MASTER

THEORY OF THERMIONIC CONVERTER OPERATION
WITH APPLICATIONS TO THERMIONIC REACTOR ANALYSIS

D. R. Wilkins
C. D. Sawyer
P. R. Hill

LEGAL NOTICE

This report was prepared as an account of Government sponsored work. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission

A. Makes any warranty or representation, expressed or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately owned rights, or

B. Assumes any liabilities with respect to the use of, or for damages resulting from the use of any information, apparatus, method, or process disclosed in this report.

As used in the above, "person acting on behalf of the Commission" includes any employee or contractor of the Commission, or employee of such contractor, to the extent that such employee or contractor of the Commission, or employee of such contractor prepares, disseminates, or provides access to, any information pursuant to his employment or contract with the Commission, or his employment with such contractor.

Nuclear Thermionic Power Operation
General Electric Company
Pleasanton, California
United States of America

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

THEORY OF THERMIONIC CONVERTER OPERATION WITH APPLICATIONS TO THERMIONIC REACTOR ANALYSIS

D. R. Wilkins, C. D. Sawyer, P. R. Hill
General Electric Company, Pleasanton, California
United States of America

ABSTRACT

Fundamental principles of molecular chemistry, statistical mechanics, and plasma physics are used to derive theoretical output current and efficiency characteristics of vapor thermionic converters. The results are obtained in terms of basic physical parameters which describe the converter electrodes and interelectrode gas and are in good agreement with corresponding experimental measurements for a broad range of converter operating conditions.

The theoretical formalism is employed to study the thermal and electrical performance characteristics of a nuclear thermionic fuel element. It is shown that, with realistic axial fission profiles, fuel void fractions, and temperature limits, over-all fuel element efficiencies in the vicinity of 12 to 14% can be achieved.

INTRODUCTION

A theoretical description of thermionic converter operation is important in developing thermionic power plants. In particular, accurate converter theory greatly facilitates the design, testing, and evaluation of prototype converters, and is fundamental in analytical studies which lead to an optimum power plant design.

An analytical description of the thermionic converter which adequately fulfills these needs must incorporate three key features: (1) be formulated in terms of basic data which characterizes the converter materials and operating conditions, (2) be applicable to the entire domain of practical thermionic converter operation, (3) yield results which are in agreement with experimental data.

The development of a useful analytic description of thermionic converter performance requires that due consideration be given to both electrode surface and interelectrode volume phenomena and to Schottky effects which occur at the electrode surface - interelectrode volume interfaces. Phenomena in each area have been separately considered in previous theoretical studies, many of which are cited in the literature ^(1, 2). These studies have served to isolate and to clarify many of the individual physical processes which are significant in thermionic converter operation. No attempt has been made, however, to combine and extend the previous analyses to provide a unified, practical theoretical description of thermionic converter operation.

In this study, a unified theoretical description of thermionic converter performance characteristics is developed, programmed for digital computer studies, and the theoretical results compared with appropriate experimental data. Significant features of the analysis are that it: (a) simultaneously accounts for the influence of surface and volume phenomena and Schottky effects on converter operation, (b) contains no restrictions concerning the "mode" of converter operation, (c) deals with the plasma sheath polarities self-consistently, (d) applies to converters with elevated collector temperatures, (e) provides for the determination of converter efficiency, and (f) is not restricted to Cs converters. Theoretical output current characteristics

are obtained for a W emitter, Mo collector converter and exhibit good agreement with corresponding experimental characteristics for a broad range of emitter and Cs reservoir temperatures, and interelectrode spacings.

As an illustrative practical application, the theoretical formalism is employed to optimize the thermal and electrical performance characteristics of a nuclear thermionic fuel element (TFE). The influences of different design constraints on the optimized performance characteristics are discussed.

