A generalized Jaeger $\mathscr{I}(01 ; t)$ integral, resulting from mathematical modelling in electroanalytical chemistry

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#### Abstract

Eighty years ago J. C. Jaeger et al. introduced a class of improper integrals, currently called "Jaeger integrals" that occur in theoretical models of diverse physical phenomena characterized by cylindrical geometry. One application area is electroanalytical chemistry, where, in particular, the limiting Faradaic current in a potential step chronoamperometric experiment at a cylindrical electrode is described by the Jaeger $\mathscr{I}(0,1 ; t)$ integral. In a recently published paper the first author determined the Laplace transform of the nonlimiting Faradaic current for a reversible charge transfer between members of a redox couple characterized by different diffusion coefficients. In this study we invert the novel Laplace transform and observe that, while it cannot be expressed by any of the Jaeger integrals, it can be perceived as a generalization of the $\mathscr{I}(0,1 ; t)$ integral. We also describe how to compute this integral with the modulus of the relative error close to $10^{-16}$ or smaller, using a $\mathrm{C}++$ code employing exclusively standard floating point variables, without resorting to quad precision or other external high precision libraries. keywords: Jaeger integrals; Bessel functions; contour integration; Laplace transform; potential step chronoamperometry; cylindrical microelectrodes; computational electrochemistry


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## 1 Introduction

In 1942, Jaeger and Jaeger and Clarke [1, 2] introduced a class of improper integrals de ned by

$$
\begin{equation*}
\mathscr{I}(p \quad q ; t)=\int_{0} \frac{1}{\left[p u J_{1}(u)+q J_{0}(u)\right]^{2}+\left[p u Y_{1}(u)+q Y_{0}(u)\right]^{2}} \frac{e^{u^{2} t}}{u} \mathrm{~d} u \tag{1}
\end{equation*}
$$

where $t>0$, and $J_{\nu}(u)$ and $Y_{\nu}(u)$ with $=01$, are Bessel functions of the rst and second kind, respectively, of order . The integrals resulted from theoretical solutions of the heat conduction or di usion partial di erential equations (PDEs), in spatial domains possessing a cylindrical geometry. Later, they were identi ed in mathematical models of diverse physical phenomena, including, for example, heat transport in solids [3], thermal engineering [4], marine hydrogeology [5], land-atmosphere interactions [6], wellbore hydraulics [7], biomedical modelling [8], animal abundance evaluations [9], polymer physicochemistry [10], and electroanalytical chemistry [11]. A number of authors also investigated various mathematical properties of these integrals [11, 12, 13].

In electroanalytical chemistry, the Jaeger integrals can be used to describe some aspects of the di usional transport of reactants at cylindrical wire electrodes. An example which motivated the present communication, is the dependence of the Faradaic current on time, observed in the so-called potential step chronoamperometric experiments. It has been known for some time (see, in particular Refs. [14, 15, 16, 17, 11, 18]) that, under limiting current conditions, this dependence can be expressed using the $\mathscr{I}(01 ; t)$ integral:

$$
\begin{equation*}
I(t)=\frac{4}{2} \mathscr{I}(0 \quad 1 ; t) \tag{2}
\end{equation*}
$$

In (2) it is assumed that $t$ is a dimensionless time de ned as a product of the dimensional time and the parameter $=\bar{D} r_{0}$, where $D$ is the di usion coe cient of the electroactive species, and $r_{0}$ is the electrode radius. The quantity $I(t)$ is a dimensional current normalised by $\mathrm{n} F A c^{\star} \bar{D}$, where n is the number of electrons transferred in an electrochemical reaction, $F$ is the Faraday constant, $A$ is the electrode area, and $c^{\star}$ is the initial concentration of the electroactive species (see [18] for details). Equation (2) refers to a single chemical species (satisfying a single di usion PDE) consumed in a single electrochemical reaction. The limiting current conditions mean that the concentration of the species is forced to be zero at the electrode, so that the Faradaic current is the largest possible (in absolute value).
Electrochemists often use the Laplace transform method to obtain solutions of the evolutionary di usion PDEs describing electroanalytical experiments. By applying this ap-
proach, an alternative formula for the limiting current was obtained $[14,15]$ :

$$
\begin{align*}
I(t) & =\mathscr{L}^{1}\{f(s)\} \\
& =\mathscr{L}^{1}\left\{\frac{K_{1}(\bar{s})}{\bar{s} K_{0}(\bar{s})}\right\} \tag{3}
\end{align*}
$$

where $K_{\nu}(\bar{s})$ with $=01$, are the modi ed Bessel functions of the second kind, and the Laplace transform is between the domains of $t$ and $s$. Note we shall employ $f(s)$ to express a generic Laplace transform, either in the form of (3) or (6) below. The proof of the equivalence:

$$
\begin{equation*}
\frac{4}{2} \mathscr{I}(0 \quad 1 ; t)=\mathscr{L}^{1}\left\{\frac{K_{1}(\bar{s})}{\bar{s} K_{0}(\bar{s})}\right\} \tag{4}
\end{equation*}
$$

can be deduced from Carslaw and Jaeger ([3], Ch. 13). A numerical C++ procedure, combining various series expansions and tted polynomials, initially described in [17], and improved in [18], can be used to calculate $\mathscr{I}(01 ; t)$ values with relative error moduli close to $10{ }^{19}$.

