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Barium Oxide Depletion from Hollow-Cathode Inserts: Modeling and Comparison with Experiments

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In this paper, the results of a barium oxide depletion model are compared with some experimental results. The model is used to simulate the T5 and T6 cathodes and the NSTAR discharge cathode. A comparison with the experimental data is performed. For the T5 and T6 cathodes, good qualitative agreement is found, but for the NSTAR cathode, the agreement is not as good. In both cases, the agreement is improved when the boundary conditions are modified to better reflect the experimental conditions. The model presented is the first three-dimensional axisymmetric insert model that includes the dependency of BaO depletion from both the impregnant chemistry and the diffusive motion inside the insert.

I. Introduction

HOLLOW cathodes are some of the most important devices in the field of electric propulsion. They are currently used as electron emitters/neutralizers in gridded and radio-frequency ion thrusters and in Hall-effect thrusters. At present, hollow cathodes have demonstrated a lifetime of 30,000 h [1], and no experimental data exist above this limit. With the use of gridded ion engines or Hall-effect-thruster-based solar electric propulsion subsystems for deep space missions, hollow-cathode lifetime is becoming a growing issue: in particular, when the required lifetime is in excess of 30,000 h or when operating conditions differ significantly from those used in the 30,000 h test.

Hollow-cathode lifetime is considered to be limited by various phenomena such as low-work-function material depletion from the insert, orifice erosion, poisonous compounds, and sputtered tungsten deposition on the insert surface. Barium oxide (often combined with CaO and Al_2O_3) is one of the most common impregnants used in the preparation of hollow-cathode inserts. A model to predict barium oxide depletion from hollow-cathode inserts has been already developed by the authors [2], starting from the knowledge of the BaO-CaO-Al_2O_3 ternary system chemistry and including the evaporation-rate dependence on the local BaO content and the diffusive motion of barium inside the insert. In this paper, the model results will be compared with the experimental measurements relative to the T5 and T6 cathodes [3,4] and the NSTAR discharge cathode [1].

Regarding the modeling of BaO depletion from hollow-cathode inserts, other papers have been published in the past. In those studies, the chemistry of BaO evaporation was often reduced to a single evaporation reaction, neglecting any dependence of the evaporation rate on the local impregnant composition [5,6] and hence, in certain cases, overestimating the BaO evaporation rate up to several orders of magnitude [2]. In those studies in which the complicated chemistry of the BaO-CaO-Al_2O_3 system has been taken into account [7,8], it seems that the processes leading to barium oxide diffusion from the insert core to the surface have been neglected, assuming that all the BaO contained in the insert is instantaneously available at the surface for evaporation. In the model developed by the authors, both the chemistry of the BaO-CaO-Al_2O_3 system and the diffusion processes leading to BaO migration are taken into account. Regarding the importance of barium oxide depletion from the insert, some interesting results have been obtained by Polk [9], according to which the barium evaporated from the insert does not escape from the cathode. This leads to the build up of a high Ba partial pressure, preventing further Ba evaporation from the insert, except from a small region in which the ionization reduces the neutral barium pressure. Considering these results to be correct, the modeling of barium oxide depletion from the insert might look less important than before. However, the results presented in [9] are dependent on the knowledge of the partial pressures produced by the barium evaporation from the insert, and this (as shown in [2]) depends on the local barium content that in turn depends on the barium and barium oxide diffusive motions inside the insert. The model that will be presented in this paper is therefore still valid, and if the results in [9] are confirmed by further investigation, it can be easily modified (through a change in the boundary conditions) to adapt to the scenario presented in [9].

This paper will be divided into two parts: in the first, a comparison with the data relative to the T5 and T6 cathodes [3,4] will be performed, and in the second, the comparison will be performed using the data measured relative to the NSTAR cathode [1].

