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Meta-Analysis of Gas Flow Resistance Measurements Through Packed Beds

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ARL-TR-301   November 1993

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REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE November 1993	3. REPORT TYPE AND DATES COVERED Final, Sep 92 - Sep 93

4. TITLE AND SUBTITLE

Meta-Analysis of Gas Flow Resistance Measurements Through Packed Beds

5. FUNDING NUMBERS

CC: 4B592392510000

6. AUTHOR(S)

Malcolm S. Taylor and Csaba K. Zoltani

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

U.S. Army Research Laboratory
ATTN: AMSRL-CI-S
Aberdeen Proving Ground, MD 21005-5067

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)

U.S. Army Research Laboratory
ATTN: AMSRL-OP-CI-B (Tech Lib)
Aberdeen Proving Ground, MD 21005-5066

10. SPONSORING / MONITORING AGENCY REPORT NUMBER

ARL-TR-301

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION / AVAILABILITY STATEMENT

Approved for public release; distribution unlimited.

12b. DISTRIBUTION CODE

13. ABSTRACT (Maximum 200 words)

Measurements of the resistance to flow through packed beds of inert spheres have been reported by a number of authors through relations expressing the coefficient of drag as a function of Reynolds number. A meta-analysis of the data using improved statistical methods is undertaken to aggregate the available experimental results. For Reynolds number in excess of 10^3 the relation $\log F_v = 0.49 + 0.90 \log Re'$ is shown to be a highly effective representation of all available data.

14. SUBJECT TERMS

gas flow resistance, packed beds, meta-analysis, bootstrap, regression, gas flow, Reynolds number

15. NUMBER OF PAGES

19

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT UNCLASSIFIED	18. SECURITY CLASSIFICATION OF THIS PAGE UNCLASSIFIED	19. SECURITY CLASSIFICATION OF ABSTRACT UNCLASSIFIED	20. LIMITATION OF ABSTRACT UL

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TABLE OF CONTENTS

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LIST OF FIGURES

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1. INTRODUCTION

Experimental results are cumulative if in aggregate they unify and extend empirical relations and theoretical structures that may be obscured in individual investigations. Empirical cumulativeness, which Hedges (1987) describes as "... the degree of agreement among replicated experiments or the degree to which related experimental results fit into a simple pattern that makes conceptual sense," is the focus of this report. Glass (1976) was among the first to recommend the use of quantitative procedures in integrative research reviews and to introduce the term "meta-analysis" to cover the collection of such procedures. Meta-analysis claims certain classical statistical procedures, as well as approaches developed specifically for research synthesis, and has found application in the social and biological sciences. The unification of experimental results obtained by different investigators operating independently with their own experimental protocol and sometimes using different methods of analysis, is the kernel of meta-analysis. A comprehensive treatment of this subject is given by Hedges and Olkin (1985).

Measurement in the physical sciences is generally regarded as highly accurate, and although some variability is inevitable, the variation itself is thought to be insignificant from a practical standpoint. Counterexamples to this notion are plentiful, even in carefully conducted experiments. Consider, for instance, the situation described by Touloukian (1975) involving two sets of measurements taken on the thermal conductivity of gadolinium. These data, shown in Figure 1, "... are for the same sample, measured in the same laboratory two years apart in 1967 and 1969. The accuracy of curve 1 was stated as within 1% and that of curve 2 as 0.5% ..." and yet, the curves differ by more than several hundred percent at higher values of temperature.

Physical scientists normally bring a careful qualitative analysis to their research studies. If prudently employed, interrogative statistics, which are part of meta-analysis, have a contribution to make in the physical sciences as well.

