4. TITLE AND SUBTITLE
Heat Transfer Modeling of a Charring Material Using Isoconversional Kinetics (Pre-Print)

6. AUTHOR(S)
Mark Ewing, Brian Pincock

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
ATK Launch Systems, Inc.
P.O. Box 707
Brigham City, UT 84302

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)
Air Force Research Laboratory (AFMC)
AFRL/RQRM
4 Draco Drive
Edwards AFB, CA 93524

12. DISTRIBUTION / AVAILABILITY STATEMENT
Approved for public release; distribution unlimited

14. ABSTRACT
An isoconversional modeling approach has been considered in the modeling of heat transfer and pyrolysis in a charring material. The isoconversional approach is appealing due to the use of only a single reacting component as opposed to the multi-component model typically used. This reduces the number of required field variables which reduces numerical demands in large multi-dimensional models. In this study, isoconversional parameters have been reduced from available test data for a generic ablative material. The results were evaluated by implementing the approach into a one-dimensional ablation heat transfer program and modeling the thermal and decomposition response of a charring material subjected to an elevated surface temperature. The results were compared to the same modeling using a traditional multi-component Arrhenius approach. Modeling outputs showed that the two methods produced very similar results when proper care was taken in the tabulated parameters of the isoconversional model which is susceptible to variations in supporting test data and insufficient table resolution. The results of this study indicate that the isoconversional model provides a viable alternative to the widely used multi-component approach.

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:
a. REPORT Unclassified
b. ABSTRACT Unclassified
c. THIS PAGE Unclassified

17. LIMITATION OF ABSTRACT SAR

18. NUMBER OF PAGES 31

19. NAME OF RESPONSIBLE PERSON

20. DISTRIBUTION / AVAILABILITY STATEMENT
Approved for public release; distribution unlimited

21. SECURITY CLASSIFICATION OF:
a. REPORT Unclassified
b. ABSTRACT Unclassified
c. THIS PAGE Unclassified

22. LIMITATION OF ABSTRACT SAR

23. NUMBER OF PAGES 31

24. NAME OF RESPONSIBLE PERSON

25. DISTRIBUTION / AVAILABILITY STATEMENT
Approved for public release; distribution unlimited

26. SECURITY CLASSIFICATION OF:
a. REPORT Unclassified
b. ABSTRACT Unclassified
c. THIS PAGE Unclassified

27. LIMITATION OF ABSTRACT SAR

28. NUMBER OF PAGES 31

29. NAME OF RESPONSIBLE PERSON

30. DISTRIBUTION / AVAILABILITY STATEMENT
Approved for public release; distribution unlimited

31. SECURITY CLASSIFICATION OF:
a. REPORT Unclassified
b. ABSTRACT Unclassified
c. THIS PAGE Unclassified

32. LIMITATION OF ABSTRACT SAR

33. NUMBER OF PAGES 31

34. NAME OF RESPONSIBLE PERSON

35. DISTRIBUTION / AVAILABILITY STATEMENT
Approved for public release; distribution unlimited

36. SECURITY CLASSIFICATION OF:
a. REPORT Unclassified
b. ABSTRACT Unclassified
c. THIS PAGE Unclassified

37. LIMITATION OF ABSTRACT SAR

38. NUMBER OF PAGES 31

39. NAME OF RESPONSIBLE PERSON

40. DISTRIBUTION / AVAILABILITY STATEMENT
Approved for public release; distribution unlimited

41. SECURITY CLASSIFICATION OF:
a. REPORT Unclassified
b. ABSTRACT Unclassified
c. THIS PAGE Unclassified

42. LIMITATION OF ABSTRACT SAR

43. NUMBER OF PAGES 31

44. NAME OF RESPONSIBLE PERSON

45. DISTRIBUTION / AVAILABILITY STATEMENT
Approved for public release; distribution unlimited

46. SECURITY CLASSIFICATION OF:
a. REPORT Unclassified
b. ABSTRACT Unclassified
c. THIS PAGE Unclassified

47. LIMITATION OF ABSTRACT SAR

48. NUMBER OF PAGES 31

49. NAME OF RESPONSIBLE PERSON

50. DISTRIBUTION / AVAILABILITY STATEMENT
Approved for public release; distribution unlimited
Heat Transfer Modeling of a Charring Material Using Isoconversional Kinetics

M. Ewing* and B. Pincock†

ATK Aerospace Group, Brigham City, UT, 84302

Abstract

An isoconversional modeling approach has been considered in the modeling of heat transfer and pyrolysis in a charring material. The isoconversional approach is appealing due to the use of only a single reacting component as opposed to the multi-component model typically used. This reduces the number of required field variables which reduces numerical demands in large multi-dimensional models. In this study, isoconversional parameters have been reduced from available test data for a generic ablative material. The results were evaluated by implementing the approach into a one-dimensional ablation heat transfer program and modeling the thermal and decomposition response of a charring material subjected to an elevated surface temperature. The results were compared to the same modeling using a traditional multi-component Arrhenius approach. Modeling outputs showed that the two methods produced very similar results when proper care was taken in the tabulated parameters of the isoconversional model which is susceptible to variations in supporting test data and insufficient table resolution. The results of this study indicate that the isoconversional model provides a viable alternative to the widely used multi-component approach.