II. Comparison with the Experimental Results Relative to the T5 and T6 Cathodes

The T5 cathode and the T6 cathodes were tested in representative discharge chamber conditions for, respectively, 15,000 and 800 h [3,4]. At the end of the test, the inserts and cathode tubes of these cathodes were destructively analyzed. The external surface of the T5 insert was found to be covered in a greenish-white crust that an energy-dispersive x-ray (EDX) analysis indicated to be mainly barium containing impregnated material. The same kind of deposition has also been found on the T5 cathode tube, hence providing the evidence that BaO evaporation occurs also from the external surface of the cathode. The insert of the T5 cathode has been fractured and analyzed using a scanning electron microscope EDX to map the $L\alpha$ lines of barium. The result of this analysis is reported in Fig. 1, in which the region extending 1.6 mm upstream of the orifice plate (downstream end of the cathode) is presented.

In Fig. 1 the darker zones indicate areas in which barium has been depleted, and the brighter zones indicate areas in which a high content of barium is still present. In particular, it shows that the depletion takes a tongue shape at the downstream end of the cathode, with a depletion depth of 435 μm from the orifice plate. Unfortunately, no quantitative depletion data are present in the literature for the T5 insert; hence, a qualitative comparison between experimental and numerical data will be done using the map reported in Fig. 1. The T6 cathode operated for 800 h has been sectioned and

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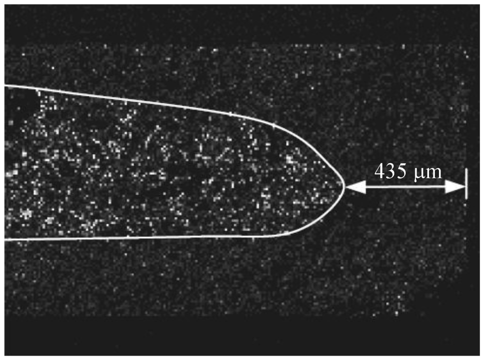

Fig. 1 EDX mapping of barium *Lα* line of the T5 cathode [4].

analyzed using EDX scanning. This cathode has been reported to show, as expected, no appreciable depletion [3,4].

The T5 and T6 cathodes have been simulated for 15,000 h with the model reported in [2]. The insert temperature profiles used to run these simulations have been taken from [10], in which using thermocouples placed inside the insert the temperature profiles of the T5 and T6 has been characterized for different current levels, including those used in the 800 and 15,000 h tests. These temperature profiles are shown in Fig. 2, in which 0 and 1 indicate, respectively, the upstream and downstream end of the insert.

We will assume that the barium oxide content inside the insert is maximum at the beginning of life, with the insert perfectly filled by the impregnant and with homogeneous barium oxide distribution. This assumption is justified by the fact that even if the composition inside the insert will be most probably nonhomogeneous, given the impregnation process, no measurements relative to the initial impregnated composition in the T5 and T6 cathodes have been reported in the literature; hence, the only reasonably feasible assumption is that of homogeneous content.

We will impose boundary conditions so that evaporation occurs from the internal and external surfaces of the cathode, as shown by the experimental observations. The contour map relative to barium oxide depletion from the insert of the 800 h T6 cathode test is reported in Fig. 3, in which 0 indicates the upstream end of the cathode and 1 indicates the downstream end.

As shown in Fig. 3, the model predicts a very low level of depletion, as expected and as observed in the experimental analysis. To have a better comparison between numerical and experimental data, the computed barium contour map relative to the whole T5 insert after 15,000 h of functioning is shown in Fig. 4.

To verify the presence of any similarities between the numerical and the experimental depletion profiles, the computed depletion profile relative to the area extending 1.6 mm upstream of the orifice plate (the same area of the insert presented in Fig. 1) is shown in Fig. 5.

Figure 5 shows a tongue shape similar to that present in Fig. 1. To better judge the agreement between the profiles in Fig. 1 (experimental) and Fig. 5 (computed), we will take the barium

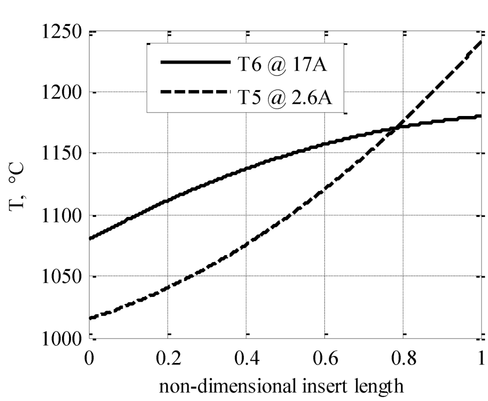

Fig. 2 T5 and T6 insert temperature profiles [10].

