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REVIEW OF METHODS APPLICABLE
TO THE CALCULATION OF GAP CONDUCTANCE
IN ZIRCALOY-CLAD UO_2 FUEL RODS

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GAP CONDUCTANCE IN ZIRCALOY-CLAD UO_2 FUEL RODS

by
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April 1975

On January 19, 1975, research and development programs of the U.S. Atomic Energy Commission (AEC) became part of the newly formed Energy Research and Development Administration (ERDA). In this report, since it refers to work done in 1974, most references are to AEC programs.

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REVIEW OF METHODS APPLICABLE TO THE CALCULATION OF GAP CONDUCTANCE IN ZIRCALOY-CLAD UO_2 FUEL RODS

INTRODUCTION

The program GAPCON-THERMAL-1 solves for the steady-state temperature distribution in a reactor fuel rod by iterating on converging choices for the gap conductance. This conductance is calculated via a modification of the Ross-Stoute model.^(1,2) In a continuing effort to update and improve the program, a review was made of data and calculational methods (in addition to those of Ross and Stoute) which are applicable to gap conductance. Our concern was to determine if modifications would be needed to use GAPCON-THERMAL-1 in ranges of temperature, gas pressure, and interfacial gas types not covered by the Ross-Stoute data. Specifically, note the following:

<u>Parameter</u>	<u>Range of Interest in Power Reactor Calculations</u>	<u>Range of Ross-Stoute Data</u>
Mean Temperature in Gap	300 - 1000°C	200 - 360°C
Fill Gas Pressure	2 - 300 atm (abs.)	0.5 - 1 atm (abs.)
Contact Pressure	0 - 3000 psi	1400 - 7000 psi
Gas Type	<u>Mixed</u> He, Xe, Kr, H ₂ , N ₂ , and CO ₂	<u>Pure</u> He, Ar, Kr, Xe

When fuel is not contacting the cladding the thermal conduction is primarily through the gas. When fuel does contact the cladding, 5 - 20% of the heat may flow through the contact points, depending on the contact pressure, the gas mix in the gap, and the surface profiles. In no practical case however, does heat flow due to radiation exceed ~2% of the total. Therefore, our review is limited to conduction through the gas and through

the contact points. This report summarizes the results of that review and presents our recommendations for modification of the GAPCON program.

The first two sections of this report present, discuss, and numerically compare various approaches to calculating the conductance through the gas (h_{gas}), and the conductance through contact points (h_{solid}), respectively. Conclusions and recommendations for the GAPCON program are presented in the third section, page 20. The symbols and metric engineering units used throughout are listed in Appendix A. The equations for temperature jump distance and for h_{solid} are put into standardized formats and units in Appendices B and C, respectively.

PART I - HEAT CONDUCTION THROUGH THE INTERFACIAL GAS

I.A. INTRODUCTION OF TERMS AND CONCEPTS

As indicated in Figure 1, the temperature drop across the fuel-clad gap due to conduction through the gas can be represented by two components:

- 1) The temperature drop through the bulk of the gas, which depends upon the gas conductivity, K , according to the Fourier equation,

$$-K \frac{dT}{dx} = \text{surface heat flux (S.H.F.)}$$

(For K constant, this temperature drop is linear in x .)

- 2) A temperature drop at each surface which arises from imperfect energy exchange between the gas and the surface. This drop is called the "temperature jump."

These two components are combined into one equation by extrapolating the linear fall of temperature through the gas to incorporate the true temperature at the surfaces. The length of this extrapolation is called the "temperature jump distance," g .

The Fourier conditions can then be integrated to form

$$\frac{K\Delta T}{\Delta X} = \text{S.H.F.}$$

FIGURE 1. Temperature Drop Across the Fuel-Clad Gap
(Jump distances are exaggerated)

where

$\Delta T = T_1 - T_2$ = fuel surface temperature - clad inner temperature.

$\Delta X = d + g_1 + g_2$ = physical gap size + temperature jump distance.

The defining equation for $h_{Tot.}$ is $h_{Tot.} = \frac{S.H.F.}{\Delta T}$

Combining, we have

$$h_{Tot.} = h_{gas} = \frac{K_{gas}}{d + g_1 + g_2}$$

Now, $g_1 + g_2$ is estimated to be on the same order as the mean free path of the fill gas, which in typical power reactor situations is on the order of the surface roughness of the fuel ($5 \times 10^{-5} - 2 \times 10^{-4}$ cm).

Thus, for operating gaps of 10^{-3} cm or greater, h_{gas} can be approximated simply as

$$h_{gas} = \frac{K_{gas}}{d}$$

where d is the nominal gap size.

However, as fuel and clad approach contact, several complications arise: the temperature jump distance must be accounted for, and the effective distance between the surfaces, $d_{eff.}$ is some complicated function of the actual surface profiles of fuel and clad; in addition there is some conductance through the contact points, so that $h_{Tot.} = h_{gas} + h_{solid}$.

One way to circumvent these difficulties would be to define the "total effective distance," $\Delta X_{eff.}$, of the gap to be

$$\Delta X_{eff.} = d_{eff.} + g_1 + g_2 = K_{gas}/h_{gas}$$

and then determine K_{gas}/h_{gas} * at sufficient points to span the ranges of interest of surface temperatures, surface conditions, gas temperatures and

* Note that h_{gas} is not measureable directly for surfaces in contact. The measureable quantities, S.H.F. and ΔT , yield $h_{Tot.}$ In the Ross-Stoute experiments, the conductance was measured in vacuo, then gas introduced with the surfaces held in contact, and the conductance remeasured. The difference of the two measurements was called " h_{gas} ."

pressures, and gas mixes. This simply has not been done. Referral to the ranges of interest in the Introduction gives an indication of the difficulty and expense of such a project.

In the absence of sufficient data for ΔX , one must estimate d_{eff} and $g_1 + g_2$ by theory and models which do account for the available data and extrapolate conservatively into the unknown regions. It should be kept in mind that no model will be theoretically "exact" because the estimation of d_{eff} will depend on the surface profiles of the fuel and clad. The few published profile measurements^(2,10,11) demonstrate that d_{eff} cannot be characterized with any exactitude. It is also clear that the surface profiles will change due to fuel cracking, plastic clad strain, and deformation of contact points.

