathbf{v}^* , respectively, and the distribution functions f_1 and f_1^* are evaluated at the collision partner's pre-collision velocity \mathbf{v}_1 and post-collision velocity \mathbf{v}_1^* , respectively. Also in the collision term, $c_r = |\mathbf{v} - \mathbf{v}_1|$ is the relative speed of the colliding molecules, σ is the cross section of the binary collision, and Ω is the solid angle. The details of the binary collision are included in the collision cross section.⁷

B. The BGK collision-term model

The complexity of the integral collision term led to the development of simplified models that retain some of its properties but are not derived directly from it. Bhatnagar, Gross and Krook² (BGK) proposed a simplification that takes the form

$$\left[\frac{\partial}{\partial t}(nf) \right]_{\text{collision}} = nv(f_o - f), \quad (2)$$

where f_o is the Maxwellian distribution corresponding to the local temperature and average velocity, and v is the relaxation rate of the initial distribution to the equilibrium distribution. In this model, the term nvf_o represents the collisions replenishing the distribution, and the term nvf represents the collisions depleting the distribution. The physical interpretation of the BGK model is that post-collision molecules are selected from a Maxwellian distribution at the local average velocity and temperature. Examination of the BGK model indicates that it reproduces the equilibrium solution $f = f_o$ and the conservation equations of mass, momentum, and energy at equilibrium (Vincenti and Kruger⁷). The BGK model also satisfies the H-theorem and leads to the Navier-Stokes equations when the Chapman-Enskog expansion is applied.

One difficulty with the BGK model involves the specification of the relaxation rate v , which is not necessarily the same as the equilibrium collision frequency of the gas. One way to specify the relaxation rate is in terms of the coefficient of viscosity μ :

$$\mu = \frac{nkT}{v}, \quad (3)$$

where T is the temperature and k is the Boltzmann constant. Alternatively, the relaxation rate can be specified using the coefficient of thermal conductivity K :

$$K = \frac{5}{2} \left(\frac{k}{m} \right) \frac{nkT}{v}, \quad (4)$$

where m is the mass of a molecule. Equations (3) and (4) lead to different relaxation rates unless the Prandtl number of the gas is unity. Since the Prandtl number of most gases differs appreciably from unity, this feature of the BGK model can be a disadvantage.

It should be noted that the above choices for the relaxation rate do not depend on the molecular velocity \mathbf{v} directly but only on the local number density and temperature. This behavior is different from the collision frequency for all molecular models apart from Maxwell molecules. The use of a velocity-dependent relaxation rate in the BGK model is possible. However, the BGK model is usually applied with a velocity-independent relaxation rate. Following most previous applications of the BGK model^{5,7}, the velocity-independent relaxation rate based on the viscosity, given by Equation (3), is used in this study.

C. The BGKC collision-term model

Cercignani³ proposed a modification to the BGK model (herein termed the BGKC model) that allows it to reproduce the viscosity and thermal conductivity inherent in the integral collision term by introducing the Prandtl number as an explicit parameter. The BGKC generalization of the BGK model is obtained by replacing the Maxwellian distribution with an anisotropic Gaussian distribution, referred to as the ellipsoidal statistical (ES) distribution:

$$f_o = \pi^{-3/2} (\det \mathbf{A})^{1/2} \exp(-\mathbf{c}^T \mathbf{A} \mathbf{c}). \quad (5)$$

In this expression, the molecular thermal velocity \mathbf{c} is given by $\mathbf{c} = \mathbf{v} - \mathbf{u}$, where \mathbf{v} and \mathbf{u} are the molecular velocity and the average molecular velocity, respectively. In the ES distribution, the matrix \mathbf{A} is given by the relation:

$$\mathbf{A}^{-1} = \frac{2}{3} \text{trace} \left[\frac{\mathbf{P}}{\rho \text{Pr}} \right] \mathbf{I} - 2(1 - \text{Pr}) \frac{\mathbf{P}}{\rho \text{Pr}}, \quad (6)$$

where \mathbf{I} is the identity tensor, Pr is the Prandtl number, ρ is the mass density, and \mathbf{P} is the pressure tensor:

$$\frac{\mathbf{P}}{\rho} = \int \mathbf{c} \mathbf{c}^T f d\mathbf{v}. \quad (7)$$

Note in passing that the temperature T is related to the trace of the pressure tensor \mathbf{P} :

$$\frac{3kT}{m} = \text{trace} \left[\frac{\mathbf{P}}{\rho} \right] \quad (8)$$

The BGKC model is an extension of the BGK model and reproduces the BGK model for a Prandtl number of unity. Andries *et al.*⁸ have shown that the BGKC model satisfies the H-theorem and reproduces the correct moments of the Boltzmann equation just as the original BGK model does.