After data have been collected according to a carefully constructed experimental design (e.g., see Montgomery 1991) the main reason for determining a correlation (a regression analysis) is to examine the effects that some variables exert, or appear to exert, on others. Even when no intuitive physical relationship is apparent, regression analysis may provide a convenient summary of the data. The summary can be accomplished in a number of ways and has been an active area of investigation since the time of A. M. Legendre (1752–1833), who published the first account of regression by least squares in 1805. Section 2 of this report reviews the correlations that have been advanced for steady flow through inert
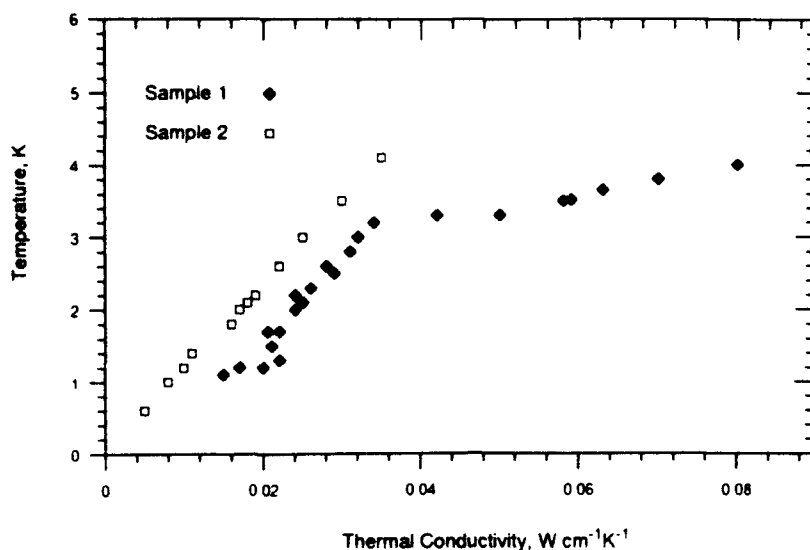
Figure 1. Thermal conductivity of gadolinium.

spherically packed beds and some of the consequences of the attendant data analysis. In Section 3, a meta-analysis of the gas flow resistance measurements is undertaken. Section 4 contains a summary and main conclusions.

2. REGRESSION ANALYSIS OF GAS FLOW RESISTANCE MEASUREMENTS

Ergun (1952), Kuo and Nydegger (1978), and Jones and Krier (1983) have proposed models relating coefficient of drag to Reynolds number for steady flow through packed beds of inert spheres. However, the correlations were developed under different experimental regimens. Robbins and Gough (1978) also investigated coefficient of drag at a high Reynolds number but presented their results in terms of a friction factor $f_s' = F_v/[Re/(1 - \phi)]$, which is the ratio of coefficient of drag F_v, and Reynolds number Re scaled by a solids loading factor $(1 - \phi)$.

In comparing Ergun's relation

$$F_v = 150 + 1.75 \left(\frac{Re}{1 - \phi} \right) , \tag{1}$$

2

to that of Kuo and Nydegger

$$F_v = 276.23 + 5.05 \left(\frac{Re}{1 - \phi} \right)^{0.87} , \tag{2}$$

or of Jones and Krier

$$F_v = 150 + 3.89 \left(\frac{Re}{1 - \phi} \right)^{0.87} , \tag{3}$$

a slight notational difference portends substantial complications. Equation 1 is a simple linear model. Equations 2 and 3 are nonlinear in the sense that one or more parameters appear nonlinearly. Nonlinearity complicates the statistical analysis of the data since determining appropriate choices for the parameters in Equations 2 and 3 becomes a computationally intensive optimization procedure, and inference about the resultant relation and parameters becomes much more tentative. The mathematical underpinnings of nonlinear regression will not support as much in the way of statistical inference or hypothesis testing as is available for linear regression. In general, nonlinear models should be avoided unless there is a compelling reason for their use. Draper and Smith (1981) discuss this issue in greater detail.

Standard regression procedures are developed under several assumptions. Fundamental among these is that the response (here, F_v) is measured with error but the predictor(s) (here, Re and ϕ) are measured without error. Jones and Krier provide estimates of error for F_v, Re, and ϕ, confirming that this assumption is not met, and call into question the efficacy of the resultant correlations. Sometimes an attempt to circumvent this requirement is undertaken by arguing that the error in predictor measurement is sufficiently small as to be ignored when compared to the range of the predictor variable. If this claim is invoked, reliance upon any resultant representation must be tempered accordingly.