Two distinct models were considered for ΔX : that used by Shlykov⁽³⁾ and the more familiar one used by Kennard,⁽⁴⁾ Cetinkale and Fishenden⁽⁵⁾ and many later authors including Ross and Stoute. (This latter model is referred to as the "standard" model.) Three distinct ways of calculating temperature jump distance were considered: Kennard's classical approach,⁽⁴⁾ GAPCON's⁽¹⁾ present simplified approach, and an approach by Lloyd⁽⁶⁾ derived from transport theory. Combining the two models for ΔX with each of the three calculations of $g_1 + g_2$ yields six different approaches to calculate ΔX . These various models and methods are described and compared in Sections I.B and C. In Section I.D. are presented the results of linear regression of all 6 different approaches for calculating ΔX , as applied to the Ross and Stoute data.

I.B. DESCRIPTION OF MODELS FOR ΔX

1) The "standard" model (as presently used in GAPCON-THERMAL-1)

The "standard" model is simply the extension of Figure 1 to the contact situation:

$$\Delta X_{\text{eff.}} = d_{\text{eff.}} + g_1 + g_2$$

where $d_{\text{eff.}}$ is some effective value for the physical separation of the surfaces due to their roughness.

It might be expected that $d_{\text{eff.}}$ would be a function of the interfacial pressure as well as surface roughness. Cetinkale and Fishenden⁽⁵⁾ did not find such a dependence during measurement of conductance through metal-metal pairs at pressures up to 800 psi. Their measurements indicated

$$d_{\text{eff.}} = 0.61 (R_1 + R_2)$$

(where R_1 and R_2 are roughnesses of surface 1 and 2, respectively.)

The Ross and Stoute data seems to indicate a slight dependence on pressure for UO_2 - Zr pairs in the pressure range of 1400 to 7000 psi and a fit of their data indicates

$$d_{\text{eff.}} = C(R_1 + R_2)$$

$$\text{where } C = 2 \exp \left[-1.25 \times 10^{-3} P_a \right],$$

P_a is interfacial pressure in kgf/cm^2 .

In the standard model $d_{\text{eff}} = C(R_1 + R_2)$ with C defined as above. The factor 2 is an attempt to incorporate the effect of "waviness" of the surface and distribution of peak heights on the conductance.^(3,10) The exponential term seeks to model the reduction of these effects with increasing contact pressure.

2) The Shlykov Model

An empirical version of the standard model comes from the Russian literature on contact conductance. Shlykov demonstrated excellent correlation of several hundred data points for metal-metal pairs in air and other gases from the following considerations:

The mathematical definition of $\Delta X_{\text{eff.}}$ is

$$\frac{1}{\Delta X_{\text{eff.}}} = \frac{1}{S} \int_{\text{Surface of interest}} dS / [d(\vec{r}) + g_1 + g_2]$$

where $d(\vec{r})$ is the physical separation of the surfaces at position $\vec{r}$. If one defines V as $\Delta X_{\text{max}} / (g_1 + g_2)$ and y as $\Delta X_{\text{max}} / \Delta X_{\text{eff.}}$, then the above definition can be rewritten as

$$Y = \int_0^1 dA / (e + 1/V)$$

where A is the relative area of true contact and e is $d(\vec{r}) / \Delta X_{\text{max}}$, the relative gap height.

From examining surface profiles of typically machined surfaces, Shvets and Dyban⁽⁷⁾ developed a correlation for Y as a function of V . This so-called "bearing-surface curve" is

$$Y = 3.33 + \frac{10}{V} + \frac{4}{V^2} - 4 \left(\frac{1}{V^3} + \frac{3}{V^2} + \frac{2}{V} \right) \ln(1 + V)$$

Shlykov used this correlation, coupled with his estimate that $\Delta X_{\text{max}} = 2(R_1 + R_2)$, to correlate the metal-metal contact conductance data. To summarize, his calculation of $\Delta X_{\text{eff.}}$ proceeds as follows:

- a) Calculate $V = 2(R_1 + R_2) / (g_1 + g_2)$
- b) Calculate Y from V by the bearing-surface curve
- c) Calculate $\Delta X_{\text{eff.}} = 2(R_1 + R_2) / Y$

I.C. METHODS FOR CALCULATING THE TEMPERATURE JUMP DISTANCE

Tabulated below are the three methods for calculating temperature jump distance, g , mentioned earlier. The methods have been put in a standardized format, that is,

$$g = A \left[\frac{K_{\text{gas}} \sqrt{T_{\text{gas}}}}{p} \right] F(a_i, f_i, M_i)$$

where g is in cm., A is a constant, and F is a function of thermal accommodation coefficients a_i , mole fractions f_i , and molecular weights M_i of the components of the gas. Please refer to Appendix A for a complete definition of symbols and units, and to Appendix B for derivation of the forms presented here.

TABLE 1. Equations for Temperature Jump Distance*

Method	The Constant A (for g in cm.)	The Function F for Mixed Gases	The Function F for Pure Gases
Kennard	2878.	$\left(\frac{2 - a_{\text{mix}}}{a_{\text{mix}}} \right) \sqrt{\frac{1}{\sum f_i / M_i}}$	$\left(\frac{2 - a}{a} \right) \sqrt{M}$
GAPCON	25220.	$\left(\frac{\sum_i f_i M_i k_i / \sum_j \phi_{ij} f_j}{\sum_i f_i k_i / \sum_j \phi_{ij} f_j} \right) \sqrt{\frac{1}{\sum f_i M_i}}$	$\sqrt{M}$
Lloyd	2875.	$\frac{1}{\sum a_i f_i / \sqrt{M_i}}$	$\frac{\sqrt{M}}{a}$

One can see that the methods are rather similar for pure (monatomic) gases, but differ considerably for mixed gases.** Notice also the methods

* In the above equations "a" is the thermal accommodation coefficient for the gas on a given surface. As discussed in Appendix B, we prefer recent measurements by Ullman et al.⁽⁸⁾ for estimating "a." These measurements show "a" to be dependent on the temperature of the surface, so that g_1 and g_2 should in general be calculated separately and not considered equal. It is true, however, that $g_1 + g_2 \approx 2[g(T_{\text{avg}})]$, where $T_{\text{avg.}} = (T_1 + T_2)/2$.