* Senior Technical Fellow, Thermal and Aerothermal Analysis, ATK Aerospace Group, UT40-252, P.O. Box 707, Brigham City, UT, 84302. (435) 863-2492, (435) 863-6223 fax, mark.ewing@atk.com
† Graduate Research Assistant, Stanford University

Distribution A: Approved for Public Release; Distribution Unlimited.
PA Case Number: 15273
Introduction

Ablative materials are commonly used in aerospace components such as rocket motor insulation and thermal protection systems of re-entry vehicles. These materials ablate at the surface due to thermochemical convective interaction with reactive boundary gases [1]. In addition, these materials often lose mass as they pyrolyze (char) internally, causing pyrolysis gases to escape through the porous char structure. As a result, accurate modeling of ablation heat transfer often requires submodels to capture the extent and effects of in-depth charring. Various models are available that include pyrolysis submodels. Notably the Charring Material Thermal Response and Ablation (CMA) [2] program has been available for decades, along with various derivatives of that program. Recently, the Insulation Thermal Response and Ablation Code (ITRAC) [3] has been made available for general modeling of ablative insulators. Both the CMA and ITRAC programs are one-dimensional and provide multi-component Arrhenius submodels to account for in-depth charring. The multi-component model has provided a successful modeling approach for some time, primarily within the framework of one-dimensional codes. However, with recent developments of advanced multi-dimensional codes such as the Heat Transfer and Erosion Analysis Program (Hero) [4,5], models with hundreds of thousands and even millions of elements are common, putting high demand on computational power. Successful reduction of computational expense in the numerical model is therefore of great value, and that is the primary impetus behind the work described here.

For typical ablation heat transfer modeling in aerospace applications, three primary field variables are solved for within the ablative material. These variables are
temperature $T$, internal pore pressure $P$, and degree-of-char (or extent-of-reaction) $\alpha$.

With the multi-component model, the extent-of-reaction is quantified as a combination of individual component reactions $\alpha_i$, typically three, with a field solution for each. A less-known approach for modeling reaction kinetics is available that requires only a single overall extent-of-reaction $\alpha$. Use of this approach in the modeling of a charring material would therefore provide a reduction in the number of field variables, thereby reducing numerical demand. The approach, referred to as an “isoconversional” method [6], is described below following a review of the familiar multi-component model.

**Degree-of-Char (Extent-of-Reaction) Models**

The extent of material pyrolysis can be quantified using an overall extent-of-reaction $\alpha$ based on the bulk density of the decomposing solid $\rho_s$ related to densities in the fully-virgin and fully-charred conditions $\rho_v$ and $\rho_c$. The relationship is [3]

$$\alpha = \frac{\rho_v - \rho_s}{\rho_v - \rho_c} \quad (1)$$

Traditionally, the overall extent-of-reaction is cast in terms of multiple components, each with its own set of reaction kinetics. Alternatively, the isoconversional approach is based only on the overall extent-of-reaction. Each of these approaches is discussed below.

**Multi-component Approach**

Here the pyrolysis process is modeled as a combination of multiple reactions, each with its own extent-of-reaction $\alpha_i$. The fraction of the total virgin mass loss as a result of the $i$th reaction is denoted as $x_i$. Assuming that the material volume is constant
during the decomposition process, the bulk density of the decomposing solid is related to the component reactions by

\[ \rho_s = \rho_v - \rho_v \sum_{i} x_i \alpha_i \]  

(2)

A fully-charred condition corresponds to a value of unity for each \( \alpha_i \) giving the following for the char density

\[ \rho_c = \rho_v - \rho_v \sum_{i} x_i \]  

(3)

Combination of Equations (1) through (3) gives the following expression for the overall extent-of-reaction

\[ \alpha = \frac{\sum_{i} x_i \alpha_i}{\sum_{i} x_i} \]  

(4)

The rate for each reaction is based on both temperature \( T \) and the component extent-of-reaction \( \alpha_i \). It is common to use an Arrhenius function for the \( T \)-dependence with a reaction-order model for the \( \alpha_i \)-dependence as follows

\[ \frac{\partial \alpha_i}{\partial t} = A_i e^{-E_{a,i}/RT} (1 - \alpha_i)^{m_i} \]  

(5)

The kinetic parameters in Eq. (5) are a pre-exponential factor \( A_i \), an activation energy \( E_{a,i} \), and a reaction order \( m_i \). These are determined using complex fitting approaches against experimental data such as thermogrammetric analysis (TGA), providing mass loss versus time at various heating rates.
**Isoconversional Approach**

