A New Weighting Scheme Approach for Two-phase Condensation Modeling

Rakesh Kumar and D. A. Levin

Pennsylvania State University, University Park, PA 16802

Abstract. In this work, we develop a new species weighting scheme to reduce the computational effort associated with the study of freely expanding homogeneous condensation flows. The present work is an extension of our previous work[Kumar *et al.*, AIAA Paper 2010-818 (2010)], in which, we developed CO_2 condensation models in the statistical BGK framework to simulate the experimental data [Ramos *et al.*, Phys. Rev. A72, 3204 (2005)] for stagnation pressures up to 5 bar. The present work is aimed at the development of a numerically efficient numerical scheme that will extend the range of applicability of the present condensation models to the more challenging flow regimes of higher stagnation pressures. The accuracy and efficiency of the new species weighting factor method is compared with simulations performed without weighting factors. Numerical results are found to be in agreement, with the new approach shown to significantly reduce the computational effort.

Keywords: Weighting scheme, Condensing flow, Statistical BGK
PACS: 05.20.Jj

INTRODUCTION

In our previous work,[1] the homogeneous condensation of CO_2 was studied in the statistical BGK based computational framework. The work involved the development of a condensation model suitable for BGK that included the processes of nucleation, cluster-monomer sticking and non-sticking collisions, coalescence and cluster evaporation[1]. Simulations using the BGK based condensation model were compared with measurements of gas rotational temperature, cluster size and number density distributions[2] and were found to be in good agreement. These solutions were however obtained without a species weighting scheme, the use of which can potentially reduce the computational effort and in turn extend the range of applicability of BGK based condensation model to even higher pressure flows. Moreover, there are also situations in condensing flows where the condensate is a trace species compared to the monomer gas, making the former difficult to resolve without the use of species weighting factors. In the present work, we aim to incorporate species dependent weighting scheme in the condensation and evaporation models to develop a computationally efficient model.

A species-oriented weighting scheme was first proposed by Bird [3], in which an attempt was made to ensure almost equal number of particles of each species in the computational domain. This was achieved by assigning a different weight to particles of different kinds. The procedure enables one to dramatically increase the sample size of trace species. Since the particles now carry different weights, the collisional procedure needs to be revisited to take into account an artificially increased number of particles of trace species in the computational domain. Bird found that the weighting scheme mainly affects the computation of collisions. One of many examples for the use of species weighting factors is its use in modeling trace species that produce sensible radiation. Ultraviolet radiation from the the bow shock of a hypersonic rocket was measured and from an onboard spectrometer the source was determined to be trace amounts of nitric oxide (NO) molecule formed in the bow shock chemistry.[4] In fact the amount of NO that existed in the flowfield was computed to be on the order of a mole fraction less than 10^{-5}, which would present a major difficulty and computational constraint for a particle method. This is because in order to simulate one particle of NO in a computational cell, 100,000 other particles would be needed and if this approach were followed, at least 100 million particles would be needed making a simulation that should have been of modest size extremely expensive. To avoid this problem, species weighting factors were used and the computational particles representing the NO molecule were given a lower weight than those particles that represented the abundant species of N_2 and O_2.[5]

For all of the simulated cases, two kind of species are chosen to fill the flowfield, CO_2 gas and CO_2 clusters. As CO_2 clusters are produced from the gas as a result of nucleation, it can be assumed that the number of clusters may be considerably small in number as compared to the gas particles. In the new weighting scheme, a cluster has been assigned a weighting factor of 0.1 as compared to that of unity for the gas, so as to have comparable number of simulated cluster and gas particles in the computational domain. The fidelity of the new condensation model (with species dependent weighting scheme) is checked against the numerical results obtained in our previous work using a BGK based species independent condensation model.

DEVELOPMENT OF A NEW SPECIES WEIGHTING SCHEME FOR THE CONDENSATION MODEL IN THE BGK FRAMEWORK

Existing Weighting Scheme in the DSMC Framework

In the weighting scheme proposed by Bird [3], each particle in the computational domain is assigned a weight, W_i, with all particles of the same chemical species having the same weight. The incorporation of this scheme in the DSMC algorithm translates into affecting the computation of collisions in two ways. First, it affects the computation of the number of collisions and second, it affects the collision outcome.

