Numerical Simulation of the Insert Chemistry of the Hollow Cathode from the Deep Space 1 Ion Engine 30,000 Hrs Life Test

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M. Coletti* and A. Grubisic†
University of Southampton, Southampton, SO17 1BJ, United Kingdom

S.B. Gabriel‡
University of Southampton, Southampton, SO17 1BJ, United Kingdom

Using a model for the insert chemistry developed by the authors and based on the knowledge of the BaO – CaO – Al₂O₃ ternary system the ELT discharge cathode insert from the Deep Space 1 life test has been simulated. The computed data show a good agreement with the experimental one; the agreement increase with the imposition of boundary conditions closer to the experimental evidence. Tungsten deposition effect have been introduced into the model using experimental data and further improving the agreement between computed and measured data. The deposition trend found suggests the possibility of a link between barium depletion and tungsten deposition.

Nomenclature

\[ A = \text{Al}_2\text{O}_3 \]
\[ B = \text{BaO} \]
\[ BC = \text{boundary conditions} \]
\[ C = \text{CaO} \]
\[ D_a = \text{diffusion coefficient} \]
\[ E_{Da} = \text{activation energy of the diffusion process} \]
\[ IDS = \text{inner diameter surface of the insert} \]
\[ k = \text{Boltzman constant} \]
\[ ODS = \text{outer diameter surface of the insert} \]
\[ OP = \text{orifice plate surface of the insert} \]
\[ q = \text{electron charge} \]
\[ s.s. = \text{solid solution} \]
\[ T = \text{temperature} \]
\[ t = \text{time} \]
\[ US = \text{upstream surface of the insert} \]
\[ \Delta w = \text{length of the insert covered by tungsten deposition starting from the OP} \]
\[ \Pi = \text{insert porosity} \]

* PhD Student, Astronautic Research Group, School of Engineering Sciences, Coletti@soton.ac.uk
† PhD Student, Astronautic Research Group, School of Engineering Sciences, a.grubisic@soton.ac.uk
‡ Prof. of Aeronautics and Astronautics and Head of the Astronautic Research Group, School of Engineering Sciences, sbg2@soton.ac.uk.
I. Introduction

HOLLOW cathodes are one of the most important components in the field of electric propulsion. They are used as electron sources and neutralizers inside ion thrusters and Hall effect thrusters and in the future probably as stand alone microthrusters\(^1\)\(^{-4}\) hence their lifetime is a key factor in all the application mentioned above.

One of the most important life limiting mechanism in hollow cathodes is depletion of low work function compounds from the insert. In a paper recently presented by the authors\(^5\) a model to predict barium depletion from a hollow cathode’s insert has been developed.

In this paper the model will be used to simulate barium depletion from the ELT discharge cathode and the numerical result will be compared to the experimental evidence collected during the Deep Space 1 Ion Engine 30,000 Hrs Life Test\(^6\).

II. The chemical model\(^5\)

Barium oxide diffusion and evaporation from the insert has been numerically modelled\(^5\) starting from the knowledge of the behavior of the ternary system BaO – CaO – Al\(_2\)O\(_3\)\(^7\)\(^{-9}\).

![BaO-CaO-Al\(_2\)O\(_3\) ternary diagram](image)

Figure 1. BaO-CaO-Al\(_2\)O\(_3\) ternary diagram. (a) the whole diagram at 1250 °C, (b) particular of the diagram

Each point of the diagram in Fig. 1 (a) represents a state of the system where the concentration of \(A\), \(B\) and \(C\) are inversely proportional to the distance of the point from each corner. Each area in the diagram represents a different state of the system hence which compounds are present.

The list of compounds present in each area is reported below\(^9\),\(^10\)
Table 1 Compounds present in each area of the ternary diagram. The up lined formulas refers to a well define composition of the corresponding solid solution

<table>
<thead>
<tr>
<th>Area N°</th>
<th>Compounds</th>
<th>Area N°</th>
<th>Compounds</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>B₁₃₄ s.s. and B₁₂₃ s.s.</td>
<td>8</td>
<td>B, C and B₁₂₃ s.s.</td>
</tr>
<tr>
<td>2</td>
<td>B₁₂₃ s.s., B₁₂₄ s.s. and B₁₂₃CA</td>
<td>9</td>
<td>C and B₁₂₄ s.s.</td>
</tr>
<tr>
<td>3</td>
<td>B₁₂₃ s.s. and B₁₂₃CA s.s.</td>
<td>10</td>
<td>C, B₁₂₄ s.s. and B₁₂₃CA s.s.</td>
</tr>
<tr>
<td>4</td>
<td>C, B₁₂₃ s.s. and B₁₂₃CA s.s.</td>
<td>11</td>
<td>C and B₁₂₃CA s.s.</td>
</tr>
<tr>
<td>5</td>
<td>B₁₂₄ s.s. and B₁₂₃ s.s.</td>
<td>12</td>
<td>C, B₁₂₃ and BA</td>
</tr>
<tr>
<td>6</td>
<td>B and B₁₂₄ s.s.</td>
<td>13</td>
<td>C, BA and C₁₂₃</td>
</tr>
<tr>
<td>7</td>
<td>B₁₂₄ s.s. and B₁₂₃ s.s.</td>
<td>14</td>
<td>AB, C₁₂₃ and CA</td>
</tr>
</tbody>
</table>