** The equations in Table 2 are derived for pure and mixed monatomic gases only. Introducing more complicated gases complicates the derivation beyond the scope of this simple comparative study.

vary in the amount of input information required preliminary to the calculation of g . The Kennard approach requires an estimate of " a_{mix} " for mixed gases in addition to a_i for pure cases. As Ullman notes,⁽⁸⁾ only Godesar has put forth an explicit method for deducing a_{mix} from a_i , and no basis is provided for that method. The Lloyd method requires an estimate of " a " for each of the components individually, but not for the mix as a whole; and the GAPCON-THERMAL model requires no estimate of " a " whatsoever. Because the Ullman data and that compiled by Trilling⁽¹⁴⁾ indicate that " a " is dependent on the species of gas and the temperature of the surfaces, we question whether the present GAPCON equation is theoretically sound, even though it may account for presently available (and highly scattered) data for ΔX , as will be seen in section I.D.

To make the difference in the equations more graphic, they were each used to calculate the temperature jump distance for He-Xe mixtures at 1 atm. and 260°C (the approximate conditions of the Ross-Stoute measurements). We used the Ullman data for a_{He} and a_{Xe} (see Appendix B) and estimated " a_{mix} " by linear interpolation between the two. The results are presented in Figure 2.

I.D. RESULTS OF LINEAR REGRESSION ON ROSS-STOUTE DATA

One way to evaluate the various possibilities of calculating ΔX is to fit them to measurements of ΔX such as the Ross-Stoute data. Figure 3 presents the Ross-Stoute data for ΔX as compared to the calculated values from the GAPCON model. The purpose of Figure 3 is two fold: to display the data for reference, and to show what linear regression of a model on this data involves. A linear regression code sets the measured values of ΔX equal to " Y " and the calculated values equal to " X " and finds the least squares estimate for the line " $Y = A X + B$ ". The least squares estimate of ΔX would then be

$$\Delta X_{\text{regression}} = A \Delta X_{\text{calc.}} + B.$$

FIGURE 2. Temperature Jump Distance for Xe-He Mixtures at 260°C and 1 atm. Pressure

FIGURE 3. Ross-Stoute Data for ΔX Versus
 Calculated Values from the GAPCON Model

If the model from which $\Delta X_{\text{calc.}}$ is calculated fits the data ideally, the slope, A, would be close to 1.0, the intercept, B, would be relatively small, and the correlation coefficient, ρ , would be close to 1.0 and the residual standard deviation, σ , would be relatively small. Thus, A and B are measures of how much the model must be adjusted to fit the data in the least squares sense, and ρ and σ are measures of how good the fit is. In Figure 3, the line of 1-1 correspondence is drawn for regression of the GAPCON model on the Ross-Stoute data ($A = 1.0$, $B = 0.0$). Also shown is the line of best fit ($A = 1.7$, $B = -3.3 \times 10^{-4}$ cm) and the 95% upper bound on that line.

Table 2 summarizes the results of linear regression listed on the Ross-Stoute data for all 6 possible combinations of model and g calculations.

TABLE 2. Results of Regression
on Ross-Stoute Data

Model	Method for Calc. g	Slope	Intercept. $\times 10^{-4}$ cm	Corr. Coef.	Res. Std. Dev. $\times 10^{-4}$ cm
Shlykov	GAPCON	2.0	2.4	0.74	4.3
	Kennard	1.5	+1.4	0.71	4.5
	Lloyd	2.5	-1.0	0.76	4.1
"Standard"	GAPCON	1.7	-3.3	0.77	4.1
	Kennard	1.5	-1.1	0.78	4.0
	Lloyd	1.8	-1.2	0.75	4.2

The above results, while not very conclusive, are interesting. The structure of the data (slope of best fit line) is dominated by helium and argon points, for which $g_1 + g_2$ is a significant fraction of ΔX , yet all six methods for calculating ΔX demonstrate similar regression results! Two conclusions can perhaps be drawn at this point.

- 1) The Shlykov model appears to be as applicable to the Ross-Stoute data as the standard model. (This may be the first comparison of this model to nonmetallic interfaces.)

- 2) The differences in the models for $g_1 + g_2$ do not significantly affect the outcome of ΔX calculations for typically rough interfaces, and these calculations appear qualitatively correct.

PART II - HEAT CONDUCTANCE THROUGH CONTACT POINTS

II.A. BASIC TERMS AND CONCEPTS

In addition to heat flow through the interfacial gas, there is some heat flow through points of contact. Measurements of this conductance for UO_2 on metal have been made in vacuo by Rapier et al.,⁽¹⁰⁾ and by Ross and Stoute, and in argon by Dean.⁽¹³⁾ Measurements for metal-metal pairs have been made and/or correlated by Cetinkale and Fishenden,⁽⁵⁾ Fenech and Rohsenow,⁽¹¹⁾ and Shlykov,⁽³⁾ among others. Todreus⁽¹²⁾ reexamined UO_2 -metal data in the light of the Mikic model.⁽¹⁵⁾

All seven above-mentioned references have put forth models which attempt to correlate general or specific measurements of surface profiles plus apparent contact pressure with their measurements of h_{solid} , the solid-solid contact conductance. All the models have the same basic form:

$$h_{solid} = AK_m F(L_i \text{ and/or } R_i)(P_a/H)^n, \quad i = 1, 2$$

where A is a constant and

K_m = mean conductivity, $2K_1K_2/(K_1 + K_2)$

F = a function of roughness R and "wavelength" L

(L is the mean peak-peak distance on a surface)

P_a = apparent interfacial pressure

H = Meyer hardness of the softer material (chosen for its direct connection to the yield strength of a metal under a load on a point.)

n = an exponent, discussed below.

The exponent "n" is taken generally as 0.5 or 1.0, depending on whether, as contact pressure increases, the contact points are assumed to remain constant in number (but increase in area) or to remain constant in area

(but increase in number). The dependence of "n" on these two assumptions can be seen from the following considerations:

The assumption is always made that the actual pressure on a contact point will not exceed the Meyer hardness of the softer material. As pressure increases, the actual area of contact will increase to maintain the equation,

$$\frac{\text{Actual contact area}}{\text{Apparent contact area}} = \frac{P_a}{H}.$$

Now assume N equally spaced contact points per unit area. Associated with each point is an equivalent cylinder for heat (axis perpendicular to the interface), with cross-section radius r_e determined from $N\pi r_e^2 = 1$. The actual radius of the contact spot, "r," is determined from the relation,

$$\frac{\text{Actual contact area}}{\text{Apparent contact area}} = \frac{P_a}{H} = \frac{\pi r^2}{\pi r_e^2}$$

Now if N increases with pressure, the ratio r/r_e does not change, and the so-called constriction resistance, arising from the constriction of heat flow through the contact points, remains constant. Hence h_{solid} varies as N, which varies as $(P_a/H)^{1.0}$. If N remains constant on the other hand, r/r_e increases and the (inversely proportional) constriction resistance decreases, such that h_{solid} varies as $(P_a/H)^{0.5}$. Refer to the paper by Cetinkale and Fishenden⁽⁵⁾ for more complete discussion.