The $\mathscr{I}(0 \quad 1 ; t)$ integral also describes the chronoamperometric current under non-limiting current conditions, if the electrochemical reaction is reversible (which in the electrochemical terminology means that the reaction is in a permanent virtual equilibrium), provided that the di usion coe cients $D_{\mathrm{O}}$ and $D_{\mathrm{R}}$ of the chemical species O and R (that represent a redox couple) are identical [18]. In such a case the normalised Faradaic current is [18]

$$
\begin{equation*}
I(t)=(1+\quad)^{1} \frac{4}{2} \mathscr{I}(0 \quad 1 ; t) \tag{5}
\end{equation*}
$$

where $\quad=\exp (U)$, with $\quad<U<$, is a nonnegative parameter. Parameter $U$ is de ned as $U=\frac{\mathrm{n} F}{R T}\left(E_{\text {step }} \quad E^{0}\right)$, where $R$ is the gas constant, $T$ is the absolute temperature, $E_{\text {step }}$ is the imposed electrode potential step, and $E^{0}$ is the conditional potential of the electrochemical reaction. From the mathematical point of view, is the ratio of the concentrations of O and R at the electrode surface, so that it represents a coupling of two di usion PDEs by a linear Dirichlet boundary condition. The coupling vanishes under limiting current conditions, when $0(U)$

A di erent situation occurs when the electrochemical reaction is reversible, but $D_{\mathrm{O}}$ is not equal $D_{\mathrm{R}}$. As was shown in [18], in this case the current is given by the inverse Laplace transform:

$$
\begin{align*}
I(t) & =\mathscr{L}^{1}\{f(s)\} \\
& =\mathscr{L}^{1}\left\{\frac{K_{1}(\bar{s})}{\bar{s} K_{0}(\bar{s})}\left[1+-\frac{K_{1}(\bar{s}) K_{0}(\bar{s})}{K_{1}(\bar{s}) K_{0}(\bar{s})}\right]^{1}\right\} \tag{6}
\end{align*}
$$

where $=D_{\mathrm{O}} D_{\mathrm{R}}$. Formula (6) cannot be expressed by any of the Jaeger $\mathscr{I}(p q ; t)$ integrals, which will become evident later. Attempts to design a practical $\mathrm{C}++$ procedure for calculating $I(t)$ from (6) with relative error moduli close to $10{ }^{16}$ or smaller, were only partially successful in Ref. [18]. A numerical Laplace transform inversion had to be used in a large domain of $t$, and , and despite the employment of quad precision variables, the accuracy of the inversion was not entirely satisfactory.

In the present communication we show that although (6) is not expressible in terms of $\mathscr{I}(p q ; t)$, it can be rewritten in the form of (1), but with a more complicated expression multiplying $e^{u^{2} t} u$ in the integrand. Thus, the resulting integral can be viewed as a speci c generalization of the $\mathscr{I}(01 ; t)$ integral, which reduces to $\mathscr{I}(01 ; t)$ when $\quad 0$ and 1. Having a representation of the formula (6) in terms of an integral of a realvalued integrand is potentially very useful. As we shall demonstrate, numerical evaluation of such an integral can be performed very accurately using exclusively standard oating point variables, so that it is more advantageous for computing $I(t)$ than the numerical Laplace transform inversion. The latter is often ill-posed (see, for example, [19]). It may require multiple precision that is rarely available as a standard in programming languages (in particular, the standard C++ essentially relies on the IEEE-754-compliant oating point variables [20] and does not involve multiple precision). Or, it may require the use of complex variables and functions.

## 2 The generalized $\mathscr{I}(01 ; t)$ integral

In order to derive the integral representing the inverse Laplace transform (6), it is instructive to rst reconsider the simpler inverse transform (3).

The Bessel functions $K_{0}(\bar{z})$ and $K_{1}(\bar{z})$ both tend to as $z$ tends to zero, and both tend to zero as $z$ tends to . In particular, we have

$$
\begin{array}{ll}
K_{0}(\bar{z}) & \ln \bar{z} \\
K_{1}(\bar{z}) & \frac{1}{\bar{z}} \tag{8}
\end{array}
$$

as $z \quad 0$, while

$$
\begin{equation*}
K_{\nu}(\bar{z}) \sqrt{\overline{2} \bar{z}} \exp (\quad \bar{z})\left[1+\frac{4^{2} 1^{1}}{8 \bar{z}^{2}}+\right]=01 \tag{9}
\end{equation*}
$$

as $z \quad[21,22]$.
We rst notice that a branch point (of type $\ln \bar{z}$ ) occurs at $z=0$. Furthermore, it is noted that $K_{0}(\bar{z})$ has no zeros in the left-hand plane [23, 24]. Thus the appropriate


Figure 1: Bromwich contour

Bromwich contour is given by the Figure 1, where $R$ is the radius of the large circle and is the radius of the small circle.

Cauchy's theorem implies that

$$
\begin{align*}
f(t) & =\mathscr{L}^{1}\{f(s)\} \\
& =\lim _{\epsilon} 00 \frac{1}{2} \int_{A B} e^{s t} f(s) \mathrm{d} s \\
& =\lim _{R} \frac{1}{2}\left\{\int_{B C}+\int_{C D}+\int_{D E F}+\int_{F G}+\int_{G A}\right\} e^{s t} f(s) \mathrm{d} s \tag{10}
\end{align*}
$$

We next observe that when $s=R e^{\imath \theta}, f(s) \quad O\left(\frac{1}{R^{1 / 2}}\right)$ as $R \quad$ so that clearly $\quad M k>0$, independent of $R$, such that

$$
f(s)<M R^{k}
$$

for large $R$, implying that the integrals around BC and GA converge to zero as $R$ [25].