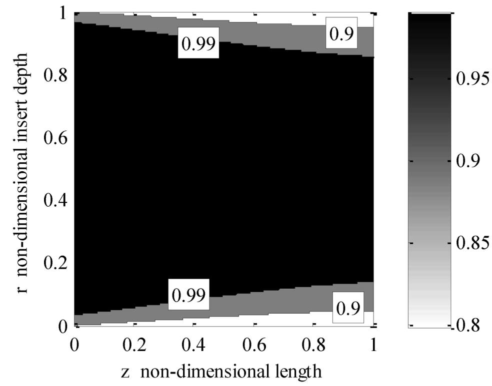

Fig. 3 Barium contour map of the T6 cathode after 800 h at 17.1 A.

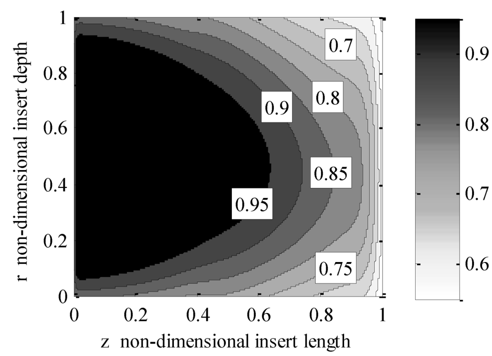

Fig. 4 Barium contour map of the T5 cathode after 15,000 h at 2.6 A.

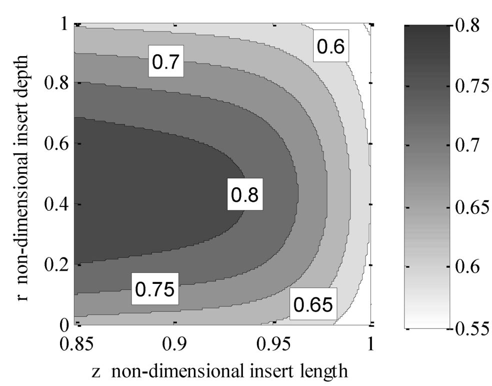

Fig. 5 BaO color map corresponding to the measurements in Fig. 1.

isodepletion contour relative to 435 μm of depletion from the orifice plate and superimpose it on Fig. 1.

As shown in Fig. 6, the barium oxide isodepletion line closely follows the experimentally derived depletion profile. The line follows the experimental results very closely in the top part (corresponding to

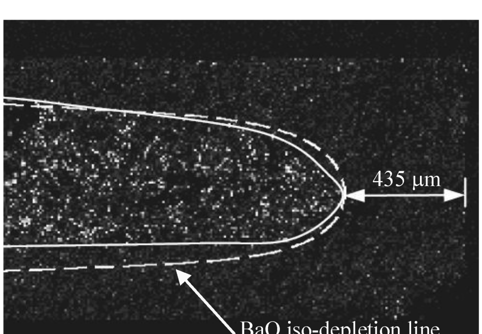

Fig. 6 Comparison between the experimental depletion profile (solid line) and the corresponding BaO isodepletion contour (dashed line) calculated numerically.

the insert external surface), whereas the bottom one (corresponding to the insert internal surface) is a bit more distant. The reason for this could be that the model, having the outer and inner diameter surfaces perfectly free to evaporate BaO, presents a strong symmetry. This symmetry might be nonrealistic, since the outer surface of the cathode is still enclosed by the cathode tube, hence allowing evaporation of barium oxide until the deposition over the cathode tube will fill the gap existing between it and the insert and hence occluding the insert pores and preventing further evaporation.

III. Comparison with the Data from the NSTAR Cathode

As part of the Deep Space 1 life test, the NSTAR discharge cathode has been run for 30,372 h at different throttle levels, as depicted in Table 1 [1].

