ISBN: 978-3-95450-184-7 doi:10.18429/JACoW-IPAC2018-MOPML060

SELF-CONSISTENT SIMULATION AND OPTIMIZATION OF SPACE-CHARGE LIMITED THERMIONIC ENERGY CONVERTERS *

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Abstract

Thermionic energy converters (TEC) are an attractive technology for modular, efficient transfer of heat to electrical energy. The steady-state dynamics of a TEC are a function of the emission characteristics of the cathode and anode, an array of intra-gap electrodes and dielectric structures, and the self-consistent dynamics of the electrons in the gap. Proper modeling of these devices requires self-consistent simulation of the electron interactions in the gap. We present results from simulations of these devices using the particle-in-cell code Warp, developed at Lawrence Berkeley National Lab. We consider the role of individual energy loss mechanisms in reducing device efficiency, including kinetic losses, radiative losses, and dielectric charging. We discuss the implementation of an external circuit model to provide realistic feedback. Lastly, we illustrate the potential to use nonlinear optimization to maximize the efficiency of these devices by examining grid transparency.

INTRODUCTION

Thermionic energy converters (TECs) operate by using an external heat source to drive thermionic emission of electrons across a narrow vacuum to be collected on an opposing conductor. A traditional TEC is comprised of narrowly-separated plates; thermionic emission at the cathode releases electrons which travel to the anode, producing a current which may generate electrical power [1]. Simple structures are often space-charge limited as operating temperatures may produce currents exceeding the corresponding Child-Langmuir limit. To overcome space charge limitations an accelerating grid can be used to boost the amount of current that can be extracted. A magnetic field may be added to constrain electron trajectories and limit losses on the grid. The ideal voltage drop across the load in the circuit will be equal to the difference in work functions for the emitter and collector. In this paper, we describe a self-consistent simulation model implemented using the Warp particle-in-cell framework [2].

EFFICIENCY MODEL

Thermionic conversion efficiency is a function of kinetic, thermal, radiative, and resistive losses. We have implemented a model that is well-established from literature [3] that has also shown good results in experimental validation studies [4].

This model is based on four main loss mechanism of power from the TEC system: power carried by electrons leaving the emitter P_{ec}, net radiative power from the emittance P_r, conductive heat loss in the TEC circuit P_{ew}, and finally power lost from holding the voltage on the gate P_{gate}. We note that the simulations assume periodic boundaries, and so the current and corresponding power quantities are normalized by area. If the power that is generated from circuit load is P_{load}, the efficiency η is:

$$\eta = \frac{P_{load} - P_{gate}}{P_{ec} + P_r + P_{ew}}. \tag{1}$$

The calculation of loss mechanisms in the simulation is then based on a combination of quantities calculated directly from the simulation state and analytic relationships. To begin, the electron power takes the form:

$$P_{ec} = P_{em} - tJ_{coll}\left(\phi_{em} + 2k_b T_{coll}\right) \tag{2}$$

Here P_{em}, the power carried by electrons from the emitter, is known exactly from the simulation based on monitoring emitted particles. The second term stems from any return current present due to electrons streaming towards the emitter. The factor of t accounts for the geometric transparency of the grid. Because the collector is normally assumed to be held at < 500 K, the emitted current is orders of magnitude lower than the cathode emission, and we analytically compute J_{coll} assuming Richardson-Dushman emission.

The radiative heat loss is based on an analytic calculation for infinite parallel plates with shielding placed between them, representing the grid. This is calculated as:

$$P_r = \epsilon_{eff}\sigma_{sb}\left(T_{em}^4 - T_{coll}^4\right) \tag{3}$$

where ϵ_{eff} is an effective emissivity, estimated from material and number of intervening grids (in the case where focusing and acceleration grids are present), σ_{sb} is the Stefan-Boltzmann constant, and T_{em} and T_{coll} are the emitter and collector temperature respectively.