Here, the Arrhenius function of temperature is still used, but no assumption is made about the functional relationship with $\alpha$. Instead, the reaction rate is written as the following function of $T$ and generic function of $\alpha$

$$\frac{\partial \alpha}{\partial t} = Ae^{-E_a/Rt} f(\alpha) \quad (6)$$

The activation energy $E_a$ along with the combined parameter $Af(\alpha)$ are assumed to be functions of $\alpha$. In order to determine the functional relationship, the full range of possible $\alpha$ values (0 to 1) is divided into segments, and the values for $E_a$ and $Af(\alpha)$ are assumed to be constant over each interval. The variables in Eq. (6) can then be separated and the equation rewritten as

$$\frac{1}{A} \int_{\alpha_{\text{start}}}^{\alpha_{\text{end}}} f(\alpha) \, d\alpha = \int_{t_{\text{start}}}^{t_{\text{end}}} e^{-E_a/Rt} \, dt \quad (7)$$

where $\alpha_{\text{start}}$ and $\alpha_{\text{end}}$ are the two endpoints of a particular $\alpha$-segment, and $t_{\text{start}}$ and $t_{\text{end}}$ are the corresponding times from TGA testing at a given heating rate. The right-hand-side of Eq. (7) can be numerically integrated with a given value for $E_a$, and the result is referred to as an “Arrhenius integral,” $I(E_a)$. Integrating the left-hand-side gives

$$\frac{\alpha_{\text{end}} - \alpha_{\text{start}}}{Af(\alpha)} = I(E_a) \quad (8)$$

At least two temperature rise rates are required from the testing. With the $\alpha$-segments defined, $I(E_a)$ can be evaluated for a selected $E_a$ value associated with that interval; note that $t_{\text{start}}$ and $t_{\text{end}}$ are different for each temperature rise rate for the given $\alpha$-segment. The activation energy $E_a$ is then selected to minimize differences between the Arrhenius integrals for the various temperature rise rates. Once $E_a$ has been established for a
particular \( \alpha \)-segment, the corresponding \( I(E_a) \) follows, and \( Af(\alpha) \) can be found from Eq. (8); the average value of \( I(E_a) \) for the various temperature rise rates is used.

The resulting model is then Eq. (6) with tabular values for \( E_a \) and \( Af(\alpha) \) for each \( \alpha \)-segment. The equation is rewritten in the form of Eq. (9) below to emphasize the combined parameter \( Af(\alpha) \) and the functional relation of the activation energy on the extent-of-reaction \( E_a(\alpha) \). Note that the \( \alpha \)-dependent values are fixed over each segment and are not interpolated between \( \alpha \) values.

\[
\frac{\partial \alpha}{\partial t} = e^{-E_a(\alpha)/RT} Af(\alpha)
\]

Since no functional relation is assumed for the \( \alpha \)-dependence, the approach is sometime referred to as “model free” [7,8].

**Program Implementation**

Numerical solution of the thermal and charring response of on ablative material using the multi-component model in the ITRAC program has been described by Ewing et al. [3]. The approach involves the coupling of solutions for the \( \alpha \)-response (solutions of the extent-of-reaction equations), the \( P \)-response (solutions of a mass/momentum equation), and the \( T \)-response (solutions of an energy equation). We have incorporated the option for the isoconversional method for the \( \alpha \)-response into the ITRAC program. This was accomplished by replacing the standard calculations of Eqs. (1) – (6) with that of Eq. (9) along with tabulated look-up tables for \( E_a(\alpha) \) and \( Af(\alpha) \). Resulting calculations for \( \partial \alpha/\partial t \) were then incorporated into energy and mass-momentum equations which are simultaneously solved to provide the in-depth response. We have compared the two methods on a representative problem using kinetic data available for a
charring ablative from the open literature. A description of the comparison is given below.

**Example Material Characterization**

Representative material property data were needed to support the evaluation of the isoconversional method against the traditional approach. The properties of a “theoretical” material were used that has been formulated for ablation model comparisons in the open literature. The material has been named Theoretical Ablative Composite for Open Testing (TACOT) [9], and it corresponds to a lightweight ablative composite. Properties required for typical ablation heat transfer modeling have been compiled. These include the thermal properties of fully-virgin and fully-charred material, pyrolysis kinetic properties, and properties of resulting pyrolysis gases. Densities in the fully-virgin and fully-charred materials for the TACOT material are provided in Table 1.

*Pyrolysis Kinetic Data*

TACOT pyrolysis kinetics are based on the data of Goldstein [10] who provides experimental TGA data for model development of a phenolic material at heating rates of 3 and 18°C per minute (DPM). In addition, Goldstein provides experimental data for model comparison at a heating rate of 100 DPM. The Goldstein data thereby provides experimental data at three separate heating rates. Figure 1 provides an illustration of the data which are used as the basis for comparisons in this paper between the multi-component and isoconversional methods.
Multi-component Model

Table 2 provides previously derived kinetic modeling inputs for the TACOT material. These have been converted into the format required by the ITRAC program. Figure 2 provides an illustration of the use of these parameters in the model of the Goldstein data from which they were derived. The results indicate good correlation between the model and data, as expected. However, it can be seen that the apparent fluctuations in the data are not reflected by the model, the trend of which is driven by the $T$- and $\alpha$-based multi-component model of Eq. (5).

