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WHAT IS INDUSTRIAL MATHEMATICS?

(modeling, industrial applications, non linear problems)

AVNER FRIEDMAN*

* Department of Mathematics, University of Minnesota, 206 Church St. SE, Minneapolis, MN 55455.

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ABSTRACT

The purpose of this paper is to explain what is industrial mathematics and to describe some mathematical models and results that were developed toward solving problems that arose in industry.

1. INTRODUCTION AND DEFINITIONS

As the complexity of processes and products in the manufacturing and service industries increases, industry must shorten the time from concept into product. Experiments are too costly and lengthy, and the demand for mathematical/statistical modeling and simulation increases. The creation of mathematical/statistical models and the development of algorithm for computer simulation to obtain solutions for problems in industry is what we call **industrial mathematics** (see[5] for more details).

How does industrial mathematics differ from «applied mathematics»?

First, you must travel to industry and talk to its scientists and engineers in order to identify their mathematical problems; you cannot pick up problems just from the literature. Secondly, you cannot tell industry people: «Sorry, I cannot help you with your mathematical problems since I specialize in another field of mathematics»; when in industry, your specialty is mathematics, all of it! Thirdly, you have a limited time for solving problems; sometimes just a few weeks. However, you need not provide a full mathematical solution; partial timely solutions are usually all that is required. Finally you need to be aware of the fact the goals in university and in industry are different; whereas university's goals are teaching, research and publications, industry's goal is to make profits.

What is the difference between industrial mathematics and engineering?

(a) Engineers build tools and products. They use any scientific knowledge, theoretical or experimental, available to them. They may use physics, chemistry, mathematics, biology, etc., but the are not experts in any one of these disciplines, (b) Not every industrial/engineering problem can be formulated as a mathematical problem, (c) The most fundamental component in industrial mathematics is the development of a mathematical model of a problem from industry, after which mathematical analysis and numerical algorithms are used, or developed, to solve the problem. (d) Industrial mathematicians are strong in mathematics. Mathematicians in industry are viewed as having highly developed skills in abstraction, analysis of underlying structures, and logical thinking; as having the best tools for formulating and solving problems. They are often viewed as consultants; for more details see [12].

A number of Mathematics Departments in the U.S. are developing programs in industrial mathematics. The goals of these programs are to help industry by solving problems, to develop new mathematics as needed, and to broaden career opportunities for students and postdocs. A blue print how to start such a program is described in [5].

In the following sections we give examples of challenging mathematical problems that came from industry.

2. PARTICLES IN A DIESEL ENGINE

In order to design the shape of some components of a diesel engine or of its exhaust, researches in General Motors wish to find out the inception rate I(t) of soot particles that are formed in flat flame. These particles, assumed to be spherical, grow by means of surface reactions whose rate k(t) is another unknown function that need to be found. The particles also grow by coagulation: a collision of size u particle with size v particle forms a size u + v particle; here «size» means volume. The smallest size particle is $v_1 = 10^{-21}$ cm³ and the largest size particle is typically $v_2 = 10^{-16}$ cm³, so that if we normalize v_1 to 1

$$C[n](v,t) = \frac{1}{2} \int_{1}^{v-1} \beta(v-u,u) \ n(v-u,t) \ du - n(v,t) \int_{1}^{\infty} \beta(u,v) \ n(u,t) \ du$$

where $\beta(u,v)$ is the rate of collision between particles of sizes u and v. The evolution of n(u,t) is then (see[11]):

$$\frac{\partial n(u,t)}{\partial t} = -Bk(t)\frac{\partial}{\partial v} \Big[v^{2/3} n(v,t) \Big] + C[n](v,t)$$

for $1 < u < \infty$, and the boundary condition is

$$n(1,t) = \frac{1}{B} \frac{I(t)}{k(t)}$$

where B is a known positive constant. We also have the initial condition

$$n(v,0) = 0.$$

Optical measurements of absorption and scattering provide, respectively, the values of the first and second moment of n:

$$\int_{1}^{\infty} v n(v,t) dv = f(t),$$
$$\int_{1}^{\infty} v^2 n(v,t) dv = g(t).$$

The problem is then: Given f and g, determine the functions I and k.

This is an inverse problem; it requires us to first solve for n(v, t), not knowing be data *I*, *k*, and then determine these data from the knowledge of the first two moments of n(v, t).