After 30,372 h, the test was stopped intentionally and the cathode was then sectioned and analyzed by means of EDX scanning to measure the Ba/W ratio at various points of the insert (see Fig. 7). This signal can be related to the BaO content inside the insert, since barium reacts with the rest of the impregnant material (CaO and Al_2O_3), forming compounds in which barium always appears bonded with oxygen, producing compounds that have the general form of $(BaO)_x$-$(CaO)_y$-$(Al_2O_3)_z$ [11]. Hence, considering the W content to be constant, the signal is directly proportional to the barium/barium oxide content in the insert (for details regarding the chemistry of the BaO-CaO-Al_2O_3 system, please refer to [2,11]).

The barium-over-tungsten ratio has been also measured before the beginning of the test, as shown by the black points in Fig. 7a. From these data, two hypotheses relative to the initial barium content in the insert have been formulated. The first hypothesis is that the insert is completely filled with the impregnant at the beginning of the test, and hence the initial BaO profile (including not only molecular BaO, but also all the compounds formed inside the impregnant in which BaO is present [2]) is flat (dashed line in Fig. 8), with a value that is the average of the measured values. The second hypothesis is that, due to the impregnation process, the BaO profile is not flat along the insert depth; in this case, its trend has been derived by interpolating the measurements (solid line in Fig. 8). It must be noted that in [1] it is not reported where along the insert length the points relative to the unused insert have been taken, and hence that the interpolated profile might then not be valid for the whole insert.

The temperature profiles needed to simulate the insert chemistry have been taken directly from the literature [12] when possible. Otherwise, they have been derived interpolating the published data, assuming a linear trend of the insert temperature with the discharge current. The insert has been simulated with both the flat and the interpolated initial BaO profiles and assuming evaporation to always occur from the inner diameter surface, whereas different simulations have been performed regarding the conditions of the outer diameter and orifice-plate surface. The complete set of boundary conditions used is reported in Table 2. The closest agreement has been obtained using boundary condition (BC) sets 1 and 2, in which no evaporation occurs from the orifice-plate surface.

To judge the trends reported in Figs. 9 and 10 for every set of numerical data [1.5, 6.5, 13.5, and 23.5 mm from the orifice plate (OP) with both the interpolated and flat profile and with both BC set 1 and set 2], the value of the error with respect to the experimental data has been defined as the average of the absolute value of the errors calculated between the experimental points and the calculated points at the same radial position.

Table 1 Extended-life-test discharge cathode throttle settings [1]

Throttle level	Accumulated hours	Discharge current, A
12	500	9.9
15	4,800	13.5
8	10,500	7.6
15	15,500	13.5
0	21,500	4.9
15	25,500	13.5
5	30,000	6.9

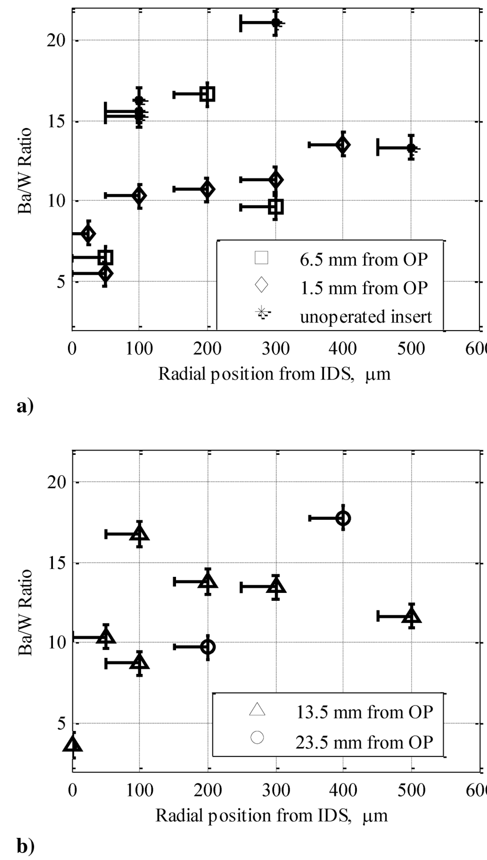

Fig. 7 Ba/W ratio value for different radial and axial positions [1].