In the present work, we use SMILE [6] as our baseline DSMC code which utilizes the majorant frequency scheme (MFS) to efficiently select potential collision pairs. The collision frequency is defined as follows:

$$\omega_{ij}^{MFS} = n_j \left[\sigma_c v\right]_{max} W_j \tag{1}$$

where σ_c is the collision cross-section of simulated molecules and is related to σ_c', the true physical cross section by

$$\sigma_c = \sigma_c' \cdot F_{num} \tag{2}$$

where F_{num} represents the ratio of the number of true to simulated particles. In Eq. 1, n_j represents number density of simulated molecules and W_j is the weight of species j, having a numerical value between zero and unity. Once a pair is selected, the probability that a collision occurs is evaluated by an acceptance-rejection test of the ratio of $P = \frac{\sigma_c v}{[\sigma_c v]_{max}}$. The number of collisions between pairs (i,j) is then

$$Z_{i,j}^{coll,MFS} = n_i \omega_{ij}^{MFS} \delta t P = n_i \omega_{ij}^{MFS} \delta t \left[\frac{\overline{\sigma_c v}}{[\sigma_c v]_{max}}\right] \tag{3}$$

where the bar represents the averaging over the cell.

If the two colliders have different weights, a second acceptance-rejection test is then performed to determine if the particle participate in an elastic collision $P_{i,j}'$ represents the probability that the a particle of species i is selected to collide with a particle of species j where

$$P_{i,j}' = \frac{W_j}{W_{max}}, \text{ and } W_{max} = max(W_i, W_j) \tag{4}$$

This probability accounts for the fact that when particles of different weights collide, the amount of change in the properties of the particle with the larger weight is reduced. To be more precise, when two particles of different weights collide, the probability that the properties of particle of lower species weight, i.e., the trace particle, would change is unity. On the other hand, the velocities of the particle with the higher weight i would change with a probability given by the ratio of the particle weights, $\frac{W_j}{W_i}$, if species j is the trace particle [5, 7]. This procedure was also extended to our previous DSMC simulations of homogeneous condensation for a freely expanding supersonic flow of CO_2 [8]. In that work, a weighting scheme was used in the study with a cluster species weighting factor of 0.04 with respect to a unity value of CO_2 gas weighting factor to resolve the presence of carbon dioxide cluster which becomes low as the plume expands.

New Weighting Scheme in the BGK Framework for Condensing Flows

In a recent study of homogeneous condensation of CO_2 in an expanding flow, a statistical BGK based condensation model [1] was developed and was shown to be able to simulate high pressure flows previously not possible with the DSMC method due to huge computational cost. The solutions obtained by the BGK method showed good agreement with the experiments, but, at a high computational cost because a cluster-species weighting scheme was not used. In presenting our new results with species weighting factors, we will refer to these solutions as the baseline results obtained by the BGK based condensation model without species weights.

In the present study, we continue to use the statistical BGK method [9] to model condensation of CO_2 but with a new weighting scheme which makes the method numerically efficient and in turn allows the simulation of even higher pressure flows. In order to understand the new weighting scheme, it is important to emphasize that in the BGK approach the actual collisions between molecules and clusters are not modeled. Instead the effect of such monomer-cluster collisions is approximated by an equilibration rate equation [10] which obviates the need for use of the acceptance-rejection tests that are used in the DSMC method. Moreover, in a condensing flow there are collisions which involve phase changes and the energy transformation associated with them. In addition to gas-gas interactions, condensing flows include the processes of nucleation, cluster-growth and evaporation processes, and coalescence. If one is to model all of these four processes in BGK, the weighting scheme approach must provide consistent results without the use of the acceptance-rejection technique. Note however that only the cluster-growth (or sticking) and evaporation

processes involve the simultaneous exchange of energy between the monomer and the cluster and a change of cluster size. Therefore, the weighting scheme for the nucleation model in the BGK framework is the same as in the DSMC method [8] and will not be described here. The coalescence model, which involves, cluster-cluster interactions, is also not described here because it does not require any change in the weighting scheme since the interacting cluster-particles have the same weighting factors. The non-sticking interactions of cluster-monomer computational particles are modeled by the same procedure as used in the recent work [1]. The implementation of weighting factors for the cluster-growth and evaporation models in the BGK framework however require a new weighting scheme, as described below.