The power dissipated from the circuit is calculated as:

$$J_{ec}\left(\left(\phi_{em} - \phi_{coll}\right) - \rho_{cw}J_{ec} - \rho_{ew}\left(J_{ec} - tJ_{coll}\right)\right) \tag{4}$$

where J_{ec} is the current density from the emitter that reaches the collector, known exactly from the simulation and J_{coll} is the analytically calculated current flow from the collector. The resistivities ρ_{ew} and ρ_{cw} account for the emitter and collector side wiring respectively and are calculated as a function of temperature. Finally, ϕ_{em} and ϕ_{coll} are the emitter and collector work functions.

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* This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research under Award Number DE-SC0017162.

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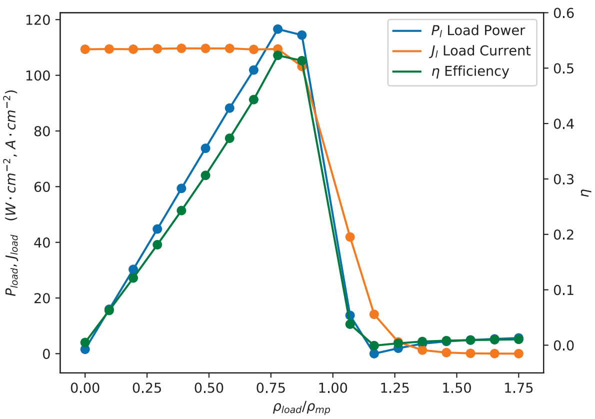

Figure 1: Varying the resistance, ρ, of the load on the external circuit varies the voltage drop at the collector due to current crossing the gap, and the power extracted from the collector. When the resistance is below optimal, $\rho < \rho_{mp}$, the load current is removed at a discounted voltage, leading to a reduced efficiency. When the resistance is above the optimal value, a retarding potential develops at the collector, leading to a reduction in the current across the gap and a reduction in the power across the load.

The power lost in the gate is calculated based on the grid voltage V_{grid}, the current density striking the grid J_{grid} and an estimate from the analytic calculation of collector back current:

$$P_{gate} = V_{grid}\left(J_{grid} + tJ_{coll}\right) \quad (5)$$

Finally, the power generated by the TEC is simply calculated from net current at the collector J_{ec} and the load voltage V_{load}:

$$P_{load} = J_{ec}V_{load}. \quad (6)$$

External Circuit Effects

For a traditional TEC, any current drawn through a load prompts a subsequent decrease in the effective voltage across the gap. The aim of an external circuit model is to permit these time-varying adjustments to maintain an accurate, self-consistent current value as the device reaches steady-state.

In our implementation, these adjustments can be made with arbitrary stride, meaning that for fast fluctuations in the current driven by noise in the simulation, we may period average over the noise to obtain a steady-state correction. The resistance of the load is pre-computed based on the expected temperature and work functions of the emitter and collector as well as the resistance of the wiring connecting the emitter and collector. We tested our implementation by running simulations with incremental changes to the resistance through the load, thereby producing an effective I-V characteristic curve. Figure 1 displays this curve for one benchmark configuration.

Simulation Procedure

The described efficiency model is only valid in the limit of steady-state operation. In order to reach steady state, a simulation must be run for enough time to eliminate transient effects at the cathode due to space charge while also permitting saturation of particles in different regions of the device within which the electron velocity distribution is large. To do this, we have devised a procedure which ensures that each simulation reaches a steady-state phase before efficiency measurements commence.