II.B. STANDARDIZED EQUATIONS FOR h_{solid}

The models proposed for h_{solid} by the seven references noted in part II.A were placed in standard format and (metric) units. Please refer to Appendix C for details of the derivations. The standardized equations appear in Table 4, in terms of the format.

$$h_{\text{solid}} = AK_m \left(\frac{P_a}{H} \right)^n F(R_i \text{ and or } L_i), i = 1,2$$

TABLE 3. Equations for h_{solid}			
Authors	Values for A (for h_{solid}) in $\text{W/cm}^2 - ^\circ\text{C}$	The Function "F"	Values of N
Cetinkale- Fishenden	132.6	$1/(L_1 + L_2)$	1.33
Rapier-Jones	1.0	$1/L_1$	0.5
Ross-Stoute	1.189	$1/(R_1^2 + R_2^2)^{1/4}$	1.0
Ferech-Rohsenow (Approximated)	1.89	$\left[1.89(R_1 + R_2) + \sqrt{\frac{P_a}{H}} L_1 \right]^{-1}$	1.0
Mikic-Todreas	2.314	$R_1/(R_1^2 + R_2^2)^{1/2} L_1$	1.0 or 0.5
Shlykov	118.9	$Q^{0.86}$	0.86
Dean	11.67	$1/(L_1 L_2)^{1/2}$	1.0

The surprising variety of the above models is even more apparent when they are cast in comparable format, as has been done here. This variety probably arises because the models are really just correlations of the data which the various authors developed or chose to examine. These data sets differ considerably in surface condition, pressures and materials involved, as is pointed out in the table below.

TABLE 4. Experimental Conditions for h_{solid} Data

Authors	Materials	Surface Roughness $\times 10^{-6}$ cm	REL. PRESS. Range, P_a/H
Cetinkale- Fishenden	Various metals	25-650	>0.2
Rapier	UO_2 -SS	9-1600	1.5×10^{-4}
Ross- Stoute	UO_2 -Zirc	25-400	.01-0.07
Fenech- Rohsenow	Iron- Aluminum	260-465	0.001-0.08
Mikic- Todreas	UO_2 -Zr, UO_2 -SS	(See Rapier, Dean, and Ross-Stoute)	
Shlykov	Various Metals	1000-2000	<0.03
Dean	UO_2 -Zirc	30-290	0.002-0.006

II.C. NUMERICAL COMPARISONS OF EQUATIONS FOR h_{solid}

As can be seen from Table 5, much of the data for h_{solid} involves pairs of metals, and is not directly comparable to UO_2 -metal data. The three references presenting UO_2 -metal data are so scattered in experimental conditions, and the results so scattered in magnitude, as to make regression analysis difficult to apply.

We therefore picked seven cases spanning the full range of (P_a/H) and roughness values, and applied each of the seven models to each of the cases. The cases are distributed in (P_a/H) and roughness as shown below:

	REL. PRESSURE $\xrightarrow{(P/H)}$		
	Low	Nom.	High
↓ Roughness R_1 , 10^{-6} cm	~ 0.001	~ 0.01	~ 0.1
Extremely Smooth $R_1 = \sim 1-10$	Rapier 1-7	Ross- Stoute 3-1	Ross- Stoute 3-5
Nominally Rough $R_1 = 10-100$	No data	Ross- Stoute 1-1	Ross- Stoute 1-5
Very Rough $R_1 = 100-1000$	Rapier 1-1	Dean 1-7	No data

It would be revealing to work examples from each of the 9 cells shown above; but, as noted, data is lacking.

The relevant parameters for each of the seven cases chosen are tabulated as follows (most numbers are taken from the tabulation by Todreas and Jacobs).⁽¹²⁾

TABLE 5. Input for Numerical Comparisons

Case	$(P_a/H)^*$	K_m W/cm ² - °C	R_1 Cm x 10 ⁻⁶	R_2 Cm x 10 ⁻⁶	L_1 cm	L_2 cm
Rapier 1-1	0.00015	0.112	1370	940	0.015	0.0079
Rapier 1-7	0.00015	0.112	16	6	0.0018	0.00099
R&S 1-1	0.014	0.078	100	48	0.0045**	0.0032**
R&S 1-5	0.071	0.078	100	48	0.0045**	0.0032**
R&S 3-1	0.014	0.078	24	18	0.0033**	0.0025**
R&S 3-5	0.071	0.078	24	18	0.0033**	0.0025**
Dean 1-7	0.005	0.078	290	120	0.061	0.0032**

* Nominal H-values were chosen: 600,000 psi for Rapier cases

100,000 psi for Dean and R&S cases

** L-values are assumed, not measured; could be in error by a factor of 2.

Values for h_{solid} were calculated for these cases via all seven models, and the results are tabulated below. The experimental results are listed in the last column for reference.

TABLE 6 Calculated Results for h_{solid} (W/cm² - °C)

Case	Cetinkale-Fishenden	Rapier-Jones	Ross-Stoute*	Fenech-Rohsenow	Mikic-Todreas	Shlykov	Dean	Experimental
Rapier 1-1	0.0053	0.091	0.0006	0.0068	0.23**	0.00045	0.018	0.08
Rapier 1-7	0.045	0.80	0.0050	0.50	1.6	0.021	0.15	0.42
R&S 1-1	4.8	2.0	0.14	2.6	0.51	0.15	3.5	0.12
R&S 1-5	40.3	4.6	0.64	6.8	2.6	0.62	17.0	0.70
R&S 3-1	6.0	2.8	0.21	4.3	0.61	3.1	4.4	0.032
R&S 3-5	52.4	6.3	1.0	11.0	3.1	12.3	23.0	1.0
Dean 1-7	0.14	0.091	0.023	0.15	1.5**	0.0022	0.33	0.66

* Assuming $A_0 = 1.0 \text{ cm}^{1/2}$

** In these cases the Zircaloy is the "controlling surface."

If the Todreas-Mikic values are reduced by a factor of 4, they come into rather good agreement overall with the experimental values, granted the uncertainty in L_f for the Ross-Stoute data. For no other model considered can such a simple change effect such good overall agreement among these cases.

