DSMC Simulations of Hypersonic Flows and Comparison With Experiments

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Abstract. This paper presents computational results obtained with the direct simulation Monte Carlo (DSMC) method for several biconic test cases in which shock interactions and flow separation-reattachment are key features of the flow. Recent ground-based experiments have been performed for several biconic configurations, and surface heating rate and pressure measurements have been proposed for code validation studies. The present focus is to expand on the current validating activities for a relatively new DSMC code called DS2V that Bird (second author) has developed. Comparisons with experiments and other computations help clarify the agreement currently being achieved between computations and experiments and to identify the range of measurement variability of the proposed validation data when benchmarked with respect to the current computations. For the test cases with significant vibrational nonequilibrium, the effect of the vibrational energy surface accommodation on heating and other quantities is demonstrated.

INTRODUCTION

Shock/shock and shock/boundary layer interactions continue to receive considerable attention because of their impact on the performance and design requirements of hypersonic vehicles. Because these interactions produce very challenging problems for experimental measurements and numerical simulations, several experiments [1,2] have recently been performed with the objective of providing code validation data while minimizing some of the additional complexities that occur in flight; that is, avoiding three-dimensional effects by using axisymmetric model configurations at zero incidence and conducting the tests such that the flow is laminar and free of chemical reactions. References [2–4] provide recent results of computational studies obtained with both continuum and DSMC methods for several of these experimental test cases, including the four test cases considered in the present study. The flow conditions simulated are those for three experimental conditions performed by Holden and Wadhams [1] in the Calspan-University at Buffalo Research Center (CUBRC) 48-Inch Shock Tunnel for Mach 11 to 16 nitrogen flow about a 25°/55° biconic. The fourth test case simulated is the one for the experiments performed by Chanetz, Pot, and Benay [2] in the ONERA R5Ch low density wind tunnel for Mach 10 air flow about a 25°/65° biconic.

Results from several DSMC codes are included in the present paper, but the primary emphasis is on testing the accuracy of a relatively new DSMC code called DS2V [5], that has been developed by Bird. The DS2V code is a general 2D/axisymmetric code that provides time accurate simulations. The current paper extends the study presented in Ref. [6] by expanding on the range of test cases and by including additional comparisons with other DSMC solutions, particularly the solutions obtained by Markelov with the SMILE [7] (Statistical Modeling In Low-density Environment) code. The code-to-code comparisons are shown to be good (heating rate differences of less than 10 percent), while the code-to-experiment comparisons are shown to range from poor (differences greater than 15 percent in heating) to good. By comparing with several sets of experimental results, one can establish the range of variability that exists for the experiments when they are compared with computations, as is done in the present paper.

TABLE 1. Free-stream and surface[a] conditions for biconic test cases.

Condition	V_∞, m/s	$\rho_\infty \times 10^4$, kg/m^3	$n_\infty \times 10^{-22}$, m^{-3}	T_∞, K	$T_{\infty,V}$, K	p_∞, N/m^2	Gas	M_∞	Re_∞ m^{-1}	T_W, K
48-Inch Run 7	2 072.6	1.757	0.378	42.61	1986	2.23	N_2	15.6	137 467	297.2
48-Inch Run 35	2 587.8	6.030	1.297	101.11	2610	18.13	N_2	12.6	222 769	296.1
48-Inch Run 28	2 542.3	7.164	1.540	137.78	2535	29.30	N_2	10.6	191 273	295.0
ONERA R5Ch	1 382.6	4.520	0.940	48.5	—	6.30	Air	9.9	202 067	290.0

[a] Diffuse with either full thermal accommodation or zero vibrational accommodation.

The three CUBRC test cases have an elevated free-stream vibrational temperature, and the current calculations show that there is a significant vibrational nonequilibrium in the shock layer. Experimental evidence [8] suggests that when there is significant vibrational nonequilibrium within the shock layer, the vibrational energy does not accommodate itself to the surface temperature when the molecules impact the surface. Calculated results for these three test cases show a reduction of approximately 12 percent in surface heating rate when the surface is assumed to have zero rather than full thermal accommodation for the vibrational energy, which is in agreement with a similar study by Markelov et al. [9]

Results obtained for the ONERA test case using both DS2V and SMILE are shown to differ substantially from the results obtained and reported by Moss et al. [10] with the DAC (DSMC Analysis Code) code [11], but did agree reasonably well with the results, reported in the same reference [10], obtained by using an earlier code of Bird [12] called G2. Results of these findings led to the discovery of a deficiency in the axisymmetric version only of the DAC code. The current results from three different DSMC codes give similar values for both the extent of separation and the heating rate distributions, but the calculated heating values are about 30 percent higher than the experimental values [2] .