A sticking collision between a cluster and a monomer is referred to as cluster growth event and an estimation of the cluster growth rate is as follows. For a spherical cluster of average radius r_c, the molecular flux to the cluster surface per unit time for a cluster immersed in a gas of number density n with mean molecular thermal velocity $\overline{c}$ is given by $b = \frac{1}{4}n\overline{c}$, where $\overline{c}$ is the mean molecular gas velocity. A cluster of size r_c is therefore bombarded by the gas molecules at a rate $4\pi r_c^2 b$ and the cluster growth rate, C, can then be given by the following equation:

$$C = \frac{4\pi r_c^2 \cdot q \cdot P}{\sqrt{2\pi m k T_t}} \tag{5}$$

where P is the condensible gas pressure, T_t is the gas temperature, m is the molecular mass and q is the sticking probability.

From the cluster growth rate relationship, Eq. 5, the number of cluster growth events per time step can be obtained for a cell. For each cluster growth event, a gas monomer is deleted from the computational domain, and added to a set of randomly chosen $1/W_c$ number of clusters, so that the size of each of the chosen clusters increases by 1. A schematic of the weighting scheme is shown in Fig. 1, in which a sticking interaction (condensation) between a gas monomer and cluster computational particles is modeled. The LHS of the figure shows a computational gas monomer particle (in blue) and a computational cluster particle (in red) interacting with each other. The middle figure shows that due to the use of a cluster species weighting factor, $W_c = 0.1$, the effective number of cluster particles participating in the interaction will be $1/W_c$ times the original number of cluster particles. On the RHS of Fig. 1, it is shown that the condensing gas monomer is virtually split into $1/W_c$ parts with each part interacting with one of $1/W_c$ clusters and carrying an equal fractional amount of momentum and energy. Note that the collision cross-section of each of such imaginary split gas monomer remains the same as the original one, as shown in the RHS of the figure. For each of the $1/W_c$ number of clusters, the velocity and temperature are modified by following the momentum and energy conservation principles. In other words, it is assumed that the momentum and energy carried by the condensing gas monomer gets equally distributed to every chosen cluster.

One could consider an alternative procedure too, in which we allow a gas monomer computational particle to condense on only one of $1/W_c$ randomly chosen simulated cluster particles and increase its size by unity. However, the procedure would be inconsistent, because in the nucleation stage [8, 1], the cluster species weighting factor results in an increased number of clusters, while in the cluster growth stage, it would increase the size of a cluster rather than the number. A solution using such a weighting scheme was obtained by this alternative approach and was found to be weighting factor dependent and to differ from that obtained by a BGK based condensation simulation without species weighs. On the other hand, the procedure, as described above, was found to agree well with the baseline results as will be shown in the next section.

Using the weighting scheme approach, the momentum and energy conservation for a cluster growth event are given as

$$W_c \cdot m\vec{v}_{m1} + mj\vec{v}_{c1} = m(j+1)\vec{v}_{c2}, \tag{6}$$

$$W_c \cdot \frac{1}{2}mv_{m1}^2 + W_c \cdot \frac{\xi}{2}kT_{m1} + \frac{1}{2}mjv_{c1}^2 + jC_pmT_{c1} + W_c \cdot H_v m = \frac{1}{2}m(j+1)v_{c2}^2 + (j+1)C_pmT_{c2}. \tag{7}$$

where ξ represents the number of degrees of freedom of gas monomer, subscripts m and c refer to monomer and cluster respectively, and 1 and 2 refer to pre and post cluster growth properties. The velocities and temperatures of the gas monomer and the chosen clusters of size j are known before the collision. The cluster size increases by unity after the collision becoming $j+1$. Therefore, the post-collisional velocities and temperatures of cluster can be calculated using Eqs. 6 and 7. The latent heat of condensation,H_v, associated with the cluster growth process is adjusted in the heat accommodation model [1].

In the evaporation process, monomers are removed from clusters and are returned to the computational domain as gas monomers. The evaporation rate is obtained assuming that the the cluster is in a metastable state where its size remains at the critical limit and is in steady state with the condensation process. The evaporation rate is given by the following equation,

$$E = \frac{4\pi r_c^2 \cdot P_s}{\sqrt{2\pi m k T_c}} \exp\left(\frac{2\sigma}{\rho R T_c r_c}\right) \tag{8}$$

where σ is the cluster surface tension and T_c is the cluster temperature. For each computational cell, a cluster surface area corresponding to the sum of the surface area of all the clusters in the cell is computed and an average temperature is used to obtain the evaporation rate.

