The Effect of Spatially Correlated Roughness on the Conduction of Heat through a Slab

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Abstract: Heat conduction through a slab, $0 \leq x \leq W$ is one dimensional. However, if one of the edges, say x=0, is rough the conduction will be two dimensional. The two dimensionality varies with the correlation length with a maximum at a length approximately 10% of the slab width. The maximum percentage standard deviation of the flux is of the order of 3 time that of the roughness.

Keywords: *Surface Roughness, Correlation length, Stochastic Conduction*

1. Introduction:

Consider the conduction of heat through a slab of thickness W and unit depth whose rough surface at $x = 0$ is presumed to be locally random with a correlation length $\mathcal{L}$, Figure 1. Because of the two dimensional nature of the surface, both x and y components of heat will exist. For a value of $\mathcal{L}$ that is small in relation to the slab width W, i.e., approaching white noise, the effects are intuitively expected to attenuate quickly with increasing distance into the slab. For larger values of $\mathcal{L}$, implying smoother variations with respect to y, the effects are expected to propagate with little change through the thickness.
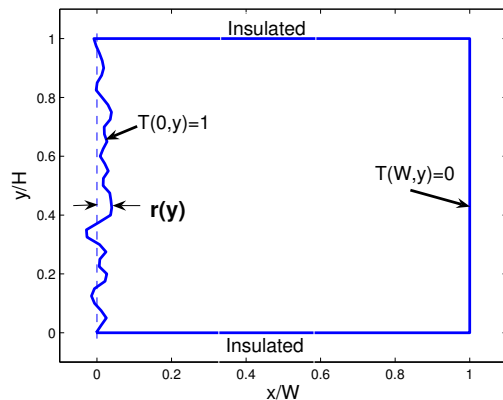

Figure 1 Schematic of a Slab with a Rough Surface

Let the deviation of the edge from the nominal value of $x = 0$, defined as $r(y)$, be characterized by the random field, $\xi(y)$, such that

$$r(y) = \sigma\xi(y) \qquad (1)$$

where $\xi(y)$ is a random field whose mean at any specific value of y is zero with a standard deviation of unity and σ is the standard deviation of the field. $\xi(y)$ has a spatial correlation length of $\mathcal{L}$. If $\mathcal{L} = 0$, i.e., $\xi(y)$ is characterized by white noise, we expect that the region in which the conductive flux is two dimensional will be very thin and to approach zero in extent while if $\mathcal{L}$ is large in comparison to H, $\xi(y)$ will be nearly constant with respect to y, i.e., be a random variable with $\xi(y) = \overline{\xi}$ and the heat transfer will approach that of one dimensional conduction with values per unit depth of

$$\overline{q}_x = \frac{k\ \Delta T}{\overline{W}} \qquad \text{with} \ \ \sigma(q_x) \approx \overline{q}_x \frac{\sigma(\xi)}{\overline{W}} \ \ (2)$$

where the overbars represent averages. Without detailed analysis, it might then be reasonable to assume that the region in which two dimensional conduction is important will gradually diminish in size as $\mathcal{L}$ decreases. As will be shown this is not the case and there is actually an amplification of the uncertainty in a region near the rough edge.

Because of the random nature of the surface, this system is stochastic in nature and the evaluation of the net heat transfer will involve the solution of a partial differential equation over a random region. In most of the reported literature, the stochasticity is associated with a property such as the thermal conductivity or a boundary condition, usually the temperature. The two problems, that of a random roughness and that of a random boundary condition, are fundamentally different and require different approaches.

There are very few reported results for random regions. Lin et al. [1] solve the problem of a rough leading edge on a wedge in supersonic flow by mapping the region. However, the mapping technique is valid only for Neumann boundary conditions. References 2 and 3 suggest a method in which a coordinate system is embedded in an elastic domain whose shape is that of the mean region being studied. The embedded coordinate system is similar to that used for deterministic irregular surfaces [4]. Forces are applied to the domain and using the distorted coordinate system the field equations are solved for the desired quantity, temperature in our case. These forces are determined by solving the inverse elasticity problem, with the distorted grid being a natural consequence of the solution of the coupled equations of elasticity. For each simulation, solving for the temperature requires the evaluation of the conductance matrix based upon the movement of the embedded nodal points. This approach is both complex and computationally expensive and it is not clear that it is less expensive than using the highly efficient mesh generators available in commercial software.