Another way to compare these models is to plot h_{solid} (calculated) as a function of P_a/H for some nominal values of roughness and K_m . This has been done in Figure 4 for models of Dean, Ross and Rapier, and Mikic and Shlykov for reference. Also included on Figure 4 are qualitative estimates of the ranges of Dean Rapier and Ross-Stoute data, (shaded areas) normalized to the nominal conditions indicated. Such a normalization is of course somewhat qualitative, but the major trends are clear:

- 1) Each author's model correlates his own data well but does not extrapolate to include the data from each of the other two.
- 2) The Dean data is relatively high. (This may be due to the relatively high values they report for L_f/R_f , which may not be typical of the other two sets.)*
- 3) The Mikic-Todreas model (modified by a factor of 1/4) is conservative with respect to all the data sets.

Figure 5 presents a plot of the ratio L_f/R_f for the measured values reported by Rapier and by Dean. Since this ratio is not controlled in the production and operation of reactor fuel (and since h_{solid} may be inversely proportional to it, according to the Mikic model.), we think it best to remain conservative in the estimation of h_{solid} . We thus prefer the Mikic model at this point, modified as indicated. We propose to estimate L_f from R_f via the correlation of the data points noted on Figure 5.

* The effect of this, according to the Mikic model, is to make the Zircaloy the controlling surface, which raises the conductance. In normalizing the Dean data L_f/R_f values typical of the other two data sets were assumed.

FIGURE 4. Comparison of Models for Solid-Solid Conductance
(Data is normalized for

$$R_m = \sqrt{\frac{R_1^2 + R_2^2}{2}} = 1 \times 10^{-4} \text{ cm}$$

$$K_m = 0.08 \text{ W/cm} \cdot ^\circ\text{C}$$

FIGURE 5. Data for R_1 and L_1 for UO_2

PART III - CONCLUSIONS AND RECOMMENDATIONS FOR GAPCON-THERMAL-2

III.A. CALCULATION OF THE TEMPERATURE JUMP DISTANCE g

Both Kennard and Lloyd indicate that temperature jump distance should be a function of the accommodation coefficient. Furthermore, Ullman has shown that the accommodation coefficient is dependent on the species of gas and the temperature of the surface. All of the models do correlate the Ross-Stoute data significantly. However, only the Lloyd model takes variation of the accommodation coefficient into account. For this reason, and because the Lloyd model is more attractive in the calculation of g for mixed gases, we chose it as the basic model for the temperature jump distance.

III.B. CALCULATION OF EFFECTIVE GAP WIDTH, ΔX

As indicated in Table 3, the use of the Lloyd temperature jump distance with either the standard or Shlykov model leads to nearly identical regression results with the Ross-Stoute data for ΔX . We recommend the use of the standard model, not because it is any more theoretically satisfying but because we encountered convergence problems when the Shlykov model was used in GAPCON-THERMAL. Note that the regression model for input is

$$\Delta X_{\text{reg.}} = 1.8 \Delta X_{\text{calc.}} - 0.00012$$

where $\Delta X_{\text{calc.}} = C (R_1 + R_2) + (g_1 + g_2)_{\text{Lloyd}}$

and $C = 2 \exp \left(-0.00125 P_a \right)$ as before (here, P_a is in kgf/cm^2 and R_1, R_2 are in cm.)

III.C. CALCULATION OF h_{solid}

As noted at the end of Part II, the Mikic-Todreas model (reduced by a factor of 4) is conservative compared to available data for h_{solid} in UO_2 -metal pairs. We recommend its use until more data becomes available for h_{solid} in as-fabricated and irradiated fuel rod materials.

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APPENDIX A

DEFINITIONS AND UNITS FOR SYMBOLS USED IN EQUATIONS

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DEFINITIONS AND UNITS FOR SYMBOLS USED IN EQUATIONS

The metric units for various material properties and calculated parameters listed below were chosen to facilitate dimensional analysis and use of equations appearing in this report. For example, because the specific heat capacities of gases are usually tabulated in cal/g-°C, and because the ratio of gas conductivity to specific heat capacity appears in the equations for temperature jump distance, gas conductivities, K_i , are in cal/sec-cm-°C. On the other hand, the mean solid-solid conductivity, K_m , appears in the equation for h_{solid} as

$$h_{\text{solid}} (\text{W/cm}^2\text{-}^\circ\text{C}) = K_m \left(\frac{P_a}{H} \right)^n F (\text{cm})^{-1}$$

so that for K_m , the least cumbersome units are W/cm-°C.

<u>Symbol</u>	<u>Meaning</u>	<u>Units</u>
a_i	The thermal accommodation coefficient of the i^{th} gas in a mixture	Dimensionless
a_{mix}	The accommodation coefficient for a gas mixture as a whole	Dimensionless
C_p, C_v	The specific heat capacities of a gas at constant pressure and volume, respectively	cal/g-°C
d	The physical fuel-clad or solid-solid gap dimension	cm
$d_{\text{eff.}}$	The effective solid-solid separation for solids in contact, due to their roughness	cm
f_i	The mole fraction of the i^{th} component in a gas mixture	Dimensionless

Symbol	Meaning	Units
g_1, g_2	The temperature jump distance at the fuel and cladding, respectively	cm
h_{gas}	The conductance per unit area through the interfacial gas	$\text{W/cm}^2\text{-}^\circ\text{C}$
h_{solid}	The conductance per unit area through points of solid-solid contact	$\text{W/cm}^2\text{-}^\circ\text{C}$
h_{total}	Total conductance per unit area	$\text{W/cm}^2\text{-}^\circ\text{C}$
H	The Meyer Hardness of the softer material in contact	kgf/cm^2
K_i	The conductivity of the i^{th} component in a gas mixture	$\text{cal/sec-cm-}^\circ\text{C}$
$K_{\text{mix}}(K_{\text{gas}})$	The conductivity of a gas mixture (or pure gas) as a whole	$\text{cal/sec-cm-}^\circ\text{C}$
K_1, K_2	Thermal conductivities of fuel and clad materials, respectively, evaluated at T_1 and T_2	$\text{W/cm-}^\circ\text{C}$
K_m	The mean solid-solid conductivity, given by $2K_1K_2/(K_1 + K_2)$	$\text{W/cm-}^\circ\text{C}$
L_1, L_2	The distance between peak heights on fuel and clad materials, respectively	cm
M_i	The molecular weight of the i^{th} gas in a mixture	g/mole
P	The pressure of the interfacial gas	dyne/cm^2
P_a	The apparent interfacial pressure	kgf/cm^2
Pr	The Prandtl number for a gas (defined as $C_p u/K$)	Dimensionless
R	The gas constant. (8.317×10^7)	$\text{ergs/mole-}^\circ\text{C}$
R_1, R_2	The arithmetic mean roughnesses of fuel and clad, respectively	cm
s_1, s_2	The standard deviations of peak heights of fuel and clad	cm