THERMIONIC CONVERTER THEORY

VOLUME PHYSICS

The neutral interelectrode plasma in a thermionic converter may be analyzed by using a previously derived set of transport differential equations.⁽³⁾ Since plasma electron temperatures are nearly uniform,⁽⁴⁾ these equations may be written in the well-known approximate form:

$$(dJ_e/dx) = (dJ_i/dx) = e(\nu_1 n - \beta_r n^3) \quad (1)$$

$$J_e = -e\mu_e [\theta_e (dn/dx) + nE]; J_i = -e\mu_i [\theta_i (dn/dx) - nE] \quad (2)$$

where J_α , μ_α , and θ_α are the current density, mobility, and temperature (in electron volts) for the electrons ($\alpha=e$) and ions ($\alpha=i$), respectively, n is the charged particle density; E is the electric field; ν_1 is the ionization frequency, and β_r is the three-body recombination coefficient.

The source terms in Eq. (1) describe a multistage volume ionization-recombination process. The recombination coefficient for Cs is assumed to have a form similar to that for hydrogen,⁽⁶⁾ since both atoms have a valence of unity and similar binding energies for the higher excited states. The ionization frequency ν_1 is computed from the recombination coefficient β_r to satisfy certain thermodynamic equilibrium requirements.⁽²⁾

The electron and ion mobilities in Eq. (2) are computed by using relations previously developed for three-component plasmas.⁽³⁾ Both charged particle and charged particle - neutral particle collisions are accounted for in the electron and ion mobilities. The former collisional processes are represented by a Coulomb interaction potential, while the latter are described in terms of effective hard sphere cross sections. The plasma electron temperature, which is assumed to uniform, must satisfy the energy balance equation

$$q_{e1} - q_{e0} = JV_p - (J_{i1} - J_{i0}) V_i \quad (3)$$

where q_e is the electron kinetic energy flux; V_p is the voltage drop across the interelectrode plasma, and the subscripts "0" and "1" are used to denote a quantity evaluated at the emitter and collector edges of the plasma, respectively.

Equations (1) and (2) are integrated to yield, in terms of Jacobi elliptic functions, the charged particle density and electrostatic potential distributions in the interelectrode plasma.⁽²⁾ The integration constants which arise and the electron kinetic energy fluxes q_{e0} and q_{e1} are evaluated from sheath analyses as discussed in the following paragraphs.

The electrostatic sheaths at the plasma-electrode interfaces are analyzed by writing electron and ion current and electron kinetic energy flux balances across the sheaths; i. e., between each electrode and the adjacent edge of the interelectrode plasma. The exact form of these balances for a given sheath depends upon its polarity, which is referred to here as accelerating or retarding if the sheath accelerates or retards, respectively, an electron traveling toward the collector. Electron and ion current and electron kinetic energy flux balances are given in Table 1 for accelerating and retarding emitter and collector sheaths. In this table, J_M and I_M are the electron and ion emission current densities, respectively, for the emitter (M-E) and collector (M=C); V_M are the sheath voltage drops at the emitter (M-E) and collector (M-C) edges of the plasma; and J_r and I_r are the electron and ion random current densities, respectively, in the interelectrode plasma. Note that the sheath voltage drops are treated as negative and positive for accelerating and retarding sheaths, respectively. The equations presented in Table 1 contain terms, derived from first order transport theory, to account for the non-Maxwellian, anisotropy of the plasma electron and ion distribution functions. These terms become appreciable if the net particle currents near the sheaths are comparable to the corresponding random currents.

The electron and ion emission current densities from the emitter and collector (Table 1) are governed by surface phenomena and Schottky effects. The theoretical determination of these quantities is discussed in the following two sections.

SURFACE PHYSICS

The field-free, electron work function ϕ_M of a substrate metal (M) partially coated by an adsorbate film depends upon the substrate and adsorbate properties, the substrate temperature T_M , and the adsorbate reservoir temperature T_R . In other words, for a specified substrate and adsorbate: $\phi_M \sim \phi_M(T_M, T_R)$. The theoretical prediction of this relation for thermionic emitters (M-E) and collectors (M-C) is the objective of thermionic converter surface physics studies.