Let us now consider the three remaining integrals. For integral around DEF let $s=e^{\imath \theta}$
so that

$$
\left.\begin{align*}
&\left|\int_{D E F} e^{s t} f(s) \mathrm{d} s\right|=\left|\lim _{\epsilon} \int_{\pi \epsilon}^{\pi+\epsilon} f\left(e^{\imath \theta}\right) e^{\imath \theta} e^{\epsilon e^{\imath \theta} t} \mathrm{~d}\right| \\
&= \left\lvert\, \lim _{\epsilon} \int_{\pi \epsilon}^{\pi+\epsilon} \frac{K_{1}\left({ }^{1 / 2} e^{\imath \theta / 2}\right) e^{\imath \theta} e^{\epsilon e^{\imath \theta} t}}{1 / 2} e^{\imath \theta / 2} K_{0}\left(1 / 2 e^{\imath \theta / 2}\right)\right. \\
& \mathrm{d}
\end{align*} \right\rvert\,
$$

Consider the integral along CD , and let $s=x e^{\imath \pi}=x$, so that $\bar{s}=\bar{x} e^{\imath \pi / 2}=\bar{x}$. Then

$$
\begin{align*}
\frac{1}{2} \int_{C D} e^{s t} f(s) \mathrm{d} s & =\lim _{\epsilon} \frac{1}{2} \int_{R}^{\epsilon} \frac{K_{1}\left(s^{1 / 2}\right) e^{s t}}{s^{1 / 2} K_{0}\left(s^{1 / 2}\right)} \mathrm{d} s \\
& =\lim _{\epsilon} \frac{1}{2} \int_{R}^{\epsilon} \frac{K_{1}(\bar{x}) e^{x t}(\mathrm{~d} x)}{\bar{x} K_{0}(\bar{x})} \\
& =\frac{1}{2} \int_{0} \frac{K_{1}(\bar{x}) e^{x t}}{\bar{x} K_{0}(\bar{x})} \mathrm{d} x \tag{12}
\end{align*}
$$

Consider the integral along FG, and let $s=x e^{\imath \pi}=x$, so that $\bar{s}=\bar{x} e^{\imath \pi / 2}=\bar{x}$. Then a similar argument shows that

$$
\begin{equation*}
\left.\frac{1}{2} \int_{F G} e^{s t} f(s) \mathrm{d} s=\frac{1}{2} \int_{0} \frac{K_{1}(\quad \bar{x})}{K_{0}( } \quad \bar{x}\right) \frac{e^{x t}}{\bar{x}} \mathrm{~d} x \tag{13}
\end{equation*}
$$

Thus we obtain the inverse Laplace transform:

$$
\begin{equation*}
\mathscr{L}^{1}\left\{\frac{K_{1}(\bar{s})}{\bar{s} K_{0}(\bar{s})}\right\}=\frac{1}{2} \int_{0}\left[\frac{K_{1}(\quad \bar{x})}{K_{0}(\bar{x})}+\frac{K_{1}(\quad \bar{x})}{K_{0}(\quad \bar{x})}\right] \frac{e^{x t}}{\bar{x}} \mathrm{~d} x \tag{14}
\end{equation*}
$$

The integral in (14) admits simpli cation. From Appendix III of Carslaw and Jaeger [3] we have:

$$
\begin{align*}
K_{\nu}(z) & =\frac{1}{2} e^{\frac{1}{2} \nu \pi v}\left[J_{\nu}(z)+Y_{\nu}(z)\right]  \tag{15}\\
K_{\nu}(z) & =\frac{1}{2} e^{\frac{1}{2} \nu \pi v}\left[J_{\nu}(z) \quad Y_{\nu}(z)\right] \tag{16}
\end{align*}
$$

Now

$$
\begin{align*}
\frac{K_{1}(\quad \bar{x})}{K_{0}(\quad \bar{x})}+\frac{K_{1}(\quad \bar{x})}{K_{0}(\quad \bar{x})} & =\frac{K_{1}(\bar{x}) K_{0}(\bar{x})+K_{1}(\quad \bar{x}) K_{0}(\bar{x})}{K_{0}(\bar{x}) K_{0}(\bar{x})}  \tag{17}\\
& =\frac{\frac{\pi^{2}}{4} 2\left[J_{0}(\bar{x}) Y_{1}(\bar{x}) \quad J_{1}(\bar{x}) Y_{0}(\bar{x})\right]}{\frac{\pi^{2}}{4}\left[J_{0}(\bar{x})^{2}+Y_{0}(\bar{x})^{2}\right]} \tag{18}
\end{align*}
$$

using the above identities (15) and (16) for $K_{\nu}(z)$ and $K_{\nu}(z)$ with $z=\bar{x}$.
Furthermore, $J_{1}(\bar{x})=J_{0}(\bar{x})$ and $Y_{1}(\bar{x})=Y_{0}(\bar{x})$ and the Wronskian (see, e.g. [3]) provides

$$
\begin{equation*}
J_{0}(\quad \bar{x}) Y_{0}(\quad \bar{x}) \quad Y_{0}(\bar{x}) J_{0}(\quad \bar{x})=\frac{2}{\bar{x}} \tag{19}
\end{equation*}
$$

Thus the expression (17) becomes

$$
{ }^{4} \frac{1}{\bar{x}} \frac{1}{\left[J_{0}(\bar{x})^{2}+Y_{0}(\bar{x})^{2}\right]}
$$

and so (14) can be written as

$$
\begin{align*}
\mathscr{L}^{1}\left\{\frac{K_{1}(\bar{s})}{\bar{s} K_{0}(\bar{s})}\right\} & =\frac{2}{2} \int_{0} \frac{1}{\left[J_{0}(\bar{x})^{2}+Y_{0}(\bar{x})^{2}\right]} \frac{e^{x t}}{x} \mathrm{~d} x \\
& =\frac{4}{2} \int_{0} \frac{1}{\left[J_{0}(u)^{2}+Y_{0}(u)^{2}\right]} \frac{e^{u^{2} t}}{u} \mathrm{~d} u \tag{20}
\end{align*}
$$

after the transformation $\bar{x}=u$. This proves the equivalence (4).
For practical applications of the electrochemical theory it is useful [17] to decompose $f(s)$, as de ned by (3), into two terms, the rst of which is characteristic of planar geometry, and the second represents the e ect of electrode cylindricity:

$$
\begin{equation*}
f(s)=\frac{1}{\bar{s}}+g(s) \tag{21}
\end{equation*}
$$

where

$$
\begin{equation*}
g(s)=\frac{K_{1}(\bar{s}) \quad K_{0}(\bar{s})}{\bar{s} K_{0}(\bar{s})} \tag{22}
\end{equation*}
$$

and the inverse transform $\mathscr{L}^{1} g(s)$ is identical with the function icylw $(\bar{t})$ introduced in [17], where icylw is a shortcut for $\underline{\underline{i}}$ (or current) for cylindrical wire. In this paper we employ a more compact notation and rename the function $(0 \quad \overline{;})$, as a special case of the function ( $\quad ; t)$ to be considered later.