Assuming that f(t), g(t) are continuously differentiable for $t \ge 0$, that f''(0), g''(0) exist, and that f'(0) > 0, g''(0) > f''(0), Friedman and Reitich [8] derived a nonlinear nonlocal integral equations for *I*, *k*:

(1)
$$I(t) = \Phi(I,k,f,g),$$
$$k(t) = \Psi(I,k,f,g).$$

They proved:

Theorem 1: The system (1) has a unique continuous solution for all $0 \le t < T$, where either $T = \infty$, or else, $T < \infty$ and k(t) or I(t) become negative at $t = T + \varepsilon$, for any small $\varepsilon > 0$.

The conditions f'(0) > 0, g''(0) > f''(0) are essentially necessary conditions if the inverse problem can be solved.

Theorem 1 shows that the inverse problem has a unique solution as long as the physical assumptions $k \ge 0$, $I \ge 0$ are valid.

The proof of Theorem 1 has two parts: First we solve the system for a small time interval, and then we extend the solution step-by-step using some a priori estimates on I and k. This procedure resembles a method of proof which occurs in an entirely different problem arising in optics (see [6], [7]): Given points A, B and x_1 , x_2 on the line connecting them, design an axially symmetric lens passing through x_1 , x_2 such that any ray from A which falls on the lens passes through B after being refracted. If the lens occupies the region.

$$|x_1 - \beta| \le F\left(\left(x_2^2 + x_3^2\right)^{1/2}\right),$$

then, setting $y = (x_2^2 + x_3^2)^{1/2}$, the refraction law leads to a system of nonlinear nonlocal integral equations for the functions F(y), $\phi(y)$ (see Figure 1). This system has a unique solution as long as the points (F(y), y) on the lens can be «seen» by A.



3. PHOTOGRAPHIC FILM

A color photografic film is made up of several emulsion layers separated by gelatin layers and coated over a polymeric base. Each emulsion layer contains silver halide grains and oil droplets in gelatin. The oil droplets contain a chemical called coupler, which forms color dye with the oxidized developer of exposed silver halide grains, when the film is developed. In order to maintain the «freshness» of the film, from the time of manufacturing to the time when the film is exposed, it is necessary to control the size of the oil droplets. This is achieved by introducing certain coagulation-preventing chemicals. An important problem arises: how to measure coalescence rates of such droplets?

Droplets are formed by an homogenization process such as rotating plates, driving a mixture through an orifice, or stirring with a motor. In all these processes both rupture and coalescence take place, so that the number density n(x, t) (x represents volume of the droplets, assumed to be spherical) satisfies the evolution equation.

$$\frac{d}{dt}n(x,t) = \frac{1}{2}\int_0^x K(x-\xi,\xi) n(x-\xi,t) n(\xi,t) d\xi + \int_x^\infty B(\xi,x) n(\xi,t) d\xi - \frac{1}{2}n(x,t)\int_0^x B(x,\xi) d\xi - n(x,t) \int_0^\infty K(x,\xi) n(\xi,t) d\xi;$$

here $K(x, \xi)$ is the probability, per unit time, that a particle of (volume) x and a particle of size ξ coalesce, and $B(x, \xi)$ (for $x > \xi$) is the probability, per unit time, that a particle of size x ruptures to produce one particle of size ξ another of size $x - \xi$. In order to measure coalescence rates, researches at Eastman Kodak wait until equilibrium has been reached. Then they take a portion of the emulsion (typically 20%) and add to it chemiluminescent species, and introduce it back into the mixture. They continue the homogenization process and measure, as time progresses, the luminescent signal. They want to use this signal to determine the coalescence rate.

If we denote by n(x, c, t) the number density of droplets of volume x and chemiluminescent concentration c, then, according to David Ross from Eastman Kodak,

$$\frac{d}{dt}n(x,c,t) = \frac{1}{2} \int_0^x \int_0^\infty K(x-\xi,\xi) n\left(x-\xi, \frac{xc-\gamma\xi}{x-\xi}, t\right) n(\xi,\gamma,t) \left(\frac{x}{x-\xi}\right) d\gamma d\xi + \int_x^\infty B(\xi,x) n(\xi,c,t) d\xi - \frac{1}{2}n(x,c,t) \int_0^x B(x,\xi) d\xi -n(x,c,t) \int_0^\infty \int_0^\infty K(x,\xi) n(\xi,\gamma,t) d\gamma d\xi.$$

The signal, which is the number of photons emitted per unit time from a droplet, is a function f(x, c), typically xc^2 . The measured signal is

$$S(t) = \int_0^\infty \int_0^\infty f(x,c) n(x,c,t) dx dc$$

and the degree of coalescence is

$$D(t) = \int_0^\infty \int_0^\infty (c - c_\infty) n(x, c, t) \, dx \, dc$$

where c_{∞} is the limiting concentration, unknown in advance.