2. Representation of the Random Edge

The random edge is represented through the Karhunen-Loeve expansion

$$\xi(y) = \sum_{i=1}^{\infty} \sqrt{\lambda_i} f_i(y) u_i \qquad (3a)$$

where u_i are uncorrelated random variables and λ_i and $f_i(y)$ are the eigenvalues and orthogonal eigenfunctions that satisfy

$$f_i(y) = \frac{1}{\lambda_i} \int C(y, y') f_i(y') dy' \quad (3b)$$

$$\int f_i(y) f_j(y) dy = \delta_{ij} \qquad (3c)$$

where $C(y, y')$ is the covariance function and δ_{ij} is the Kronecker delta. Eq. (3a) defines a realization of $\xi(y)$ as the sum of the deterministic functions $f_i(y)$, that are ordered in terms of their eigenvalues, multiplied by multiple random variables, u_i, and in our case are taken as having a zero mean Gaussian distribution. The series, Eq. 3a, is usually terminated at N terms and the combined variance of the first N vectors is given by

$$\sigma^2(\xi) = \sum_{i=1}^{N} \lambda_i^2 \qquad (4)$$

The number of such random variables, u_i, needed will depend upon the desired accuracy. For a mesh with $\Delta y = 1/140$ over $0 \leq y \leq 1$, the number of vectors needed to achieve 99.9% of the total variance is shown in Figure 4. Our computed results did not show adequate convergence unless more than 99.9% of the variance of the rough edge was accounted for.
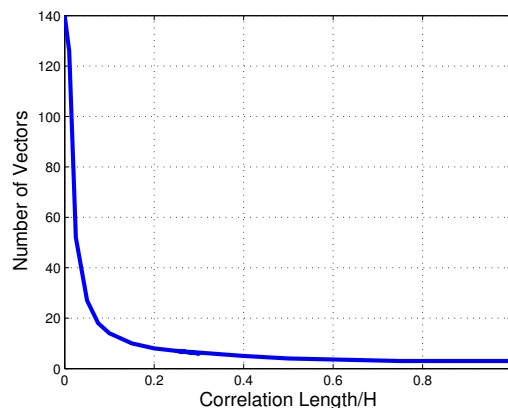

Figure 4 Number of Vectors, N, using Eq. 3a needed to achieve 99.9% of the true variance as a function of the correlation length $\mathcal{L}/H$ (the number approaches infinity as $\mathcal{L} \to 0$ (white noise))

The covariance function was

$$C(y, y') = exp(-(y - y')^2/\mathcal{L}^2) \qquad (5)$$

and Eq. 3a was solved numerically. When done on a finite grid, the K-L expansion is usually referred to as Principal Component Analysis [5].

The question of the appropriate mesh size is difficult to determine. One suggestion is that the correlation length $\mathcal{L}$ should span 2-3 elements [6]. Experience solving deterministic problems has also shown that reasonable results are found when using of the order of 3 elements per wave length. The eigenvectors diminish in wave length as i increases and the shortest wavelength was found to be of the order of $1.5\mathcal{L}$ for all values of $\mathcal{L}$ examined from 0.01H to 3H. This suggests that an adequate mesh would be one in which $\Delta y \approx 0.5\mathcal{L}$.

3. Solving the Problem

Realistically there are only a limited number of techniques to solve the energy equation:

1 Direct simulation (Monte Carlo) which is simple and straight foward, but computationally expensive

2 The Neumann approach in which the conductance matrix is in the form $\mathcal{K}_0(\mathcal{I} + \Delta\mathcal{K})$ and the inverse is an infinite series $\mathcal{I} - \Delta\mathcal{K} + (\Delta\mathcal{K})^2 - (\Delta\mathcal{K})^3....$

3 Polynomial Chaos [7] in which both the stochastic field and the solution are represented as a sum of orthogonal functions of u_i. Most published solutions have used only a few terms in the series with each term a function of only one or two of the u_i. Preliminary calculations indicate that several terms are needed and that the functions be of the form $f(u_i, u_j, u_k)$. As a consequence the final set of equations to be solved involves a very large number of coupled equations. Because of the high value of N, we estimate that of the order of 5000 coupled equations need to be solved.