III. NUMERICAL IMPLEMENTATION

A. DSMC method

The DSMC method is a well-established technique for simulating gas flows in which mean-free-path effects are significant. The particular DSMC method used in this study is that of Bird¹, the implementation of which is described more fully by Bartel *et al.*⁶

In brief, the DSMC method is applied as follows. The computational domain is populated with "computational molecules", each of which typically represents a large number of identical real molecules (*e.g.*, 10^{10}). During one time step, computational molecules move from one location to another, interact with boundaries, experience collisions, and are sampled to accumulate statistics. During a move, computational molecules travel at constant velocity for the entire time step or until a boundary is encountered. In the latter situation, the appropriate boundary condition is applied. Typical boundary conditions are "inflow" (computational molecules enter the domain with a prescribed Maxwellian distribution), "outflow" (computational molecules crossing this boundary are deleted, appropriate for supersonic applications), "diffuse wall" (computational molecules are reflected with a prescribed Maxwellian distribution), and "specular wall" (computational molecules are reflected with

mirror symmetry). Following movement and boundary interactions, computational molecules experience collisions, which change their velocities. It should be noted that computational molecules have three-dimensional velocity vectors for collision purposes even if a two-dimensional geometry is considered. After the collision phase, statistics (*e.g.*, number density, velocity, and temperature) are accumulated on the computational mesh, which exists only for this purpose and for determining possible collision pairs. To preclude nonphysical behavior, the mesh cells are constrained to be well less than a mean free path, and the time step is similarly constrained to be well less than a mean collision time.¹

B. Selection of post-collision velocities

The selection of post-collision velocities differs for the BGK, BGKC, and VHS collision-term models. In the VHS model,¹ pairs of computational molecules are randomly selected as possible collision partners, and pairwise collisions are performed at the physically appropriate rate. The collision probability is determined by the pair's relative velocity, and the post-collision velocity distribution in the center-of-mass frame is isotropic in solid angle. When a collision is performed, post-collision velocities that conserve mass, momentum, and energy are selected from the prescribed velocity distribution.

The BGK and BGKC models use a somewhat different approach for performing collisions. In these two models, every computational molecule has the possibility of undergoing a collision. As in the VHS collision term, these collisions are performed at the physically appropriate rate. In contradistinction to the VHS collision term, post-collision velocities are selected randomly from a prescribed velocity distribution that reproduces certain moments of the actual velocity distribution. The BGK model uses a Maxwellian distribution that reproduces the local number density, the average velocity, and the temperature, whereas the BGKC model uses

an ES distribution, which reproduces these quantities but allows the Prandtl number to be different from unity, as previously discussed.

The following approach is used to select post-collision velocities in the BGK and BGKC models. Since a Maxwellian distribution is used in the BGK model, the approach described in Bird¹ for the VHS collision term can be used without modification. For the ES distribution used in the BGKC model, the approach of Bird can be generalized in the following manner. Since by construction the matrix A^{-1} in the ES distribution is symmetric and non-negative definite (actually positive definite except for pathological cases), a symmetric matrix S can be found such that $A^{-1} = SS$ (e.g., Press *et al.*⁹). Defining a normalized thermal velocity vector C using the linear transformation

$$c = SC, \quad (9)$$

the argument of the exponential function in Equation (6) becomes

$$c^T A c = (SC)^T (S^{-1} S^{-1}) (SC) = C^T C. \quad (10)$$

Since C satisfies a Maxwellian distribution, the approach of Bird¹ for the VHS collision term is used to select post-collision values of C , and the corresponding c values are determined from Equation (9).

Computation of the matrix S can be accomplished in a variety of ways. For example, the eigensystem corresponding to matrix A^{-1} can be solved, and S can be directly constructed from the resulting eigenvectors and eigenvalues (actually their square roots, as in Press *et al.*⁹). Alternatively, a Taylor-series approach can be used, for which the first term is given by:

$$S = \left(\frac{2kT}{m} \right)^{1/2} \left[I - \frac{1}{2} \left(\frac{1 - Pr}{Pr} \right) \left\{ \frac{m}{kT\rho} P - I \right\} \right]. \quad (11)$$

For the situations examined here, both methods are found to produce virtually identical results.