From the knowledge of the compounds present it is possible to calculate the evaporation rate of barium oxide from the insert surface⁶,⁹,¹⁰. This evaporation creates a barium oxide concentration gradient generating a BaO motion from the insert core to the insert surface.

The motion of barium oxide from the interior part of the insert to the surface is the result of various processes: Knudsen flow of gaseous Ba and BaO through the pores, solid diffusion of BaO inside the BaO-CaO-Al₂O₃ impregnate, solid diffusion of BaO inside tungsten and surface diffusion of BaO along the pores surfaces.

These processes, being too complicated to be modelled separately, were represented globally with a single diffusion coefficient reducing the BaO depletion problem to a diffusion problem where the evaporation rate represents one of the boundary conditions.

The diffusion coefficient trend with temperature and insert porosities has been derived by comparison with experimental data¹¹. The diffusion coefficient formula is reported below:

\[
D_a = (b \Pi + c) e^{-\frac{qE_d a}{kT}}
\]

\[
b = 0.1165 \text{ m}^2/\text{s}
\]

\[
c = -0.01653 \text{ m}^2/\text{s}
\]

\[
E_{da} = 3.5 \text{ eV}
\]

III. Numerical analysis

In Ref. 6 by means of EDX scanning the Ba/W ratio has been measured in various point of the insert after 30372 hours of operation (Fig 2).
The barium-over-tungsten ratio has been also measured before the beginning of the test as shown by the black points in Fig 2. Looking at these data two hypotheses relative to the initial barium content in the insert have been made.

The first hypothesis is that at the beginning of the test the insert is completely filled with the impregnate, hence the initial BaO profile is flat (dashed line in Fig. 3) 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; in this case its trend has been derived interpolating the measurements (solid line in Fig. 3).

The two profiles are represented below

![Figure 3. Different initial BaO profile.](image)

During the destructive test of the ELT cathode\textsuperscript{6} barium oxide deposits were found on the internal surface of the cathode tube and on the external surface of the insert showing how BaO evaporation occurs also from the outer diameter surface.

The insert chemistry has been simulated using the temperature profiles given in Ref 12 and with both the flat and the interpolated initial BaO profile.

Evaporation has been assumed to occur always from the inner diameter and from the upstream surface while different simulation have been done regarding the conditions of the outer diameter and orifice plate surface.

The complete set of boundary conditions used is reported in Table 2 where with “open” we indicate a surface where evaporation occurs and with “closed” a surface where it does not.

<table>
<thead>
<tr>
<th>Boundary Conditions set 1</th>
<th>Boundary Conditions set 2</th>
<th>Boundary Conditions set 3</th>
<th>Boundary Conditions set 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flat BaO profile</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>IDS = open</td>
<td>IDS = open</td>
<td>IDS = open</td>
<td>IDS = open</td>
</tr>
<tr>
<td>US = open</td>
<td>US = open</td>
<td>US = open</td>
<td>US = open</td>
</tr>
<tr>
<td>ODS = closed</td>
<td>ODS = open</td>
<td>ODS = closed</td>
<td>ODS = open</td>
</tr>
<tr>
<td>OP = closed</td>
<td>OP = closed</td>
<td>OP = open</td>
<td>OP = open</td>
</tr>
<tr>
<td>Interpolated BaO profile</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>IDS = open</td>
<td>IDS = open</td>
<td>IDS = open</td>
<td>IDS = open</td>
</tr>
<tr>
<td>US = open</td>
<td>US = open</td>
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</tr>
</tbody>
</table>

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The best results were obtained with BC set 1 and 2 where the orifice plate surface is “closed”. Comparing Fig. 4 and 5 it can be seen how imposing that the external surface of the insert is “open” improve the results accuracy, as could be expected from the experimental evidence6.