DSMC CODES

Results from several DSMC codes are included in the present paper with references to each noted in the introduction. A brief description of the DS2V program is included because it was used to generate the major portion of the results. The DS2V program of Bird [5,13] is a general 2D/axisymmetric code that provides both time accurate unsteady flow and time-averaged steady flow simulations. Molecular collisions are simulated with the variable hard sphere molecular model. Energy exchange between kinetic and internal modes is controlled by the Larsen-Borgnakke statistical model [14]. For the present study, the simulations are performed by using nonreacting gas models while considering energy exchange between translational, rotational, and vibrational modes. The molecular gas constants used in the current study are those given in Ref. [13]. Also, a rotational relaxation collision number of 5 and a temperature dependent vibrational collision number (Eq. 6.53 of Ref. [13]) was used. Two options are exercised concerning surface thermal accommodation: one in which all energy modes are fully accommodated and one in which all energy modes, except for vibration, are fully accommodated ($a_{C,V} = 0$). An indicator of the resolution achieved in a given simulation is the ratio of the mean collision separation between collision partners to the local mean free path (mcs/mfp), which should be less than 1. The magnitude of mcs/mfp is reduced by increasing the number of simulated molecules.

RESULTS OF CALCULATIONS FOR FLOW ABOUT SHARP BICONICS

Table 1 presents a summary of the free-stream conditions for the four test cases investigated. The Mach and Reynolds numbers listed are those provided for the respective test facilities and are based on the free-stream translational temperatures. Figure 1 provides information on the size of the two biconic models used in the current study: the 25°/55° model for the CUBRC tests (a maximum diameter d of 261.8 mm with a forecone running length of 101.59 mm) and the 25°/65° model for the ONERA tests (a maximum diameter of 60 mm with both forecone and second cone running length equal 22.57 mm). Also shown in Fig. 1 are the outline of the computational domains used and selective density contours that are normalized by their corresponding free-stream values. The calculated locations for flow separation and reattachment are noted by S and R, respectively.

CUBRC Run 7 Test Conditions

More extensive details regarding the simulations and results for this test case are included in Ref. [6]. Results presented in both Table 2 and Fig. 2 summarize some of the key features for this test case where there is a

TABLE 2. DS2V numerical parameters and results for sharp biconic (25°/55°), Run 7 test conditions.

Solution	$\triangle$ time, ms	mpc[a]	Molecules	mcs/mfp	Vib. Accom.	x_S, mm	x_R, mm	$\triangle x$, mm
a0	1.27 to 1.91	10	0.514E+6	0.944	0.0	82.8	99.4	16.6
b0	3.30 to 3.65	10	1.980E+6	0.441	0.0	81.2	100.4	19.2
c0	3.84 to 3.97	40	8.136E+6	0.214	0.0	80.3	100.7	20.4
d0[b]	3.97 to 4.41	40	8.114E+6	0.213	0.0	80.4	100.8	20.4
a1	1.03 to 2.02	10	0.528E+6	0.946	1.0	82.6	99.6	17.0
b1	3.30 to 3.65	10	1.980E+6	0.441	1.0	81.1	100.4	19.3
c1	3.83 to 3.96	40	8.133E+6	0.214	1.0	80.4	100.8	20.4
d1	3.96 to 4.40	40	8.114E+6	0.213	1.0	80.4	100.8	20.4
e1	4.81 to 4.93	40	16.482E+6	0.147	1.0	80.1	101.0	20.9

[a] mpc = molecules per cell (target number that is user specified)
[b] SMILE solution with 79.4E+6 molecules, $x_S = 79.6$, $x_R = 101.1$, and $\triangle x = 21.5$
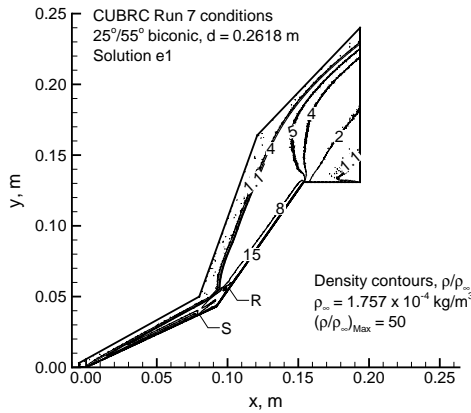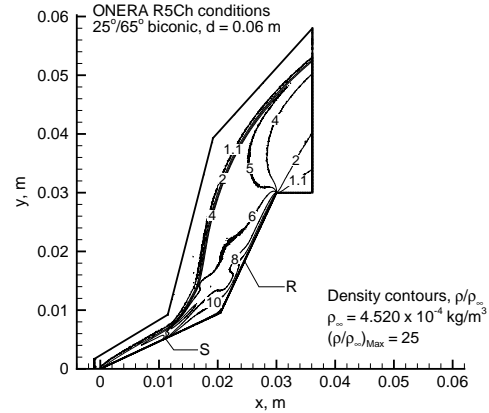

