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Technical Note
Numerical evaluation of the Graetz series

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Nomenclature

A, B coefficients in series (11) and (13), respectively
F eigenfunction [Eq. (4)]
J Bessel function of the first kind
M confluent hypergeometric function
n^* order to switch to asymptotic approximations
Pe Peclet number
r', r dimensional, dimensionless radial coordinate, $r=r'/R_0$
R derivative $(\partial F/\partial r)_{\lambda=\lambda_n}^{r=1}$
R_0 tube radius
x', x dimensional, dimensionless axial coordinate, $x=x'/(R_0\,Pe)$.

Greek symbols
ε absolute error, defined by Eqs. (21) or (23)
η similarity variable, $\eta = 9x/2$
θ dimensionless temperature
λ eigenvalue
ξ similarity variable, $\xi = (1-r)\eta^{-1/3}$
Λ derivative $(\partial F/\partial \lambda)_{\lambda=\lambda_n}^{r=1}$.

1. Introduction

The Graetz problem describes the temperature (or concentration) field in fully-developed laminar flow in a circular tube where the wall temperature (or concentration) profile is a step-function. A great deal of analysis has been performed on this fundamental problem: a detailed survey of the relevant abundant literature may be found in [1].

The infinite series solution of the problem, referred to as the Graetz series, is

$$\theta(x,r) = -2\sum_{n=1}^{\infty}\frac{\exp(-\lambda_n^2 x)F(r,\lambda_n)}{\lambda_n\Lambda_n} \tag{1}$$

whereas the series solutions for the bulk average temperature and the local Nusselt number are

$$\theta_{\mathrm{av}}(x) = 8\sum_{n=1}^{\infty}\frac{R_n\exp(-\lambda_n^2 x)}{\lambda_n^3\Lambda_n} \tag{2}$$

and

$$Nu(x) = \frac{1}{2}\frac{\sum_{n=1}^{\infty}R_n\exp(-\lambda_n^2 x)/\lambda_n\Lambda_n}{\sum_{n=1}^{\infty}R_n\exp(-\lambda_n^2 x)/\lambda_n^3\Lambda_n}. \tag{3}$$

As first demonstrated by Lauwerier [2], the eigenfunctions $F(r, \lambda_n)$ can be expressed in terms of the confluent hypergeometric function $M(a, b, z)$ (or Kummer's function) as follows

$$F(r,\lambda_n) = \exp\left(-\frac{\lambda_n r^2}{2}\right)M\left(\frac{2-\lambda_n}{4},1,\lambda_n r^2\right). \tag{4}$$

Moreover, due to the boundary conditions, the eigenvalues λ_n are the zeros of the transcendental equation.

$$M\left(\frac{2-\lambda_n}{4},1,\lambda_n\right) = 0. \tag{5}$$

For the numerical evaluation of series (2) and (3) one disposes a vast set of computational means [1]. However, a well defined method that enables the numerical evaluation of series (1) with known accuracy does not exist. Such an evaluation is important in many applications, for example, in the interpretation of nucleation experiments in flow diffusion chambers [3, 4], where, due to the extreme sensitivity of the supersaturation ratio on temperature, a detailed knowledge of the temperature field near the entrance is required.

The obvious way to compute series (1) is first to calculate accurately a finite number of terms, say up to order n^*, and then calculate as many high-order terms as necessary for convergence with the help of known

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asymptotic approximations [5]. However, important information is missing on the following points:

—What is precisely the order n^* to switch to asymptotic approximations and, more importantly, how does its value affect the accuracy of the final result.
—In the asymptotic regime ($n > n^*$) there does not exist a 'ready to use' asymptotic formula for the eigenfunctions, uniform throughout the whole interval $0 < r < 1$.
—Even for orders $n < n^*$, the accurate numerical evaluation of the eigenfunctions is not always evident.

