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An Introduction to System Level Steady-State and Transient Modeling and Optimization of High Power Density Thermoelectric Generator Devices Made of Segmented Thermoelectric Elements

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Abstract

High power density, segmented, thermoelectric (TE) elements have been intimately integrated into heat exchangers, eliminating many of the loss mechanisms of conventional TE assemblies, including the ceramic electrical isolation layer. Numerical models comprised of simultaneously solved, non-linear, energy balance equations have been created to simulate these novel architectures. These models begin at the element level and progress to the device and finally to the system level. Both steady state and transient models have been created in a MATLAB/Simulink environment. The models predict data from experiments in various configurations and applications over a broad range of temperature, flow, and current conditions for power produced, efficiency, and a variety of other important outputs.

The ability to accurately and precisely model such devices allows devices to be extensively studied without additional experimentation. Using the validated models, the devices and systems can be optimized using advanced multi-parameter optimization techniques for different operating conditions. Optimization objectives such as

maximum power output, power density, and efficiency can be pursued with numerous different constraints being considered such as pressure drop and temperature limitations. Devices optimized for particular steady state conditions can then be dynamically simulated in a transient operating model. This transient model incorporates system and device thermal time constants that affect performance. The transient model can be operated for a variety of operating conditions including automotive and truck drive cycles.

Key Words

thermoelectric, power generation, modeling, waste heat recovery, steady state, transient

Introduction

In the last few years, there has been important work done in the area of thermoelectric (TE) power generation modeling. This work has included analyzing thermoelectric elements with finitie element analysis (FEA)[1, 2], which also involved the addition of a thermoelectric module to the finite element (FEA) package, ANSYS[3]. It has also comprised work done using the mathematical package SPICE for numerical modeling[4-6]. Quasi-steady state modeling of thermoelectric generators (TEG) integrated into automotive systems in ADVISOR was also conducted[7, 8]. Numerical optimization studies have also been executed for segmented elements[9]. Hendricks et al.[10-12] have used stochastic and probablistic approaches for optimization of advanced thermoelectric conversion systems. While this work has been important and has continued to improve the ability to predict TE performance, there is still room for further improvement.

The current work builds off of previous thermoelectric modeling work done in a MATLAB/Simulink environment[13, 14]. Previous papers by the author have discussed modeling of thermoelectrics in heating and cooling[15]. They have also discussed initial modeling of the building blocks for power generation[16]. The current paper takes this previous work and extends the validated heating and cooling device and system level models to power generation and takes the validated building block models in power generation and extends those to device and system level models. These initial models are steady state models. Advanced optimization tools are discussed in relation to these models. With optimized designs in steady state for nominal design conditions, the TE models are further extended as the introduction of transient operating models are discussed. This paper is an introduction to these models. Full validation of these models is not complete yet, but what validation has been completed will be reported in the context of this paper.

Steady State Model Development

The thermoelectric device being modeled in this paper is unique in its design as it integrates high power density TE material directly into the heat exchanger device. Different aspects of these designs have been described and discussed extensively in previous papers[16-20] and will only be summarized and generally discussed here.

Each TE element (alternating between p- and n- legs) is sandwiched between connectors or shunts as shown in Figure 1. These connectors serve as a means of both thermal and electrical energy transport. The connectors provide an electrical path from one TE element to another completing the necessary TE p-n couple. The connectors also provide a thermal path from the hot and cold fluid-carrying channels to the TE elements. The connectors are joined to the TE elements using a high electrical and thermal conductivity interface.

The shunts are connected to the channels carrying hot and cold fluids using high thermal conductivity and electrically isolating interfaces. The device is placed in compression separately in both the thermal and electrical flow directions. The benefits of this design concept, which are significant, have been elaborated in previous papers[17, 18, 21, 22] and will not be restated here.

Previously introduced in Crane et al.[16, 17], the equations used to model the TE elements were defined in Snyder[23]. Looking at the TE element in the direction of heat flow, a temperature gradient across the element is predefined. This temperature gradient is then subdivided into smaller equal temperature steps. The three basic thermoelectric material properties, Seebeck coefficient, electrical resistivity, and thermal conductivity, which are defined as functions of temperature, are calculated at each of these temperature steps across the entire temperature gradient. The reduced current density, which is the ratio of the electric current density to the conduction-driven heat flux[23] is calculated at each temperature step using the calculated TE material properties.