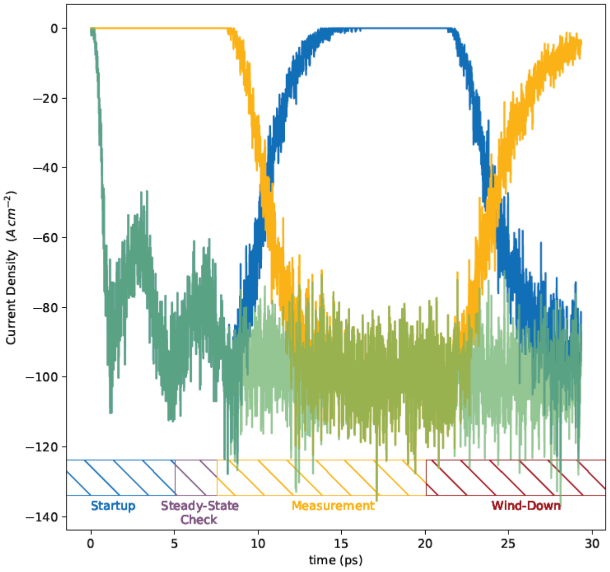

Figure 2: The procedure for determining steady state and then measuring device performance consists of four phases, for which the measurement phase (gold-colored current) requires approximately half the total simulation time.

The procedure consists of four phases, as documented in figure 2. First, the "startup" phase consists of particle emission at the originally specified operating conditions. This initial emission is subject to virtual cathode oscillations [5] from the beam space charge and circuit feedback on the collector potential. As a result, the current in the gap will oscillate as these feedback mechanisms change the field at the emitter. After several crossing times have commenced, the "steady-state check" phase begins, wherein the the current at the collector is gated and measured for consistency across reasonable intervals. Once steady-state has been reached within the defined tolerances, the measurement phase begins. During this phase, specially tagged measurement particles are emitted for a number of crossing times. These particles are used for computing the efficiency of the device, and are flagged by Warp to distinguish them from other macroparticles. Once measurement particles have been released for enough time, the "wind-down" phase begins, and standard electron macroparticles are emitted to maintain the steady-state conditions for the remaining measurement particles. Once a sufficient fraction of the measurement particles exit the domain (though collisions with emitter, collector, or grid), the simulation ends, and the efficiency is computed for that run.

OPTIMIZATION TOOLS

As an initial test of our interface, a series of optimization routines were performed with the goal of optimizing the grid transparency for a simple 3D gridded TEC configuration. Figure 3 shows the efficiency of the TEC as a function of iteration number for both Nelder-Mead and for LBFGS. Here it is interesting to see that the LBFGS algorithm converged close to the final solution much faster than the Nelder-Mead run. Both methods test the parametric constraints prior to taking guided steps, but in the LBFGS instance, those constraints lie close to the optimum working point, hence a large initial improvement is seen prior to the computation of an estimated Hessian, and further iterations do not result in significant improvements.

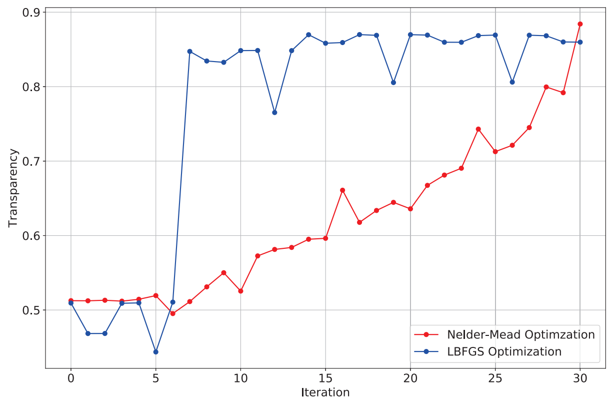

Figure 3: Efficiency as a function of iteration number for the Nelder-Mead and LBFGS optimization methods.

CONCLUSION

We have developed self-consistent tools using the Warp code to model thermionic energy converters. We implemented and tested a well-established efficiency model for computing the individual loss channels and overall efficiency of TEC devices. An external circuit model was also included, which adjusts the potential at the collector to provide realistic feedback. To improve fidelity of the efficiency evaluation, we devised a four-phase simulation strategy to limit our measurements to a well-defined steady-state. Lastly, we explored optimization of these devices using different optimization techniques. Our results suggest that optimization techniques should be effective at generating device designs with realistic efficiencies.

ACKNOWLEDGMENTS

We would like to acknowledge the Warp development team, from the Accelerator Technology & Applied Physics group at Berkeley Lab. We would also like to thank Tony Pan, Eric Clark, Arvind Kannan, and Andrew Koch from Modern Electron, LLC for helpful discussions.

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