Isoconversional Model

The Goldstein data at the three heating rates were used to calculate a high resolution table of $E_a(\alpha)$ and $Af(\alpha)$ for use in the isoconversional model. Resulting values are listed in Table 3. These results were used along with the ITRAC program to evaluate the isoconversional method against the data upon which the model parameters were derived. The results are illustrated in Figure 3. The model-free method results in an excellent match against the data from which it was derived. The better mathematical fit against the data is due to this increased freedom in the model associated with the lack of an assumed model for the $\alpha$-dependence. This may appear to be a strength in the approach; however, it makes the model subject to inherent variations in measurement data. This can result in poor extrapolation as illustrated in the next section.
**Extrapolation**

Figure 4 shows results of the two modeling approaches applied to heating rates of 10, 100, 1,000, and 10,000 DPM. The results show that the two models agree favorably at 10 and 100 DPM, but when extrapolated to the higher rates of 1,000 and 10,000 DPM the models deviate. The accuracy of extrapolated models is always a concern, but the isoconversional model appears to suffer from unrealistic results associated with the effects of variation in the lower heating rate data upon which it was based. The quality of the extrapolated application is clearly affected by the quality of the lower heating rate data upon which the model is based. In the next sections, we explore improvements in model consistency through the use of higher fidelity data upon which the isoconversional parameters are based.

**Model Consistency**

Here we force improved model consistency between the isoconversional and the multi-component models. In order to accomplish this, we use results directly from the multi-component model to generate the isoconversional parameters. In other words, the isoconversional model is based directly on output from the multi-component model (as if it were the experimental TGA data). The resulting isoconversional parameters are shown in Table 4. Analyses were performed in ITRAC with these inputs and the results are compared to the multi-component model in Figure 5. As seen in Figure 5, the isoconversional model is capable of precisely mimicking the multi-component model within the heating rate range of the input data. Extrapolation is considered in the next section.
Re-extrapolation with Consistent Models

As before, the two models were run in ITRAC with heating rates of 10, 100, 1,000 and 10,000 DPM. The results are shown in Figure 6. While the comparison is improved, the results indicated divergence of the models at extrapolated heating rates. This suggests that if consistency with the multi-component model is of importance, then isoconversional parameter generation should be done covering heating rates consistent with the intended application.

Input Table Resolution

Another issue for consideration is related to resolution in the parameter input table for the isoconversional model; for example the resolution of Tables 3 and 4 is based on 100 $\alpha$-increments. For comparison, we considered a reduction to 20 increments and noticed a scalloping effect in modeling results as shown in Figure 7. This figure corresponds to modeling results at a heating rate of 100 DPM. The high-resolution results correspond to 100 increments, and the low to 20 increments. The observed scalloping effect is associated with upward concavity over the input data $\alpha$-increments. This can be explained by considering Eq. (9), whose second derivatives with temperature are always positive resulting in the upward concavity. The scalloping effects are diminished with increased resolution, which should be considered much like grid resolution in the discretization of the numerical model.
Charring Material Model Application

In order to evaluate the model applied to a typical charring material application, we considered a test case that has been defined to support discussion in the open literature. In this test case, a 3-cm slab of the charring TACOT material is subjected to a surface temperature of 1,644 K for 60 sec. This elevated temperature drives heat transfer into the material along with subsequent charring. The test case was run with ITRAC using both the multi-component and the isoconversional approach for modeling the decomposition. For the isoconversional modeling, two cases were considered. The first case used the parameters of Table 3 (with isoconversional parameters derived using the data from Goldstein), the second used the data from Table 4 (with isoconversional parameters based on the multi-component model). The modeling results are presented in Figures 8 through 11. Each figure shows results from both the isoconversional and the multi-component models. Parts a) and b) show results corresponding to isoconversional parameters from Table 3 and Table 4, respectively. Results from the models are discussed below.

Material density profiles at simulation times of 20, 40, and 60 sec are shown in Figure 8. Results from the Table 3 simulation show variations in the contours that have been influenced by variations in the original data. The results from the Table 4 simulation more closely match those from the multi-component simulation as expected. Similar comparisons are seen in Figure 9 which shows temporal plots of the depth of the pyrolysis front (location where $\alpha = 0.02$), the depth of the char front (location where $\alpha = 0.98$), and the mass flux of pyrolysis gases leaving the surface. The influence of the different isoconversional parameters; however, on the resulting temperature solutions is
much less pronounced. Figure 10 shows the temperature response at various positions throughout the domain, and the temperature responses are very similar in the cases from the Table 3 and Table 4 results. Although the TACOT material properties account for changes in the char conditions, the impact of the differences in the charred conditions on the temperature solutions is minor.