We note that

$$
\begin{equation*}
\mathscr{L}^{1}\{f(s)\}=\frac{1}{=}+\frac{4}{2} \int_{0} \frac{1 \quad \frac{\pi}{2} u\left[J_{0}(u)^{2}+Y_{0}(u)^{2}\right]}{\left[J_{0}(u)^{2}+Y_{0}(u)^{2}\right]} \frac{e^{u^{2} t}}{u} d u \tag{23}
\end{equation*}
$$

since

$$
\underline{2} \int_{0} e^{u^{2} t} d u=\frac{1}{\bar{t}}
$$

Therefore

$$
\begin{equation*}
f(s)=\frac{1}{\bar{s}}+\mathscr{L}\left\{\frac{4}{2} \int_{0} \frac{1 \quad \frac{\pi}{2} u\left[J_{0}(u)^{2}+Y_{0}(u)^{2}\right]}{\left[J_{0}(u)^{2}+Y_{0}(u)^{2}\right]} \frac{e^{u^{2} t}}{u} d u\right\} \tag{24}
\end{equation*}
$$

that is,

$$
\begin{equation*}
(0 \quad ; t)=\mathscr{L}^{1} g(s)=\frac{4}{2} \int_{0} \frac{1 \frac{\pi}{2} u\left[J_{0}(u)^{2}+Y_{0}(u)^{2}\right]}{\left[J_{0}(u)^{2}+Y_{0}(u)^{2}\right]} \frac{e^{u^{2} t}}{u} d u \tag{25}
\end{equation*}
$$

We are now in a position to consider the inversion of the more general expression (6). We need essentially to invert the following Laplace transform:

$$
\begin{equation*}
f(s)=\frac{K_{1}(\bar{s}) K_{1}(\bar{s})}{\left.\bar{s}\left[K_{1}(\bar{s}) K_{0}(\bar{s})+-\overline{K_{1}( } \bar{s}\right) K_{0}(\bar{s})\right]} \tag{26}
\end{equation*}
$$

For $s$ real the function $f(s)$ is always positive and behaves as $O\left(\frac{1}{(1+\bar{\delta}) \bar{s}}\right)$ as $s$
. Furthermore, the expression $K_{1}(\bar{s}) K_{0}(\bar{s})+{ }^{-} K_{1}(\bar{s}) K_{0}(\bar{s})$ is also always positive for positive $s$, and consequently does not cross the $x$-axis; it also tends to zero at in nity. There is a branch point $\left(\begin{array}{ll}1 & \bar{s}\end{array}\right)$ at zero. In theory, of course, zeros could exist in the complex plane $s \quad \mathbb{C}, \quad s<0, \quad s=0$. We make the assumption that no zeros exist in this part of the complex plane and this is borne out by the computation of Section 3 and the earlier paper [18]. We can therefore employ the same Bromwich contour given by Fig. 1 .

As in the previous case we observe that when $s=R e^{\imath \theta}, \quad M k>0$, independent of $R$, such that

$$
|f(s)|<M R^{k}
$$

implying that the integrals around BC and GA converge to zero as $R$
The integral round the small circle DEF when $s=e^{\imath \theta}$ can be shown to be zero as
0. Thus, using the previous arguments we obtain

$$
\begin{equation*}
\mathscr{L}^{1}\{f(s)\}=\frac{1}{2} \int_{0}[X(\bar{x})+X(\quad \bar{x})] \frac{e^{x t}}{\bar{x}} \mathrm{~d} x \tag{27}
\end{equation*}
$$

where

$$
\begin{equation*}
X(\bar{x})=\frac{K_{1}(\quad \bar{x}) K_{1}(\quad \bar{x})}{K_{1}(\quad \bar{x}) K_{0}(\quad \bar{x})+\quad-\quad K_{1}(\quad \bar{x}) K_{0}(\quad \bar{x})} \tag{28}
\end{equation*}
$$

It is convenient to introduce the following notation:

$$
\begin{align*}
& A(\bar{x})=K_{1}(\quad \bar{x}) K_{1}(\quad \bar{x})  \tag{29}\\
& B(\bar{x})=K_{1}(\bar{x}) K_{0}(\bar{x})  \tag{30}\\
& C(\bar{x})=K_{0}(\quad \bar{x}) K_{1}(\bar{x}) \tag{31}
\end{align*}
$$

This allows us to rewrite the integral (27) as

$$
\begin{equation*}
\mathscr{L}^{1}\{f(s)\}=\frac{1}{2} \int_{0} \frac{N(x)}{D(x)} \frac{e^{x t}}{\bar{x}} \mathrm{~d} x \tag{32}
\end{equation*}
$$

with

$$
N\left(\begin{array}{c}
\bar{x})=A( \\
\bar{x}) B(
\end{array} \overline{\bar{x}}\right)+A(\quad \bar{x}) B(\quad \bar{x})+{ }^{-}\left[A \left(\begin{array}{ccc}
\bar{x}) C( & \bar{x})+A( & \bar{x}) C(\bar{x})]
\end{array}\right.\right.
$$

and


Now it can be readily shown, using the relationships (15) and (16), and the Wronskian (19), that