Our objective is to provide explicit responses to the above issues, and thus establish a useful method for the evaluation of the local solution. As an aside, the domain in which the Lévêque solution should be used is precisely specified.

Note that today with the help of sophisticated software systems such as *Mathematica* [6] it is possible to evaluate all the required high-order parameters and functions via their exact mathematical expression, without resorting to asymptotic methods. In fact, we have used *Mathematica* to quantify the accuracy of our results. However, this procedure requires computing time that is excessive, if not prohibitive, for practical applications. Therefore, notwithstanding the availability of such powerful tools, the present method is of value due to its computational economy: it requires little programming effort, and the resulting algorithm can be executed quickly with modest computing power.

2. Evaluation of the eigenvalues and constants

The first 11 eigenvalues λ_n and derivatives R_n and Λ_n have been calculated and tabulated with 10 decimal point accuracy by Brown [7]. Sellars et al. [5] provided asymptotic formulae for all parameters λ_n, R_n and Λ_n, whereas Newman [8] obtained the following improved asymptotic formula for λ_n

$$\lambda_n = \omega_n + S_1\omega_n^{-4/3} + S_2\omega_n^{-8/3} + S_3\omega_n^{-10/3} + S_4\omega_n^{-11/3} + O[\omega_n^{-14/3}], \quad n = 1, 2, \ldots \tag{6}$$

where

$$\omega_n = 4n - 4/3, \quad n = 1, 2, \ldots$$
$$S_1 = 0.159152288, \quad S_2 = 0.0114856354,$$
$$S_3 = -0.224731440, \quad S_4 = -0.033772601. \tag{7}$$

We have extended Newman's method to obtain improved asymptotic expressions for the derivatives R_n and Λ_n. The approach consists of substituting Eq. (6) for λ_n into Lauwerier's [2] asymptotic expressions for $\partial F/\partial r$ and $\partial F/\partial\lambda$; then, a MacLaurin expansion with respect to $z = \omega_n^{-1/3}$ about the point $z = 0$ is performed (hence, in the limit $\omega_n \to \infty$) to obtain the following asymptotic expressions

$$R_n = (-1)^n P\lambda_n^{1/3}(1 + P_1\omega_n^{-4/3} + P_2\omega_n^{-2} + P_3\omega_n^{-8/3} + P_4\omega_n^{-10/3} + P_5\omega_n^{-11/3} + O[\omega_n^{-4}]), \quad n = 1, 2, \ldots \tag{8}$$

$$\Lambda_n = (-1)^n Q\lambda_n^{-1/3}(1 + Q_1\omega_n^{-4/3} + Q_2\omega_n^{-2} + Q_3\omega_n^{-7/3} + Q_4\omega_n^{-8/3} + Q_5\omega_n^{-10/3} + Q_6\omega_n^{-11/3} + O[\omega_n^{-4}]), \quad n = 1, 2, \ldots \tag{9}$$

The constants that appear in Eqs. (8) and (9) are:

$$P = 0.7116134100, \quad P_1 = 0.0721675797,$$
$$P_2 = 0.0577777781 \quad P_3 = -0.0026040798,$$
$$P_4 = -0.0977347533, \quad P_5 = -0.0153141806$$
$$Q = 0.7026286927, \quad Q_1 = -0.0721675799,$$
$$Q_2 = -0.0577777778 \quad Q_3 = 0.2122030514,$$
$$Q_4 = 0.0078122394, \quad Q_5 = 0.1060741183$$
$$Q_6 = 0.0306283612. \tag{10}$$

Note that the leading-order terms of expansions (8) and (9)— as well as the leading term of Newman's expansion (6)—are just the asymptotic expressions given in [5], namely $\lambda_n = 4n - 4/3$, $R_n = (-1)^n 2^{2/3}\lambda_n^{1/3} 3^{-5/6}/\Gamma(4/3)$ and $\Lambda_n = (-1)^n \pi\lambda_n^{-1/3} 6^{-2/3}/\Gamma(2/3)$. However, the additional terms in (6), (8) and (9) improve accuracy substantially: at $n = 11$ their agreement with the exact results of Brown is to 8 decimal places, whereas the formulae of [5] are accurate only to two decimal places.