TABLE 1. Emitter and Collector Sheath Analyses

ACCELERATING EMITTER SHEATH ($V_E \leq 0$)		ACCELERATING COLLECTOR SHEATH ($V_C \leq 0$)	
1.	$J_{e0} = J_E - (J_{r0} - 1/2 J_{e0}) \exp(V_E/\theta_e)$	1.	$J_{e1} = (J_{r1} + 1/2 J_{e1}) - J_C \exp(V_C/\theta_C)$
2.	$J_{i0} = I_E \exp(V_E/\theta_E) - (I_{r0} - 1/2 J_{i0})$	2.	$J_{i1} = (I_{r1} + 1/2 J_{i1}) \exp(V_C/\theta_C) - I_C$
3.	$q_{e0} = 2 J_E (\theta_E - \theta_e) + J_{e0} (2 \theta_e - V_E)$	3.	$q_{e1} = 2 J_{r1} (\theta_e - \theta_C) + J_{e1} (\theta_e + \theta_C)$
RETARDING EMITTER SHEATH ($V_E \geq 0$)		RETARDING COLLECTOR SHEATH ($V_C \geq 0$)	
1.	$J_{e0} = J_E \exp(-V_E/\theta_E) - (J_{r0} - 1/2 J_{e0})$	1.	$J_{e1} = (J_{r1} + 1/2 J_{e1}) \exp(-V_C/\theta_e) - J_C$
2.	$J_{i0} = I_E - (I_{r0} - 1/2 J_{i0}) \exp(-V_E/\theta_E)$	2.	$J_{i1} = (I_{r1} + 1/2 J_{i1}) - I_C \exp(-V_C/\theta_C)$
3.	$q_{e0} = 2 J_{r0} (\theta_E - \theta_e) + J_{e0} (\theta_E + \theta_e)$	3.	$q_{e1} = 2 J_C (\theta_e - \theta_C) + J_{e1} (2 \theta_e + V_C)$

Notes

1. Electron Current Balance 2. Ion Current Balance 3. Electron Kinetic Energy Flux Balance

In this analysis, the recently developed Steiner-Gyftopoulos formalism⁽⁷⁾ is employed to determine the field-free, emitter and collector work functions. This formalism is an extension of earlier work⁽⁸⁾ and is based upon principles of molecular chemistry and statistical mechanics; it yields the relation $\phi_M = \phi_M(T_M, T_R)$ once a set of parameters which characterize the substrate and adsorbate are specified.

SCHOTTKY EFFECTS

The field-free work functions do not always prevail at the emitter and collector electrodes in a thermionic converter. In particular, if the emitter sheath is accelerating or the collector sheath is retarding, the electric field at the corresponding electrode surface depresses the effective electrode work function as shown in Fig. 1

The effective lowering of an electrode work function by an imposed electric field (Fig. 1) was first analyzed by Schottky who obtained

$$\Delta \phi_M = \phi_M - \phi'_M = \sqrt{[e/(4\pi\epsilon_0)] E_M} \quad (4)$$

where ϕ_M and ϕ'_M are the field-free and effective work functions of electrode M, respectively, e is the electronic charge, ϵ_0 is the vacuum permittivity, and E_M is the magnitude of the electric field existing at the surface of electrode M

Hansen^(9, 10) employed Eq. (4) to demonstrate the importance of Schottky effects in thermionic converters. The analyses were performed for limited domains of converter operation, and they cannot readily be extended to apply to the broad range of converter operating conditions under present consideration. Therefore, an alternate approach to the analysis of Schottky effects in thermionic converters is utilized here. Significant features of the present analysis are that it is mathematically simple, and yet can be expected to yield reasonably accurate results for the entire range of converter operating conditions of practical interest.