4 Transformation of the coordinates such that

$$s(y) = x/W(y) \qquad 0 \le s(y) \le 1 \quad (6a)$$
$$t = y/H \qquad 0 \le t \le 1 \qquad (6b)$$

In terms of s, t the problem is one of a constant region and the two dimensional conduction equation

$$\left(2\left(\frac{W'}{W}\right)^2 - \frac{W''}{W}\right)\frac{\partial T}{\partial s} + \left(\frac{sW'}{W}\right)^2\frac{\partial^2 T}{\partial s^2}$$
$$-2\frac{sW'}{W}\frac{\partial^2 T}{\partial s \partial t} + \frac{\partial^2 T}{\partial t^2} = 0 (6c)$$

Although COMSOL can solve Eq. 6c, since $W(y)$ must be expressed by Eq. 3a, the derivatives W' and W'' will involve N terms, each of which will have a randomly selected coefficient, u_i. In other words, a Monte Carlo sampled set of pdes.

4. COMSOL and Monte Carlo Sampling

Monte Carlo simulation, while expensive, proved to be the best approach. This was particularly true because of the high efficiency of the mesh generator and solver in COMSOL. Values of u_i were chosen using a Latin Hypercube based upon dividing the cdf into 50 equal probability increments. For each sample, a new mesh was generated and the energy equation solved.

There proved to be an unusual problem caused by COMSOL's very efficient mesh generator. Suppose that the rough edge was defined by 5 boundary segments and let them be numbered 1-5 with the top edge being 6, the right edge 7, and the bottom edge 8. Clearly edges 6,7 and 8 have fixed thermal boundary conditions, namely insulated, isothermal, and insulated respectively. Unfortunately, as the coordinates of the boundary points on the rough edge change with each sample, the edge number that COMSOL assigns to the edges changes. We spent quite a bit of time plumbing the secrets of the structure of 'fem' before finding a way to fix the edge numbers. We present the algorithm to help other users.

Let Ney be the number of edges on the rough edge and define the coordinates of the vertices of the edges by

E_X1=[Edge(1,1:Ney+1) 1 1];
E_Y1=[Edge(2,1:Ney+1) 1 0];

Then in the script for COMSOL insert these commands

```
% create bounding lines of the rough edge
CC(1)=curve2([E_X1(1),E_X1(2)],
   [E_Y1(1),E_Y1(2)],[1,1]);
for Iedge=2:Ney+2
CC(Iedge)=curve2([E_X1(Iedge),E_X1(Iedge+1)],
   [E_Y1(Iedge),E_Y1(Iedge+1)],[1,1]);
end
CC(Ney+3)=curve2([E_X1(Ney+3),E_X1(1)],
   [E_Y1(Ney+3),E_Y1(1)],[1,1]);
[g1,ctx]=geomcoerce('solid',CC,'out','ctx');
clear bnd
bnd.type = 'q0','T','T';
bnd.T0 = 273.15,1,0;
afeX=[2*ones(1,Ney) 1 3 1];
afe.bnd=afeX;
for il=1:Ney+3
afeY(find(ctxil))=afeX(il);
end
bnd.ind=afeY;
```

The boundary conditions on edges 6,7 and 8 will be correct.

The problem was solved for a unit thermal conductivity (all results presented are normalized by the value of q_x for a smooth edge) and a roughness of 2% of the slab width, $\overline{W}$. The value of 2% was chosen as representing a reasonable degree of roughness. Using a Gaussian distribution truncated at $\pm 4\sigma$, the maximum deviation is 0.08% of W, giving a range of thermal resistance of a one dimensional smooth slab from 0.92 to 1.08. Computations were made with $H = W$, $3W$ and $5W$. Little effect was found on the behavior of $q_x(x)$ in the vicinity of $y = H/2$ and only the case of $H = W$ is reported. The number of simulations to achieve a converged result was a weak function of the correlation length $\mathcal{L}$, usually in the order of 1500 to 3500. This number is a function of the number of random variables, $u_i, i = 1, \cdots, K$. The values of u_i were found using the Latin Hypercube approach [8].