In conclusion, by using the values of Brown [7] for $n \leqslant 11$ and the expressions (6), (8) and (9) for $n > 11$, an accuracy by more than eight decimal places is always achieved for the eigenvalues λ_n and the constants R_n and Λ_n.

3. Evaluation of the eigenfunction

As can be seen from Eq. (4), the evaluation of the eigenfunctions $F(r, \lambda_n)$ involves the computation of the confluent hypergeometric function. A fast algorithm for the computation of $M(a, b, z)$ over a wide range of parameters a, b and argument z, does not seem to exist. Computational difficulties arise as soon as z becomes large and $|a| \gg |b|$, as is precisely the case at high orders n.

For small or moderate values of z, the function $M(a, b, z)$ can be evaluated from its series expansion. We have considered two different series expansions: one in terms of Bessel functions (as originally considered in [9]), and one in terms of powers of r. Employing the expansions available in Abramowitz and Stegun [10], and on account of Eq. (4), the following computational expressions are derived:

—In terms of power series:

$$F(r,\lambda_n)=\exp\left(-\frac{\lambda_n r^2}{2}\right)\sum_{m=0}^{\infty}A_m(\lambda_n r^2)^m \tag{11}$$

with the coefficients A_m determined from the following recurrence relation

$$A_0=1,\quad A_m=\frac{4m-2-\lambda_n}{(2m)^2}A_{m-1},\quad m=1,2,\ldots \tag{12}$$

—In terms of Bessel function series:

$$F(r,\lambda_n)=\sum_{m=0}^{\infty}B_m r^m J_m(\lambda_n r) \tag{13}$$

with the coefficients B_m determined from the following recurrence relation

$$B_0=1,\quad B_1=0,\quad B_2=1/2$$

$$B_m=\frac{m-1}{m}B_{m-2}-\frac{\lambda_n}{2m}B_{m-3},\quad m=3,4,\ldots \tag{14}$$

At small orders n, and with double precision floating point arithmetics, the numerical errors in the summation of series (11) or (13) remain tolerable. With increasing n the errors increase, and ultimately become catastrophic. Hence, asymptotic approximations become unavoidable beyond some order n^*. Given that when n increases the numerical error increases, whereas the error of an asymptotic approximation decreases, there exists a point where the two errors become comparable. This must be precisely the optimum order to invoke asymptotic methods.

Before identifying the order n^*, a uniform asymptotic expression for $F(r, \lambda_n)$ has to be established. This can be done with the help of the analytical results of Sellars et al. [5]. They provided a WKB asymptotic expansion valid for intermediate r (F_3), and two approximations to the exact solution valid for r near the centreline (F_1) and for r near the wall (F_2), as follows

$$F_1=J_0(\lambda_n r) \tag{15}$$

$$F_2=(-1)^{n-1}\sqrt{\frac{2(1-r)}{3}}J_{1/3}\left(\frac{\lambda_n\sqrt{8}}{3}(1-r)^{3/2}\right) \tag{16}$$

$$F_3=\sqrt{\frac{2}{\pi\lambda_n r}}\frac{\cos\left[(\lambda_n/2)r\sqrt{1-r^2}+(\lambda_n/2)\arcsin r-\pi/4\right]}{(1-r^2)^{1/4}}. \tag{17}$$