$$
\begin{align*}
& A\left(\begin{array}{cc}
\bar{x}) B(\quad \bar{x})+A(\quad \bar{x}) B(\quad \bar{x})=\frac{3}{4 \bar{x}}\left[J_{1}(\bar{x})^{2}+Y_{1}(\bar{x})^{2}\right] \\
A(\bar{x}) C( & \bar{x})+A(\quad \bar{x}) C(\bar{x})=\frac{3}{4 \bar{x}}\left[J_{1}(\bar{x})^{2}+Y_{1}(\bar{x})^{2}\right] \\
B(\bar{x}) B(\quad \bar{x})=\frac{4}{16}\left[J_{1}(\bar{x})^{2}+Y_{1}(\bar{x})^{2}\right]\left[J_{0}(\bar{x})^{2}+Y_{0}(\bar{x})^{2}\right] \\
C(\bar{x}) C(\quad \bar{x})=\frac{4}{16}\left[J_{0}(\bar{x})^{2}+Y_{0}(\bar{x})^{2}\right]\left[J_{1}(\bar{x})^{2}+Y_{1}(\bar{x})^{2}\right]
\end{array}\right. \tag{33}
\end{align*}
$$

Calculating $B(\bar{x}) C(\quad \bar{x})+B(\quad \bar{x}) C(\bar{x})$ requires a little more work, but can be shown to be

$$
\begin{equation*}
\frac{4}{16}\left\{\frac{8}{2-x}+2\left[J_{0}(\bar{x}) J_{1}(\bar{x})+Y_{0}(\bar{x}) Y_{1}(\bar{x})\right]\left[J_{0}(\bar{x}) J_{1}(\bar{x})+Y_{0}(\bar{x}) Y_{1}(\bar{x})\right]\right\} \tag{37}
\end{equation*}
$$

Using (33)-(37) the integral (32) then becomes

$$
\begin{equation*}
\mathscr{L}^{1}\{f(s)\}=\frac{2}{2} \int_{0} \frac{J_{1}(\bar{x})^{2}+Y_{1}(\bar{x})^{2}+\left[J_{1}(\bar{x})^{2}+Y_{1}(\bar{x})^{2}\right]}{(\bar{x})} \frac{e^{x t}}{x} \mathrm{~d} x \tag{38}
\end{equation*}
$$

where

$$
\begin{align*}
(\bar{x})= & {\left[J_{1}(\bar{x})^{2}+Y_{1}(\bar{x})^{2}\right]\left[J_{0}(\bar{x})^{2}+Y_{0}(\bar{x})^{2}\right] } \\
& +-\left\{\frac{8}{2-x}+2\left[J_{0}(\bar{x}) J_{1}(\bar{x})+Y_{0}(\bar{x}) Y_{1}(\bar{x})\right]\right. \\
& {\left.\left[J_{0}(\bar{x}) J_{1}(\bar{x})+Y_{0}(\bar{x}) Y_{1}(\bar{x})\right]\right\} } \\
& +{ }^{2}\left[J_{0}(\bar{x})^{2}+Y_{0}(\bar{x})^{2}\right]\left[J_{1}(\bar{x})^{2}+Y_{1}(\bar{x})^{2}\right] \tag{39}
\end{align*}
$$

The transformation $\quad \bar{x}=u$ then yields

$$
\begin{equation*}
I(t)=\mathscr{L}^{1}\{f(s)\}=\frac{4}{2} \int_{0} \frac{J_{1}\left({ }^{-} u\right)^{2}+Y_{1}\left({ }^{-} u\right)^{2}+\left[J_{1}(u)^{2}+Y_{1}(u)^{2}\right]}{(u)} \frac{e^{u^{2} t}}{u} \mathrm{~d} u \tag{40}
\end{equation*}
$$

The integral in (40) presents the generalization of the Jaeger $\mathscr{I}(01 ; t)$ integral that is the object of our study.

Observe that (40) cannot be expressed as any of the Jaeger $\mathscr{I}(p q ; t)$ integrals when $=1$, as we previously stated, since $J_{\nu}\left({ }^{-} u\right)$ and $Y_{\nu}\left({ }^{-} u\right)$ are not then expressible as functions of $J_{\nu}(u)$ and $Y_{\nu}(u)$. This can happen only when $=1$. In particular, when $=1$ and 0 (40) reduces to

$$
\begin{align*}
\mathscr{L}^{1}\{f(s)\} & =\frac{4}{2} \int_{0} \frac{\left[J_{1}(u)^{2}+Y_{1}(u)^{2}\right]}{\left[J_{1}(u)^{2}+Y_{1}(u)^{2}\right]\left[J_{0}(u)^{2}+Y_{0}(u)^{2}\right]} \frac{e^{u^{2} t}}{u} \mathrm{~d} u \\
& =\frac{4}{2} \int_{0} \frac{1}{J_{0}(u)^{2}+Y_{0}(u)^{2}} \frac{e^{u^{2} t}}{u} \mathrm{~d} u \tag{41}
\end{align*}
$$

that is, to the expression (2) involving $\mathscr{I}(01 ; t)$, for the limiting current, as it should do. When $=1$ and $>0$ we obtain

$$
\begin{gather*}
B\left(\begin{array}{cc}
\bar{x}) C( & \bar{x})+B( \\
\bar{x}) C\left(\begin{array}{cc}
\bar{x}
\end{array}\right)= \\
2\left[K_{1}(\quad \bar{x}) K_{1}( \right. & \bar{x})]\left[K_{0}( \right. \\
\bar{x}) K_{0}( & \bar{x})]= \\
\frac{4}{8}\left[J_{1}( \right. & \bar{x})^{2}+Y_{1}( \\
\left.\bar{x})^{2}\right]\left[J_{0}( \right. & \bar{x})^{2}+Y_{0}( \\
\bar{x})^{2}
\end{array}\right]
\end{gather*}
$$