5. Convergence of Computations

Figure 5a shows the convergence of the numerical computations for the standard deviation of the flux, $\sigma(q_x)$, at x=0.1W and y=0.5H (similar results were found for other quantities of interest) for $\mathcal{L}/H$=0.075 as a function of the number of simulations for meshes using quadratic Lagrangian triangles and whose number of nodes ranged from 1000 to 68000 with maximum element areas ranging from 10^{-2} to 10^{-4} and element areas near the rough surface ranging from 10^{-4} to $2.5\ 10^{-6}$ respectively.
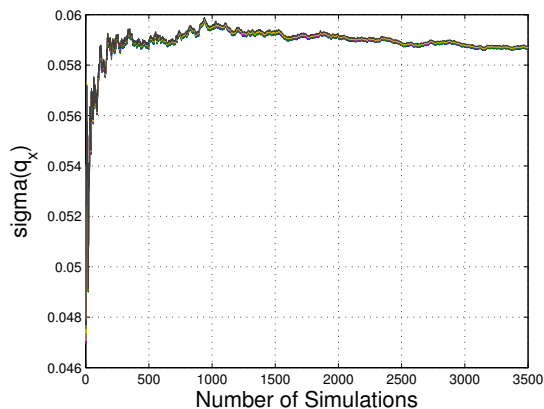

Figure 5a Convergence for $\mathcal{L}$=0.075
For meshes with degrees of freedom
ranging from 1000 to 68000

The results are seen to converge to a steady value after circa 3500 and to be insensitive to the mesh used. The mean value of $\sigma(q_x)$ over the range MC=3500 to 5000 changed by less than 0.001 with a variation of ± 0.0002 over the different meshes.

The effect of the number of the number of elements on the edge $x = 0, 0 \leq y \leq H$ is shown in Figure 5b. As suggested by the figure, all computations for $\mathcal{L}/H > 0.05$ were performed with 120 elements on the edge except for $\mathcal{L}/H = 0.01$ for which 140 were used. Convergence was checked by monitoring the value of $\sigma(q_x)$ at $x = 0.1W$ and $y = 0.5H$. Computations were carried out for 1300 iterations and thereafter at ever 100 simulations the mean value of $\sigma(q_x)$ and its standard deviation over the preceding 100 simulations examined. Convergence was achieved when the mean changed by less than 0.001 and the standard deviation was less than 0.05%. Execution times are lisrted in Table 1.
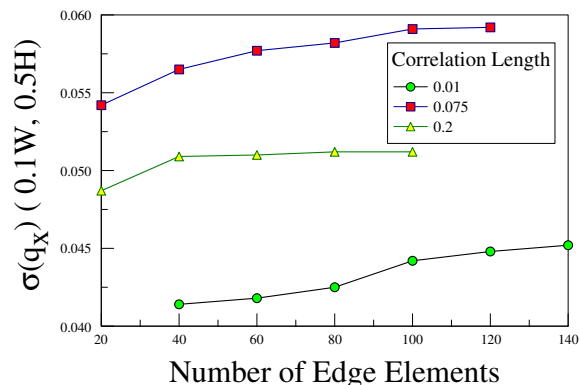

Figure 5b Effect of the Number of Edge
Elements on the value of $\sigma(q_x)$
at x=0.1W and y=0.5H

Computations made using meshes that had 4000 dof and 2000 elements and ones that had 68000 dof and 25000 elements with minimum element areas of $3\ 10^{-5}$ to $2.5\ 10^{-6}$ respectively gave results that differed by less than 1%.

Table 1

Execution times on a 2.8 GHz cpu with 1GB of ram
for 1000 simulations: forming mesh 970 sec; solving 3900 sec,
extracting T, q_x, q_y; 2100 sec

$\mathcal{L}/W$	average number of dof	average number of elements	mesh quality	
			minimum	average
0.01	13474	6614	.443	.988
0.10	13784	6777	.786	.989
1.0	14209	6990	.813	.986

The results presented in the following figures were obtained using the next to finest mesh (of the order of 14000 degrees of freedom, 7000 quadratic triangular elements with a minimum area of approximately $8 \ 10^{-5}$) and between 3200 and 3500 Monte Carlo simulation. Figure 6 shows the contours for q_x and q_y for an edge roughness of 2%. Near the right edge, the conduction is essentially one dimensional since the flux in the y direction at all values of y has approached zero and as a consequence the standard deviation of the x flux approaches from below the value obtained from Eq. 2 . Near the rough edge, there is a substantial disruption of the heat flow with large values of q_y that are of the order of q_x. Consequently, the standard deviations of both fluxes are significantly larger than that of the edge roughness. In the central portion, $0.2H \le y \le 0.8H$ the y flux is unconstrained, but near the
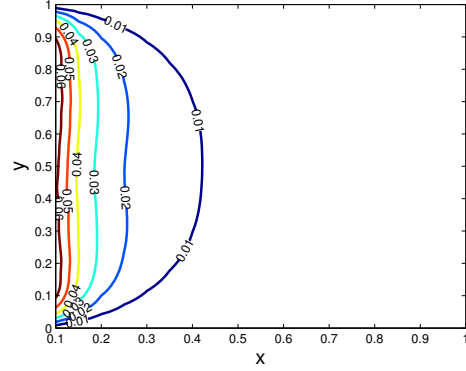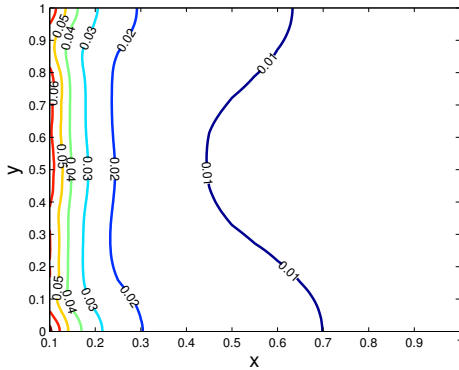
$\sigma(q_y)$