C. Conservation of momentum and energy

If applied as described in the previous section, the BGK and BGKC models would conserve momentum and energy only in a statistical sense, which could introduce an undesirable random walk into the calculation.¹ This effect is minimized in the limit that the number of computational molecules in a cell becomes very large. However, this approach is undesirable from a computational point of view. An alternative approach is to calculate the total momentum and energy in a cell before the collisions and to adjust the velocities of the computational molecules in the cell after the collisions to ensure that momentum and energy are exactly conserved. This can be accomplished as follows. The average velocity and the temperature of each cell are determined for the pre-collision conditions (\mathbf{u} and T) and for the provisional post-collision conditions (\mathbf{u}_p and T_p). The final post-collision velocity \mathbf{v} of each computational molecule is determined from its provisional post-collision value \mathbf{v}_p according to:

$$\mathbf{v} = \mathbf{u} + (\mathbf{v}_p - \mathbf{u}_p) \left(\frac{T}{T_p} \right)^{1/2} \quad (12)$$

This approach is used in all of the following BGK and BGKC simulations.

D. DSMC code

The DSMC code Icarus is used for the simulations presented in the following section. Icarus was developed by Bartel *et al.*⁶ and implements Bird's approach¹ for two-dimensional and axisymmetric simulations on massively parallel computers. The simulations presented here are performed on 512 nodes of ASCI Red, a teraflop-capable parallel computer. A simulation typically uses 3,500,000 computational molecules and requires 3.5 hours of run time to produce statistically acceptable results. The BGK, BGKC, and VHS collision-term models are separate options of Icarus.

IV. COMPUTATIONAL APPLICATION

A. Test problem

A test problem has been developed and analyzed using the BGK, BGKC, and VHS models. The problem involves supersonic flow of a monatomic gas over a wedge with a specular surface (see Figure 1). In this situation, a finite-thickness oblique shock wave emanates from the wedge vertex, and analytical results are available for the shock angle β and the downstream conditions in terms of the wedge angle θ and the upstream conditions (*e.g.*, Anderson¹⁰):

$$\tan \theta = \frac{\cot \beta (M^2 \sin^2 \beta - 1)}{\frac{\gamma + 1}{2} M^2 - (M^2 \sin^2 \beta - 1)}, \quad (13)$$

where M is the upstream Mach number and γ is the specific heat ratio. Of the two possible solutions, the weak solution is obtained. Since these analytical results depend only on the conservation of mass, momentum, and energy for a perfect gas, comparing computational and analytical results enables verification that conservation is properly enforced. A full-flow-field comparison of the BGK and BGKC simulations to the corresponding VHS simulations is a more stringent test because the precise details of the flow field depend on the collision term.

Two cases are simulated with all three collision terms. The gas is taken to be argon, with molecular collision parameters and a temperature-dependent viscosity as given by Bird¹ and with upstream conditions as given in Table 1. In the BGKC simulations, the Prandtl number is set equal to $2/3$, as appropriate for a monatomic gas. Two values of the wedge angle θ are examined: 5° and 10° . Table 1 shows the analytical results for the corresponding downstream conditions.

The computational domain is shown schematically in Figure 1. The left side of the domain is an inflow boundary: computational molecules enter the domain along this side with a

Maxwellian velocity distribution corresponding to the upstream conditions. The right side of the domain is an outflow boundary: computational molecules crossing this boundary are deleted from the calculation, as is appropriate for supersonic outflow. The remaining boundaries are all specular walls: molecules are reflected from these sides with mirror symmetry. The top boundary is positioned far enough from the wedge so that the oblique shock wave does not reach this boundary. The domain is initially populated everywhere with computational molecules at the upstream conditions.

The following values for numerical parameters are used in all three types of simulations. The time step is 10 ns, and about 30 computational molecules per cell are used on average. The mesh cells are approximately square, with a side length of about 0.025 mm. The wedge vertex is 1 mm from the inflow boundary, 10 mm from the outflow boundary, and 6 mm from the boundary opposite the wedge. Increasing or decreasing each of these values by at least a factor of 2 is found to produce nearly identical flow fields. Since the upstream mean free path is 0.1 mm, the cells and time step are small enough to satisfy the criteria¹ that computational molecules travel less than a mean free path per time step and that cell sizes are less than a mean free path (even downstream of the shock wave).