Fig. 1a. CUBRC model, Run 7 conditions.　　Fig. 1b. ONERA model, R5Ch conditions.

FIGURE 1. DS2V computational domain and computed density profiles for CUBRC and ONERA test cases.

small but distinct separation region with significant thermal nonequilibrium within the shock layer; that is, the vibrational temperature is essentially frozen at the elevated free-stream condition.

Table 2 presents a summary of some of the numerical parameters used in the DS2V calculations for the Run 7 test conditions, along with results for the locations (x_S and x_R) and the extent ($\triangle x$) of the separation region. Two separate series of calculations are made where the surface thermal accommodation for the vibrational energy is the only variable; zero accommodation for the lettered solutions with a "0" extension, and full accommodation for the lettered solutions with a "1" extension, as listed in Table 2. Results for these time accurate solutions are included for flow times of approximately 1 to 5 ms. The time accurate calculations suggest that the flow, with boundary layer separation, stabilizes rather quickly, on the order of a millisecond. The longer run time used in the present study occurred because several numerical perturbations (grid adaption and/or increase in the number of simulated molecules) were imposed as the simulation evolved in time. The simulations were monitored to ensure that a steady state was achieved, followed by the generation of a significant time-averaged sample for the results listed in Table 2. The steady state aspect of the simulations is demonstrated in Table 2 for the c0/1 and d0/1 solutions, both with and without surface vibrational accommodation, where sequential time-averaged solutions yield essentially the same results for the separation region. Also, the current simulation approach has used computational cells that are coarse in relation to the local mean free path, but the simulation has used the transient subcell feature [15] of the DS2V code, along with a large number of simulated molecules per cell, to promote small values of the local mcs/mfp parameter. For the most resolved
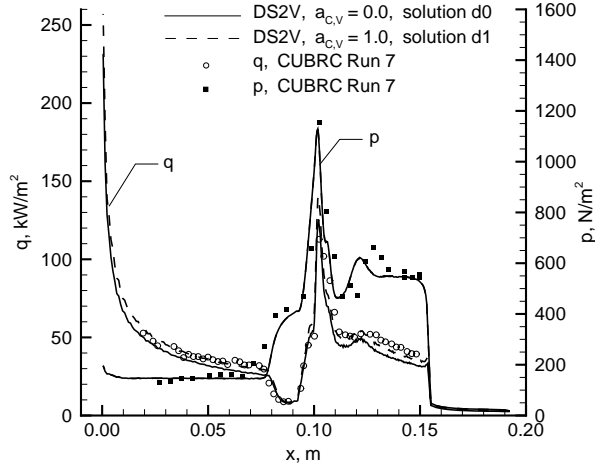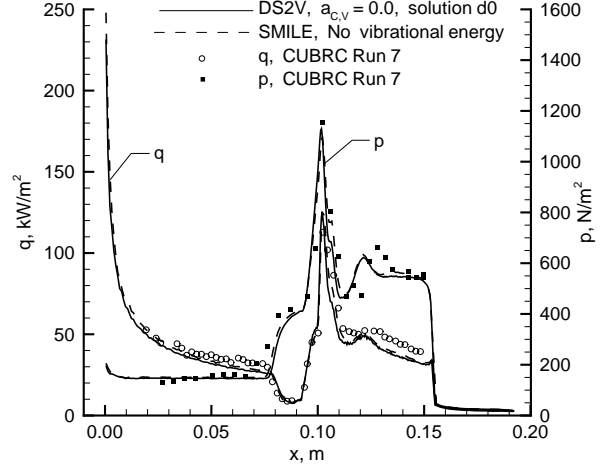
Fig. 2a. Effect of surface accommodation.

Fig. 2b. DS2V and SMILE results.

