NASA CONTRACT NSR 52-112-002

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FINAL REPORT on Contract NSR 52-112-002, for "Calculations of higher order collision integrals for use in the determination of transport coefficients of high temperature gases"

Publications

1. To be published in The Computer Journal :

   H. O'Hara and F. J. Smith, "The evaluation of definite integrals by interval subdivision".

2. Submitted to J. Computational Physics :

   H. O'Hara and F. J. Smith, "The efficient computation of the transport properties of a dilute gas to a prescribed accuracy".

3. To be submitted shortly to Comp. Phys. Comm. :

   H. O'Hara and F. J. Smith, "A program for the calculation of the transport properties of a dilute gas".

4. To be submitted shortly (Journal not decided yet) :

   A. Allison, A. Dalgarno and F. J. Smith, "The viscosity and thermal conductivity of atomic hydrogen at low and thermal temperatures".

Work in past quarter (1 January 1969 - 31 March 1969)

In the last quarter we put together the work of the previous three quarters. In particular, we used the method we described in our paper "The evaluation of definite integrals by interval subdivision" to evaluate all of the integrals. This gave correct, reliable results. Unfortunately, they were over-reliable at the expense of computer time. We quickly realised that our new splitting techniques would barely meet the time requirements laid down in the contract. At the same time, we realised that there was another approach to the evaluation of the badly behaved integrals, which was much more efficient: the use of changes of variable which force a concentration of the abscissas in the region where the integrand was largest and changed

most rapidly. The new methods we adopted are described in the enclosed preprint, "The efficient computation of the transport properties of a dilute gas to a prescribed accuracy". As we explain there, because of the difficulty of making error estimates in the more traditional methods, we adopted a Chebyshev curve-fitting technique for the purpose of interpolation.

These unexpected changes took us a few weeks into April to complete, and we used 20.3 hours of computer time more than we had planned. The extra cost is borne by the University. The resulting program benefited considerably from this extra effort, and a more efficient and reliable program was produced at the end than we could possibly have hoped for at the beginning.

The program was finally tested with runs on the (12-6), (12-6-3), (12-6-5) and e^{-r}/r potentials. These runs were all successful. As a final test we ran it for the gerade and ungerade potentials of atomic hydrogen, potentials fitted by many parameter functions at long and short ranges, and by a table at intermediate ranges. The results are also enclosed.

Results

A listing of the program with sample data and corresponding results is attached. Also included is a report of our work on the transport properties of atomic hydrogen and a preprint of our paper describing the numerical methods used in our program.

All of the contract provisions were fully met or surpassed. The program calculates a complete set of collision integrals at 40 temperatures to an accuracy greater than 1 in 1000 in $4\frac{1}{2}$ minutes on our ICT 1907 computer (similar to an IBM 7090). The contract specifies 20 minutes. It is possible to calculate collision integrals to an accuracy 1 in 10,000 or probably 1 in 100,000 with the program; the contract specifies 1 in 1000 only.

The flexibility of the program is demonstrated by one possible set of calculations of $\Omega^{(1,1)*}$ and $\Omega^{(2,2)*}$ at ten temperatures to an accuracy better than 1 in 100 in only one minute. The same program could calculate a complete set of collision integrals to an accuracy better than 1 in 10,000 in 10 minutes.

The Viscosity and Thermal Conductivity of Atomic Hydrogen

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The gerade and ungerade interaction potentials, $V_g(r)$ and $V_u(r)$, for the interaction of two ground-state hydrogen atoms have been calculated accurately by Kolos & Wolniewicz (1965) out to an internuclear distance $r = 10$ atomic units. The long range potentials are also known accurately (Walch and Bernstein, 1967; Chan and Dalgarno, 1969). Thus we know $V_g(r)$ and $V_u(r)$ over the whole range of r.

Since the weights of the gerade and ungerade states are 1 and 3 respectively the mean collision integral is given by

$$\overline{\Omega^{(l,s)*}(T)} = \frac{1}{4}\Omega_g^{(l,s)*}(T) + \frac{3}{4}\Omega_u^{(l,s)*}(T) \qquad (1)$$

where $\Omega_{g,u}^{(l,s)*}(T)$ are the collision integrals for the gerade and ungerade potentials on their own (Smith, 1967). These mean collision integrals replace the simple collision integrals in the Chapman-Enskog theory where there is only one interaction potential (Mason et al. 1959).

We curve fitted the potentials accurately using splines to fit the tables given by Kolos and Wolniewicz, making small changes in their tables to make the second and third derivatives smooth. These potentials were then put into the transport collision integral program of O'Hara and Smith (1969) and the collision integrals $\Omega_{g,u}^{(l,s)*}(T)$ were calculated. From these, using (1), we calculated the third order Chapman-Enskog approximation to the Viscosity and Thermal Conductivity of Atomic Hydrogen. This replaces previous less accurate calculations (Smith and Dalgarno, 1962). These are given in the Table over a range of temperatures. The results are correct to a few parts in 1,000 if the potentials are as accurate as this. They are likely to be correct within 1%.

At high temperatures, because of ionization, these results will be incorrect for a real gas. At low temperatures quantum effects will be dominant. These quantum effects are at present being calculated.

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References

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Table

Viscosity, η, and Thermal Conductivity, μ, of Atomic Hydrogen. The symbols η_1 and η_3 refer to the 1st and 3rd Chapman-Enskog approximations.

T(°K)	η_1 micropoise	η_3 micropoise	μ_3 10^{-3} cal. $cm^{-1} s^{-1} {}^{o}K^{-1}$
20	8.02	8.05	0.0596
50	15.5	15.6	0.115
100	25.0	25.2	0.187
150	33.3	33.4	0.248
200	40.7	41.0	0.304
250	47.8	48.0	0.356
300	54.4	54.7	0.405
350	60.8	61.1	0.453
400	67.0	67.3	0.499
500	78.9	79.2	0.587
600	90.3	90.7	0.672
700	101.0	102.0	0.753
800	112.0	112.0	0.833
900	122.0	123.0	0.910
1000	133.0	133.0	0.986
1500	182.0	182.0	1.35
2000	228.0	229.0	1.70
2500	274.0	274.0	2.03
3000	317.0	318.0	2.35
4000	400.0	401.0	2.97
5000	481.0	482.0	3.57
6000	562.0	563.0	4.16
7000	644.0	644.0	4.77
8000	727.0	728.0	5.38
9000	820.0	820.0	6.06
10000	913.0	914.0	6.75
20000	2090.0	2110.0	15.7
40000	5690.0	5790.0	43.3
60000	10800.0	11000.0	82.6
80000	17200.0	17700.0	133.0
100000	24900.0	25700.0	193.0
200000	81600.0	84500.0	637.0
400000	278000.0	289000.0	2190.0