Then for each evaporation event, a gas monomer is randomly placed in the computational cell, with velocity components sampled from a Maxwellian distribution at the local cell temperature. Likewise the rotational and vibrational energies of the gas monomer are randomly assigned corresponding to the local cell temperature, T_t. To account for the species dependent weighting factors, it is assumed that whenever an evaporation event takes place, an equivalent number of $1/W_c$ clusters participate such that the size of each of the $1/W_c$ clusters decreases by unity. If the arrows are reversed, Fig. 1 also shows the evaporating interaction between a gas monomer and a cluster. The velocity and temperature of each of the $1/W_c$ clusters are determined by the use of momentum and energy conservation, given by the following equations, while assuming that the momentum and energy of evaporated gas monomer is derived equally from every cluster.

$$mj\vec{v}_{c1} = W_c \cdot m\vec{v}_{m2} + m(j-1)\vec{v}_{c2}, \tag{9}$$

$$\frac{1}{2}mjv_{c1}^2 + jC_pmT_{c1} - H_vm = \frac{1}{2}m(j-1)v_{c2}^2 + (j-1)C_pmT_{c2} + W_c \cdot \frac{1}{2}mv_{m2}^2 + W_c \cdot (RE+VE)_{m2}. \tag{10}$$

where v_{m2} is the velocity of gas monomer sampled from Maxwellian distribution at local cell temperature, v_{c2} is the post evaporation cluster velocity, $(RE+VE)_{m2}$ are the sum of rotational and vibrational energies of gas monomer evaporated from the cluster. Once v_{m2} is known, the post evaporation velocity of cluster v_{c2} can be obtained from momentum conservation, Eq. 9. Likewise, the post evaporation temperature of the cluster, T_{c2}, can be determined once the last term of the Eq. 10 is obtained by randomly assigning the gas monomer rotational and vibrational energies at the local cell temperature.

VALIDATION RESULTS FOR THE CONDENSATION MODEL IN BGK FRAMEWORK AND EFFICIENCY

The accuracy and efficiency of the new condensation weighting scheme was tested by comparison of condensation results obtained without any species dependent weighting factors. The latter simulations were shown to compare well with the experimental data of Ramos *et al.* [2] in our previous work [1]. Three cases were studied corresponding to the stagnation pressures of 1, 3 and 5 bars. The computational domain used in our work is shown in Fig. 2. The domain is 10-by-2 nozzle diameters from the starting surface at the nozzle exit, *i.e.,* from x = 0 to 0.0032 m and from y = 0 to 0.006 m. Further details about the procedure to obtain starting surface can be found in Ref. [1]. The BGK numerical parameters used are given in Table 1.

Figure 3-(A) compares the variation of cluster number density along the plume centerline obtained by the BGK method with and without the species weighting factors for pressures of 1, 3 and 5 bars. It can be seen that the two schemes agree well with each other and capture the condensation physics. The cluster number density decreases after reaching a maximum value because as clusters move through the flowfield, they have a tendency to collide and merge with other gas monomers and clusters. Cluster particles can also evaporate because of the extra energy gained during a collision with the other particle. These two effects along with the nucleation rate variation with gas number density result in the cluster number density profile as shown in Fig. 3-(A).

Figure 3-(B) compares the new weighting scheme with the baseline BGK results for the cluster size variation along the plume centerlines for different pressure cases. It is evident that the two schemes are in good agreement with each other. It can be seen that the cluster size increases along the plume centerline for all of the cases. This is expected because as a cluster moves along the flowfield, it can consume gas particles or it can merge with other clusters, resulting in cluster growth. At the same time, a cluster size may decrease because of evaporation. Therefore cluster growth, coalescence, and evaporation affect the cluster size along its trajectory. All these effects become less significant further downstream as the flow expands. Accordingly, the figure shows that the cluster size, on a log scale, increases linearly initially with the axial distance for all of the cases, and then starts saturating at the middle of the computational domain, i.e., at $x/D = 5$.