Steady-state flow fields are obtained in the following manner. Steady-state conditions are achieved throughout the domain by 20,000 time steps (0.2 ms). The flow field is averaged for an additional 120,000 time steps (1.2 ms) to obtain statistically accurate results. It should be noted that during the first 20,000 time steps the computational-molecule population of the domain is purged and renewed almost 25 times.

B. Simulation results

Figures 2 and 3 show number-density and temperature contours, respectively, for the 5° wedge obtained using the BGK, BGKC, and VHS collision terms, and Figures 4 and 5 show the corresponding results for the 10° wedge. As expected, all simulations yield oblique shock waves emanating from the wedge vertex, and the shock angle and downstream number density and temperature are seen to increase with increasing wedge angle. For both wedge angles, the BGK, BGKC, and VHS collision terms all obtain the correct shock angle and the correct downstream conditions (see Table 1), indicating that the BGK, BGKC, and VHS collision terms properly conserve momentum and energy.

From comparing the full flow fields, it is clear that the BGKC results agree quite closely with the VHS results but the BGK results do not. Moreover, the discrepancy between the BGK results and the VHS results becomes larger as the shock strength is increased (by increasing the wedge angle). In the number-density and temperature plots (Figures 2-5), the BGK collision term is seen to produce slightly thinner shock waves than the BGKC and VHS collision terms. Also, the temperature contours along the wedge surface are more closely spaced in the BGK results than they are in the BGKC and VHS results. These observations are in harmony with the fact that the thermal conductivity in the BGK model, which has a Prandtl number of unity, is two-thirds of the value used by the BGKC model, which has a Prandtl number of $2/3$.

V. CONCLUSIONS

The BGK and BGKC (Bhatnagar, Gross, Krook, and Cercignani) collision-term models have been examined and compared to the more rigorous variable-hard-sphere (VHS) model for the integral collision term of the Boltzmann equation. Simulations of supersonic flow of a monatomic gas over a wedge indicate that the BGKC model, which explicitly incorporates the

Prandtl number of the gas, produces results that are in close agreement with the VHS results. The BGK results differ systematically from the VHS results in a manner that is attributed to the spurious value of unity for the Prandtl number. The BGKC model thus offers the possibility of a simplified collision term that yields good agreement with the rigorous form.

Future research should focus on several areas. First, the limit of validity for the BGKC model needs to be firmly established. Second, it is desirable to extend the BGKC model to include molecules with internal degrees of freedom, such as diatomic molecules. Third, the possibility of improving the BGKC model by using a velocity-dependent relaxation rate should be investigated.

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Quantity	Variable	Upstream	Downstream	Downstream
Wedge angle	θ	–	5.0°	10.0°
Shock angle	β	–	14.6°	19.6°
Number density	n	$1.00 \times 10^{22} \text{ m}^{-3}$	$1.54 \times 10^{22} \text{ m}^{-3}$	$2.11 \times 10^{22} \text{ m}^{-3}$
Temperature	T	180. K	246. K	336. K
Pressure	p	24.9 Pa	52.3 Pa	97.7 Pa
Sound speed	a	250. m/s	292. m/s	341. m/s
Velocity	u	1365. m/s	1340. m/s	1304. m/s
Mach number	M	5.463	4.591	3.823

Table 1. Parameters for simulation cases: argon, mass $m = 6.63 \times 10^{-26}$ kg, $\gamma = 5/3$.

