New Mathematical Functions for Vacuum System Analysis

Michael S. Woronowicz

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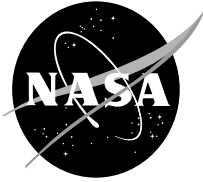
New Mathematical Functions for Vacuum System Analysis

Michael S. Woronowicz
SGT, Inc., Greenbelt, MD

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Abstract

A new bivariate function has been found that provides solutions of integrals having the form $u^{-\eta}e^{u}\,du$ which arise when developing predictions for the behavior of pressure within a rigid volume under high vacuum conditions in the presence of venting as well as sources characterized by power law transient decay over the range [0,1) for η and for $u \geq 0$. A few properties of the new function are explored in this work. For instance the $\eta =$ ½ case reproduces the Dawson function. In addition, a slight variation of the solution technique reproduces the exponential integral for $\eta = 1$. The technique used to generate these functions leads to an approach for solving a more general class of nonlinear ordinary differential equations, with the potential for identifying other new functions that solve other integrals.

Introduction

The evolution of pressure versus time $p(t)$ within a rigid volume V with venting in free molecule flow becomes governed by the behavior of gas sources Q contained within the volume. Based upon a mass conservation statement for an ideal gas at room temperature T [1]

$$V\frac{dp}{dt} = Q - C(p - p_{\infty}).\tag{1}$$

Venting is described by conductance C to exhaust pressure p_{∞}. For molecular flow conditions, C is not a function of pressure, and for this discussion it is assumed $p_{\infty} = 0$. Dividing by C and defining characteristic time $\tau \equiv V/C$ and reduced gas load $q \equiv Q/C$,

$$\tau\frac{dp}{dt} = q(t) - p.\tag{2}$$

Let $s \equiv t/\tau$. For sources associated with diffusion-limited outgassing, classical theoretical behavior yields $q \propto 1/\sqrt{s}$, [2] while for those associated with surface desorption $q \propto 1/s$. [3] While these sorts of behaviors are often observed experimentally, it appears more generally one must deal with [4]

$$q(s) = \frac{c}{s^{\eta}},\tag{3}$$

where c and τ are constants for a given system and $0.5 \leq \eta \leq 1.0$, although this parameter range does not represent hard limits. Rearranging and introducing integration factor e^{s}

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$$\frac{d}{ds}\left(pe^s\right) = c\,\frac{e^s}{s^{\eta}}.\tag{4}$$

The solution to this ordinary differential equation for pressure $p(t)$ with some initial value p_1 at t_1 becomes

$$p(t) = p_1 e^{-\Delta s} + c\left[\left(e^{-s}\int_0^s \frac{e^u}{u^{\eta}}\,du\right) - e^{-\Delta s}\left(e^{-s_1}\int_0^{s_1}\frac{e^u}{u^{\eta}}\,du\right)\right].\tag{5}$$

The matter now becomes one of evaluating the parenthetical expressions.

Analytical Development

It appears no general solutions for integrals of the type highlighted in Eq. (5) have ever been published, as they are conspicuously absent from references on mathematical functions. When η is a positive integer their behavior is governed by the exponential integral Ei(s), [5-7] and the Dawson function $D\left(\sqrt{s}\right)$ describes η = ½. [7-9] For this integral there also appears to be a relationship with the lower incomplete gamma function under certain conditions. [10-12]

The procedure for direct numerical solution of this integral seems to be quite problematic. The integrand has a singularity at s = 0, and for large arguments both the numerator and denominator increase without bounds. On the other hand the scaling factor ahead of the integral counteracts some of this behavior overall.

When $0 \le \eta < 1$, let $x \equiv \sqrt[b]{u}$, where $b \equiv 1/(1-\eta)$. Then

$$e^{-s}\int_0^s \frac{e^u}{u^{\eta}}\,du = be^{-x^b}\int_0^X e^{x^b}\,dx \equiv bG(\eta, x).\tag{6}$$

It happens that $G(\eta, x)$ satisfies its own ordinary differential equation:

$$\frac{\partial G}{\partial x} + bx^{b-1}G = 1.\tag{7}$$

Properties of Bivariate Function $G(\eta, x)$

The solution of Eq. (6) may be accomplished much more easily numerically using Eq. (7) than it can by attacking the integral directly. Eq. (7) may be explored to discover a variety of properties of G.