Figure 11 shows post-processed heating rates from the model at various depths and times. The results show peak heating rates over 12,000 DPM, well above the range of data for which the isoconversional parameters were determined. This confirms that even with extrapolated heating rates, the isoconversional model can produce comparable results to the multi-component model.

**Summary and Conclusions**

An isoconversional kinetic modeling approach has been incorporated in the ablation heat transfer modeling program ITRAC, and the resulting approach has been evaluated by comparing modeling outputs from the isoconversional method and the more common multi-component approach. A generic test case was used, making use of a fictitious charring material based on published decomposition TGA data. Isoconversional parameters were determined using the data directly, and also by using corresponding weight versus time output by the ITRAC program using the multi-component model. It was found that the lack of an assumed $\alpha$-dependence in the isoconversional approach resulted in modeling behavior that was sensitive to variations in the test data. This effect was diminished when the isoconversional parameters were based on data generated from the multi-component model.
It was also found that numerical irregularities could be seen in the form of a scalloping effect in the output when resolution in the isoconversional input table was too low. As a result, the importance of table resolution should be considered in much the same way as domain discretization of the numerical model. It was found that sensitivities in temperature solutions were low for this particular case, even when density profiles significantly deviated. This indicates potential forgiveness in the thermal solution for this type of modeling. Overall, the isoconversional method was able to closely duplicate the results of the multi-component model. As a result, the method appears to be a viable method for pyrolysis modeling in heat transfer applications. Since the model is based on a single extent-of-reaction, it has the potential for significantly reducing numerical demand in large multi-dimensional charring heat transfer models.

Acknowledgements

This work was sponsored by the Air Force Research Laboratory (AFRL) under the program management of Mr. Lester Knox. We would like to thank AFRL and Mr. Knox for their continued support in advancing the state-of-the-art in engineering modeling and simulation.
Nomenclature

\[ A = \text{Pre-exponential coefficient, sec}^{-1} \]

\[ \alpha = \text{Extent-of-reaction (degree-of-char), unitless} \]

\[ E_a = \text{Activation energy, J/kmol} \]

\[ f(\alpha) = \text{Function of } \alpha, \text{ unitless} \]

\[ I = \text{Arrhenius integral, sec} \]

\[ m = \text{Reaction order, unitless} \]

\[ m'' = \text{Mass flux, kg/m}^2 \text{-sec} \]

\[ P = \text{Pore pressure, Pa} \]

\[ \rho = \text{Density, kg/m}^3 \]

\[ t = \text{Time, sec} \]

\[ T = \text{Temperature, K} \]

\[ x = \text{Fraction of virgin mass loss due to pyrolysis, unitless} \]

Subscripts

\[ c = \text{Fully charred} \]

\[ end = \text{The end of the } \alpha \text{-interval} \]

\[ g = \text{Pyrolysis gas} \]

\[ i = \text{The } i \text{th reaction} \]

\[ s = \text{The decomposing solid material} \]

\[ start = \text{The start of the } \alpha \text{-interval} \]

\[ v = \text{Fully virgin} \]
References


Figure 1 Pyrolysis data of Goldstein [10]
Figure 2  Multi-component model compared with test data
Figure 3  Isoconversional model compared with test data
**Figure 4** Data-fit models compared at various heating rates
Figure 5 Model comparisons with isoconversional fit to multi-component results
Figure 6  Correlated model outputs at various heating rates
Figure 7  Effect of low table resolution
(a) Isoconversional model directly based on test data

(b) Isoconversional model fit to multi-component model

Figure 8 Density profile comparisons
(a) Isoconversional model directly based on test data

(b) Isoconversional model fit to multi-component model

Figure 9  Ablation comparisons
(a) Isoconversional model directly based on test data

(b) Isoconversional model fit to multi-component model

Figure 10  In-depth temperature comparisons
Figure 11  Heating rate versus depth at various times
<table>
<thead>
<tr>
<th>$\alpha$</th>
<th>$\rho \text{ (kg/m}^3\text{)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>280</td>
</tr>
<tr>
<td>1</td>
<td>220</td>
</tr>
</tbody>
</table>

**Table 1** Density of the TACOT material
<table>
<thead>
<tr>
<th>$x_i$</th>
<th>$m_i$</th>
<th>$E_i$ (J/kmol)</th>
<th>$A_i$ (sec$^{-1}$)</th>
<th>$T_{crit}$ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.10714</td>
<td>3.0</td>
<td>7.1137E+07</td>
<td>1.2000E+04</td>
<td>333.3</td>
</tr>
<tr>
<td>0.10714</td>
<td>3.0</td>
<td>1.6994E+08</td>
<td>4.9778E+08</td>
<td>555.6</td>
</tr>
</tbody>
</table>