An initial reduced current density is defined as

$$u_1 = \frac{I}{Q_h - \alpha_1 I T_1}$$

Equation 1

This equation is negative if an n-type material is being evaluated. The temperature variation along the length of the element is then calculated as a function of the reduced current density, with the sum being equal to the current density times element length[23].

Using these now defined equations, the model makes initial assumptions for heat flow and current. Using the optimization function, FMINCON, in MATLAB, the model iteratively solves for the heat flow and current that maximizes TE element efficiency. A constraint for the optimization is that the TE elements must match a predefined element length. Another input to the model is the electrical resistance at the TE element interfaces. This resistance has been indirectly measured in validated TE heating and cooling experiments and is similar to those reported in the literature[24]. The thermal interfacial resistance is related to this electrical contact resistance using the Wiedmann-Franz law [25]. A reduced current density is also evaluated at the temperature step created by the electrical contact resistance and the temperature drop caused by the thermal contact resistance. In this way, the metallization and other interfacial attributes of the elements are evaluated. To model segmented or multi-material elements, more interfaces were added, but the evaluation method remained the same. Validation of this model was described for both single material and segmented material TE elements in Crane et al.[16]. This element and couple-level model was adjusted to fit into a larger model that integrated these TE elements into a TE device, including shunts, heat exchangers, and fluid flows.

Building on previous work of validated TE numerical simulation[15], a MATLAB-based, numerical, steady-state model was created, comprised of simultaneously solved, non-linear, energy balance equations. These energy balance equations simulate the high-power density, segmented element TE assemblies discussed above. The numerical model of the TE heat exchanger uses a finite volume approach with discretization in the axial direction of both hot and cold flows. A first-order upwind differencing scheme is implemented for the convective derivatives. Downwind differencing can also be chosen as an option. Transverse or radial heat transfer is modeled using standard conduction equations that incorporate central differencing discretization for the gradients. Each segment of the fluid-carrying channel is separated into four control volumes. Since the temperature gradients across each segment and from one segment to another are small, this level of discretization was determined to be adequate. Differential algebraic equations model the energy balances for each control volume.

Convective heat transfer coefficient and pressure drop correlations were derived from experimental and simulation[26] data. The thermal resistances of the device are rigorously modeled. These resistances include thermal contact resistances at each TE element interface, including between different material segments of a segmented element as well as the interfacial resistance between the TE element and the shunts on both the hot and cold side of the elements. The metallization layer(s) on the elements are lumped into this contact resistance both thermally and electrically. The thermal contact resistance is also simulated between the shunts and the heat exchangers. Temperature drops are also calculated from the fluid through the fins to the wall of the heat exchanger. These drops continue through the heat exchanger wall and through any interface materials, which can include electrically insulating coatings such as anodize and thermal grease. The thermal resistance of the shunts, based on geometry and material, are then accounted for culminating in a surface temperature at the metallization layer of the TE.

Heat loss factors are also rigorously accounted for in the model. Convective, conductive, and radiative heat losses are considered. Heat can be lost to the outside environment or it can be transferred from a hot surface to a cold surface within the device or system. The geometry of the components is considered when determining where the heat is being transferred to. Different environments can be modeled, including air, argon, xenon, or vacuum. Different insulations can also be modeled, such as microporous insulation and Aerogel. The emissivity and absorbtivity of the exposed surfaces is also accounted for.

Different fin correlations can be chosen for the fluid channels. The choices include straight, offset, wavy, annular, as well as other more specialized correlations. The shape of the fluid channels can also be specified as square (rectangular), hexangonal, or circular. Radiation heat transfer is also computed with the convective heat transfer coefficient within the fluid channels. Temperature dependent fluid properties for many different fluids are also part of the model. The user can choose from air, water, glycol/water, helium/xenon, oil, exhaust gas, CO2, argon, as well as other specialized fluids. The temperature dependent properties modeled include density, thermal conductivity, specific heat, and dynamic viscosity.

Many different TE materials can be chosen for simulation, including Bi2Te3, PbTe, TAGS, half heusler, and skutterudite. These materials can be chosen as single material or as a part of segmented TE elements. Material properties, Seebeck coefficient, electrical resistivity, and thermal conductivity, as a function of temperature are taken from measured data or are supplier-provided. To simulate improved TE materials, base TE material properties can be scaled to a desired ZTavg. The model allows the user to choose how this will occur, either by changing the Seebeck coefficient, electrical resistivity, or thermal conductivity.