Figure 9 shows that the trends derived with the flat and interpolated initial profiles show a comparable level of agreement with the experimental data, with a relative error difference of 9%, in favor of the data obtained with the flat profile. The same cannot be said for Fig. 10, in which the error obtained with the flat profile is about two-thirds of that obtained with the interpolated profile.

It can also be seen (Figs. 9a and 10a) that the change in boundary conditions relative to opening the external surface to evaporation (moving from BC set 1 to BC set 2) strongly increases the error relative to 1.5 and 6.5 mm from the OP, whereas a smaller impact can be found on the data relative to 13.5 and 23.5 mm (Figs. 9b and 10b). In particular, at the upstream end of the insert, the improvement is increased with the use of BC set 2. In fact, Fig. 9b shows that with the external surface closed, the numerical data relative to 13.5 mm show a Ba content that continuously increases with the radial position, and in Fig. 10b, in which the external surface is open, the numerical data

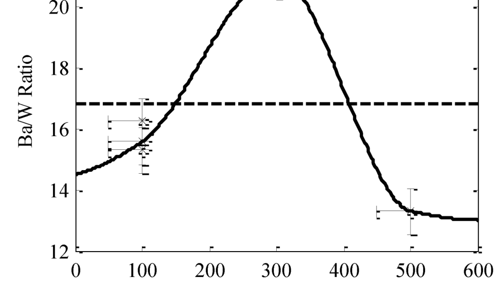

Fig. 8 Different initial BaO profiles; flat profile (dashed line) and interpolated profile (solid line).

Table 2 Different sets of boundary conditions

Boundary conditions	Descriptions
BC set 1	Evaporation from the inner surface only
BC set 2	Evaporation from all the surfaces but the orifice plate and upstream surface
BC set 3	Evaporation from all the surfaces but the external and upstream surface
BC set 4	Evaporation from all the surfaces

better follow the experimental data, decreasing after about 300 μm from the internal diameter surface. This translates to a relative reduction of 15% of the error relative to 13.5 mm from the OP, when the external surface is considered open to evaporation.

Considering what has been reported above, it can be seen that the downstream end of the cathode is better represented when the external surface is closed, whereas the upstream part is better represented when the external surface is open. This can be explained by noting that the internal part of the cathode tube has been reported to be covered in a Ba-containing crust [1], hence allowing for the assumption that evaporation occurs for the external surface of the insert. This evaporation is possible only if a small gap exists between the insert and the cathode tube. When the evaporated material fills this gap, it will occlude the insert pores, hence avoiding further evaporation from that location. This will happen much sooner at the cathode downstream end, where the temperature and, hence, the evaporation rates are higher than at the upstream end. To include this effect in the simulation, we will assume a size for the gap existing between the insert and the cathode tube, and we will allow evaporation to occur from a point on the external surface until the gap between insert and cathode tube at that point gets filled by the evaporated impregnant. This boundary condition will produce an external surface that is completely open to evaporation at the beginning of life and that gradually becomes closed, starting from the downstream end of the insert and moving upstream.

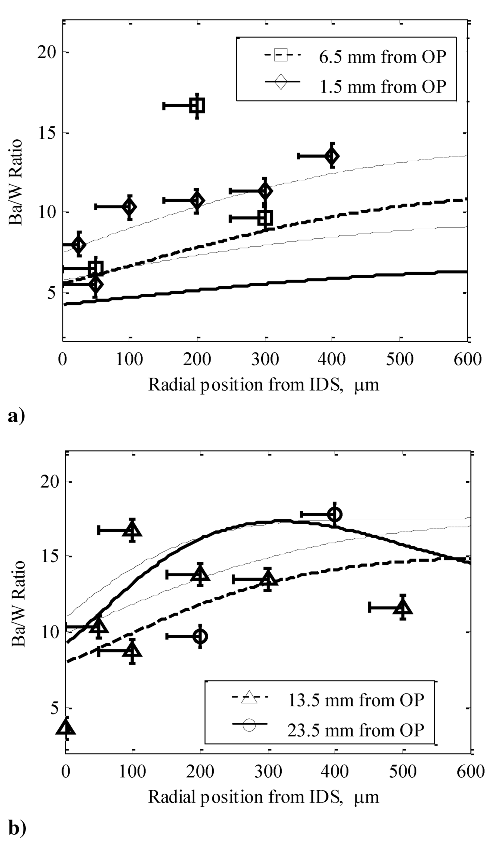

Fig. 9 Comparison between numerical and experimental results BC set 1.