Problem. Determine the relation of D(t) to S(t), and the behavior of D(t) as $t \to \infty$.

To solve this problem Friedman and Reitich [9] established the following conservation law, for any function bounded by c(1 + x) for all $x \ge 0$, $c \ge 0$:

$$\frac{dS(t)}{dt} = \frac{1}{2} \int_0^\infty dx \int_0^\infty d\xi \int_0^\infty dc \int_0^\infty d\gamma K(x,\xi) n(x,c,t) n(\xi,\gamma,t)$$
$$\times \left[f\left(x+\xi, \frac{xc+\xi\gamma}{x+\xi}\right) - f(x,c) - f(\xi,\gamma) \right]$$
$$+ \int_0^\infty dx \int_0^\infty dc \int_0^\infty B(\xi,x) n(\xi,c,t) \left[f(x,c) - \frac{x}{\xi} f(\xi,c) \right] d\xi$$

It enabled them to prove the following:

Theorem 2: If $c_{\infty} = M_1/M_0$ where

$$M_0 = \int_0^\infty \int_0^\infty xn(x,c,0) \, dx \, dc,$$
$$M_1 = \int_0^\infty \int_0^\infty xcn(x,c,0) \, dx \, dx,$$

then $D(t) \to 0$ as $t \to \infty$.

In case $f(x, c) = xc^2$, D(t) is related to S(t) by

$$D(t) = S(t) - 2c_{\infty}M_1 + c_{\infty}^2M_0$$

and thus measurements of S(t) determine D(t). They also proved that, as $t \to \infty$,

$$xcn(x,c,t)dx dc - xn(x,t)dx \rightarrow 0$$

in the sense of weak convergence of measures.

4. ELECTROPHOTOGRAPHY

Traditional photography produces images using light and chemical processes. Electrophotography produces images using light and electric images. The electrophotographic cycle consists of several steps: Charge the photoconductor; expose the photoconductor using flash; develop electrical image to a visible one; transfer the visible image to a paper; fuse the visible image permanently on the paper, and, finally, clean the photoconductor. Here we shall concentrate only on the step of developing the electrical image into a visible image. This is done by means of charged toner particles which stream into an electric field between a magnetic brush and the photoconductor. If we consider just one pixel, and an electric image corresponding to a black square within the pixel, then the electric potential -u will satisfy (we take for simplicity a 2-dimensional model):

$$\Delta n = \begin{cases} \rho & \text{in } D(t) \\ 0 & \text{in } \Omega \setminus D(t) \end{cases}$$

where D(t) is the region filled by the toner concentration ρ (assumed to be constant); here Ω is a rectangle $\{-a \le x \le a, -b \le y \le h\}$ with y = 0 representing the surface of the photoconductor, and D(t) lies in $0 \le y \le h$. The electric image is represented by the condition

$$\frac{\partial u(x,0+)}{\partial y} - \frac{\partial u(x,0-)}{\partial y} = -\sigma, \quad -a_1 < x < a_1,$$

where $0 < a_1 < a$ and σ is a positive constant. We also impose boundary conditions

$$u = M$$
 on $y = h$, $u = 0$ on $y = -b$,
 $\frac{\partial u}{\partial x} = 0$ on $x = \pm a$.

Finally, the velocity V of the (free) boundary $\Gamma(t)$ of D(t) in $\{y > 0\}$ satisfies:

$$V = \frac{\partial u}{\partial n}.$$

Problem. Show that this system, with the initial condition that D(0) is empty, has a solution for some time interval $0 \le t \le T$, and find the shape of D(t).

Friedman and Velazquez [10] solved this problem. They parametrized $\Gamma(t)$, taking

$$\Gamma(t)$$
: $x = x(t, \lambda), y = y(t, \lambda)$

with $x(0, \lambda)$, $y(0, \lambda) = 0$, subject to the dynamical system

(2)
$$\frac{dx}{dt} = -u_x(x, y, t), \quad \frac{dy}{dt} = -u_y(x, y, t)$$

which captures the free boundary condition.

Their procedure is as follows: Given a family of curves $\Gamma(t)$, solve the elliptic problem for u (where now D(t) is given), and then define a new family of curves by (2). Using potential theoretic estimates they proved that this mapping from one family of curves $\Gamma(t)$ to another has a unique fixed point, which is then precisely the solution of the free boundary problem.

Their calculation also shows that the profile of $\Gamma(t)$, for small t, is as shown in Figure 2.