Symbol	Meaning	Units
T_1, T_2	The surface temperatures of fuel and clad materials	$^{\circ}\text{C}$
T_{gas}	The average temperature of the interfacial gas	$^{\circ}\text{K}$
u_i	The viscosity of the i^{th} component in a gas mixture	g/cm-sec
u_{mix}	The viscosity of a gas mixture as a whole	g/cm-sec
ΔX	The total effective width of solid-solid separation, such that $h_{\text{gas}} = K_{\text{mix}}/\Delta X$	cm

APPENDIX B

DERIVATION OF STANDARDIZED EQUATIONS FOR TEMPERATURE JUMP DISTANCE

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DERIVATION OF STANDARDIZED EQUATIONS FOR TEMPERATURE JUMP DISTANCE

1. NOTES ON CALCULATION OF K_{gas} , K_{mix} , " a_i " and " a_{mix} "

The calculation of gas conductivity, K_{gas} , is performed according to Chapman-Enskog theory as recommended in Reference 9.

$$K_{\text{gas}} = \frac{1.989 \times 10^{-4}}{\sigma_{\text{gas}}^2 \Omega(z)} \sqrt{\frac{T_{\text{gas}}}{M}}$$

where $z = e_{\text{gas}} T_{\text{gas}} / k$

with $k = \text{Boltzman's constant}$

e_{gas} Leonard-Jones potential for the gas

and σ_{gas} = an interaction distance characteristic of the gas

Values for σ_{gas} , e_{gas}/k , and $\Omega(z)$ are tabulated in Reference 9.

The conductivity of a mixture of gases, K_{mix} , is calculated by weighting and adding the conductivities of the components:

$$K_{\text{mix}} = \sum_i \left(f_i K_i / \sum_j f_j \phi_{ij} \right)$$

The weighting function ϕ_{ij} is defined as

$$\phi_{ij} = \frac{1}{\sqrt{8}} \left(1 + \frac{M_i}{M_j} \right)^{-1/2} \left[1 + \left(\frac{u_i}{u_j} \right)^{1/2} \left(\frac{M_j}{M_i} \right)^{1/4} \right]^2$$

where the u_i are the viscosities of the components.

It is worthwhile to note that the u_i are proportional to the K_i for monatomic gases. (The derivation of the correct proportionality constant is, in fact, a major accomplishment of the Chapman-Enskog theory.) The relation is

$$u_i = 0.1343 K_i M_i$$

The calculations of the accommodation coefficient "a" used in this report are based on recent measurements by Ullman, et al.⁽⁸⁾ of the accommodation coefficients of helium and xenon on UO_2 and on stainless steel. Their data span a temperature range from 500 to 1000 °K, and suggest equations of the form:

$$\begin{aligned} a_{He} &= 0.425 - 2.3 \times 10^{-4} T_i \\ a_{Xe} &= 0.749 - 2.5 \times 10^{-4} T_i \end{aligned} \quad i = 1, 2$$

These equations can be compared with a compilation of data listed by Trilling⁽¹⁴⁾ for helium, neon, argon, krypton and xenon on clean tungsten wire, for temperature up to 500°K. Ullman's data for a_{Xe} in the overlapping temperature region agrees quite well with Trilling's compilation, but Ullman's data for a_{He} is one order of magnitude greater than comparable data from Trilling's sources. This may be due to difference in surface condition between clean tungsten wire and the rough, uncleaned surfaces deliberately used by Ullman. Because the latter surfaces are more typical, and because Ullman's a_{He} leads to larger (more conservative) estimates of temperature jump distance, we prefer to use Ullman's data until the discrepancy is resolved.

We calculated a_{mix} (for the Kennard equation) and a_i for gases other than helium and xenon by linear interpolation between a_{He} and a_{Xe} based on molecular weight. The effective molecular weight of a gas mixture was taken to be

$$\sum_i f_i M_i.$$

At least for pure argon and krypton, this procedure is borne out by qualitative agreement with clean-wire data in Trilling's compilation.

2. THE KENNARD EQUATION

Kennard defines the accommodation coefficient as the ratio of the net average energy transfer from the gas molecules to a surface compared to

that which would occur if impinging gas molecules came into thermal equilibrium with the surface. He then proceeds to derive the temperature jump distance in a straightforward way using classical mechanics. His final equation can be reduced for a pure gas to

$$g = \left(\frac{2 - a}{a} \right) \left(\frac{1}{1 + C_p/C_v} \right) \left(\frac{K_{\text{gas}}}{C_v P} \right) \left(\frac{2\pi RT_{\text{gas}}}{M} \right)^{1/2}$$

Note that $C_v = (3/2) (R/M)$ for a pure monatomic gas so that the equation can be written

$$g = \left(\frac{2 - a}{a} \right) \left(\frac{1}{1 + C_p/C_v} \right) \left(\frac{K_{\text{gas}}}{P} \right) \left(\frac{4\pi T_{\text{gas}}}{3 C_v} \right)^{1/2} \times 4.188 \times 10^7$$

$$\text{Now } C_v = \sum_i f_i C_{v_i}$$

for monatomic gases, as a consequence of equipartition of energy. Hence, the term under the radical can be written

$$\frac{4\pi T_{\text{gas}}}{3 \sum f_i C_{v_i} \times 4.188 \times 10^7} = \frac{8\pi T_{\text{gas}}}{9R \sum f_i/M_i \times 4.188 \times 10^7} = 3.358 \times 10^{-8} \frac{T_{\text{gas}}}{\sum f_i/M_i}$$