Figure 6b Contours of $\sigma(q_y)$
for an Edge Roughness
of 2% and $\mathcal{L}$=0.10W

insulated edges the flow lines of the flux are forced to become aligned with the edge and the result is that q_x must vary more than it does in the central region. Consequently, the standard deviation near the insulated boundaries is of the order of 1.5 times that in the central core. Figure 7 shows how quickly the standard deviation of the heat fluxes drops with distance into the slab

Figure 8 compares the standard deviations for q_x and q_y at y=H/2. As expected, near the rough edge, the fluxes behave similarly and both approach the percentage standard deviation of the roughness as $\mathcal{L} \to 0$. However, $\sigma(q_y) \to 0$ as the isothermal right edge is approached and the flux becomes one dimensional. What is surprising is how the interaction between q_x and q_y results in a standard deviation at modest values of $\mathcal{L}$ of the order of 7% or about 3 times the value expected for large $\mathcal{L}$.
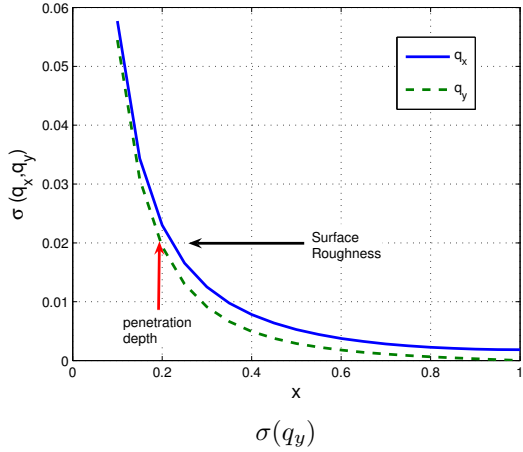
Figure 6a Contours of $\sigma(q_x)$
for an Edge Roughness
of 2% and $\mathcal{L}$=0.10W

Figure 7 σ of q at y=H/2 as a function of
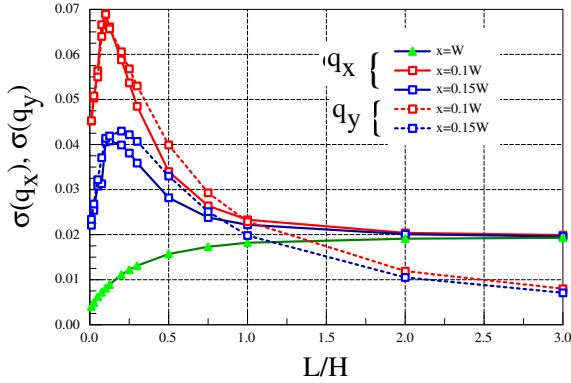depth for 2% roughness and $\mathcal{L}$=0.10W

Figure 8 Effect of $\mathcal{L}$ upon the
behavior of q_x and q_y at y=H/2
for an Edge Roughness of 2%

