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Monte Carlo uncertainty estimation for an oscillating-vessel viscosity measurement

K Horne¹, H Ban¹, R Fielding² and R Kennedy²

¹ Mechanical and Aerospace Engineering, Utah State University, 4130 Old Main Hill, Logan, UT 84322, USA
² Idaho National Lab, PO Box 1625, Idaho Falls, ID 83415, USA

E-mail: kyle.horne@aggiemail.usu.edu

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Abstract

This paper discusses the initial design and evaluation of a high temperature viscosity measurement system with the focus on the uncertainty assessment. Numerical simulation of the viscometer is used to estimate viscosity uncertainties through the Monte Carlo method. The simulation computes the system response for a particular set of inputs (viscosity, moment of inertia, spring constant and hysteretic damping), and the viscosity is calculated using two methods: the Roscoe approximate solution and a numerical-fit method. For numerical fitting, a residual function of the logarithmic decay of oscillation amplitude and oscillation period is developed to replace the residual function of angular oscillation, which is mathematically stiff.

The results of this study indicate that the method using computational solution of the equations and fitting for the parameters should be used, since it almost always out-performs the Roscoe approximation in uncertainty. The hysteretic damping and spring stiffness uncertainties translate into viscosity uncertainties almost directly, whereas the moment of inertial and vessel-height uncertainties are magnified approximately two-fold. As the hysteretic damping increases, so does the magnification of its uncertainty, therefore it should be minimized in the system design. The result of this study provides a general guide for the design and application of all oscillation-vessel viscosity measurement systems.

1. Introduction

Metallic nuclear fuels have exceptional transient behaviour, high thermal conductivity and a straightforward reprocessing path. For the development and optimal design of a casting system, viscosity information of metal fuel melts is needed. Such data can be measured using an oscillating-vessel viscometer.

Oscillating-vessel viscometers measure the viscous damping in a spring–mass–damper system from a vessel which contains the fluid to be measured as depicted in figure 1. The viscometer consists of a vessel containing the fluid to be tested which is attached to an angle encoder by a rod. Both are suspended by a thread which functions as an angular spring and the entire assembly is contained within a vacuum [1]. For the uranium–zirconium alloy viscometer, the lower components descend into a furnace which heats the vessel above the melting point of uranium (∼1600 °C), thus requiring the vessel to be composed of tantalum or tungsten [2, 3]. The rod–vessel–encoder assembly is free to rotate about its axis, and an initial displacement will result in damped harmonic motion. From the system’s response, the viscosity of the test-fluid can be computed either using an approximate analytical approach developed in the 1950s by Roscoe [4, 5] or a numerical solution method of the coupled flow–vessel oscillation equations [6].

The uncertainty resulting from such a viscometer with either viscosity-computation method is not thoroughly explored in previous works and frequently consists of order of magnitude considerations. To explore the uncertainties from such a measurement, numerical simulations of the viscometer were used in this study to estimate viscosity uncertainties using the Monte Carlo method. Such an approach is needed because of the iterative nature of the viscosity computation [7, 8]. The result of the study, the uncertainty level and the extent of the contributions from different parameters, can be used for the design and optimization of oscillating-vessel viscometers.
2. Methods

The governing differential equations of flow and oscillation are simplified by the assumption that the flow is one-dimensional inside a long, oscillating cylinder. The fluid flow and vessel oscillation equations are solved numerically to simulate the behaviour of the system after release from an initial displacement, thereby generating a system response in the form of angular oscillation verses time after release. Two methods of computing viscosity from the system response are considered: Roscoe’s approximate analytical method and a numerical-fit procedure. The expected viscosity uncertainty from each computation method from a system response is quantified using Monte Carlo uncertainty analysis.