FIGURE 2. Comparison of calculated and measured surface heating rate and pressure distributions.

simulation, solution e1, the mean value of mcs/mfp was 0.15, with local values less than 0.37 at the location of separation and with no value exceeding 0.72. As shown in Table 2, the extent of separation increases with improved spatial resolution (smaller mcs/mfp), and there is no apparent impact on the extent of separation for the assumption regarding vibrational energy accommodation at the surface. But as shown in Fig. 2a, surface vibrational energy accommodation ($a_{C,V}$) has about a 12 percent impact on the calculated heating rates but negligible influence on the calculated pressure distributions. The measured heating rate values are in good agreement with the DS2V results for the full accommodation assumption but are in only fair agreement for zero accommodation of the vibrational energy, the boundary condition assumed [8] to be the more realistic of the two .

The final comparison for the Run 7 calculations are the current DS2V results with those Markelov obtained by using the SMILE DSMC code, the same results that were included in a recent review paper by Harvey [3]. The SMILE calculations were made without accounting for the vibrational energy (vibration turned off), which should be very similar to the DS2V results with vibration included and zero accommodation for the vibrational energy at the surface. Thus the SMILE results are compared with data from solution d0. The two calculations for surface heating and pressure distributions are in very close agreement, as shown in Fig. 2b, with the SMILE results showing slightly better agreement with the experimental measurements. In the SMILE calculation, a parallel code implementation with 80 million simulated molecules was used, approximately an order of magnitude greater than that used in the single processor DS2V calculation, solution d0.

CUBRC Run 35 and Run 28 Test Conditions

The CUBRC Run 35 and Run 28 test conditions present a significant challenge for DSMC simulations because of higher density flow conditions. In the current study, DS2V solutions were obtained for only a portion of the forecone, and heating rate and pressure results are presented in Fig. 3. The computational resolution or merit parameter mcs/mfp was approximately 0.22 for both test cases, with no value greater than 0.5. As was the case for the Run 7 calculations, the impact of the boundary condition for vibrational accommodation was about 12 percent on heating rates and only 1 percent or less on pressure distributions. Contrary to the results for the Run 7 calculations (also those for the CUBRC Run 11 hollow cylinder-flare test case presented in Ref. [6]), the Run 35 and Run 28 experimental heating rate results are in better agreement with the calculations, assuming zero surface accommodation for the vibrational energy. Only the experimental data independent of separation effects are shown. Since the variability of the CUBRC experimental heating data for these four test cases (including Run 11) is approximately ±15 percent with respect to the DS2V results, it is difficult to see
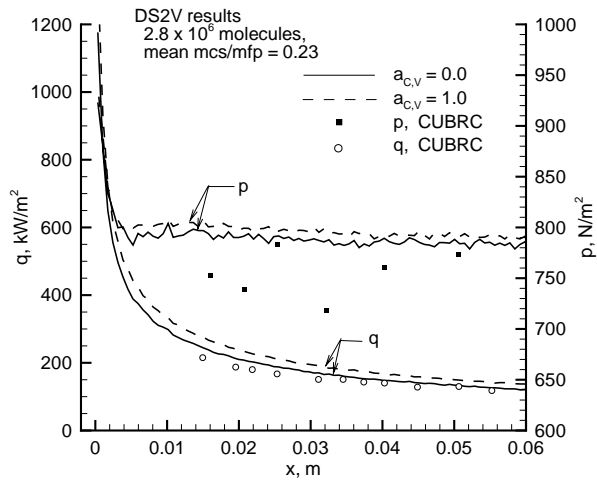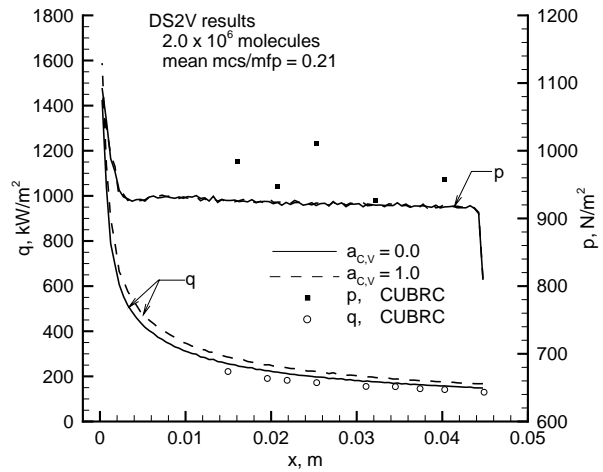
Fig. 3a. CUBRC Run 35 conditions.

Fig. 3b. CUBRC Run 28 conditions.