Since a correlation provides a convenient representation of the available data, a direct attempt at evaluating the adequacy of a regression equation involves an examination of the differences between the measurements taken and the values predicted by the equation. These differences, $F_{v_i} - F_{v_i}'$, $i = 1, 2, ..., n$, are called residuals; F_{v_i} is an experimentally determined value of drag coefficient, and F_{v_i}' is the corresponding value predicted by the regression equation. A residual plot for Equation 3 is shown in

3

Figure 2. These plots may serve as a diagnostic tool in addition to assessing the adequacy of a fitted regression model.

Figure 2 strongly suggests that another crucial regression assumption is not satisfied. The variance of the residuals does not appear constant over the range of $Re' = Re/(1 - \phi)$; moreover, the departure from the fitted equation is systematic with bead diameter, D_b. Jones and Krier recommend reverting to the relation (Equation 2) proposed by Kuo and Nydegger to describe their own measurements taken for 6-mm beads. This recommendation is data specific and is difficult to justify in general. They conjecture that an interaction between bead size and tube diameter may be present, but this requires quantitative substantiation. In general, weighted least squares, or a transformation of the observations F_{v_i} before regression, are potential corrective procedures suggested by this residual pattern.
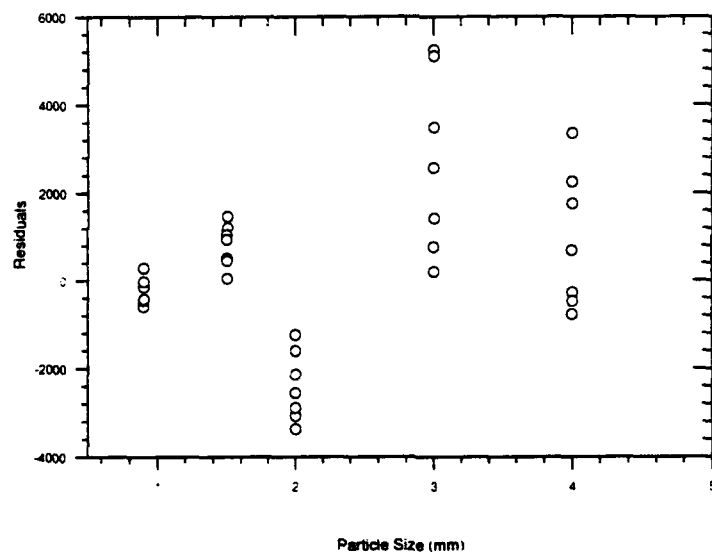
Figure 2. Residuals vs. particle diameter D_b; Jones and Krier data with 6-mm beads excluded.

Nonlinear regression algorithms normally seek to minimize the sum of the squared residuals—as in ordinary linear regression—in attempting to determine the "best" choice of parameters to model the data. These procedures have previously been cited as computationally intensive. More specifically, they are iterative and may diverge or converge to local extrema, depending upon the choice of initial conditions. Through a systematic selection of initial conditions, the authors determined that the equation

$$F_v = 61 + 2.7 \left(\frac{Re}{1 - \phi} \right)^{0.91} , \tag{4}$$

provides an improved representation of the data reported by Jones and Krier.

The root mean square error (RMSE), an estimate of the standard deviation of the residuals and a commonly used measure for adequacy of fit, is reduced by 20% compared to that corresponding to Equation 3. The measurements taken on the 6-mm beads, the chief contributor to heterogeneity of variance, have been excluded from the regression, making the comparison with Jones and Krier direct. A reduction of one-fifth in RMSE is not by itself a stunning improvement, but it does focus more sharply on the underlying physical process. The residual plot for Equation 4 still exhibits the undesirable pattern of under(over) fitting categories of bead diameter but is an improvement compared to the display in Figure 2.

The data collected by Robbins and Gough (1978, 1979), which "... correspond to several tests performed on several occasions" for beds of spheres, right circular cylinders, and multiperforated cylinders, may be transformed into units appropriate for comparison through the relationship $f_s' = F_v/[Re/(1 - \phi)]$. The authors confined the analysis to data taken on 1.27-mm-diameter lead shot and on 4.76-mm and 7.94 mm-diameter steel spheres, and determined the equation

$$F_v = -237 + 3.14 \left(\frac{Re}{1 - \phi} \right)^{0.89} , \tag{5}$$

for representation of flow through spherically packed beds. Equations 4 and 5 are shown, along with the previously established correlations (1 and 2) in Figure 3.