In applying Eq. (4) to the present problem, some uncertainty exists concerning the electric field, E_M , since the exact potential distribution within the electrostatic sheath is unknown. Generally, the sheath voltage drop occurs within several plasma electron Debye lengths of the electrode. Hence, it is reasonable to expect that the electric field at the electrode surface can be accurately approximated by

$$E_M = k_s V_M / L_M \quad (5)$$

where L_M is the electron Debye length at the edge of the plasma adjacent to the sheath; and k_s is a dimensionless constant of order unity

Equations (4) and (5) are used in this analysis to describe the Schottky reduction of the emitter work function caused by an accelerating emitter sheath, and of the collector work function caused by a retarding collector sheath. The field-free work functions ϕ_M ($M=E, C$) are computed from surface physics considerations, Eq. (4) and (5) then yield the effective work functions ϕ'_M ($M=E, C$). When the emitter sheath is retarding or the collector sheath is accelerating, no Schottky correction is applied to the corresponding electrode work function; i.e., $\phi'_M = \phi_M$.

Once the effective work function ϕ'_M is determined, emission current densities of electrons and ions from a thermionic converter electrode M (M=E, C) follow directly from the Richardson and Saha-Langmuir equations, respectively. In particular

$$J_M = A T_M^2 \exp(-\phi'_M/\theta_M), \quad \theta_M = k T_M/e \quad (6)$$

$$I_M = e p_g (2\pi m_g e \theta_M)^{-1/2} (1/2) \exp[-(V_1 - \phi'_M)/\theta_M] \quad (7)$$

where A is the Richardson constant and m_g is the mass of the adsorbate atoms. Equation (7) is an approximate form of the Saha-Langmuir equation which is valid provided the surface ionization probability is small compared to unity. This condition is always fulfilled for practical thermionic converter operating conditions.

THERMIONIC CONVERTER PERFORMANCE

The thermionic converter output voltage V for a specified output current density J is obtained by summing the voltage drops between the emitter and collector Fermi levels. Thus,

$$V = \phi'_E + V_E - V_P + V_C - \phi'_C \quad (8)$$

The several terms in this relation follow directly from the preceding analyses.

The intrinsic efficiency η_1 of a thermionic converter is defined as the efficiency in the absence of electrode, lead, and structural support losses. This efficiency is independent of detailed converter design considerations and is given by

$$\eta_1 = P / (Q_e + Q_1 + Q_r + Q_g) \quad (9)$$

where $P = JV$ is the output power density, and Q_e , Q_1 , Q_r , and Q_g are the heat fluxes removed from the emitter by electrons, ions, radiation, and gas conduction, respectively. The first three heat fluxes are given by

$$Q_e = J_{e0} (\phi'_E + V_E) + q_{e0} \quad (10)$$

$$Q_1 = J_{i0} (\phi'_E + V_E) + J_{i0} V_1 \quad (11)$$

$$Q_r = \sigma (\epsilon_E T_E^4 - \epsilon_C T_C^4) \quad (12)$$

where σ is the Stefan-Boltzmann constant, and ϵ_E and ϵ_C are effective emissivities. An expression for the interelectrode gas conduction term Q_g for Cs has been given by Kitrilakis, et al. (11). Note that Eq. (9) is readily modified to compute device efficiencies for specific converter designs by including terms to account for electrode, lead, and structural support losses.

COMPARISON OF THEORY WITH EXPERIMENT

NUMERICAL CALCULATIONS

A digital computer code has been written which incorporates the volume physics, surface physics, and Schottky effect analyses described here. The code input includes the physical parameters which characterize the converter electrodes and interelectrode gas and the converter operating conditions. With this input, the code obtains iterative solutions of the equations which

describe the surface and volume phenomena. In these computations, self-consistent sheath polarities are determined for each set of converter operating conditions, Schottky corrections are applied to the electrode work functions if appropriate. The code returns the converter output current and efficiency characteristics and other operating parameters of practical interest.

EXPERIMENTAL DATA

The experimental data chosen for comparison is a set of output current characteristics obtained by TECO⁽²⁾ for a thermionic converter with a heat-treated W emitter and polycrystalline Mo collector. The characteristics encompass a broad range of converter operating conditions and are divided into three groups to exhibit the effects of independent variations in emitter temperature, Cs reservoir temperature, and interelectrode spacing (Fig. 2).