Integration of Eq. (7) for G across various values of η and x produces curves like those presented below in Figure 1.
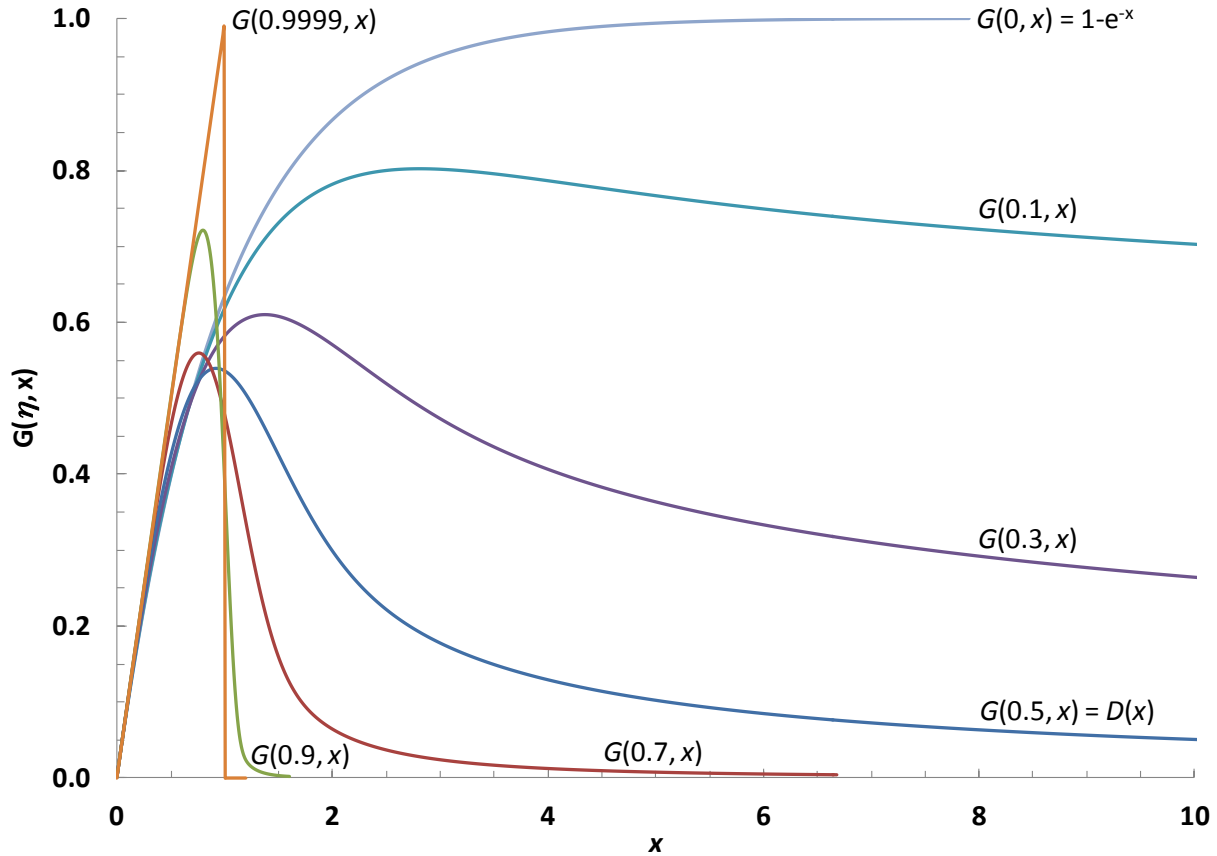
FIGURE 1. Function $G(\eta, x)$ for selected values of η.

When $(\eta, b, x) = (0, 1, s)$, $G(0, x)$ reproduces expected limiting behavior of

$$e^{-s}\int_{0}^{s} e^{s}ds = e^{-s}\left(e^{s} - 1\right) = 1 - e^{-s}, \tag{8}$$

and when $\eta = 0.5$ the function is equivalent to the Dawson function $D(x)$, with its maximum value of about 0.54 at $x \approx 0.92$. [7-9]

As $\eta \to 1$, $b \to \infty$, and the function steepens to produce a sawtooth shape with infinite slope at $x = 1$, which appears to anticipate the discontinuity associated with the exponential integral. [2]