2.1. Governing equations

Equation (1) relates the sum of the moments about the free axis of the vessel–rod structure to the angular position (θ), as a function of time, of that structure. The moment of inertia (I), thread hysteretic damping constant (C) and thread spring stiffness (k) all appear in the equation in addition to an applied moment (M):

\[ I \frac{d^2 \theta}{dt^2} + C \frac{d \theta}{dt} + k \theta = M. \]  

The viscous damping effects from the fluid are predicted by the one-dimensional Navier–Stokes equation in tangential velocity (V_θ) as a function of time t and radial position r, axisymmetric coordinates as given by (2) [9], where t is time, \( \mu \) is the dynamic viscosity and \( \rho \) is the density. By assuming one-dimensional axisymmetric behaviour, only the tangential velocity component and viscosity remain in the equation:

\[ \frac{\partial V_\theta}{\partial t} = \frac{\mu}{\rho} \left( \frac{\partial^2 V_\theta}{\partial r^2} + \frac{1}{r} \frac{\partial V_\theta}{\partial r} - \frac{V_\theta}{r^2} \right). \]  

The two governing equation are coupled through the wall shear stress which serves as a boundary condition for (2) and as a forcing function for (1) as shown in (3),

\[ M = -2\pi R^2 \rho \frac{\partial V_\theta}{\partial r} \bigg|_{r=R}, \]  

where \( R \) is the radius of the vessel, and \( h \) is the height of the liquid column.

The initial conditions for (2) are shown in (4), whereas the boundary conditions are in (5) and (6). The initial conditions for (1) are found in (7).

\[ V_\theta|_{t=0} = 0, \]  
\[ V_\theta|_{r=0} = 0, \]  
\[ V_\theta|_{r=R} = R \frac{\partial \theta}{\partial t}, \]  
\[ \theta|_{t=0} = \frac{\partial \theta}{\partial t} \bigg|_{t=0} = \frac{\partial^2 \theta}{\partial t^2} \bigg|_{t=0} = 0. \]

2.2. Numerical simulation of system response

The simulation computes the system response for a particular set of material and geometric inputs (viscosity, moment of inertia, spring constant and hysteretic damping) by numerically solving the system’s governing differential equations, shown in (1) to (3), using second-order finite differences in space and a second-order Runge–Kutta method in time.

To solve the system of equations for \( \theta(t) \) and \( V_\theta(t) \) numerically, the fluid flow (2) is discretized in the radial direction and converted to a set of linear algebra equations using second-order finite difference approximations for the spatial derivatives. The wall shear stress in (3) is computed from the discretized flow-field using a three-point finite difference at the wall for the derivative term. The time derivatives from (1) and (2) are integrated using a second-order Runge–Kutta method. The time integration of these equations provides the system response in the form of the displacement angle for the spring–mass–damper described by (1) as a function of time. The system is given an initial displacement, resulting in decaying harmonic motion; the time step and grid resolution were made fine enough that further refinement did not change the system response curve. An example of the simulation output is given in figure 2.

2.3. Roscoe’s viscosity computation

In order to obtain an analytical solution to calculate the viscosity from angular displacement using the system of
Equations (1) to (3), Roscoe used an approximation to decouple equations (1) and (2). Using a single damping coefficient to model both the hysteretic damping in the thread and the viscous damping in the fluid, the forcing function $M$ can be removed from equation (1) and a solution to the ordinary differential equation (ODE) found as equation (8) in terms of the logarithmic decrement of oscillation ($\delta$) and mean oscillatory period ($\tau$), as well as a phase-shift ($\psi$) [10]:

$$\theta = \theta_0 e^{-\frac{t}{\tau}} \cos \left( \frac{2\pi}{\tau} t + \psi \right).$$

(8)

An approximate relationship between viscosity and the observed system response in the form of $\tau$ of the logarithmic decrement of oscillation ($\delta$) and mean oscillatory period ($\tau$), as well as a phase-shift ($\psi$) [10] can be analytically derived as done by Roscoe. Equations (9) to (12) summarize the results of this solution [4, 5]:

$$Z = \left( \frac{1 + \frac{1}{4} \frac{R}{\pi^2}}{(1 - \Delta)^{-1}} \left( \frac{\sqrt{1 + \Delta^2} + 1}{2} \right) \right)^{1/2}$$

$$- \left( \frac{1 + \frac{1}{4} \frac{R}{\pi^2}}{(1 + \Delta)^{-1}} \left( \frac{\sqrt{1 + \Delta^2} - 1}{2} \right) \right)^{1/2} - \frac{1}{p} \left( \frac{3}{2} + 4 \frac{R}{\pi H} \right)$$

$$\mu = \frac{1}{\pi \rho \tau} \left( \frac{I \delta}{\pi R^3 H Z \zeta} \right)^2.$$

Equation (12) is an implicit equation for the viscosity $\mu$, in terms of given parameters and a calibration factor $\zeta$ which is determined experimentally [1, 11]. Since it is implicit, iteration is required to converge on the viscosity.