Then for a mixture of gases,

$$g = \left(\frac{2 - a_{\text{mix}}}{a_{\text{mix}}} \right) \left(\frac{1}{1 + C_p/C_v} \right) \left(\frac{K_{\text{gas}} \sqrt{T_{\text{gas}}}}{P} \right) \left(\frac{1}{\sum f_i/M_i} \right)^{1/2} \times 7675.$$

Since the ratio of heat capacities for monatomic gases is 1.667, the equation can be reduced yet more to form

$$g = \left(\frac{2 - a_{\text{mix}}}{a_{\text{mix}}} \right) \left(\frac{K_{\text{gas}} \sqrt{T_{\text{gas}}}}{P} \right) \left(\frac{1}{\sum f_i/M_i} \right)^{1/2} \times 2878.$$

and

$$g = 2878. \left(\frac{2 - a}{a} \right) \left(\frac{K_{\text{gas}} \sqrt{T_{\text{gas}}}}{P} \right) \sqrt{M}$$

for pure gases.

3. THE GAPCON EQUATION

The equations involved in the calculation for temperature jump distance in GAPCON-THERMAL-1 can be collated from the listing to form

$$(g_1 + g_2) = 5.448 \left(\frac{u_{\text{mix}}}{P} \right) \left(\frac{T_{\text{gas}}}{\sum f_i M_i} \right)^{1/2}$$

with P in psi.

Assuming $g_1 = g_2 = g$, and putting P in dynes/cm², the equation becomes

$$g = 1.87 \times 10^5 \left(\frac{u_{\text{mix}}}{P} \right) \left(\frac{T_{\text{gas}}}{\sum f_i M_i} \right)^{1/2}$$

At first this does not appear to be of the same form as the Kennard equation, but recall from the notes above that $u_i = 0.1343 K_i M_i$. Now a similar form for u_{mix} exists as for K_{mix} ⁽⁹⁾ i.e.,

$$u_{\text{mix}} = \frac{\sum_i f_i u_i}{\sum_j \phi_{ij} f_j}$$

Substituting for the u_i in the above and multiplying and dividing by K_{mix} in the above one has that

$$u_{\text{mix}} = \left[\frac{\sum_i f_i K_i M_i / \sum_j \phi_{ij} f_j}{\sum_i f_i K_i / \sum_j \phi_{ij} f_j} \right] K_{\text{mix}}$$

So for mixed gases

$$g = 25220. \left(\frac{K_{mix} \sqrt{T_{gas}}}{P} \right) \left[\frac{\sum_i f_i K_i M_i / \sum_j \phi_{ij} f_j}{\sum_i f_i K_i / \sum_j \phi_{ij} f_j} \right] \sqrt{\frac{1}{\sum_i f_i M_i}}$$

For pure gases, this reduces to a form very similar to the corresponding Kennard equation:

$$g = 25220. \frac{K_{gas} \sqrt{T_{gas}}}{P} \sqrt{M}$$

4. THE LLOYD EQUATION

A fresh outlook on the whole problem of temperature jump distance is presented by Lloyd. He developed a model from detailed consideration of the particle fluxes of each species of gas in a mixture, and the heat flux they carry from surface to gas based on P_i transport theory. His final equation can be expressed as

$$g = \frac{K_{mix}}{1.942 \sum_i^j \frac{a_i P_i}{\sqrt{M_i T'_{gas}}}}$$

where P_i are partial pressures in Torr. and K_{gas} is in Watt/cm-°C.

Note T'_{gas} is the gas temperature just ahead of temperature jump rather than the average gas temperature (the distinction is not preserved in the comparative calculations performed in parts I.C and I.D of this paper).

Recognizing $P_i = f_i P$ and changing pressure units to dynes/cm² and temperature units to cal/sec-cm-°C, the equation becomes

$$g = 2875. \left(\frac{K_{\text{mix}} \sqrt{T_{\text{gas}}}}{P} \right) \left(\frac{1.}{\sum f_i a_i / \sqrt{M_i}} \right)$$

This reduces to the familiar form for pure gases:

$$g = 2875. \left(\frac{K_{\text{gas}} \sqrt{T_{\text{gas}}}}{P} \right) \left(\frac{\sqrt{M}}{a} \right)$$

Note: The equation for K_{gas} applies without correction only for temperatures greater than 10 times the critical temperature and pressures less than 30 to 100 times the critical pressure. Reference 9 tabulates the critical values, and referral to the reduced thermal conductivity curves in the same reference will assure one that for all practical cases in power-reactor application the equation given for K_{gas} does apply.

APPENDIX C

DERIVATION OF STANDARDIZED EQUATIONS FOR h_{solid}

APPENDIX C

DERIVATION OF STANDARDIZED EQUATIONS; FOR h_{solid}

1. THE CETINKALE-FISHENDEN MODEL ⁽⁵⁾

This model assumes a fixed number N of equally spaced contact points per unit area. Associated with each contact spot is a fictitious cylinder of radius r_e . The total cross-sectional area of N of these cylinders comprise a unit area, such that $N\pi r_e^2 = 1$. The true radius of each contact spot, r , is assumed to be related to r_e by the formula,

$$r^2 = r_e^2 (P_a / H)$$

That is, as the apparent contact pressure P_a increases, the true contact pressure [which is $(r_e^2 / r^2) P_a$] is never greater than the Meyer hardness of the softer material, H . The radius r increases for each contact point to maintain this condition. Cetinkale and Fishenden derived the resistance to heat flow consequent from constricting the lines of heat flow through a contact point (as opposed to unrestricted flow through the equivalent cylinder). This so-called constriction resistance they found to be

$$\begin{aligned} R_{\text{constr.}} &= \frac{r_e^2 \tan^{-1} \left(r_e^2 / r^2 - 1 \right)}{K_m r} \\ &\approx \frac{r_e^2 \left(\pi/2 \right)}{K_m r} \end{aligned}$$

since $r_e^2 \gg r^2$

Taking the reciprocal $1/R_{\text{constr.}}$ to be h_{solid} , and using the relationship between the contact spot and equivalent cylinder radii, we have the Cetinkale-Fishenden equation for h_{solid} :

$$h_{\text{solid}} = (2/\pi) (K_m/r_e) (P_a/H)^{1/2}$$

From measurements of h_{solid} , r_e could be deduced, and the empirical relation

$$r_e = 0.0048(P_a/H)^{-5/6}(L_1 + L_2)$$

was found by Cetinkale and Fishenden to correlate their measurements. Combining this with their basic h_{solid} equation yields their final model for h_{solid} :

$$h_{\text{solid}} = \frac{132.6 K_m}{(L_1 + L_2)} \left(\frac{P_a}{H} \right)^{4/3}$$