Also apparent in Figure 1 is that $G'(\eta, 0) = 1$ at $x = 0$, independent of η. This property is also observed by setting $x = 0$ in Eq. (7). In terms of physical units, this property indicates that regardless of η and the fact that the diffusion-desorption

mechanism starts with a singularity at $t = 0$, pressure within the volume is initially well-behaved with no such influence.
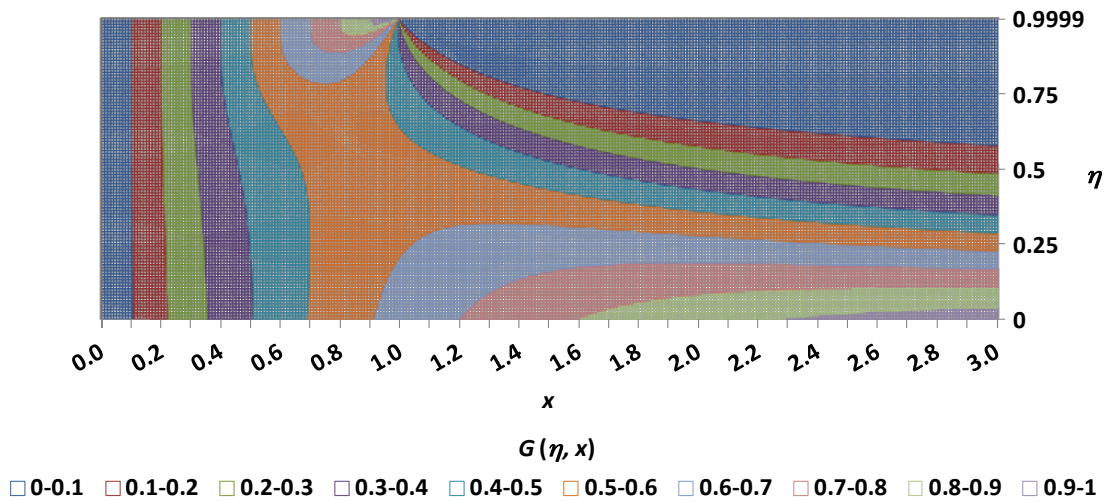
Less obvious in Figure 1 is the fact that for large values of x independent of η:

$$G(\eta, x \rightarrow \infty) \rightarrow \frac{1}{bx^{b-1}}. \tag{9}$$

In terms of satisfying Eq. (6), recall the solution for the scaled integral was defined by bG with $s = x^b$. Substitution of Eq. (9) into Eq. (5) for large $s = t/\tau$ leads to

$$p(t \rightarrow \infty) \rightarrow \frac{c}{s^\eta} = q(s). \tag{10}$$

Eq. (10) is the solution to Eq. (2) when $\dot{p} = 0$.

FIGURE 2. Contour map of function $G(\eta, x)$.

A contour map for $G(\eta, x)$ is presented in Figure 2 essentially spanning the range for η and computed for x out to three in increments of $(\Delta\eta, \Delta x) = (0.01, 0.01)$. The linear slope in the neighborhood of $x = 0$ appears as a series of equally-spaced vertical bars, and the discontinuity associated with the exponential integral is present as a node at $(\eta, x) = (1, 1)$. The prominent freeform orange cross around $x = 0.8$ is characteristic of a saddle point. Owing to the simplistic integration associated with this figure, one may say the saddle point occurs approximately at $(\eta, x) = (0.56, 0.85)$ with $G \approx 0.54$.