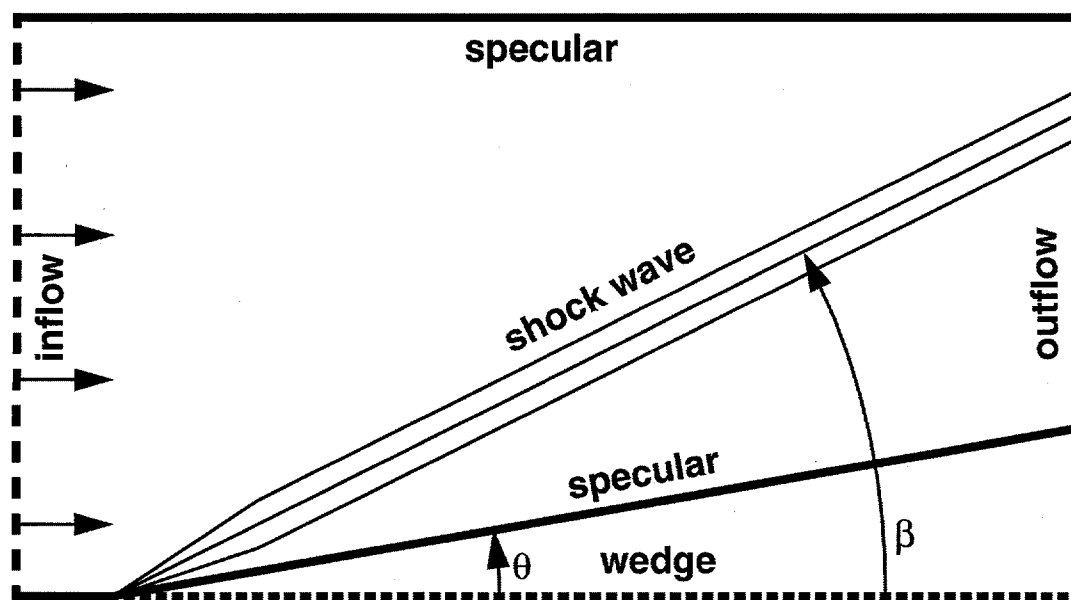


Figure 1. Schematic diagram showing supersonic flow of a monatomic gas over a wedge.