The normal experimental procedure for measuring the viscosity of a fluid using Roscoe’s method is as follows:

(i) Measure the vessel’s oscillation after an initial displacement versus time, such as in figure 2.

(ii) From the collected data, compute the logarithmic decrement and oscillation period.

(iii) Using these values and the geometry of the viscometer, iterate equations (9) to (12) until convergence of the viscosity.

2.4. Numerical-fit viscosity computation

The numerical-fit method uses a viscometer’s design parameters to generate the system’s response as a function of viscosity alone. A residual function is used to quantify the difference between the computed response for a particular viscosity and a measured response. This residual is minimized with regard to the input viscosity to find the correct value. The minimization is accomplished through a golden-search method, chosen for its robustness and simplicity.

Initially a residual function $R_\mu$ defined as the root-sum of the squares of the differences between the actual system response and the function result, as shown in (13), was tried.

$$R_\mu (\mu) = \sum_i \left[ T_i - S_i (\mu) \right]^2.$$

This residual function works very well if the viscometer’s moment of inertia ($I$) is known very accurately, but frequently fails when there is even only a 1% deviation from the true value. After computational investigation, it was found that because the moment of inertia $I$ strongly determines the period of oscillation a deviation in the assumed inertia versus the actual inertia can prevent the calculated response from ever matching the actual response, no matter what value of viscosity is used. Therefore this residual function is mathematically too stiff to be used in numerical fitting involving inertia.

Instead of using a multivariate fit procedure, an alternative residual function was chosen. The period of oscillation and logarithmic decrement for the actual response and candidate responses are computed, and the residual is the root-sum of the squares of the differences between these values for each system response. This residual does not suffer from the numerical stiffness of the previous function, and is used for the numerical-fit method. When evaluating the choice of viscosity uncertainty by Monte Carlo analysis
numerical-fit method, it was observed that the new residual is just as precise as the originally tested residual, thus making the decision to use the new method an easy one.

The numerical method is a brute-force approach to the problem, and requires significantly more computing resources than the Roscoe method. The advantage of the numerical approach is that the simulation can be made as complex as needed for the desired vessel geometry, even to the point of including full three-dimensional flow as well as body forces such as magneto-hydrodynamics or the Coriolis effect. In any case, the step size of the numerical simulation must be kept small enough so as to ensure accuracy. The grid size and time step independence study showed that the grid size needed to be $1/100$ of the radius, and the time step to be $1/1600$ of an oscillation period.

2.5. Monte Carlo uncertainty analysis

To quantify the uncertainty from indirect computational methods such as the Roscoe’s and the numerical-fit viscosity computation, Monte Carlo uncertainty analysis was performed. A particular viscometer must be considered, and the results from the analysis are only valid for that exact configuration. In this procedure, an uncertainty was assumed for one or more of the viscometer’s design parameters and from these assumed uncertainties a set of viscometer designs were generated which vary from the device of interest according to the assumed uncertainties in a Gaussian fashion. This set of theoretical viscometers served as inputs to a series of simulations to compute each viscometer’s system response for a known viscosity. Using this set of system responses as inputs to a viscosity-computation algorithm (Roscoe or numerical-fit), a set of viscosities were computed. Because the uncertainties are built into the input distribution, the resulting viscosity distribution differed from the actual viscosity; it is this difference which allowed the uncertainty to be computed. A diagram of the process is shown in figure 3.

As can be seen in figure 3, an input distribution was generated for parameters in equations (1) to (3) and used as input to series of simulations. Each simulation produced the system response for a particular value from this distribution. The set of system responses which correspond to the distribution of $C$ were used as inputs to the viscosity computation. The viscosity computation was given all the data concerning the inputs except for the parameter of interest. For that parameter, only the mean of the input distribution was given to simulate the uncertainty in that parameter. Using an inaccurate value as an input to the viscosity computation results in a error in the computed viscosity. Thus, a distribution of viscosities was produced from each computation method which corresponds to the input distribution used. Comparing the viscosity distribution against the input distribution yields important information about the uncertainty due to any particular parameter [12–14]. To ensure the validity of the results, enough points were considered in the distributions so that they accurately approximate the chosen distribution.