A three-dimensional representation of Figure 2 is depicted below in Figure 3 with the η scale reversed to better descry the approach to the singularity at $(\eta, x) = (1, 1)$. Figures 1 & 3 also reveal that another singularity is approached as $(\eta, x) \rightarrow (0, \infty)$, where $G(0, \infty) \rightarrow 1$, but $G(0+, \infty) \rightarrow 0$.
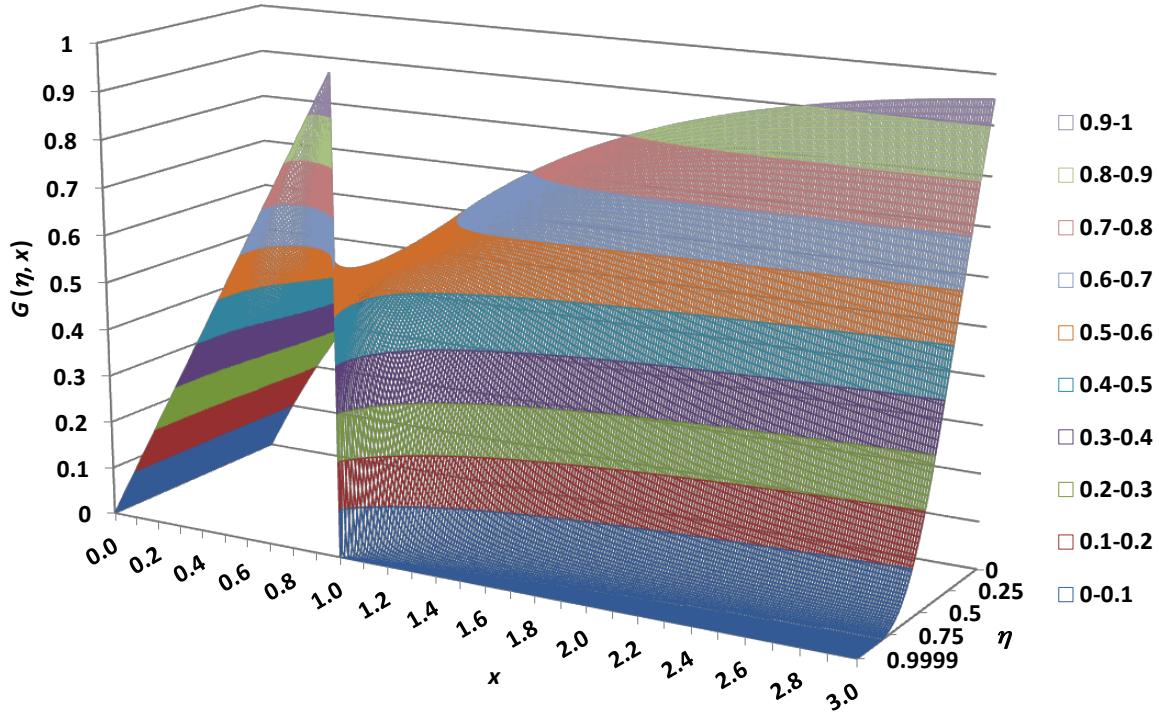
FIGURE 3. Three-dimensional contour map of function $G(\eta, x)$. (η-axis reversed from Fig. 2.)

Scaled Exponential Integral Solution *F(y)* Properties

Clearly the change of variable introduced to produce Eq. (6) will not work for $\eta = 1$, a case corresponding to surface desorption. [3] Instead let $y \equiv \ln s$. Then

$$e^{-s} \int_0^s \frac{e^u}{u} du = e^{-e^y} \int_{-\infty}^y e^{e^y} dy = F(y).$$ (11)

Eq. (11) would generally be described by an exponential integral Ei(ξ), specifically

$$F(y) \equiv e^{-e^y} \int_{-\infty}^y e^{e^y} dy = -e^{-e^y} \text{Ei}\left(-e^y\right).$$ (12)

In fashion similar to Eq. (7) it is determined that

$$\frac{dF}{dy} + e^y F = 1.$$ (13)

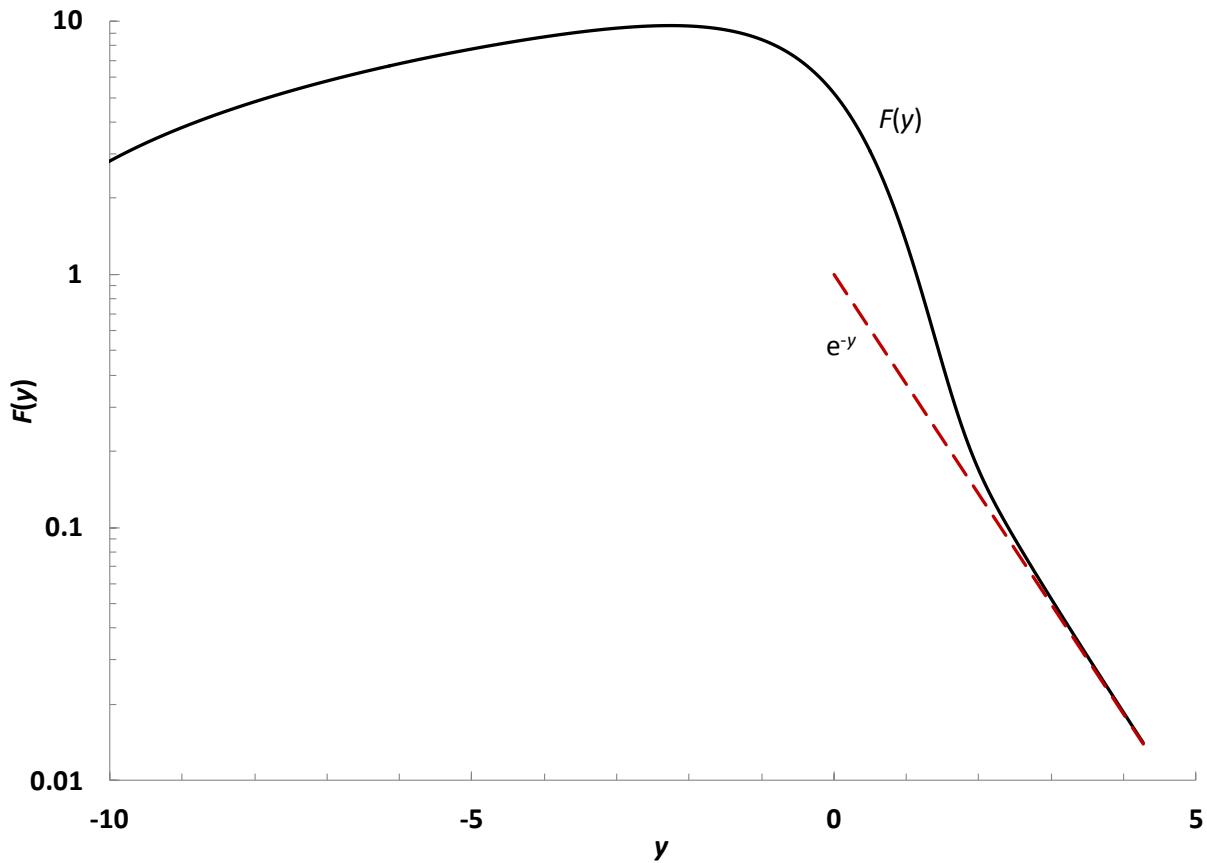From Eq. (13) it can be seen that $F'(y \to -\infty) \to 1$, which corresponds to $s \to 0$. It resembles behavior observed for $G(\eta, 0)$. Also, for large y, analogous to Eq. (9),