Now we discuss the effect of condensation on gas rotational temperature. As explained above, the latent heat release during the nucleation and cluster growth processes and latent heat removal during the evaporation process result in increased thermal motion of the gas molecules and their rotational energy modes. Figure 3-(C) compares the gas rotational temperature obtained by the new species weighting scheme with that obtained by the baseline BGK based condensation model without any species weighting scheme. It can be seen that the two schemes show very good agreement with each other. Finally we compare cumulative number density, i.e., sum of gas and cluster number density, obtained by our new scheme with the old one. Figure 3-(D) shows that the two schemes are remarkably close to each other.

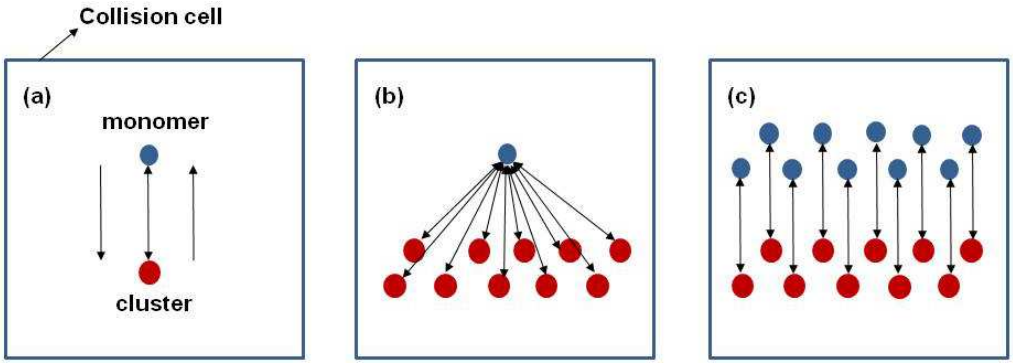

FIGURE 1. Weighting scheme for the BGK based condensation and evaporation models. (a) Physical picture, (b) Conceptual picture for a cluster species weighting factor of 0.1 , and (c) Computational picture with an imaginary break-up of a gas monomer into 10 for a cluster species weighting factor of 0.1 .

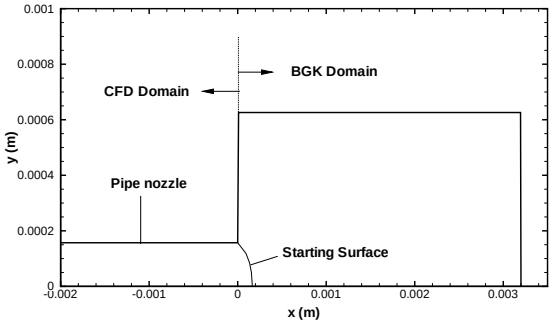

FIGURE 2. Computational domain used in the present work to simulate free expanding flows in various stagnation pressure cases.

A numerical efficiency analysis was conducted to compare the numerical performance of the two computational schemes. Table 1 shows the the comparison of computational time required for the 5 bar stagnation pressure case for a choice of CO_2 cluster species weighting factor of 0.1 versus a value of unity for CO_2 gas monomers. We also verified that the new weighting scheme is independent of the choice of the cluster species weighting factor. We used a time step of 1×10^{-9} s, which is smaller than the local mean collision time. Each of the simulated gas particle represented 5×10^7 CO_2 molecules. The simulation was carried out on Intel 3GHz Xeon processors for 5 bar case. It can be seen that the new scheme is more than two times faster than the old scheme. The computational enhancement is not directly proportional to the reduction in the number of computational particles because additional computational effort is required in the cluster growth and evaporation models.

CONCLUSIONS

A new species dependent weighting scheme was developed to reduce the computational effort associated with the study of a freely expanding homogeneous condensation flow of CO_2 for a stagnation pressure range of 1-5 bars. The new scheme was shown to perform as accurately as the scheme without any species weighting scheme, which was already shown to simulate the experimental data in our previous study. It was shown that the new scheme is about 2.5 times faster than the previous scheme. The model developed for the present work will enable us to simulate condensation flows for computationally more difficult cases in the future.