The other materials of the device can also be chosen. This includes the materials for the fluid channel structures, the connectors, and the fins, which may be different from the fluid channel. Material choices for these components include copper, aluminum, different grades of SST, molybdenum, clad materials, and various ceramic materials. For many of these materials, thermal and electrical conductivity are modeled as a function of temperature.

The TE device can be broken up into multiple temperature banks in the direction of fluid flow. Each temperature bank can have a separate set of TE elements. These elements can have different area to length aspect ratios, be segmented differently with different TE materials, or not be segmented at all. Each temperature bank can operate on its own electrical circuit or one electrical circuit can be used for all of the temperature banks. The temperature banks can be of different lengths to better match the temperature gradients and heat flows in the direction of fluid flow. In addition, each temperature bank can be modeled as having different hot side fin densities. This can be used to better match the heat fluxes and temperatures seen in a particular bank. It also can help reduce the pressure drop and weight of the fluid channel if lower density fins can be more advantageously used in different banks of the TEG.

Electrical load resistance affects the operating current and power output of the TEG at a particular set of temperature and heat flow conditions. Equation 2 shows how load resistance relates to operating current[27].

$$I = \frac{\alpha \Delta T_{TE}}{R_{TE} + R_{load}}$$

Equation 2

When designing the TEG for a particular set of temperature and heat flow conditions, the user will typically want to maximize the power output of the TEG. This condition occurs when the load resistance is equal to the internal resistance of the TEG. The model will also allow the user to run the model in off nominal conditions where the load resistance can be varied. This can be valuable in some designs since changing the current also affects the heat flow through the TE elements as can be seen in Equation 8.

To compute how all of the above attributes affect TEG operation, a set of energy balance equations have been defined.

$$Q_{h1} + \frac{1}{2} I^2 R_{conn,h} - UA_{TE-conn}(T_{cen,h} - T_{h1}) = 0$$

Equation 3

$$Q_{h2} + \frac{1}{2} I^2 R_{conn,h} - UA_{TE-conn}(T_{cen,h} - T_{h2}) = 0$$

Equation 4

$$UA_{TE-conn}(T_{cen,h} - T_{h1}) + UA_{TE-conn}(T_{cen,h} - T_{h2}) - UA_{cross,conn}(T_{sh2} - T_{cen,h}) = 0$$

Equation 5

$$hA_h(T_{fh} - T_{sh2}) - UA_{cross,conn}(T_{sh2} - T_{cen,h}) - hA_{nat}(T_{sh2} - T_{\infty}) + UA_{cross,ch,h,1-2}(\Delta T_{sh1}) - UA_{cross,ch,h,2-3}(\Delta T_{sh2}) = 0$$

Equation 6

$$\dot{m} Cp_h \Delta T_{fh} - hA_h(T_{fh} - T_{sh2}) = 0$$

Equation 7

Where

$$Q_h = \alpha I T_h + K \Delta T_{TE} - \frac{1}{2} I^2 (R_{TE} + 2R_{int})$$

Equation 8

Equation 3 and Equation 4 are energy balance equations for conductive heat transfer from the TE elements into the connectors. Equation 5 and Equation 6 are energy balance equations for conductive heat transfer from the connector through the fluid-carrying channel wall through the fins to fluid convective heat transfer. They include the losses due to natural convection, radiation, and Joule heating of the boxes. Equation 7 is an energy balance equation for the convective heat transfer into the fluid. Equation 8 is the basic equation for thermoelectric heat flow in power generation.

The model solves these governing equations simultaneously for steady-state temperatures at each node in the direction of flow using the FMINCON function in MATLAB. The number of simultaneous equations varies with the number of TE elements in the direction of fluid flow.

Outputs for the model include power output, efficiency, hot and cold outlet temperatures, hot and cold pressure drops, total mass and volume, and many others. Auxiliary power of pumps and/or fans is also computed based on the pressure drops. This output can be used to calculate a net power output instead of gross power.

Some validation has been completed for this model for low temperature (<250C) devices using single material elements with liquid heat exchangers as reported in Crane et al.[19]. The error from measurement to model was <10%. Further validation is needed on the integration of segmented elements into gas/liquid heat exchangers.

Optimization

Advanced multi-parameter optimization can be used on the steady state model for better understanding of the interactions between various design variables and parameters and to further improve the performance of the design. The TEG design problem, an example of a constrained, non-linear, minimization problem, is solved using the MATLAB function FMINCON, which uses a gradient-based optimization scheme.