The original analysis of [5] does not specify the functions that connect these three expressions. By invoking the method of asymptotic matching of piecewise WKB approximations and using some intermediate results of the original analysis in [5], we established the following matching functions

$$F_{12}=\sqrt{\frac{2}{\pi\lambda_n r}}\cos(\lambda_n r-\pi/4) \tag{18}$$

$$F_{23}=\sqrt{\frac{2}{\pi\lambda_n}}\frac{\cos\left[\sqrt{8/9}\lambda_n(1-r)^{3/2}-(\lambda_n-1)\pi/4\right]}{2^{1/4}(1-r)^{1/4}}. \tag{19}$$

These matching functions enable the uniform asymptotic approximation over the whole interval $0<r<1$ to be expressed as

$$F(r,\lambda_n)=F_1+F_2+F_3-F_{12}-F_{23}. \tag{20}$$

The absolute error in the computation of $F(r, \lambda_n)$ over the whole interval is quantified in terms of the L_2-distance between the exact and an approximate form of the function. Accordingly, for every order n the absolute error over the interval $0<r<1$ is defined by

$$\varepsilon=\left[\int_0^1|F(r,\lambda_n)-F_{\text{exact}}(r,\lambda_n)|^2\,\mathrm{d}r\right]^{1/2} \tag{21}$$

where the approximate eigenfunctions $F(r, \lambda_n)$ are obtained either from the series (11) or (13), or from the uniform asymptotic expansion (20), and the exact $F_{\text{exact}}(r, \lambda_n)$ are evaluated with *Mathematica* [6], via computing the confluent hypergeometric function with 12 decimal point accuracy, and subsequent substitution of the result in Eq. (4).

The results of the error analysis are shown in Fig. 1. Note that even for the very first orders $n=1$, 2, 3 the asymptotic evaluation of the eigenfunctions is quite successful. This remark is an extension of a similar result reported in [5] with respect to the eigenvalues. Notwithstanding that, up to moderately high n the accuracy obtained from the series calculation is clearly much better. The Bessel series expansion (13) gives more accurate results than the asymptotic expansion up to $n=24$, while the power series expansion (11) is more accurate up to $n=31$. The Bessel series expansion was found to perform better than the power series near the centre of the tube and for intermediate r, whereas close to the

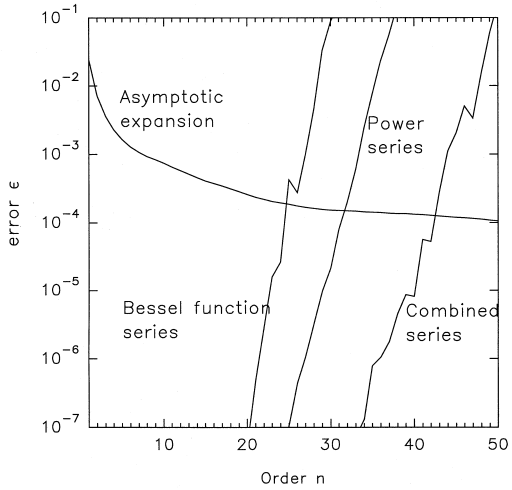

Fig. 1. Absolute error in the computation of the eigenfunctions.

wall the trend is opposite. Hence, the calculation can be optimized by suitably combining the two series. This was confirmed by a numerical experiment, from which we also determined that the optimum range to employ series (13) is the interval $0<r\leqslant 0.863$, while for $0.863<r<1$ use of series (11) should be made. As shown in Fig. 1, with such a combination of series expansions, all the eigenfunctions up to $n=42$ can be evaluated with more accuracy than that obtained with the asymptotic expressions.

4. Numerical results

The temperature field in the entrance region was calculated by keeping 150 terms in the series. Satisfactory convergence was achieved for all points (x, r) in the domain $x\geqslant 3\cdot 10^{-5}$, $0<r<1$. Eight separate calculations were performed, switching respectively to the asymptotic regime at $n^*=5, 10, 15, 20, 25, 30, 35$ and 40. The Lévêque solution was also calculated via the following extended formula

$$\theta(x,r)=\Theta_0(\xi)+\eta^{1/3}\Theta_1(\xi)+\eta^{2/3}\Theta_2(\xi) \tag{22}$$

where η and ξ are the usual Lévêque similarity variables (defined in the Nomenclature), the leading term $\Theta_0(\xi)$ is Lévêque's original solution, and the next two terms $\Theta_1(\xi)$, $\Theta_2(\xi)$ are those provided by Newman [11].