FIGURE 3. Comparison of calculated and measured results along the forecone (upstream of separation).

how the experimental data can be used to isolate a 12 percent effect on heating; that is, what is an appropriate boundary condition for the vibrational energy accommodation at the surface. Also, the experimental pressure variations with respect to the calculated values are about ± 5 percent if one assumes that the experimental pressure is the average of the respective data points for Runs 35 and 28, as shown in Fig. 3.
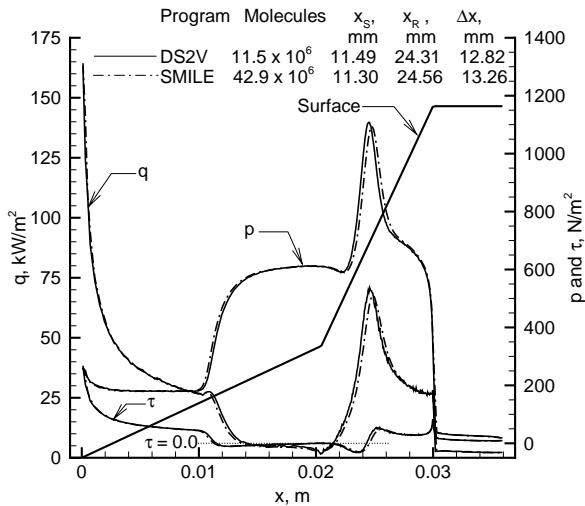
ONERA R5Ch Test Conditions
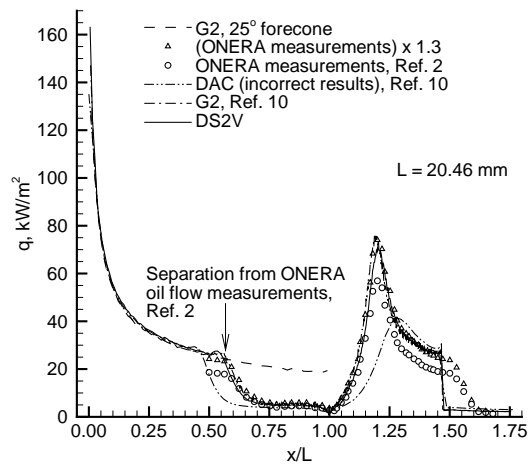

Fig. 4a. Comparison of DS2V and SMILE results.

Fig. 4b. Calculated and measured results.

FIGURE 4. Surface distributions for $25°/65°$ biconic at ONERA R5Ch conditions.

The ONERA test case (Table 1 and Fig. 1b) was included in this study because results of the experimental measurements were available [2] and continuum and DSMC solutions using both DAC and G2 had been

compared with the measurements. When the DS2V solutions were generated using 11.5 million molecules (Fig. 4) at a mean value of *mcs/mfp* equal 0.16, the calculated extent of separation was noticeably smaller than the DAC results (Fig. 4b), but was in close agreement with the G2 solution. Subsequently, Markelov, using the SMILE code, generated a solution with 42.9 million molecules, and the results for heating rate, pressure, and skin friction are in very close agreement with the DS2V results, as is shown in Fig. 4a. With three of the four DSMC codes providing similar results, Wilmoth [16] was asked to generate an independent solution with DAC and subsequently found a deficiency in the axisymmetric version of the code (not in the 2D and 3D versions) that becomes more apparent for simulations with a large radial extent. Consequently, the DAC results presented in Ref. [10] are incorrect, but the G2 results are believed to be reasonable results based on the good comparisons with both SMILE and DS2V. When the results of the three DSMC simulations are compared with the ONERA measurements, the separation location is in good agreement, but the calculated heating rates are about 30 percent greater than the measured values, as is demonstrated in Fig. 4b.

CONCLUSIONS

Results of a computational study focused on testing the accuracy of a relatively new DSMC code, called DS2V, show very good to excellent agreement with code-to-code comparisons. For the CUBRC test conditions, the variability in the experimental data with respect to the DS2V heating predictions is approximately ± 15 percent, a magnitude that would preclude any conclusions being made about vibrational accommodation. For the ONERA R5Ch biconic test case, the computed location of separation is in good agreement with the oil flow measurements, but the calculated heating values are approximately 30 percent greater than the measurements. Since the ONERA heat transfer results are inconsistent with similar measurements in other facilities when compared to the present calculations, it is believed that they are in error or there is some unexpected physical effect in the experiments that is inconsistent with the assumptions used in the current simulations.

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