Looking at Fig. 5 (b) and particularly to the data relative to 13.5 mm from the OP we can see how the interpolated profile gives better results than the flat one producing data that are much closer to the trend of the experimental point.

The data presented in Fig. 5 (a) show a poor agreement with the experimental points. In particular the predicted barium content is much lower than the measured one.

This can be explained noting that in the middle of the insert the effect of the upstream and orifice boundaries are weaker hence this part of the insert is the easiest to simulate, and that, as reported in Ref. 13 (Fig 6), close to the orifice plate there is a region of insert completely cover by tungsten deposition that, occluding the pores, prevent barium oxide evaporation.
An attempt has been done to include the tungsten deposition inside the model: to do so some hypotheses must be developed.

The first one is relative to the tungsten deposition trend on the IDS. Using the data computed before with the interpolated profile and BC set 2 the time evolution of the barium oxide content inside the insert at 1.5 mm from the OP has been analyzed. It can be noted that between 3000 and 5000 hours of operation the computed profile is quite close to the measured one after ca 31000 hours.

It can be then assumed that during this time tungsten deposition has reached this point of the insert occluding the pores and consequently stopping BaO evaporation from this site of the insert.

Hence assuming that tungsten deposition starts from the downstream end of the insert, that at 4000 hours it has reached 1.5 mm from the orifice plate and that at 30352 hours it covers 3.5 mm from the OP the deposition trend is

$$\Delta_w = 4.6783 \cdot 10^{-2} t^{0.42}$$

(2)

Where $\Delta_w$ is the length in millimetres covered by tungsten starting from the orifice plate and $t$ is the time in hours.

Noting that the barium depletion depth has been found to scale as the square root of time\textsuperscript{11}, the trend in Eq. 2, (also if derived from numerical data), is quite interesting because it shows a possible relation between barium depletion from the insert and tungsten deposition.

The second hypothesis is relative to BaO deposition on the cathode tube. The barium oxide evaporated from the external surface of the insert creates deposits on the cathode tube as observed in Ref 6. If these deposits are big
enough to fill completely the gap between the insert and the cathode tube they will occlude the insert pores preventing BaO evaporation.

Several numerical simulations have been run using the deposition trend in Eq. 2 and assuming different gap size between the insert and the cathode tube.

The gap sizes used are 25, 50, 75 and 100 μm. The best results were obtained with 75 and 100 μm.

![Graphs showing comparison between numerical and experimental results](image1)

**Figure 8. Comparison between numerical and experimental results**

IDS deposition Eq. 2, ODS – cathode tube gap = 75 μm

![Graphs showing comparison between numerical and experimental results](image2)

**Figure 9. Comparison between numerical and experimental results**

IDS deposition Eq. 2, ODS – cathode tube gap = 100 μm

The numerical results relative to 1.5 mm in Fig 8, 9 show a flat profile with a value close to the average of the measured values. The fact that the computed profile does not remain “frozen” as the one after 4000 hrs can be explained noting that in this point of the insert the diffusion motion (that is fast due to the high local value of the temperature, and hence of the diffusion coefficient) tends to move barium oxide upstream where it can evaporate and to smoothen the profile producing the flat profile computed.

Regarding the data relative to 6.5 mm from the OP it can be noted that the experimental trend is quite unusual showing a peak of barium content at one quarter of the insert thickness.

If we neglect the point relative to 6.5 mm from the OP and 200 μm from the IDS the computed data are in good agreement with the experimental ones.
Looking at the data relative to 13.5 and 23.5 mm from the OP we can note that these are not influenced by the introduction of deposition effect hence showing the same good agreement with the experimental data shown in Fig 2 by the data relative to the interpolated profile and BC set 2.

IV. Conclusions and future work

The insert chemistry of the ELT discharge cathode from the Deep Space 1 Ion Engine 30,000 Hours Life Test has been simulated using as input data the initial barium oxide content and the insert temperatures. The computed data show a good agreement with the experiments improving the agreement when the imposed boundary conditions are closer to the real functioning of the insert.

Tungsten deposition effects on the IDS and barium oxide deposition on the cathode tube were added to the model starting from the experimental measurement. This improves the model prediction accuracy producing results that are in qualitative and quantitative agreement with the measurements except the data relative to 1.5 mm from the OP where the computed results give a flat profile with a value close to the average value of the measured data.

The tungsten deposition length is found to scale with a power of the time. This trend is quite close to the trend followed by barium depletion depth hence showing the possibility of a link between these two phenomena.

Future work will consist in the development of a low work function model deposition to be added to the chemical model that will be hopefully presented at the 46th AIAA Aerospace Sciences Meeting and Exhibit in Reno.

References

4. Angelo JPC