After some manipulation (and cancellation of ${ }^{4} 8$ ) and the use of the Wronskian (19)
we obtain

$$
(\bar{x})=(1+)^{2}\left[J_{1}(\bar{x})^{2}+Y_{1}(\bar{x})^{2}\right]\left[J_{0}(\bar{x})^{2}+Y_{0}(\bar{x})^{2}\right]
$$

and thus, in this case, after substituting $\bar{x}=u$,

$$
\mathscr{L}^{1}\{f(s)\}=\frac{4}{{ }^{2}(1+)} \int_{0} \frac{1}{J_{0}(u)^{2}+Y_{0}(u)^{2}} \frac{e^{u^{2} t}}{u} \mathrm{~d} u
$$

which is equivalent to (5), again involving $\mathscr{I}(01 ; t)$.
By analogy with the decomposition (21), $f(s)$ given by (6) can be decomposed (for details see [18]) into two terms corresponding to the solution for a planar electrode and to a cylindrical correction, respectively:

$$
\begin{equation*}
f(s)=\frac{1}{1+}\left[\frac{1}{\bar{s}}+\frac{1+}{1+} g(s)\right] \tag{43}
\end{equation*}
$$

where the inverse transform $\mathscr{L}^{1} g(s)$ is identical with the function icylw ${ }_{\text {ext }}\left(\begin{array}{cc}\bar{t} & U\end{array}\right)$ introduced in [18] and which we now denote by ( $\quad ; t)$. Hence, from (43) one obvious formula for computing ( $; t$ ) (via numerical Laplace transform inversion) is

$$
\begin{equation*}
(\quad ; t)=\mathscr{L}^{1} g(s)=\frac{1+^{-}}{1+}\left[(1+-) \mathscr{L}^{1}\{f(s)\} \quad \frac{1}{t}\right] \tag{44}
\end{equation*}
$$

with $\mathscr{L}^{1}\{f(s)\}$ given by (6). However, one can also derive an integral representation of $(\quad ; t)$, by replacing $\mathscr{L}^{1}\{f(s)\}$ in (44) with the integral (40). This gives
$\mathscr{L}^{1} g(s)=\frac{1+}{1+}$

$$
\begin{aligned}
&\left\{\left(1+^{-}\right) \frac{4}{2} \int_{0} \frac{J_{1}\left({ }^{-} u\right)^{2}+Y_{1}\left({ }^{-} u\right)^{2}+\left[J_{1}(u)^{2}+Y_{1}(u)^{2}\right]}{(u)} \frac{e^{u^{2} t}}{u} \mathrm{~d} u \quad \frac{1}{t}\right\} \\
&= \frac{1+-}{1+} \\
&\left\{\left(1+^{-}\right) \frac{4}{2} \int_{0} \frac{J_{1}\left({ }^{-} u\right)^{2}+Y_{1}\left({ }^{-} u\right)^{2}+\left[J_{1}(u)^{2}+Y_{1}(u)^{2}\right]}{(u)} \frac{e^{u^{2} t}}{u} \mathrm{~d} u\right. \\
&\left.-\int_{0} e^{u^{2} t} d u\right\} \\
&= \frac{4}{2} \frac{1+{ }^{-}}{1+} \\
&\left\{\int_{0} \frac{\left(1+{ }^{-}\right)\left[J_{1}\left({ }^{-} u\right)^{2}+Y_{1}\left({ }^{-} u\right)^{2}+\left(J_{1}(u)^{2}+Y_{1}(u)^{2}\right)\right]}{(u)} \frac{\pi}{2} u \quad(u)\right. \\
&\left.\frac{e^{u^{2} t}}{u} \mathrm{~d} u\right\}
\end{aligned}
$$

Collecting terms in powers of we obtain

$$
\begin{gather*}
(\quad ; t)=\mathscr{L}^{1} g(s)=\frac{4}{2}\left(\frac{1+-}{1+}\right) \\
\int_{0} \frac{M_{1}(u)+{ }^{-} M_{2}(u)+{ }^{2} M_{3}(u)}{(u)} \frac{e^{u^{2} t}}{u} \mathrm{~d} u \tag{45}
\end{gather*}
$$

where

$$
\begin{aligned}
M_{1}(u)= & {\left[J_{1}\left({ }^{-} u\right)^{2}+Y_{1}\left({ }^{-} u\right)^{2}\right] \quad{ }_{2} u\left[J_{1}\left({ }^{-} u\right)^{2}+Y_{1}\left({ }^{-} u\right)^{2}\right]\left[J_{0}(u)^{2}+Y_{0}(u)^{2}\right] } \\
M_{2}(u)= & {\left[J_{1}\left({ }^{-} u\right)^{2}+Y_{1}\left({ }^{-} u\right)^{2}\right]+\frac{1}{=}\left[J_{1}(u)^{2}+Y_{1}(u)^{2}\right] } \\
& \quad \overline{2} u\left\{\frac{8}{2^{2-} u^{2}}\right. \\
& \left.+2\left[J_{0}(u) J_{1}(u)+Y_{0}(u) Y_{1}(u)\right]\left[J_{0}\left({ }^{-} u\right) J_{1}\left({ }^{-} u\right)+Y_{0}\left({ }^{-} u\right) Y_{1}\left({ }^{-} u\right)\right]\right\} \\
M_{3}(u)= & \frac{1}{=}\left[J_{1}(u)^{2}+Y_{1}(u)^{2}\right] \quad \overline{2} u\left[J_{0}\left({ }^{-} u\right)^{2}+Y_{0}\left({ }^{-} u\right)^{2}\right]\left[J_{1}(u)^{2}+Y_{1}(u)^{2}\right]
\end{aligned}
$$

Function ( $; t)$ then becomes

$$
\begin{align*}
(; t)= & \mathscr{L}^{1} g(s)=\frac{1+-}{1+} \\
& \frac{4}{2} \int_{0} \frac{M_{1}(u)+{ }_{-} M_{2}(u)+{ }^{2} M_{3}(u)}{(u)} \frac{e^{u^{2} t}}{u} \mathrm{~d} u \tag{46}
\end{align*}
$$

The above results (25) and (46) for (0 ;t) and ( $\quad ; t$ ) have also been obtained by using the Bromwich contour to directly invert the Laplace transforms (22), and $g(s)$ resulting from (43).