A design engineer can choose to optimize from greater than 20 different design variables, including fin and TE dimensions and include dozens of different design parameters. A variety of different constraints can also be chosen, including minimum power density, maximum hot- and cold-side pressure drops, maximum total mass, and minimum output power. Constraints can also be placed on maximum TE surface temperatures and maximum temperature gradients across the TE elements to help improve design robustness. The objective function of the analysis can also be chosen. Choices include maximum gross or net power, maximum efficiency, and maximum gross or net power density, which can be based on either total mass or TE mass. Once the design variables, parameters, constraints, and objective function have been chosen, an optimization analysis can be conducted. The result is a nominal design that can now be used in an operating model where the design conditions can vary.

Transient Model Development

The steady state model gives an effective means to choose a nominal design point and optimize the design for this set of operating conditions. However, a thermoelectric generator often may see a wide array of operating conditions, and these conditions may change frequently as a function of time. This is certainly the case when the TEG is integrated into a car or truck. An example of the mass flows and temperatures in the exhaust system, downstream of the catalytic converter, that are produced for an automotive city drive cycle (FTP-75) are shown in Figure 3. The thermal time constants of the exhaust system and of the TEG itself can have a large effect on how the TEG performs in this cycle.

In order to model the TEG in different cycles as well as other non-steady state operating conditions, the steady state models for TE couples and devices were adapted into transient models. To do this, the energy balance equations defined above were setup as differential equations based on Equation 9 and integrated into the S- Function template of MATLAB/Simulink..

$$mC_p \frac{dT}{dt} = Q_1 - Q_2$$

Equation 9

The mC_p term in Equation 9 is the thermal mass of each control volume that the equation represents. This could be a fluid, heat exchanger, connector, or TE thermal mass depending on the control volume. It is important to determine the direction of heat flow to make sure that the signs for Q_1 and Q_2 are correct. Otherwise, the differential equations will not be able to be solved correctly.

When using Simulink to solve ordinary differential equations, there is a choice of solvers made available to the user. Due to the potential rapid variation in the solution of the differential equations, the transient TEG problem is considered stiff. Ode15s, specifically designed to handle stiff problems, is the solver that most successfully solved the set of differential equations for the transient TEG problem.

A transient model was first setup for the TE couple. A validation experiment was conducted using segmented elements on a heater housing, cooled between two small cold plates. The heater housing holds a cartridge heater, which was used to provide heat to the couple. This couple setup was similar to that described in Crane et al.[16] for the 10% efficient generator. The segmented elements were made up of TAGS/PbTe and Bi2Te3. Graphs of the test results can be seen in the figure below.

The test was setup where the cartridge heater was held at a constant heat input of 35W. The hot side temperature of the TE elements was 500C and the cold water bath was set at 20C. The electrical load resistance was initially infinite making the initial current zero by Equation 2. Then the electrical load resistance was instantly changed to

30A. The electrical time constants of the couple were much faster than the thermal time constants. Thus, spikes in power and efficiency can be seen in the graphs before the thermal time constants catch up to the electrical time constants.

By adjusting the electrical load resistance, the electrical current is instantly increased. This increases the effective thermal conductivity of the elements by Equation 8. The original temperature differences of the couple no longer balance the steady state equations. The time it takes to balance these temperature differences with the new effective thermal conductance of the couple is based on the thermal mass of the elements and their connectors. This can clearly be seen in the graphs. Greater power output and efficiency are achieved initially due to the couple operating at higher temperature differences at the same heat flow. The higher temperature differences increase open circuit voltage and subsequently power output. They also increase the Carnot term of the TEG efficiency. However, these temperature differences are not sustainable in steady state, and thus the power output and efficiency eventually come down.

The cold side temperature initially increases due to the sudden increase in effective thermal conductance, transferring more heat from the hot to cold side of the TE elements. This is also what causes the hot side temperature to decrease. As the system balances, it stabilizes at a more inbetween temperature in this example. The figures show excellent correlation between the measured and simulated data, where differences are <5%.

With this validation, a transient model was created of the TEG itself, TE couples integrated directly into the heat exchangers. The optimized design from the steady state model is used as a baseline. Inputs for the model are similar to those of the steady state model. Operating condition inputs include the hot and cold side inlet temperatures and flows and the electrical load resistance. The electrical load resistance can be set to be always equal to the internal resistance of the TEG or it can be set at a particular constant load. A controller simulator can be attached to the model as an additional Simulink block in order to simulate the effects of a varying electrical load that is not necessarily optimal. Outputs for the model are again similar to those of the steady state model.