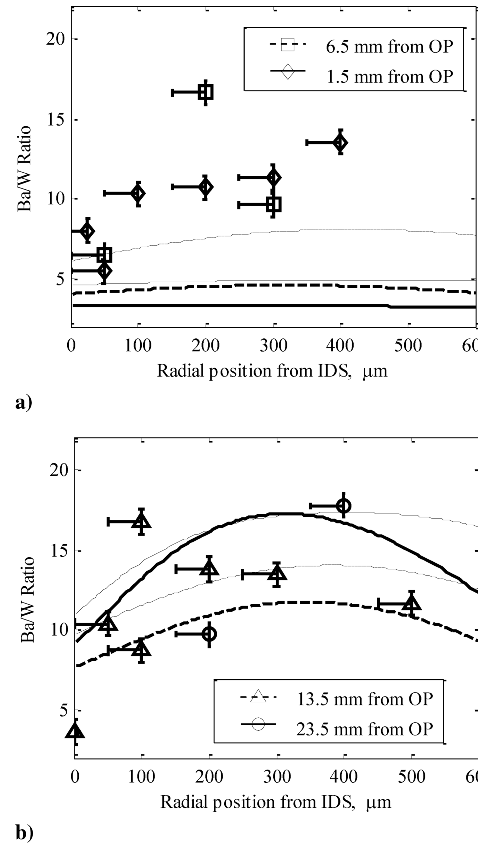

Fig. 10 Comparison between numerical and experimental results BC set 2.

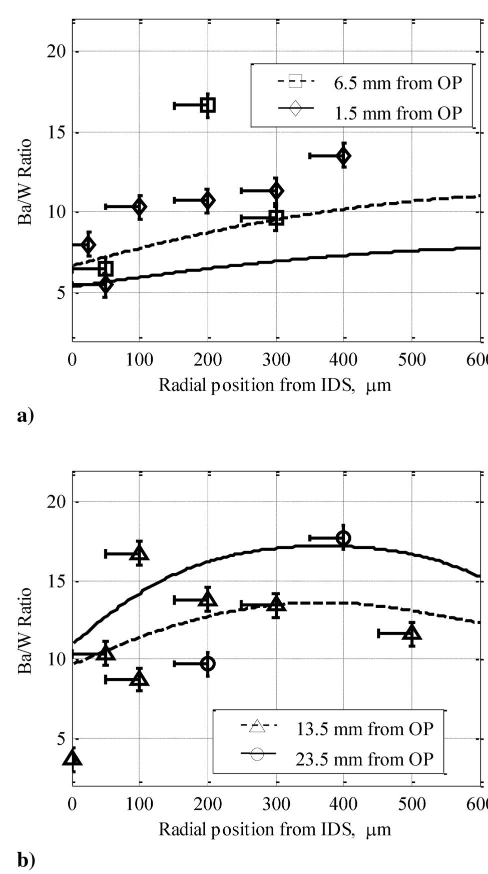

Fig. 11 Comparison between numerical and experimental results for a cathode-tube gap of 100 μm.

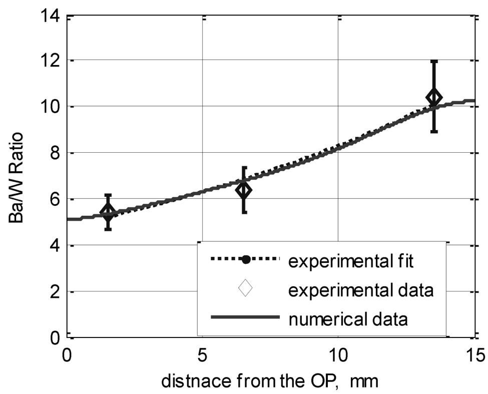

Fig. 12 Comparison with the depletion data relative to 50 μm of depth from the insert internal surface [15].