THEORETICAL INPUT PARAMETERS

The input parameters used to compute output current characteristics for comparison with the experimental data are presented elsewhere.⁽²⁾ It is shown that the values employed for the key parameters are in satisfactory agreement with the available, but sometimes limited and inapplicable, independent data.

THEORETICAL RESULTS

The theoretical output current characteristics in Figure 2 are computed for the indicated operating conditions by using the techniques and data reported here. The results are in excellent qualitative and good quantitative agreement with corresponding experimental measurements for the entire range of converter operating conditions. Even better agreement could be anticipated, however, with slight adjustments of certain input parameters.

Note that both the computed and measured output current characteristics in Fig. 2 exhibit an abrupt rise in the output current density as the output voltage is decreased and the converter enters the ignited mode of operation. The theory of this transition from the extinguished to the ignited mode has not been previously presented.

Another significant feature of the theoretical results in Fig. 2 is the nonsaturation of certain output current characteristics at low output voltage, e. g., curve 4 of Fig. 2a. The significant increase in the output current density as the output voltage is decreased is due to Schottky effects and ion currents at the emitter surface.

THERMIONIC FUEL ELEMENT ANALYSIS

In this section the theoretical formalism is employed in an investigation of the thermal and electrical performance characteristics of a nuclear TFE. The influence of fuel center and emitter temperature constraints on the performance of the fuel element is shown.

FUEL ELEMENT DESCRIPTION

A nuclear TFE is shown in Fig. 3; it consists of N series-connected cells contained within an insulated sheath tube and serviced by a single cesium reservoir. Each cell is loaded with an

identical volume fraction of UO_2 fuel, and receives a fraction f_n ($1 \leq n \leq N$) of the total TFE thermal power. In general, the f_n 's are unequal because of the nonuniformities in the axial fission profile. The fuel element is cooled externally by a liquid metal coolant.

COMPUTATIONAL PROCEDURE

The operating state of a multicell TFE is completely defined by specifying the thermal power, axial power distribution, electrical current, cesium reservoir temperature, coolant inlet temperature, and over-all coolant temperature rise. Figure 4 shows the logical structure of a digital computer program which employs this information to yield a cell-by-cell and over-all description of the TFE electrical and thermal performance characteristics. This program incorporates the thermionic converter analysis as a subroutine. Other major subroutines describe heat transfer within the fuel-emitter body, through the tri-layer collector-insulator-sheath structure, and from the TFE sheath to the liquid metal coolant.

TFE PERFORMANCE CHARACTERISTICS

A 12-cell TFE with a coolant inlet temperature of 800°K and over-all coolant temperature rise of 100°K is discussed. The axial fission profile, which is typical for a small, fast spectrum, thermionic reactor, is shown in Table 2. Note that this profile exhibits a peak-to-minimum fission ratio of 1.2 to 1.0.

TABLE 2 Axial Fission Profile

<u>Cell, n</u>	<u>Fractional Power, f_n</u>	<u>Cell, n</u>	<u>Fractional Power, f_n</u>
1	0.08020	7	0.09071
2	0.07434	8	0.08858
3	0.07933	9	0.08463
4	0.08502	10	0.07945
5	0.08899	11	0.07490
6	0.09099	12	0.08288

A summary of the performance characteristics of the 12-cell fuel element for a thermal input power P_{th} of 14.9 kWt is given in Fig. 5. Shown versus electrical current density are: (a) the optimum cesium reservoir, T_r^{opt} , (b) the cesium optimized electrical power, P_e , (c) the highest prevailing emitter temperature, T_e^{max} , and (d) the highest prevailing central fuel cavity temperature, T_f^{max} . The latter quantity is shown for several fuel void fractions, V . Note that the maximum electrical output which can be achieved for the 14.9 kWt thermal input is 2.24 kWe; which corresponds to an over-all TFE efficiency of 15%.