Transforming the variables (Re', F_v) by taking logarithms, which was suggested by the residual plot in Figure 2, effectively linearizes the data. In regression analysis, a measure of precision of the regression line which is used in addition to RMSE, is given by a statistic denoted as R^2. R^2 assumes values in the unit interval [0, 1] and quantifies the amount of variation in the response accounted for by the regression line. Values close to one are highly desirable, indicating that the regression has effectively accounted for most of the variation in the response. The regression line determined after logarithmic transformation of
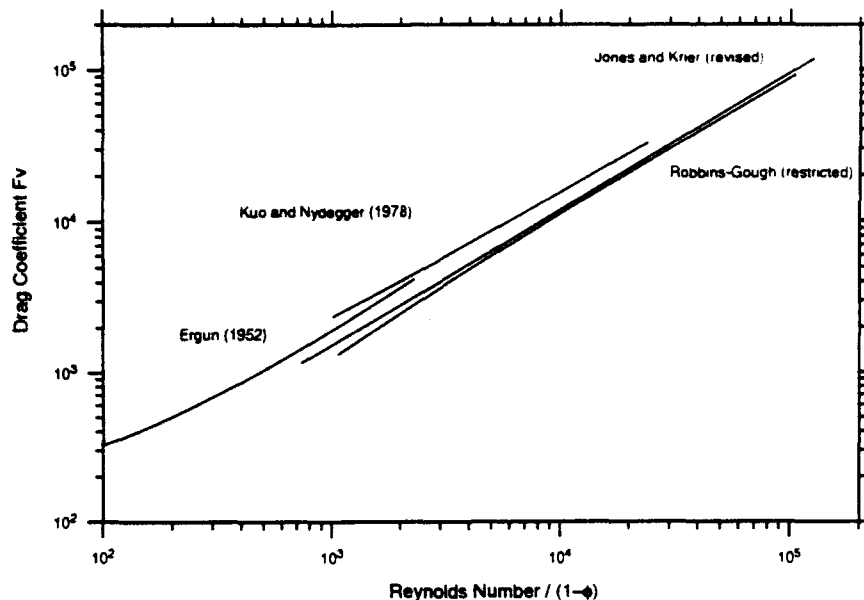
Figure 3. <u>Proposed models for relating coefficient of drag and Reynolds number.</u>

the Jones and Krier data has $R^2 = 0.98$. The transformed Robbins and Gough data have $R^2 = 0.99$. These values are so close to 1.0 that pursuit of a nonlinear model is difficult to justify mathematically.

Comparison between linear models and nonlinear models is difficult. RMSE values cannot be compared across the transformation, and a well-defined R^2 statistic for nonlinear models does not exist.

3. META-ANALYSIS OF GAS FLOW RESISTANCE MEASUREMENTS

Consider in aggregate the correlations that have been advanced for gas flow resistance measurements through spherically packed beds. For the nonlinear models, a statistical resampling plan is applied, whose goal is to extract information from a set of data through repeated inspection. The procedure is called the "bootstrap," named to convey its self-help attributes, and it tries to address an important problem in data reduction—after an estimate of some parameter is computed, what accuracy can be attached to the estimate? Accuracy here refers to the "± something" that often accompanies statistical estimates, and may

6

be conveyed through such devices as variance, RMSE, or confidence interval. For the log-linear model, the available data are directly combined.

The authors are hindered in fully exploiting a meta-analysis approach by the inability to obtain all the pertinent experimental data. It is unfortunate that experimental data are not routinely archived after collection; otherwise, additional information that it may hold is lost to extraction by subsequent investigations and by alternate statistical methods. The data of Jones and Krier and of Robbins and Gough, were accessible. With these data, this report proceeds as far as statistical prudence permits.