As before, the absolute error of the calculated radial temperature profile at x is obtained from the following L_2 norm

$$\varepsilon=\left[\int_0^1 |\theta(x,r)-\theta_{\text{exact}}(x,r)|^2\,\mathrm{d}r\right]^{1/2}. \tag{23}$$

Here again, $\theta_{\text{exact}}(x, r)$ is calculated with *Mathematica* [6], which was used to generate all 150 eigenfunctions, via the computation of the confluent hypergeometric function with 12 decimal point accuracy. Note that this reference calculation (each eigenfunction was evaluated at 100 radial points) took approximately 85 h of CPU time on a DEC-alpha workstation. The results are given in Fig. 2. It is clear that with increasing n^* the accuracy of the calculation increases considerably. At constant n^* the error, as expected, increases with decreasing x. By increasing n^*, the improvement is large for large x, while at smaller x the improvement is significantly smaller. Regarding the Lévêque solution, it can be seen that the inclusion of the extra two terms yields much higher accuracy.

Figure 2 delineates meaningfully the boundaries between Graetz series and Lévêque solution. This approach is similar to that employed by Luikov [12] in the study of conjugated heat transfer problems. Also, Fig. 2 provides useful computational guidance because it dictates how many eigenfunctions need to be calculated non-asymptotically to obtain a given accuracy. For

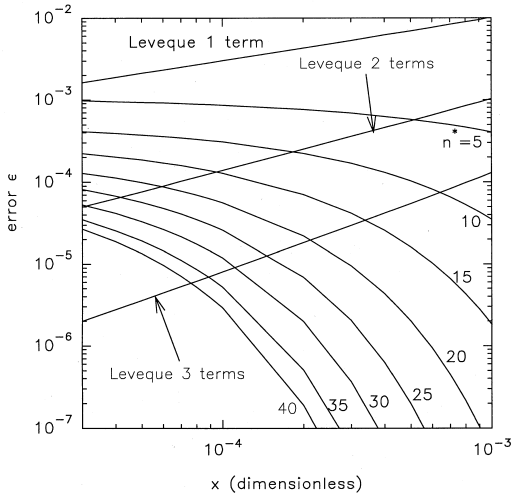

Fig. 2. Absolute error in the computation of the radial temperature profiles in the thermal entrance region.

$x\geqslant 3\cdot 10^{-5}$ the present method performs better than either the common Lévêque solution or its two-term extended form. If the comparison is made against the three-term Lévêque solution, the application limit shifts to $x=8\cdot 10^{-5}$. For smaller x the three-term Lévêque formula yields always higher accuracy, unless more than 40 eigenfunctions are computed with more accuracy than that obtained with asymptotic methods. However, $n=40$ is about the maximum order that can be evaluated non-asymptotically. It follows that the recommended application range of the present method is: $x\geqslant 8\cdot 10^{-5}$, $0<r<1$. For $x<8\cdot 10^{-5}$, use of the three-term Lévêque formula is suggested.

5. Conclusions

A method is presented that enables the thermal entrance region to be calculated easily and with known accuracy: the results are summarized in Fig. 2. New, more accurate asymptotic expressions for the derivatives R_n and Λ_n have been provided, cf. Eqs. (8) and (9). Also, we have described an approach that allows the evaluation of up to the 42nd eigenfunction with better accuracy than that obtained by asymptotic methods. This is achieved by employing Bessel series (13) and power series (11), over the intervals $0<r\leqslant 0.863$ and $0.863<r<1$, respectively. The method can be implemented with little programming effort.

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