## 3 Numerical evaluations

Integrals (40) and (46) must be evaluated numerically, but this task is not trivial. The command NIntegrate of Mathematica [26] fails to evaluate the integrals directly, when default command options are used. Variable transformation $u=1 y$ combined with the
integration along $y$ by means of the Kronrod quadrature (see e.g. [27]), available as one of the command options, turned out to be helpful in overcoming this problem, as long as (roughly) $10{ }^{40} \quad t \quad 10^{18}$. For smaller $t$ Mathematica issued error messages, and for larger $t$ incorrect results were obtained. Therefore, by following the previous practice [18], the main e ort was concentrated on designing a C++ code written in extended precision (long double C++ variables) that would provide the integral values with the smallest possible relative error in modulus. The code was prepared with the help of the freely available Bloodshed/Orwell Dev-C++ 5.7.1 programming environment [28, 29], compiled by a 32-bit release of the TDM GCC 4.8.1 compiler, and run on a laptop computer with an Intel Centrino 2 processor ( 2.4 GHz ), operating under Windows Vista. Numerical C++ procedures for calculating integrands in (40) and (46) with the modulus of the relative error not exceeding about $10^{19}-10{ }^{18}$ were devised, since standard C++ libraries do not provide procedures for the Bessel functions $J_{\nu}(u)$ and $Y_{\nu}(u)$.

In order to verify the accuracy of integration, reference values of $I(t)$ and $(\quad ; t)$ were necessary. Such values, having at least 25 accurate signi cant digits, were obtained from (6) and (44) by the numerical Laplace transform inversion. The inversion was accomplished by the GWR procedure of Valko and Abate [30], written in Mathematica. The procedure implements the Gaver-Wynn-rho method devised by Valko and Abate [31, 32]. By analogy with [18], the reference data were obtained for $\begin{array}{lllllll}60 & \log t & 60, & 3 & \log & 3\end{array}$ and $U=0, \quad 1, \quad 2, \quad 3, \quad 4, \quad 5, \quad 6, \quad 7, \quad 10, \quad 20, \quad 30, \quad 40$ and 45 . All numerical tests were limited to this choice.

The C++ numerical integration routine was based on double exponential quadratures [33] which are often characterized by an exponential convergence, and are therefore both accurate and e cient. Integral (40) was cast into the form

$$
\begin{equation*}
I(t)=\frac{2}{2} \int_{0} \frac{J_{1}\left(\sqrt{\frac{w}{t}}\right)^{2}+Y_{1}\left(\sqrt{\frac{w}{t}}\right)^{2}+\left[J_{1}\left(\sqrt{\frac{w}{t}}\right)^{2}+Y_{1}\left(\sqrt{\frac{w}{t}}\right)^{2}\right]}{\left(\sqrt{\frac{w}{t}}\right)} \frac{e^{w}}{w} \mathrm{~d} w \tag{47}
\end{equation*}
$$

from which it is seen that the integrand already involves one exponential factor $\exp (w)$. In such cases it is recommended (see e.g. [33]) to use the variable transformation

$$
w=\exp \left[\begin{array}{ll}
y & \exp (y) \tag{48}
\end{array}\right]
$$

that ensures a double exponential integrand decay in the limits of $y$ and $y$ Unfortunately, computational experiments revealed that the accuracy of such numerical integration was very low. The reason seems to lie in the nature of the integrand singularity as $w \quad 0$. Even when $w$ approaches the lower limit of the range of positive long double variables (ca. $10{ }^{4951}$ ), the transformation (48) is not able to suppress the large integrand values down to a negligible level. In order to overcome this di culty, integral (47) was
split into two integrals: one over the interval $0 \quad w \quad w_{\mathrm{b}}$, and second over the interval $w_{\mathrm{b}} \quad w<\quad$, where $w_{\mathrm{b}}=\min \left(\begin{array}{lll}1585 & \left.10{ }^{18} t 10{ }^{19}\right) \text {. In the rst interval the integrand }\end{array}\right.$ can be replaced by the rst term of its asymptotic expansion for $w \quad 0$ :

$$
\frac{J_{1}\left(\sqrt{\frac{w}{t}}\right)^{2}+Y_{1}\left(\sqrt{\frac{w}{t}}\right)^{2}+\left[J_{1}\left(\sqrt{\frac{w}{t}}\right)^{2}+Y_{1}\left(\sqrt{\frac{w}{t}}\right)^{2}\right]}{\left(\sqrt{\frac{w}{t}}\right)} \frac{e^{w}}{w}
$$

 $b=4(1+\quad)\left[(1+\quad)\left(\begin{array}{ll}\mathrm{E} & \ln 2)+\quad \ln \end{array}\right]\right.$, and $c=(1+\quad)^{2}$, with E denoting the Euler gamma constant.

Expression (49) is integrable analytically, with the result

$$
\begin{array}{r}
\int_{0}^{w_{\mathrm{b}}} \frac{2(1+)}{\left\{a+b \ln \left(\frac{w}{t}\right)+c\left[\ln \left(\frac{w}{t}\right)\right]^{2}\right\} w} \mathrm{~d} w \\
=\frac{}{1+} \operatorname{arccotan}\left\{\frac{\ln \left(\frac{w_{\mathrm{b}}}{t}\right)+2\left[\begin{array}{ll}
(\mathrm{E} & \ln 2)+\frac{\delta}{1+\delta} \ln
\end{array}\right]}{}\right\} \tag{50}
\end{array}
$$

with the inverse cotangent (arccotan) satisfying $0<\operatorname{arccotan}(z)<$ for real $z$. A well-conditioned procedure for computing arccotan for large positive arguments is needed (computations employing the standard $\mathrm{C}++$ function for inverse tangent are inaccurate due to the subtraction of almost equal numbers) and has been elaborated in this work. Transformation (48) is then applied to the numerical integration over the interval $w_{\mathrm{b}}$ $w<\quad$, after replacing the variable $w$ by $w \quad w_{\mathrm{b}}$.