The model can be operated as is in a stand-alone mode or the S-function can be cut and pasted into a larger systems-level model. Both BMW and Ford have cut and pasted versions of this model into their larger systems-level models[18]. The model can be run using single hot-side inlet flow and temperature conditions or using the hot-side inlet flow and temperature conditions for a drive cycle.

Additional systems level attributes have been added to the transient model to aid in its use as a part of a larger system. A maximum hot inlet temperature can be defined to prevent the overheating of the TE elements or any other part of the TEG device. A maximum hot flow can be defined to prevent excessive backpressure in the system. This excessive backpressure can reduce engine performance if the TEG is integrated into the exhaust system of a vehicle. In addition, to better match the thermal impedance of a dynamic thermal system as defined in Crane and Bell[20], the TEG can be broken into a number of TE sections. Having multiple TE sections can allow the TEG to operate better at low flows when the design has been optimized for higher flow rates.

Below are examples of transient simulations done with the model. Figure 5 shows the power output and hot side fluid and TE surface temperatures for the TEG being driven by a set of constant operating conditions towards steady state from an initial set of conditions. The temperature curves in these figures are at different positions in the direction of flow in the TEG as a function of time. The colder the temperatures the further they are from the inlet of the TEG. Figure 6 shows the power output and efficiency along with the hot side fluid and TE surface temperatures for the TEG for an FTP-75 (city) automotive drive cycle.

Conclusion

Steady state and transient models of thermoelectric devices have been introduced that range from element to couple to device to system level. Equations for these models have been described, and validation studies have been discussed. Further validation is needed for the gas/liquid TEG with segmented TE elements. Next steps include the testing of the newly designed and built cylindrical TEG, which is designed for hot exhaust gas on one side and automotive coolant on the other. It also includes segmented TE elements. Once tested, emprirical results can be compared to steady state and transient simulations for a more complete model validation.

With this further validation, a very powerful set of validated tools will exist that can greatly aid in the design of future thermoelectric power generation devices and systems. The tools have already been used by multiple customers to help in their design process. Hopefully, many more will use them in the future as well.

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Nomenclature

A	area (m^2)
Cp	specific heat (J/kgK)
h	heat transfer coefficient (W/m^2K)
I	electrical current (A)
K	thermal conductance (W/K)
m	mass (kg)

Q	heat flow (W)
R	electrical resistance (ohm)
t	time (s)
T	temperature (K)
u	reduced current density
U	overall heat transfer coefficient (W/m^2K)

Subscripts

1, 2, 3	location on the TEG/control volume in the direction of flow
c	cold
cen	center of
ch	channel
conn	connector
cross	cross sectional
f	fluid
h	hot
int	interfacial
load	load
nat	natural convection
s	surface
TE	thermoelectric

Greek letters

α	Seebeck coefficient
Δ, d	change in
∞	ambient

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Figure 1. TEG high power density subassembly

Figure 2. Schematic of TE subassembly with heat exchangers (HEX) showing temperature locations in the model.

Figure 3. Exhaust gas mass flow and temperature exiting the catalytic converter varying with time for the FTP-75 drive cycle for an inline 6 cylinder engine with 3.0L displacement.

Figure 4. Transient experimental and simulated performance of a TE couple.

Figure 5. Simulated outputs for the transient TEG model using constant operating conditions.

Figure 6. Simulated outputs for the automotive FTP-75 drive cycle using an optimized TEG from the steady state model.