**Table 2** Multi-component kinetic model for the TACOT material
<table>
<thead>
<tr>
<th>α</th>
<th>$E_a$ (J/kmol)</th>
<th>$Af(\alpha)$ (sec$^{-1}$)</th>
<th>α</th>
<th>$E_a$ (J/kmol)</th>
<th>$Af(\alpha)$ (sec$^{-1}$)</th>
<th>α</th>
<th>$E_a$ (J/kmol)</th>
<th>$Af(\alpha)$ (sec$^{-1}$)</th>
<th>α</th>
<th>$E_a$ (J/kmol)</th>
<th>$Af(\alpha)$ (sec$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00</td>
<td>4.16762E+07</td>
<td>9.46398E+00</td>
<td>0.05</td>
<td>5.43971E+07</td>
<td>3.08327E+08</td>
<td>0.25</td>
<td>1.08522E+08</td>
<td>2.11330E+04</td>
<td>0.75</td>
<td>9.82678E+07</td>
<td>1.32612E+02</td>
</tr>
<tr>
<td>0.01</td>
<td>3.46465E+07</td>
<td>4.68117E+00</td>
<td>0.51</td>
<td>1.21764E+08</td>
<td>1.63638E+05</td>
<td>0.76</td>
<td>1.09675E+08</td>
<td>3.06884E+03</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.02</td>
<td>3.56173E+07</td>
<td>1.57480E+00</td>
<td>0.52</td>
<td>1.41875E+08</td>
<td>3.70399E+06</td>
<td>0.77</td>
<td>1.52459E+08</td>
<td>1.00167E+06</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.03</td>
<td>3.60876E+07</td>
<td>1.09440E+00</td>
<td>0.53</td>
<td>1.50220E+08</td>
<td>1.32612E+04</td>
<td>0.78</td>
<td>1.65831E+08</td>
<td>4.94938E+05</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.04</td>
<td>4.44943E+07</td>
<td>1.17095E+00</td>
<td>0.54</td>
<td>1.68794E+08</td>
<td>3.89242E+06</td>
<td>0.79</td>
<td>1.69178E+08</td>
<td>6.61052E+06</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.05</td>
<td>5.39172E+07</td>
<td>2.0005E+02</td>
<td>0.55</td>
<td>1.66293E+08</td>
<td>8.66042E+06</td>
<td>0.80</td>
<td>1.71903E+08</td>
<td>8.46908E+06</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.06</td>
<td>6.73187E+07</td>
<td>1.83368E+02</td>
<td>0.56</td>
<td>1.53229E+08</td>
<td>1.44554E+07</td>
<td>0.81</td>
<td>1.54981E+08</td>
<td>9.19810E+05</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.07</td>
<td>7.75797E+07</td>
<td>2.34145E+02</td>
<td>0.57</td>
<td>1.56384E+08</td>
<td>2.77625E+07</td>
<td>0.82</td>
<td>1.57338E+08</td>
<td>1.14630E+06</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.08</td>
<td>8.01815E+07</td>
<td>4.06121E+02</td>
<td>0.58</td>
<td>4.05337E+08</td>
<td>4.03537E+07</td>
<td>0.83</td>
<td>1.59138E+08</td>
<td>1.31766E+06</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.09</td>
<td>9.03456E+07</td>
<td>4.24055E+02</td>
<td>0.59</td>
<td>1.65960E+08</td>
<td>7.27454E+07</td>
<td>0.84</td>
<td>1.64766E+08</td>
<td>2.36353E+06</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.10</td>
<td>5.63439E+07</td>
<td>6.43867E+02</td>
<td>0.60</td>
<td>1.87322E+08</td>
<td>7.81374E+07</td>
<td>0.85</td>
<td>1.82011E+08</td>
<td>1.79803E+07</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.11</td>
<td>1.1807E+08</td>
<td>7.50102E+02</td>
<td>0.61</td>
<td>1.67338E+08</td>
<td>7.37500E+07</td>
<td>0.86</td>
<td>1.89473E+08</td>
<td>3.98020E+07</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.12</td>