Concerning the choice between the interpolated or flat initial profile, it has been decided to use only the flat initial profile. This choice is justified by what has been noted earlier relative to BC set 2 and by the fact that the interpolated profile derived before might not be valid for the whole insert, since there is no information in [1] regarding where (along the insert) the data relative to the unused insert have been taken.

Simulations have been run with five different values of the gap size: 25, 50, 75, 100, and 125 μm. The lowest error between numerical and experimental data has been obtained with 100 μm.

The numerical results relative to 1.5 and 6.5 mm in Fig. 11 show a better agreement than those reported in Fig. 10 and are comparable with those reported in Fig. 9, confirming that the gap gets filled relatively quickly at the downstream end of the insert, hence resulting in a local boundary condition that is closed to evaporation.

The data relative to 1.5 mm still show a very poor agreement with the experimental data. A partial explanation for this poor agreement might be found by noting that the downstream area of the cathode has been reported to be influenced by tungsten deposition and erosion [13–15] that might occlude the matrix pores, hence preventing barium evaporation (in fact, there is more barium left inside the insert at 1.5 mm than at 6.5 mm, even if the temperature at 1.5 mm is about 40° higher than at 6.5 mm [12]). These processes are not included in the model, and hence a discrepancy between the numerical and the experimental data must be expected. In particular, the computed data are conservative, underestimating the barium oxide content inside the insert. Another partial explanation is that at the downstream end of the cathode, since the temperature is at its maximum, the effect produced by any simplifying assumption done regarding the chemistry in the model development [2] is stronger than in other locations along the insert.

The data relative to 13.5 mm from the orifice plate show reasonable agreement, given the uncertainties in exactly matching the temperature profiles and boundary conditions, except for the 100 μm position, whereas those relative to 23.5 mm are difficult to judge, since only two experimental points exist and the 400 μm point shows good agreement, but that at 200 μm shows poor agreement.

In [16] the depletion trend along the insert length at a depth of 50 μm from the insert inner surface is reported. A comparison between this and the numerical data is reported in Fig. 12. As shown in Fig. 12, the agreement is satisfactory in this case, and it can be confirmed by looking at the point relative to 50 μm in Fig. 11.

IV. Conclusions

In this paper, the results from a BaO depletion model have been compared with experimental data. To the best of the authors' knowledge, this is the first time that the barium content evolution inside the insert of discharge cathodes from gridded ion engines has been simulated with a 3-D axisymmetric model that takes into account both the complex BaO-CaO-Al_2O_3 impregnant chemistry and the barium oxide diffusive motion inside the insert, and the model results have been compared with actual depletion measurements

Comparisons were made with the experimental data from the T5, T6, and NSTAR cathodes. Good qualitative agreement has been found with the data from the T5 and the T6 cathodes. For the NSTAR cathode, the agreement between the experimental results and the model simulations depends on what section of the cathode is being investigated. Close to the orifice plate, where this agreement was not good, it was found that by modifying the boundary conditions to more closely represent the real functioning conditions of the cathode, including the effect of the presence of a gap between the insert and the cathode tube and how this influences the evaporation from the external surface of the insert over time, the agreement was improved (see the data relative to 6.5 mm from the orifice plate in Figs. 10 and 11). This leads us to believe that the model is a reasonably good representation of the physical and chemical mechanisms governing the barium depletion.

However, considering the difficulties related to the prediction of barium depletion (mainly the lack of chemical data regarding the kinetic of the reactions and the complexity of the diffusion motion, due to the presence of many interconnected processes), coupled with the problems of exactly matching the model to the experimental operating conditions (temperature profile and boundary conditions), the difficulties in accurately measuring the barium depletion profiles, and the paucity of experimental data, we believe that the model is capturing the essential physicochemical mechanisms that play a role in barium depletion in these hollow cathodes; however, further comparisons with high-fidelity measurements taken under controlled experimental conditions are needed to both confirm that the basis of the model is valid and suggest how it could be improved.

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