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$$F(y \rightarrow \infty) \rightarrow e^{-y} = \frac{1}{s}, \tag{14}$$

and in physical units

$$p(t \rightarrow \infty) \rightarrow \frac{c}{s} = q(s). \tag{15}$$

Function $F(y)$ is depicted in Figure 4. Its maximum value is approximately 9.60 for $y \approx -2.27$, ($s \approx 0.103$).

FIGURE 4. $F(y)$ behavior featuring function maximum and long-term trending.

General Solution Approach

The approach used to identify functions such as $F(y)$ and $G(\eta, x)$ may be formulated in a more general sense beginning with Eq. (2). Casting Eq. (1) in terms of s, the forcing term may be introduced as

$$q(s) = \frac{c}{f(s)}, \tag{16}$$

leading to

$$p(t) = p_1 e^{-\Delta s} + c\left[\left(e^{-s}\int_0^s \frac{e^u}{f(u)}du\right) - e^{-\Delta s}\left(e^{-s_1}\int_0^{s_1} \frac{e^u}{f(u)}du\right)\right]. \tag{17}$$

If it is possible to introduce the variable substitution $d\xi = du/f(u)$ such that $u = g(\xi)$ is a function in terms of the transformed variable, then the scaled integral will be

$$e^{-s}\int_0^s \frac{e^u}{f(u)}du \propto e^{-g(\xi)}\int e^{g(\xi)}d\xi \equiv H(\xi). \tag{18}$$

Function $H(\xi)$ will satisfy its own differential equation:

$$\frac{dH}{d\xi} + H\frac{dg}{d\xi} = 1. \tag{19}$$

If well-behaved, it appears these functions should all rise from some initial transformed variable zero with a slope of unity, and for large arguments will approach limiting behavior of

$$H(\xi \to \infty) \to \frac{1}{g'(\xi)}. \tag{20}$$

$H(\xi)$ will also form the core of the solution to integrals of the type arrived at in Eq. (17).

Concluding Remarks

A new mathematical function $G(\eta, x)$ has been discovered that solves integrals containing the form $u^{-\eta}e^u\,du$ through a simple transformation from u to x. The integral is solved through use of a property of G as a solution to a particular differential equation. This function is useful for describing transient behavior for pressure in vacuum systems, and several properties of this function have been explored.

It has been noted that Dawson's function is related to certain solutions of the diffusion equation used in conduction heat transfer and mass transfer studies, as well as certain investigations associated with propagation of electromagnetic radiation. Since $G(\eta, x)$ simplifies to Dawson's function for $\eta = 0.5$, it seems logical that the new function will offer at least the same level of utility.

The special case $\eta = 1$ cannot be solved with the transformation associated with development of G, but may be handled by a similar approach. The resulting function $F(\ln u)$ is related to the exponential integral.

Finally, the approach taken to generate these functions has been generalized to identify properties of solutions to integrals containing the form $\left(e^u/f(u)\right)du$. Provided certain conditions are met, these solutions will share certain features of short-period and long-period behavior.

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