Figure
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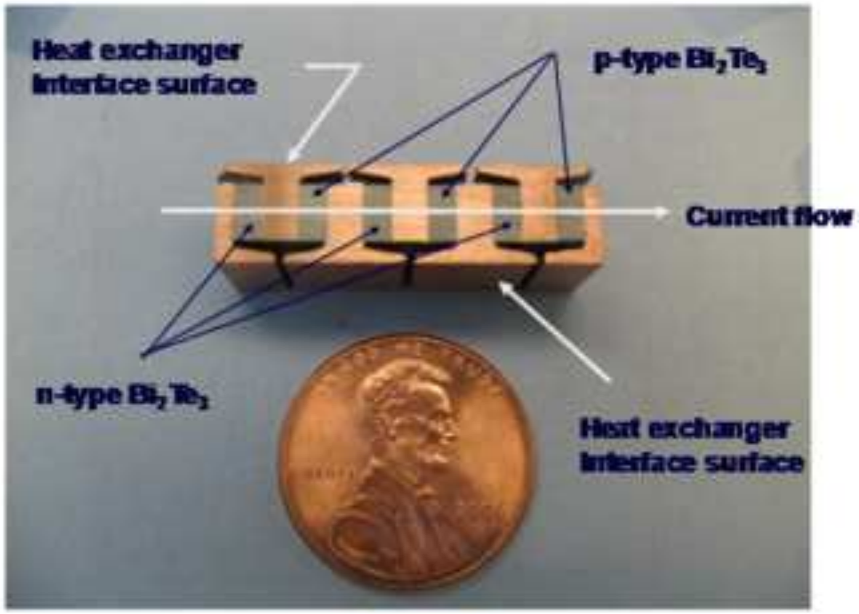

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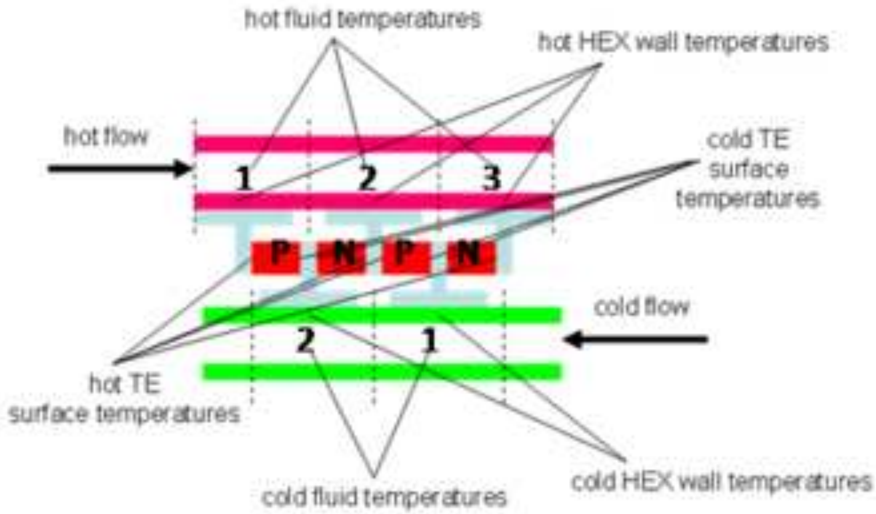

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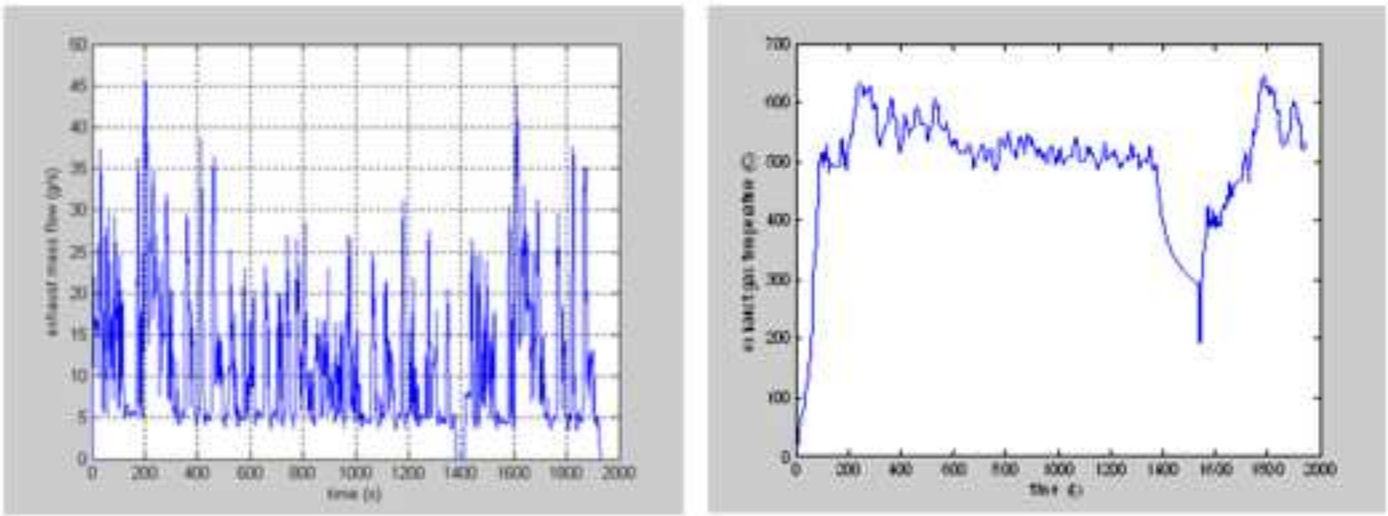