6. Correlation of the Heat Flux

The roughness of the contours of Figure 6 is
most apparent near the rough surface and di-
minishes as x approaches the right edge, $x =
W$. Both this roughness and the standard de-
viation, shown in Figure 7, are measures of
the effect of the correlation length $\mathcal{L}$. As ex-
pected for small values of $\mathcal{L}$ the roughness of
the contours diminishes quickly and the flux
q_x measured at the right edge is insensitive to
the correlation length. Figure 9 shows corre-
lation length of q_x. (see the section entitled
"Correlation Length" for the definition of $\mathcal{L}$.
In contrast to the effect of $\mathcal{L}$ on the standard
deviation of q_x, the auto correlation length
monotonically increases and becomes greater
than W when $\mathcal{L} > 0.5H$. The curve is only ap-
proximate because of the use of Monte Carlo

simulation. Repeated computations suggest a
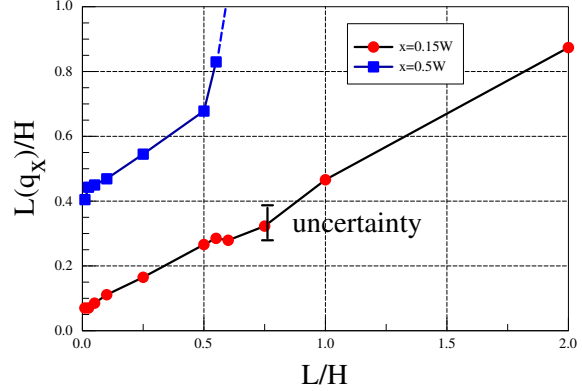range of uncertainty as indicated.

Figure 9 Effect of $\mathcal{L}$ upon the Correlation
Length, $\mathcal{L}(y)$ of q_x

7. Correlation Length

The correlation length, $\mathcal{L}$ is a measure of how
far apart y_i and y_j must be for a given de-
gree of correlation. $\mathcal{L}$ is not a physically mea-
surable quantity. Rather it is derived from
a model of the covariance. That is, the cor-
relation is expressed by an arbitrary function
$C(y_i, y_j)$ that one feels fits the measured re-
sponse. Several functions are commonly used,
$exp(-|d|/\mathcal{L}$, $exp(-d^2/\mathcal{L}^2)$, $1 - |d|/\mathcal{L}$, where
$d = y_i - y_j$. Clearly the value of $\mathcal{L}$ is dependent
on the model used and suffers from consider-
able ambiguity in its interpretation. For these
calculations, we used $C(y_i, y_j)exp(-d^2/\mathcal{L}^2)$ to
describe the random field $\xi(y)$. As expected
for this linear problem, the computed covari-
ances at different values of x were found to be
well fit by this model.

8. Conclusions

From these results it appears that it will not
be useful to treat problems of this type by us-
ing the Neumann and the Polynomial Chaos
methods. The most interesting situations are
those for which the correlated nature of the
random field causes unexpected results, i.e.,
$\mathcal{L} \leq 0.5W$. For these values of $\mathcal{L}$, ΔK is large
compared to $\mathcal{I}$ and the Neumann method does
not converge. The number of coupled equa-
tions needed for Polynomial Chaos is too large
for realistic computations.

Defining a characteristic depth of the region
directly affected by the rough edge to be the

the depth at which the percentage $\sigma(q)$ equals that of the roughness, see Figure 7, for all values of $\mathcal{L}$ is $\approx 0.1W$. The results suggest that the region in which the effects are significantly greater than for $\mathcal{L} = \infty$, as measured by the standard deviation of both q_x and q_y, does not exceed twice this characteristic depth. Figure 10 illustrates the relationship between the penetration depth and $\mathcal{L}$.
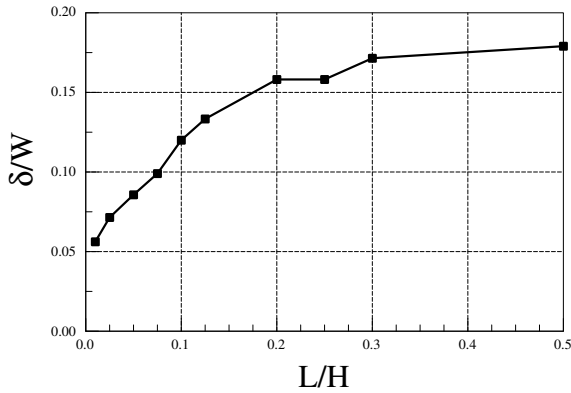

Figure 10 Effect of $\mathcal{L}$ upon the Penetration Depth

While the effect on q_x at $x = W$ can be estimated to range from 0 to $\sigma(W)$ as the correlation length varies from 0 to $\approx 0.5W$, the effects internal to the slab are not easily anticipated. Since a given slab has a unique and fixed roughness, the statistical results are to be interpreted as representing one's uncertainty about the variation of the heat flux.

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