The influence of design constraints on the fuel and emitter temperatures is readily deduced from Fig. 5. Suppose, for example, that the cell emitter temperatures are to be operated below 2073°K . This temperature restricts the permissible output current densities to values in excess of 10.6 A/cm^2 . The maximum electrical output consistent with this constraint is 2.02 kWe which corresponds to a TFE efficiency of 13.5%. For a specified fuel void fraction, constraints on the central fuel cavity temperature may be applied in a like manner.

Plots of the type shown in Fig. 5 have been computed for other TFE thermal power levels. For each thermal power, an optimum electrical output exists for a given set of design constraints.

Figure 6 shows the fully optimized TFE electrical output versus thermal input for different design limitations on the emitter and central fuel cavity temperatures. In Fig. 6 Curve 1 represents an upper limit which is achieved in the absence of temperature limitations. Curves 2 through 5 reflect the influence of both a 2073°K emitter temperature limit and a 2850°K central fuel cavity temperature limit on the results for different fuel void fractions. Note that when such temperature limits are imposed the electrical output does not increase monotonically with thermal input.

The results shown in Fig. 6 indicate that, with realistic axial fission profiles, fuel void fractions, and temperature limitations, TFE efficiencies in the vicinity of 12 to 14% can be achieved. The determinations of over-all thermionic reactor efficiencies require further optimizations involving fuel loading fractions and radial fission distributions, and is beyond the scope of this paper. Results of the type presented in Fig. 6, however, are important in such determinations.

SUMMARY AND CONCLUSIONS

A unified theoretical description of thermionic converter performance characteristics is presented. The analysis simultaneously accounts for the influence of surface phenomena, volume phenomena, and Schottky effects on converter operation; and yields theoretical output current characteristics which are in good agreement with experiment data for a very broad range of converter operating conditions. The analysis has practical applications for converter physics studies, converter performance evaluations, and thermionic power plant design.

The electrical and thermal performance characteristics of a 12-cell nuclear thermionic fuel element are described. It is shown that, with realistic axial fission profiles, fuel void fractions, and fuel and emitter temperature limitations, TFE efficiencies in the 12 to 14% range can be realized.

REFERENCES

1. Bullis, R. H., et al., Therm. Conv. Spec. Conf., San Diego, Calif., October 1965.
2. Wilkins, D. R., to be published, J. Appl. Phys., (1968)
3. Wilkins, D. R. and Gyftopoulos, E. P., Proc. Int. Conf. on Therm. Elec., Power Gen., London, England, September 1965.
4. Reichelt, W. H., Proc. Int. Conf. on Therm. Elec. Power Gen., London, England, September 1965.
5. Wilkins, D. R. and Gyftopoulos, E. P., Proc. Therm. Conf., San Diego, Calif., October 1965.
6. Hinnov, E. and Hirschberg, J. G., Phys. Rev. 125 (1962) 795-801.
7. Steiner, D. and Gyftopoulos, E. P., Proc. 27th Ann. Phys. Elec. Conf., Cambridge, Mass., March 1967.
8. Levine, J. D. and Gyftopoulos, E. P., Surface Science, 1 (1964) 171-193, 225-241, 349-360.
9. Hansen, L. K., Proc. 25th Ann. Phys. Elec. Conf., Cambridge, Mass., March 1965.
10. Hansen, L. K., Proc. Therm. Conv. Spec. Conf., San Diego, Calif., October 1966.
11. Kitrilakis, S. and Meeker, M., J. Adv. Energy Conv., 3 (1963) 59-68.
12. Howard, R., Thermo Electron Corp., Waltham, Mass., private communication, March 1966.

FIGURE 1. Influence of Electrostatic Sheath on Work Function of Thermionic Converter Electrode

FIGURE 2. Comparison of Computed and Measured⁽²⁴⁾ Output Current Characteristics For Several (a) Emitter Temperatures, (b) Cesium Reservoir Temperatures, and (c) Interelectrode Spacings

FIGURE 3. Nuclear Thermionic Fuel Element

FIGURE 4. Logical Flow Diagram for TFE Performance Computation

FIGURE 5. TFE Performance Characteristics for $P_{th} = 14.9$ kW

FIGURE 6. Fully Optimized TFE Performance Characteristics