3. Results

The Monte Carlo uncertainty program was run with both the Roscoe and numerical-fit methods to analyse the uncertainties expected from a viscometer similar to one used to measure mercury [6]. By using parameters from the mercury viscometer, the choice of values for the simulations is reasonable and relevant. Comparing the computed viscosity to the input viscosity yields the error. Many simulations are run in Monte Carlo fashion to characterize the error of each method across a range of input parameters.

3.1. Code performance

Because the numerical viscosity computation and the Monte Carlo process both require many system simulations to be executed, the total computational cost of the code is quite large. Fortuitously, the code is easily parallelized to run on a cluster computer, thereby dramatically reducing the actual real time of the computation. All computations were done on a small 12-core 64-bit AMD Athlon cluster in less than 24 h.

3.2. Predicted uncertainties

The results of the simulations are presented in figure 4 in terms of the relative uncertainty of viscosity $\mu$ as a function of one specific parameter and the uncertainty of that parameter at 1%
or 5%. Four lines are presented in each plot, two for each method of viscosity computation. The two series represent the 1% and 5% relative uncertainty of the input variable at a 95% confidence level, while the plots show the uncertainty in the computed viscosity at a given range of parameter.

A trend to consider is the increasing uncertainty of both methods with increasing hysteretic damping in the suspension thread, shown in figure 4(a). This suggests that the hysteretic damping must be either very well known or kept to a very small value to minimize the uncertainty in viscosity results. Ideally, the value of the hysteretic damping constant should be very small and accurate. The uncertainty in viscosity is shown to be almost independent of the range of values of vessel height \(h\), moment of inertia \(I\) and spring stiffness \(k\). Therefore, the design of the viscometer should only minimize the uncertainty of these parameters rather than their values.

The uncertainty due to the moment of inertia \((I)\) and the vessel height \((h)\) is approximately magnified by a factor of two as shown in figure 4, while the uncertainty from the hysteretic damping \(C\) and spring stiffness \(k\) is approximately the same as the input uncertainty. Thus, the accuracy of the first two values is critical to obtaining accurate results.

Figure 5 shows the viscosity uncertainty as the uncertainty of an input parameter changes. The increase of uncertainty in viscosity is shown to increase linearly with the parameter uncertainty. The combined overall uncertainty for the case of all inputs being equally uncertain is shown in figure 6. A major advantage of the Monte Carlo uncertainty method over the Taylor’s series method is that correlated uncertainties are included in the analysis. Additionally, even though the range of variables examined is fixed for each computation, they can be varied to explore any potential viscometer design, so long as the assumptions made in the derivation of the governing differential equations are maintained.

The results obtained from these simulations agree reasonably well with the work of Gruner and Hoyer [15]. Although the methodologies used were somewhat similar, the parameters which were varied and the combination of their effects makes it difficult to compare their results directly with those obtained in this work. If one assumes that the input uncertainties are all in the 0% to 3% range, then figure 6 suggests that their results fall in the same range as those reported here.

From these results it can be observed that the hysteretic damping in the suspension thread should be as low as possible to minimize the uncertainty increase associated therewith. Additionally, any measurement of the moment of inertia or vessel height should be very precise, since the relative uncertainty in that measurement will be effectively doubled in the computed viscosity.

Figure 4. Viscosity uncertainty computed using either Roscoe’s or the numerical method at specified parameter value and its uncertainty range of either 1% or 5%.
4. Conclusions

From the results of the uncertainty analysis, several conclusions can be drawn. First, a residual function based on oscillation period and logarithmic decay of oscillation amplitude should be used for numerical fitting. A residual function based on angular displacement is mathematically stiff. Second, the numerical-fit method generally produces better results, but the step size for actual computation of viscosity must be kept very small to ensure good results. Third, a larger value of damping generates increased uncertainty, therefore its value should be minimized as much as possible regardless of its uncertainty. The other parameters considered do not exhibit this behaviour, thus their values do not need to be minimized. The viscosity uncertainty doubles due to uncertainty in the vessel height $h$ and moment of inertia $I$, therefore these values must be known very accurately. The viscosity uncertainty varies nearly linearly with the uncertainty of either individual parameters or all the parameters. This all demonstrates that the methods used here can be used to design a viscometer that minimizes the resulting uncertainty in measured viscosities.

References

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