<td>5.93655E+07</td>
<td>2.54604E+02</td>
<td>0.62</td>
<td>1.57787E+08</td>
<td>8.21777E+07</td>
<td>0.87</td>
<td>1.94113E+08</td>
<td>6.16246E+07</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.13</td>
<td>6.47187E+07</td>
<td>7.68797E+02</td>
<td>0.63</td>
<td>1.60137E+08</td>
<td>2.36656E+07</td>
<td>0.88</td>
<td>1.84853E+08</td>
<td>1.43729E+07</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.14</td>
<td>6.59467E+07</td>
<td>8.94160E+02</td>
<td>0.64</td>
<td>1.60950E+08</td>
<td>2.30927E+07</td>
<td>0.89</td>
<td>1.91030E+08</td>
<td>2.98555E+07</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.15</td>
<td>6.79477E+07</td>
<td>1.20657E+03</td>
<td>0.65</td>
<td>1.63709E+08</td>
<td>3.13869E+07</td>
<td>0.90</td>
<td>1.97515E+08</td>
<td>5.10470E+07</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.16</td>
<td>6.91010E+07</td>
<td>1.39014E+03</td>
<td>0.66</td>
<td>1.65846E+08</td>
<td>3.99982E+07</td>
<td>0.91</td>
<td>2.04085E+08</td>
<td>9.96819E+07</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.17</td>
<td>7.16715E+07</td>
<td>2.01097E+03</td>
<td>0.67</td>
<td>1.68503E+08</td>
<td>5.36951E+07</td>
<td>0.92</td>
<td>2.18738E+08</td>
<td>4.78708E+08</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.18</td>
<td>7.13012E+07</td>
<td>2.06473E+03</td>
<td>0.68</td>
<td>1.68047E+08</td>
<td>4.50325E+07</td>
<td>0.93</td>
<td>2.65414E+08</td>
<td>9.90554E+10</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.19</td>
<td>6.88707E+07</td>
<td>1.24286E+03</td>
<td>0.69</td>
<td>1.73720E+08</td>
<td>8.66090E+07</td>
<td>0.94</td>
<td>2.85184E+08</td>
<td>3.13690E+11</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.20</td>
<td>7.01446E+07</td>
<td>1.47012E+03</td>
<td>0.70</td>
<td>1.80375E+08</td>
<td>2.15295E+08</td>
<td>0.95</td>
<td>3.13777E+08</td>
<td>6.90170E+13</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.21</td>
<td>7.40711E+07</td>
<td>1.45286E+03</td>
<td>0.71</td>
<td>1.82635E+08</td>
<td>2.81010E+08</td>
<td>0.96</td>
<td>3.43650E+08</td>
<td>4.31206E+14</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.22</td>
<td>7.22142E+07</td>
<td>1.62713E+03</td>
<td>0.72</td>
<td>1.29552E+08</td>
<td>2.45046E+08</td>
<td>0.73</td>
<td>3.73706E+08</td>
<td>6.43134E+15</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.23</td>
<td>7.23854E+07</td>
<td>1.77891E+03</td>
<td>0.73</td>
<td>1.95028E+08</td>
<td>6.87642E+08</td>
<td>0.98</td>
<td>4.93612E+08</td>
<td>3.70830E+21</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.24</td>
<td>7.31630E+07</td>
<td>1.93379E+03</td>
<td>0.74</td>
<td>1.66992E+08</td>
<td>8.87620E+08</td>
<td>0.99</td>
<td>4.28220E+08</td>
<td>7.83347E+16</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 3 Isoconversional model parameters for the TACOT material (fit to actual data)
## Table 4: Isoconversional model parameters for the TACOT material (fit to multi-component model data)