3.1 <u>Bootstrapping Regression Correlations</u>. Detailed descriptions of the bootstrap and accounts of its successful applications are amply documented (e.g., Efron [1979, 1982], Efron and Tibshirani [1985], LePage and Billard [1992]). The computational contrivance that the bootstrap procedure exploits is the generation of perturbed data sets from a single set of data through sampling with replacement. Specific to this study, the set of paired observations taken on coefficient of drag and Reynolds number, $\{(F_{v_1}, Re_1'), ..., (F_{v_n}, Re_n')\}$, that is the basis for a reported correlation, is sampled with replacement to generate another set $\{(F_{v_1}{}^*, Re_1'^*), ..., (F_{v_n}{}^*, Re_n'^*)\}$ whose elements are copies (with duplication) of the original measurements. This set is called a bootstrapped data set. The process of sampling with replacement to generate bootstrapped data sets is repeated many times.

If a correlation is determined for each bootstrapped data set and its equation plotted, a sense of the sensitivity of the regression line to perturbation of the original data comes into focus. In Figure 4, the results of 1,000 replications of this process are pictured. The outermost lines indicate boundaries within which the correlation (5) might be expected to lie if the original data set were simply perturbed. They were obtain: from the maxima and minima of the drag coefficient predicted for particular values of Re'.[1] The envelope constructed for correlation (5) contains correlation (4). This suggests that no significant difference between these empirical relations exists. Similar results are obtained if we begin with correlation (4); correlation (5) will lie within the corresponding confidence envelope. Consideration of perturbed data is highly appropriate here, since experimental results cannot be expected to be reproduced, even if the experiment is replicated under tightly controlled conditions. The theoretical justification for the use of bootstrapped data is given by Efron (1982).

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[1] More precisely, the values represent extreme quantiles after all the F_vs have been ranked; their values are not essentially different from maxima and minima.
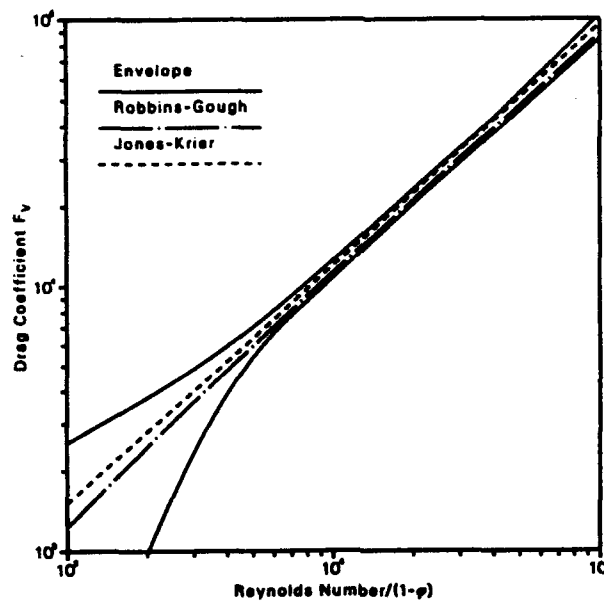
Figure 4. Bootstrapped confidence envelopes for nonlinear regression (based on Robbins-Gough data).

The relationship of Kuo and Nydegger, for which the experimental data was not accessible, was determined for a single diameter bead, $D_b = 0.83$.

3.2 Log-linear Regression. Figure 5 displays the logarithmic transformed data of Jones and Krier, and Robbins and Gough, combined. The fitted line for these data is

$$\log F_v = 0.49 + 0.90 \log Re' \; ; \tag{6}$$

included in the regression are the data taken on 6-mm beads, which were previously excluded.

Visually, the data appear linear after transformation. Statistically, the R^2-value for the regression is 0.99, making the fitted line a highly satisfactory representation of these data for ∴ practical purposes.