Figure 2A shows the current $I(t)$ calculated in the above way for $=1(U=0)$. Corresponding moduli of the relative errors of $I(t)$ are depicted in Figure 2B. The modulus of the relative error does not exceed $5096 \quad 10{ }^{18}$. This result is better than that obtained by the procedure in [18], which produced the largest relative error in modulus $584 \quad 10{ }^{15}$ for the same parameter values (cf. Fig. 2C). Results obtained for other $U$ values were similar.

The numerical C++ procedure developed in [18] was designed for computing $(\quad ; t)=$ $\operatorname{icylw}_{\text {ext }}(\bar{t} \quad U)=\mathscr{L}^{1} g(s)$ de ned by (44), and $I(t)$ was later obtained, from thus calculated ( $\quad ; t$ ), by using (Laplace inverted) (43). The procedure had a hybrid character. It combined a small- $t$ series expansion of $(\quad ; t)$ (valid for $t$ smaller than about $10^{8} \quad 10^{6}$ ) with a certain large- $t$ approximation, and a numerical Laplace transform inversion by the Stehfest method [34] used in the intermediate $t$ interval. Out of these



Figure 2: Current $I(t)$ for $\Theta=1(U=0)$, evaluated numerically by the double exponential quadrature (A); and corresponding moduli of the relative errors (B). Errors obtainable by using the hybrid algorithm from Ref. [18] are shown in subfigure C, for comparison.
three approaches to computing ( $; t)$, the Stehfest method was the least accurate, despite its implementation in quad precision, and the most expensive computationally. Interested Reader can nd a discussion of the limitations of the accuracy of the Stehfest, and related methods, caused by a nite precision arithmetic, in the recent article [35]. The results shown in Figs. 2A and 2B were obtained, in turn, at the cost of about 1200 integrand evaluations (per single $I(t)$ value), for any $t$ value from the range considered. The corresponding computational time is slightly smaller than that required by the Stehfest method (although about three orders of magnitude larger than the time needed by the small- $t$ and large- $t$ approximants).

It is therefore interesting to examine the replacement of the Stehfest method by the present numerical integration procedure, in the computational procedure described in Ref. [18]. For this purpose one can either use (44), combined with the numerical evaluation of the integral (40) followed by the subtraction of the $1 \quad \bar{t}$ term, or apply the numerical integration to the integral (46) (in the way analogous to that described above for $I(t)$ ). Both variants were tested, and in both cases a considerable error growth was observed with decreasing $t$ values, due to the loss of signi cant digits through subtraction (present in both formulae). However, the evaluation of (44) proved somewhat more accurate so that it was nally used as a replacement to the Stehfest method. In addition, the interval of applicability of the small- $t$ expansion of $(\quad ; t)$ was slightly enlarged by adding four more expansion terms (in addition to the 15 terms employed in [18]). In this way, the interval of $t$ where formula (44) had to be applied, but which gave the largest errors, was somewhat reduced.

The moduli of the relative errors of $(\quad ; t)$, obtained in the tests performed by the hybrid procedure modi ed in the above way, do not exceed about $4019 \quad 10{ }^{16}$. This error bound is about two orders of magnitude smaller than that observed in [18] (ca. $\left.3436 \quad 10^{14}\right)$. The largest error occurred for $000674(U=5)$, and results corresponding to this worst case are shown in Figs. 3A and B. For this value of the unmodi ed procedure of [18] produced the largest error of ca. $4438 \quad 10^{15}$ (cf. Fig. 3C).

Apart from the reduction of errors, the replacement of the Stehfest method by numerical integration also slightly reduces the computational times. Furthermore, these improvements are achieved without using quad precision, which was necessary in [18]. In conclusion, the integral formula (40) proves advantageous for computing both $I(t)$ and $(\quad ; t)$.

## 4 Conclusions

Summing up, the most important conclusions of this study are:



Figure 3: Function $\Xi(\Theta, \delta ; t)$ for $\Theta \approx 0.00674(U=-5)$, evaluated numerically by the hybrid procedure from Ref. [18], with the Stehfest method replaced by the double exponential quadrature for integral (40) (A); and corresponding moduli of the relative errors (B). Errors obtainable by using the unmodified hybrid algorithm from Ref. [18] are shown in subfigure C, for comparison.

The recently presented [18] model of chronoamperometry at cylindrical electrodes gives rise to an interesting, and previously unknown generalization of the real-valued Jaeger $\mathscr{I}(01 ; t)$ integral, given by (40).

The analytical derivation of this integral from the expression (6) employing inverse Laplace transforms proceeds in a way analogous to the derivation of the $\mathscr{I}(01 ; t)$ integral from its corresponding inverse Laplace transform expression (4). The same Bromwich contour can be applied.

The generalized integral (40), as well as the original $\mathscr{I}(01 ; t)$ integral, are more conveniently evaluated by means of the numerical double exponential quadratures, than by the numerical Laplace transform inversion of expressions (6) or (4), if using IEEE-754-compliant oating point variables. Although the numerical integration is not trivial, it can be accomplished with a machine accuracy, by using exclusively standard precision variables, whereas the numerical Laplace transform inversion requires multiprecision but is still less accurate. Numerical integration is also less expensive computationally.

Consequently, the numerical evaluation of the integrals (40) and (46) should be preferred in the modelling of relevant electroanalytical phenomena, over numerical Laplace transform inversion.

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