TABLE 1. Computational Efficiency

Method	New Scheme	Old Scheme
Time (CPUH)	320	750
Number of particles	2.0 mil	7.5 mil
Number of cells	0.162 mil	0.162 mil

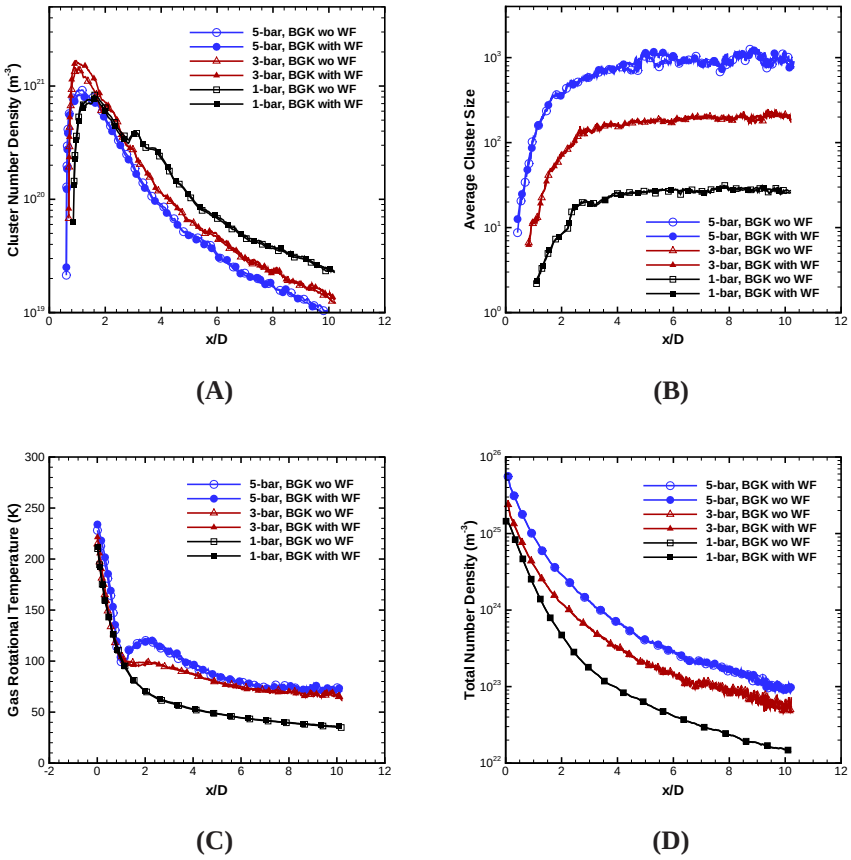

FIGURE 3. Comparison of centerline profiles obtained by the BGK method for different pressures with and without species weighting scheme, (A): cluster number density; (B): cluster size; (C): gas rotational temperature; (D): cumulative number density.

ACKNOWLEDGMENTS

The research performed at the Pennsylvania State University was supported by the Air Force Office of Scientific Research Grant No. F49620-02-1-0104 whose support is gratefully acknowledged. We thank Professor M. Ivanov of the Institute of Theoretical and Applied Mechanics, Russia for the use of the original SMILE code.

REFERENCES

1. R. Kumar, Z. Li, and D. Levin, *AIAA Paper 2010-818* (2010).
2. A. Ramos, J. M. Fernández, G. Tejeda, and S. Montero, *Physical Review A* **72**, 3204–3210 (2005).
3. G. Bird, *Molecular Gas Dynamics*, Oxford University Press, Oxford, England, UK, 1976.
4. P. Erdman, E. Zipf, C. Howlett, D. Levin, G. Candler, and R. Collins, *Journal of Thermophysics and Heat Transfer* **8**, 441–446 (1994).
5. S. Gimelshein, and D. Levin, *Journal of Thermophysics and Heat Transfer* **14**, 471–479 (2000).
6. M. Ivanov, and S. Gimelshein, "Current Status and Prospects of the DSMC Modeling of Near-Continuum Flows of Non-reacting and Reacting Gases," in *Proceedings of the Rarefied Gas Dynamics 23rd Int. Symp., AIP Conference*, 2003, vol. 663, pp. 339–348.
7. I. Boyd, *Journal of Thermophysics and Heat Transfer* **10**, 579–585 (1996).
8. Z. Li, J. Zhong, and D. Levin, *Journal of Physical Chemistry C* **114**, 5276–5286 (2010).
9. K. Nanbu, S. Igarashi, and Y. Watanabe, *Journal of the Physical Society of Japan* **57**, 3371–3375 (1954).
10. R. Kumar, E. Titov, D. Levin, N. Gimelshein, and S. Gimelshein, *AIAA Journal* **48**, 1531–1541 (2010).