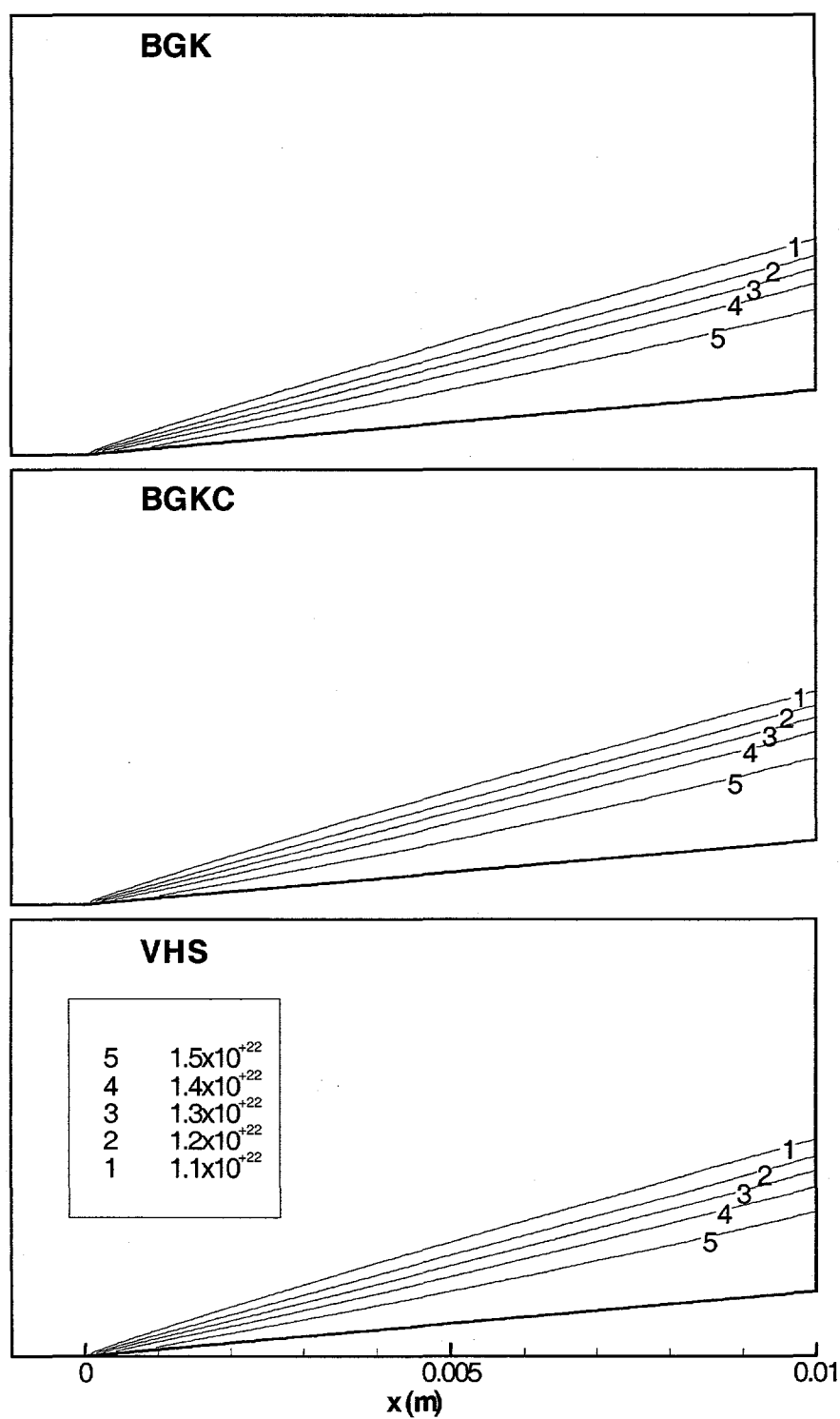


Figure 2. BGK, BGKC, and VHS number-density ($\#/m^3$) contours for a 5° wedge.