2. THE RAPIER-JONES MODEL ⁽⁷⁾

Rapier et al., developed their model along the same lines as Cetinkale and Fishenden, the difference being that they estimated r_e from the wavelength of the surface with larger wavelength. The wavelength was assumed uniform in azimuthal direction, such that

$$r_e = (\pi/2) L_1.$$

Combining this with Cetinkale-Fishenden's basic h_{solid} equation yields as modified model for h_{solid} :

$$h_{\text{solid}} = (K_m/L_1) (P_a/H)^{1/2}$$

3. THE ROSS-STOUTE MODEL ⁽²⁾

Ross and Stoute attempted to correlate their measurements of h_{solid} for UO_2 and zirconium pairs by using just one measured surface parameter, i.e., the mean surface roughnesses, R_1 and R_2 . They combined the two roughnesses as

$$R = \left(\frac{R_1^2 + R_2^2}{2} \right)^{1/2}$$

and then took the square root of R times a free parameter, A_0 , to be the correlating parameter. This procedure shifts the correlation of their data from the measured R to the chosen A_0 , and would not be very meaningful were it not for the fact that "best choices" for A_0 only ranged from about 0.5 to 1.0 for their data.

Their equation for h_{solid} is:

$$h_{\text{solid}} = \frac{1.189 K_m}{(R_1^2 + R_2^2)^{1/4}} \left(\frac{P_a}{H} \right) \text{ for } A_0 = 1.0$$

4. FENECH-ROHSENOW⁽¹¹⁾

Use of this model depends on determining the number of contact spots per unit area, n , by a graphical method. The expression for h in vacuum environment is

$$h_{\text{solid}} = \left(\frac{E^2}{1-E^2} \right) \left[\frac{\frac{1}{\sqrt{n}} [1.21 (K_1 + K_2)] + 4.26 K_1 K_2}{\left(4.26 R_1 + \frac{E}{\sqrt{n}} \right) K_2 + \left(4.26 R_2 + \frac{E}{\sqrt{n}} \right) K_1} \right]$$

where R_1, R_2 are mean heights of the surfaces

K_1, K_2 are the conductivities

and $E^2 = \frac{\text{actual contact area}}{\text{apparent contact area.}}$

If one makes the following approximations

$$E^2 = P_a/H$$

$$E^2 \ll 1$$

$$n = \frac{\pi}{4 L_1^2}, \quad \sqrt{n} \gg 1$$

$$R_1 = R_2 = (R_1 + R_2)/2$$

Then the model reduces to

$$h = \frac{4.26 K_1 K_2 E^2}{(4.26 R + \frac{2L_1 E}{\sqrt{\pi}}) (K_1 + K_2)} = \left[\frac{1.89 K_m}{1.89 (R_1 + R_2) + (P_a/H)^{1/2} L_1} \right] \left(\frac{P_a}{H} \right)$$

5. THE MIKIC-TODREAS MODEL⁽¹²⁾

The original model for contact conductance by Mikic sought to account for the fact that the conductance should be a function of the roughnesses (which somehow determine an effective roughness for the plane-on peaks model) and the slope of the asperities on the more "peaked" surface (which controls the number of actual contact spots per unit area).

The original model is

$$h_{\text{solid}} = \frac{1.45 K_m (\overline{\tan \theta})_c}{S} \left(\frac{P_a}{H} \right)^n$$

where $(\overline{\tan \theta})_c$ is the average slope of the asperities on the controlling surface, the one for which $\overline{\tan \theta}$ is larger. The exponent n is 0.5 at low pressure, reflecting the idea that a fixed number of higher peaks per unit area control the conductance. At higher pressure, n approaches 1.0, as the number of contact spots begins to increase proportionately to increasing pressure. Todreas concluded that, for UO_2 -zirconium interfaces, the transition pressure is around 1,000 psia.

The model may be put in terms of R_i and L_i by assuming*

$$\begin{aligned} \overline{\tan \theta}_i &= 2 R_i / L_i \\ S &= \left(S_1^2 + S_2^2 \right)^{1/2} \\ S_i &= \sqrt{\frac{\pi}{2}} R_i \end{aligned}$$

* See Appendix C of Mikic's paper⁽¹⁵⁾ for explanation of these assumptions. Basically a model involving equally spaced identically shaped, peaks on both surfaces is substituted for the real situation. The distribution of peak heights is assumed to be normal.

The model then becomes

$$h_{\text{solid}} = 2.314 \text{ Km} \left[\frac{R_c}{(R_1^2 + R_2^2)^{1/2} L_c} \right] \left(\frac{p_a}{H} \right)^n$$

6. THE SHLYKOV CORRELATION

The solid-solid conductance portion of the Shlykov correlation is given by

$$h_{\text{solid}} = 118.9 \text{ Km} \left(\frac{Qp_a}{H} \right)^{0.86}$$

where $Q = 1.0$ for $(R_1 + R_2) > 0.003 \text{ cm}$

$$= \left(\frac{0.0030}{R_1 + R_2} \right)^{1/3} \text{ for } 0.001 < (R_1 + R_2) < 0.003 \text{ cm}$$

$$= \frac{0.0015}{R_1 + R_2} \text{ for } (R_1 + R_2) < 0.001 \text{ cm.}$$

7. THE DEAN MODEL (13)

The solid-solid conductance portion of the Dean model is presented as

$$140 \text{ Km} \left(\frac{p_a}{H} \right) \left(\frac{1}{L_1 L_2} \right)^{1/2} = h_{\text{solid}}$$

where, for h_{solid} in $\text{Btu/hr-ft}^2\text{-}^\circ\text{F}$, K_m is $\text{Btu/hr-ft-}^\circ\text{F}$, L_1 , L_2 are in inches.

Changing K_m to $\text{W/cm-}^\circ\text{C}$ and L_1 , L_2 to cm requires the constant to change to 11.67 for h_{solid} in $\text{W/cm}^2\text{-}^\circ\text{C}$.

The derivation of this model is similar to that of Rapier's, except that the wavelengths of both surfaces are assumed to affect the number of contact points per unit area, in an equal way.

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