<table>
<thead>
<tr>
<th>α</th>
<th>$E_a$ (J/kmol)</th>
<th>$A_f(\alpha)$ (sec$^{-1}$)</th>
<th>α</th>
<th>$E_a$ (J/kmol)</th>
<th>$A_f(\alpha)$ (sec$^{-1}$)</th>
<th>α</th>
<th>$E_a$ (J/kmol)</th>
<th>$A_f(\alpha)$ (sec$^{-1}$)</th>
<th>α</th>
<th>$E_a$ (J/kmol)</th>
<th>$A_f(\alpha)$ (sec$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00</td>
<td>7.11809E+07</td>
<td>5.68656E+03</td>
<td>0.05</td>
<td>7.14003E+07</td>
<td>3.57225E+08</td>
<td>0.70</td>
<td>1.53625E+08</td>
<td>2.08476E+06</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.01</td>
<td>7.11698E+07</td>
<td>5.50475E+03</td>
<td>0.10</td>
<td>7.15144E+07</td>
<td>1.53269E+08</td>
<td>0.76</td>
<td>1.75447E+06</td>
<td>1.44500E+06</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.02</td>
<td>7.11475E+07</td>
<td>5.14312E+03</td>
<td>0.15</td>
<td>7.16763E+07</td>
<td>3.19333E+08</td>
<td>0.77</td>
<td>1.52801E+08</td>
<td>1.18845E+06</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.03</td>
<td>7.11627E+07</td>
<td>4.84446E+03</td>
<td>0.20</td>
<td>7.18817E+07</td>
<td>3.09997E+08</td>
<td>0.78</td>
<td>1.52360E+08</td>
<td>1.18845E+06</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.04</td>
<td>7.11368E+07</td>
<td>4.51092E+03</td>
<td>0.25</td>
<td>7.21778E+07</td>
<td>2.86210E+07</td>
<td>0.79</td>
<td>1.51882E+08</td>
<td>9.66457E+05</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.05</td>
<td>7.11480E+07</td>
<td>4.23233E+03</td>
<td>0.30</td>
<td>7.25741E+07</td>
<td>2.62177E+07</td>
<td>0.80</td>
<td>1.51357E+08</td>
<td>7.19750E+05</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.06</td>
<td>7.11311E+07</td>
<td>3.93930E+03</td>
<td>0.35</td>
<td>7.31273E+07</td>
<td>2.38793E+07</td>
<td>0.81</td>
<td>1.50800E+08</td>
<td>6.19070E+05</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.07</td>
<td>7.11325E+07</td>
<td>3.67500E+03</td>
<td>0.40</td>
<td>7.38796E+07</td>
<td>2.16556E+07</td>
<td>0.82</td>
<td>1.50215E+08</td>
<td>4.83816E+05</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.08</td>
<td>7.11666E+07</td>
<td>3.40977E+03</td>
<td>0.45</td>
<td>7.46709E+07</td>
<td>1.95709E+07</td>
<td>0.83</td>
<td>1.49507E+08</td>
<td>3.67704E+05</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.09</td>
<td>7.11254E+07</td>
<td>3.17649E+03</td>
<td>0.50</td>
<td>7.54313E+07</td>
<td>1.76346E+07</td>
<td>0.84</td>
<td>1.48830E+08</td>
<td>2.77992E+05</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.10</td>
<td>7.11141E+07</td>
<td>2.94033E+03</td>
<td>0.55</td>
<td>7.62114E+07</td>
<td>1.58477E+07</td>
<td>0.85</td>
<td>1.48021E+08</td>
<td>2.05532E+05</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.11</td>
<td>7.11116E+07</td>
<td>2.72150E+03</td>
<td>0.60</td>
<td>7.70114E+07</td>
<td>1.42059E+07</td>
<td>0.86</td>
<td>1.47117E+08</td>
<td>1.47506E+05</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.12</td>
<td>7.11110E+07</td>
<td>2.51525E+03</td>
<td>0.65</td>
<td>7.78434E+07</td>
<td>1.27016E+07</td>
<td>0.87</td>
<td>1.46141E+08</td>
<td>1.03269E+05</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.13</td>
<td>7.11099E+07</td>
<td>2.31948E+03</td>
<td>0.70</td>
<td>7.86864E+07</td>
<td>1.13259E+07</td>
<td>0.88</td>
<td>1.45050E+08</td>
<td>6.99666E+04</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.14</td>
<td>7.11084E+07</td>
<td>2.13390E+03</td>
<td>0.75</td>
<td>7.95447E+07</td>
<td>9.66988E+06</td>
<td>0.89</td>
<td>1.43757E+08</td>
<td>5.41914E+05</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.15</td>
<td>7.11075E+07</td>
<td>1.95884E+03</td>
<td>0.80</td>
<td>8.04018E+07</td>
<td>8.19141E+06</td>
<td>0.90</td>
<td>1.42311E+08</td>
<td>2.79193E+04</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.16</td>
<td>7.11087E+07</td>
<td>1.79446E+03</td>
<td>0.85</td>
<td>8.12266E+07</td>
<td>6.56743E+06</td>
<td>0.91</td>
<td>1.40608E+08</td>
<td>1.61874E+04</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.17</td>
<td>7.11133E+07</td>
<td>1.64072E+03</td>
<td>0.90</td>
<td>8.20615E+07</td>
<td>4.97959E+06</td>
<td>0.92</td>
<td>1.38590E+08</td>
<td>6.62989E+03</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.18</td>
<td>7.11202E+07</td>
<td>1.49664E+03</td>
<td>0.95</td>
<td>8.29015E+07</td>
<td>3.56957E+06</td>
<td>0.93</td>
<td>1.36100E+08</td>
<td>4.18316E+03</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.19</td>
<td>7.11340E+07</td>
<td>1.36315E+03</td>
<td>1.00</td>
<td>8.37543E+07</td>
<td>2.33543E+06</td>
<td>0.94</td>
<td>1.32955E+08</td>
<td>1.75235E+03</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.20</td>
<td>7.11508E+07</td>
<td>1.23835E+03</td>
<td>1.05</td>
<td>8.46180E+07</td>
<td>1.53435E+06</td>
<td>0.95</td>
<td>1.28939E+08</td>
<td>8.56672E+02</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.21</td>
<td>7.11751E+07</td>
<td>1.12291E+03</td>
<td>1.10</td>
<td>8.54861E+07</td>
<td>9.58616E+05</td>
<td>0.96</td>
<td>1.24301E+08</td>
<td>1.48953E+02</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.22</td>
<td>7.12088E+07</td>
<td>1.01647E+03</td>
<td>1.15</td>
<td>8.63637E+07</td>
<td>5.49176E+05</td>
<td>0.97</td>
<td>1.18468E+08</td>
<td>2.02585E+01</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.23</td>
<td>7.12546E+07</td>
<td>1.05683E+03</td>
<td>1.20</td>
<td>8.73283E+07</td>
<td>3.36820E+05</td>
<td>0.98</td>
<td>1.14468E+08</td>
<td>2.72111E-01</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.24</td>
<td>7.13169E+07</td>
<td>8.29785E+02</td>
<td>1.25</td>
<td>8.82852E+07</td>
<td>2.48635E+05</td>
<td>0.99</td>
<td>2.00003E+08</td>
<td>5.51718E-06</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>