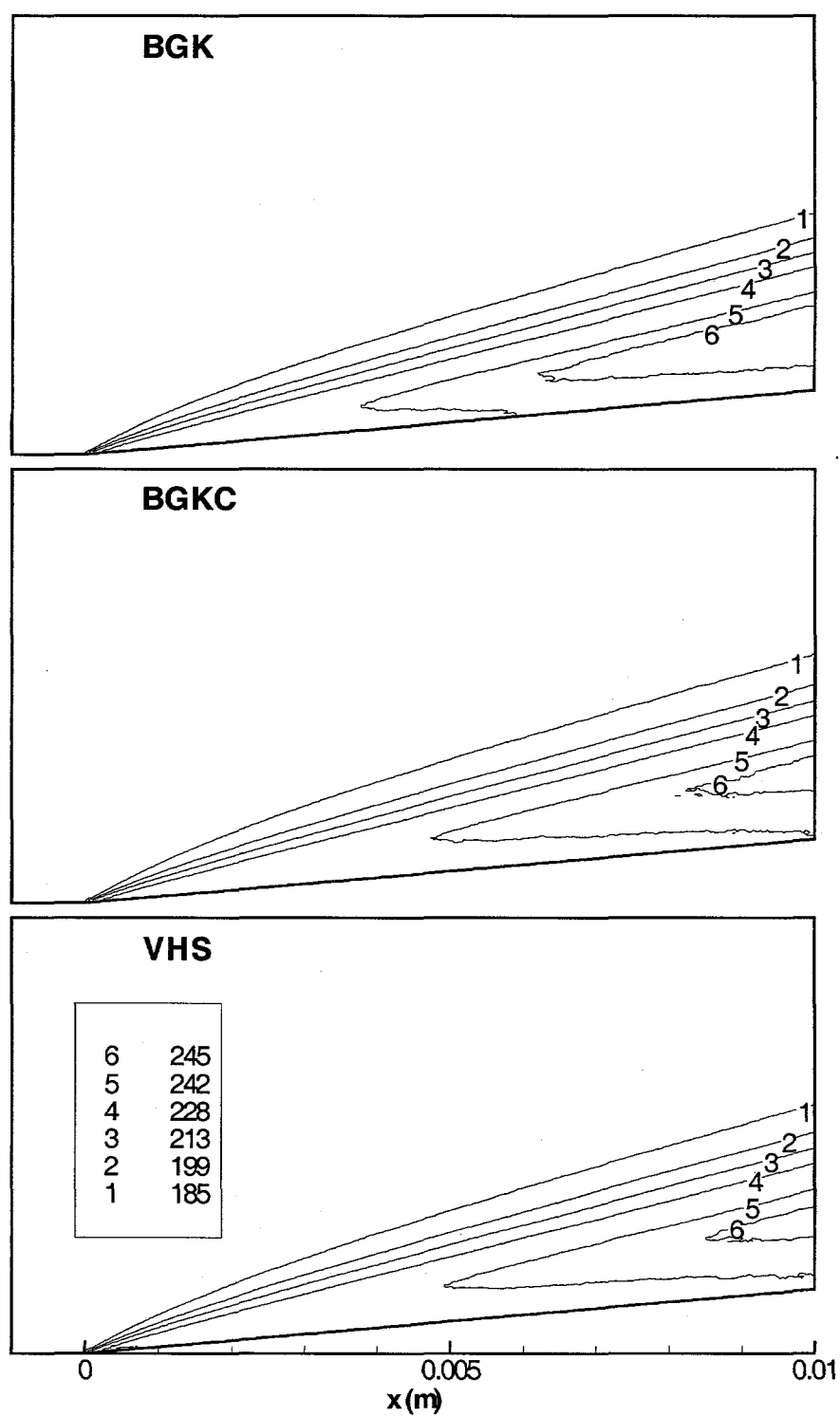


Figure 3. BGK, BGKC, and VHS temperature (K) contours for a 5° wedge.