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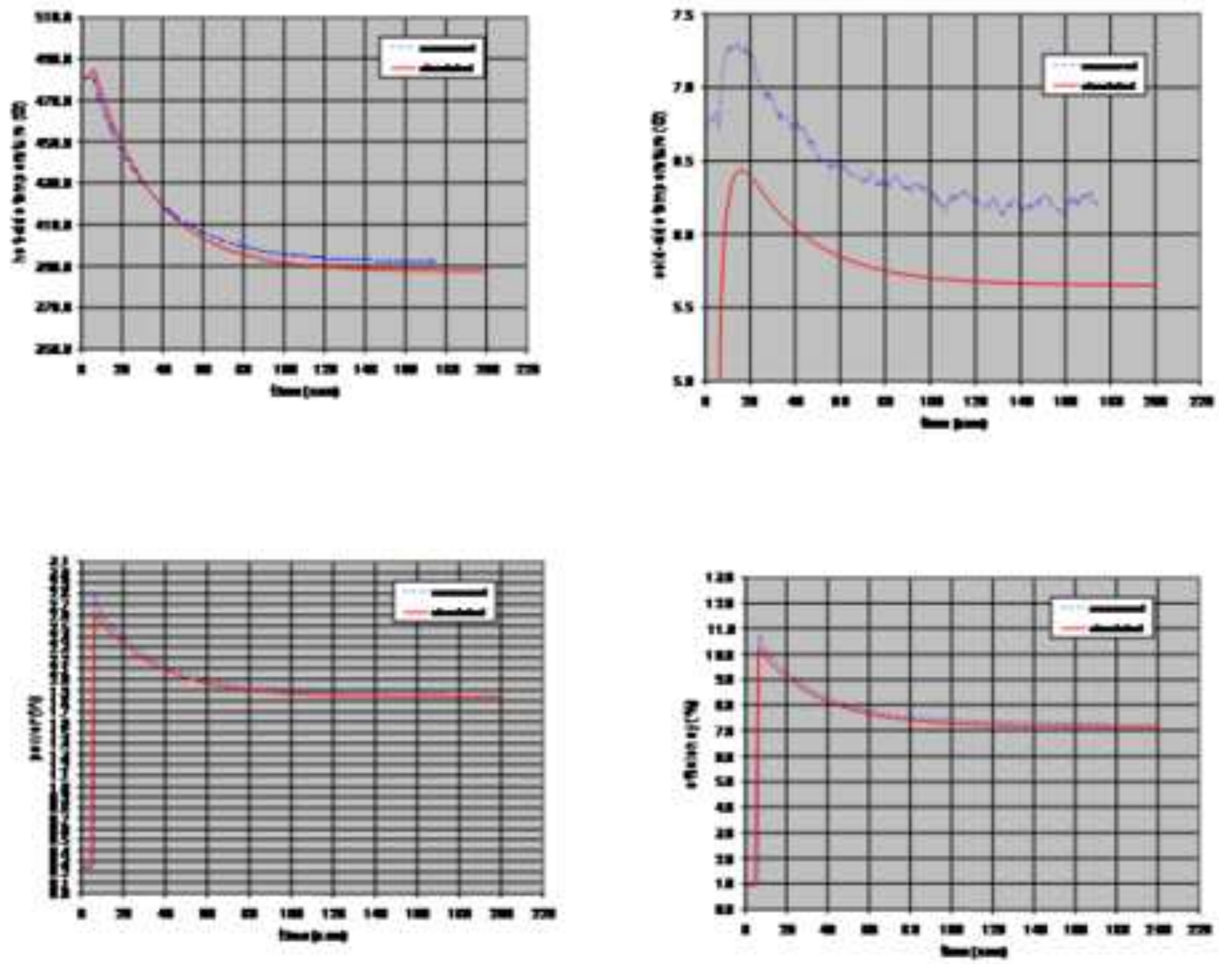

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