8
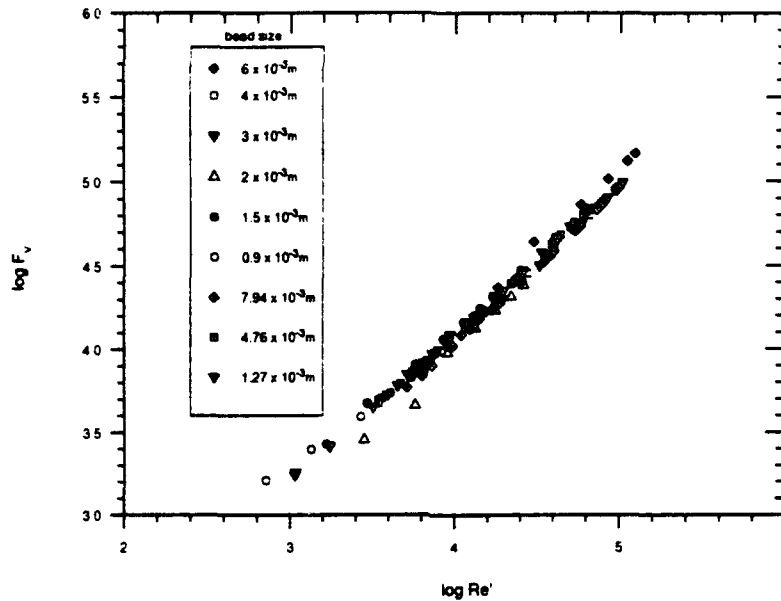
Figure 5. *Drag coefficient vs. Reynolds number/(1 − φ); Jones and Krier, Robbins and Gough data combined*

4. SUMMARY AND CONCLUSIONS

For Reynolds numbers exceeding 10^3, a more effective representation and data analysis than presently available can be obtained after logarithmic transformation of the data. This linearizes the data and removes the necessity for nonlinear regression techniques. The equation

$$logF_v = 0.49 + 0.90 \ logRe' \tag{7}$$

is an effective description of the available experimental data.

If a representation of the form

$$F_v = \beta_0 + \beta_1 \left(\frac{Re}{1 - \phi} \right)^{\beta_2} \tag{8}$$

9

is required, then Jones and Krier's results are more effectively reflected through the equation

$$F_v = 61 + 2.7 \left(\frac{Re}{1 - \phi} \right)^{0.91} , \qquad (9)$$

and Robbins and Gough's data restricted to spherically packed beds provide the relation

$$F_v = -237 + 3.14 \left(\frac{Re}{1 - \phi} \right)^{0.89} , \qquad (10)$$

but here again, approximate confidence envelopes constructed with the aid of the bootstrap suggest that these relations can be combined without loss of underlying physical insight. In total, the statistical analysis supports the combination of the various correlations, for the stated test conditions, into a single relationship.

While it is quite reasonable to suspect an interaction between the geometry of tube and packing, perhaps reflected through the ratio D_c/D_b, more extensive testing is required to establish this relation. Hopefully, this will be done in accordance with a formal statistical experimental design to minimize testing and maximize extraction of information.

G. E. P. Box, an important contemporary statistician, has remarked that "No model is correct, but some are useful." In this spirit these remarks are offered, along with the hope for an incremental move toward a more useful model.

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D_b = spherical particle (bead) diameter

D_c = test chamber diameter

f_s' = $F_v/[Re/(1 - \phi)]$, friction factor

F_v = $\dfrac{\Delta P}{L} \dfrac{D_b^2}{\mu \bar{u}} \left(\dfrac{\phi}{1 - \phi}\right)^2$, coefficient of drag

F_{v_i} = i-th observed value of the drag coefficient

F_{v_i}' = predicted drag coefficient corresponding to the i-th observed value

L = length scale

Re = $Re_p \, \phi = \rho \bar{u} D_b \phi / \mu$, Reynolds number

Re' = $Re/(1 - \phi)$

Re_p = Reynolds number based on particle size

$\bar{u}$ = average gas velocity

$\beta_i, i = 0, 1, 2$ = model coefficient

ΔP = change in pressure

ρ = density

ϕ = porosity of the packed bed

$(1 - \phi)$ = solids loading

μ = gas viscosity

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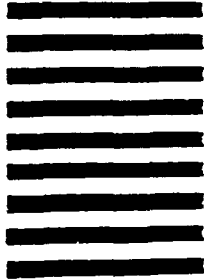
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