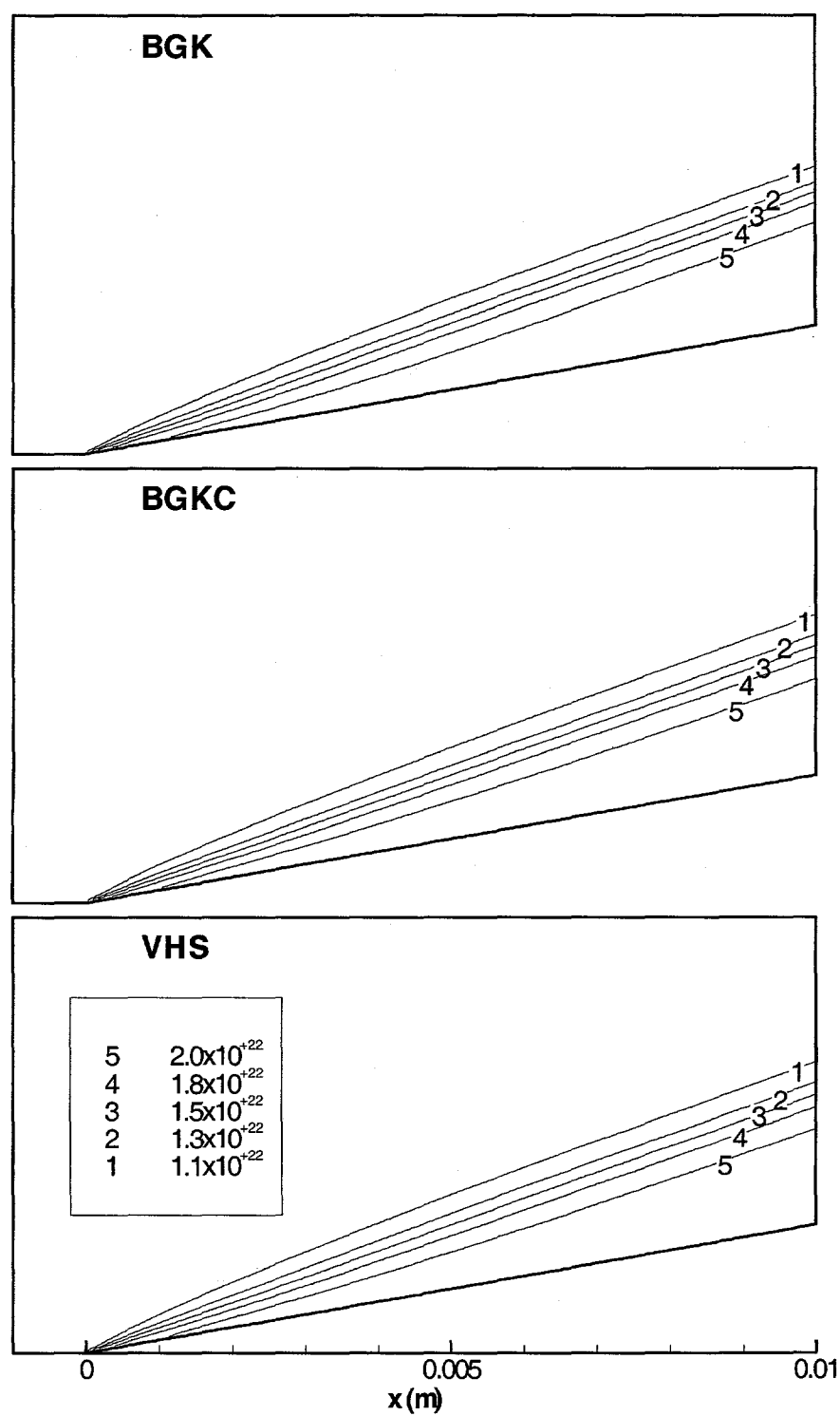
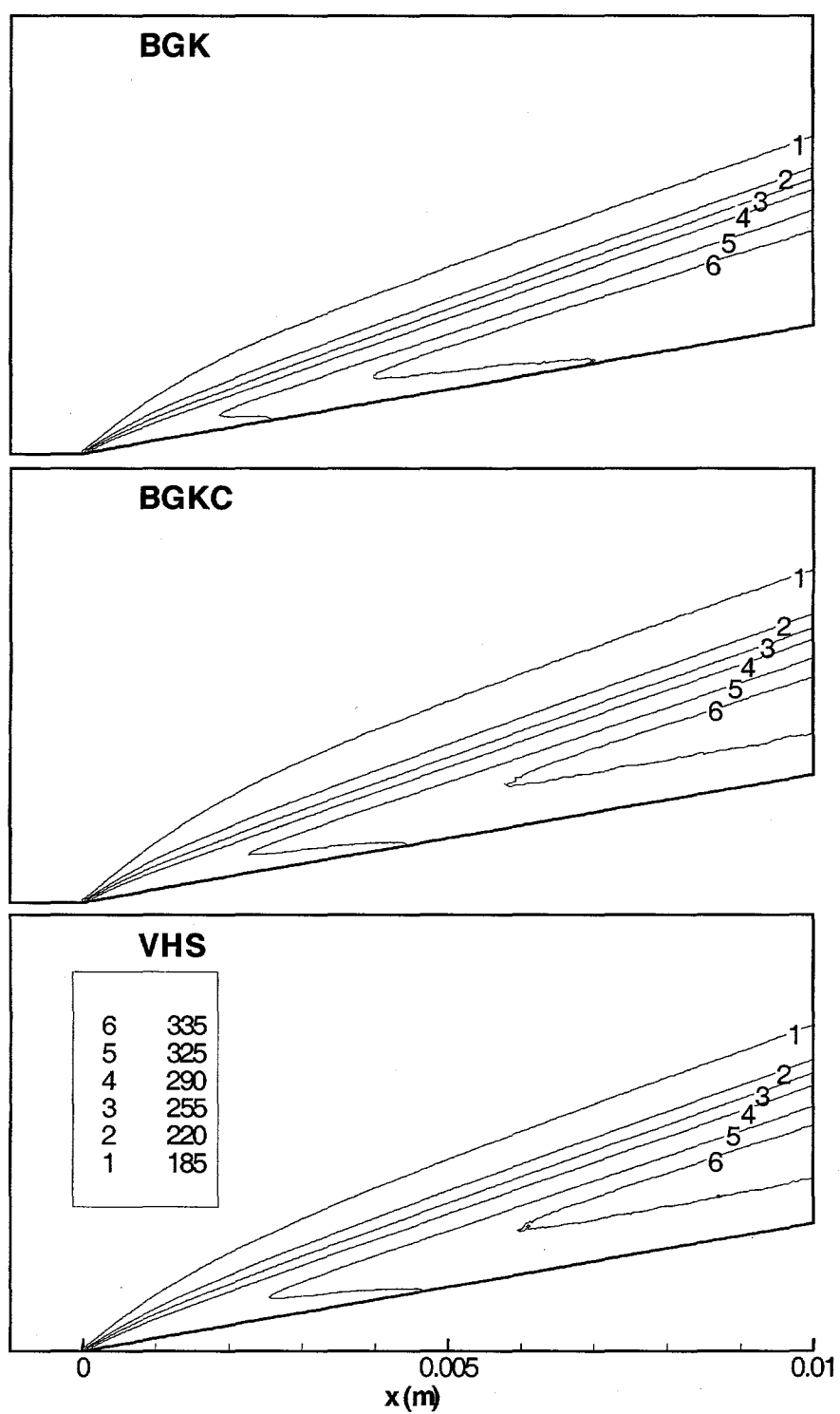


Figure 4. BGK, BGKC, and VHS number-density ($\#/m^3$) contours for a 10° wedge.

Figure 5. BGK, BGKC, and VHS temperature (K) contours for a 10° wedge.