The figure indicates that the visible image of a uniformly black interval AB ($A = (-a_1, 0)$, $B = (a_1, 0)$) is darker near the edges and lighter in the middle. This is the undesirable «edge effect» phenomenon that is well recognized in electrophotography.

5. SEMICONDUCTOR PROCESSING

In the modeling of semiconductor processing equipment companies such as Motorola encounter a difficult problem: Whereas the transistors laid on a chip are of submicron size, the tools used to produce them are of nearly 100 centimeter size, i.e., nearly six order of magnitude larger. Thus in any mathematical model that describes chemical vapor deposition, the mesh size required at the transistor level will produce unrealistically large number of finite difference or finite element equations.

To overcome this difficulty we shall «homogenize» the small scale features, i.e., average their effective contribution.

To illustrate this approach, consider a simple model of a 2-dimensional domain Ω_{ε} bounded by three lines $x = \pm a$, y = b and by fast oscillating curve $y = \varepsilon f_{\varepsilon}(x, t)$ representing the surface of the thin film, i.e., the surface of the semiconductor. In Ω_{ε} we have

$$\Delta u = 0$$

where u is the concentration of the chemical vapor, and on the boundary of Ω_{ε}

$$\frac{\partial u}{\partial n} = g \text{ on } y = b, \quad \frac{\partial u}{\partial x} = 0 \text{ on } x = \pm a$$

and

$$\frac{\partial u}{\partial n} + pu = 0$$
 on $\Gamma_{\varepsilon}(t): y = \varepsilon f_{\varepsilon}(x,t)$

We assume that

$$p = p\left(x, \frac{x}{\varepsilon}\right), \quad f_{\varepsilon}(x, 0) = f_0\left(x, \frac{x}{\varepsilon}\right)$$

where $p(x, \xi)$, $f_0(x, \xi)$ are 1-periodic in ξ , and ε is a very small parameter (e.g., $\varepsilon = 10^{-6}$). An additional complication arises from the fact that $\Gamma_{\varepsilon}(t)$ is not known in advance, for it depends on the rate of deposition of the chemical vapor on the film surface; the velocity V of the growing surface satisfies the equation

$$\frac{\partial u}{\partial n} = \varepsilon V.$$

Friedman and Hu [1] (see also [3]) proved:

Theorem 3. The above free boundary system has a unique solution, at least for some time T, independent of ε , and the free boundary $\varepsilon f_{\varepsilon}(x, t)$ satisfies:

$$\left|f_{\varepsilon}(x,t)-\hat{f}\left(x,\frac{x}{\varepsilon},t\right)\right| < C\varepsilon$$

where $\hat{f}(x,\xi,t)$ is 1-periodic in ξ ; it can be computed by solving the following problem for $(u_0(x,y,t), \hat{f}(x,\xi,t))$:

 $\Delta u_0 = 0 \quad in \ the \ rectangle \ \Omega_0 = \{ |x| < a, 0 < y < b \},\$

$$\frac{\partial u_0}{\partial x} = 0 \quad on \ x = \pm a, \quad \frac{\partial u_0}{\partial n} = g \quad on \quad y = b,$$
$$\frac{\partial u_0}{\partial n} + Pu_0 = 0 \quad on \quad y = b,$$

where

$$P(x,t) = \int_0^1 p(x,\xi) \left[1 + \left(\hat{f}_{\xi}(x,\xi,t) \right)^2 \right]^{1/2} d\xi$$

and

$$\hat{f}(x,\xi,t) = p(x,\xi) u_0(x,0,t) \left[1 + \left(\hat{f}_{\xi}(x,\xi,t) \right)^2 \right]^{1/2},$$
$$\hat{f}(x,\xi,0) = f_0(x,\xi).$$

This result was used in [2] to compute the best control g (in the condition $\partial u/\partial n = g$ on y = b) which will produce a surface with prescribed profile.

6. ELECTROSTATIC PAINTING

Electrostatic painting systems are commonly used in industry. They achieve significant saving in paint material. In the automobile industry they are used to coat the door panels and the hood. However, since these surfaces are not flat, the coated material does not cover evenly the surface, and this may cause warping of the paint layer.

In order to device painting methods that overcome this phenomenon of uneven paint covering, Ford Motor Company wanted to model and analyze the motion and deposition process of the paint on a workpiece. If the paint particles are viewed as small particles with no collision, then particles dinamics may be used; however this is computationally intensive.

An alternate approach was suggested by Friedman and Huang [4], using (instead of discrete particles) the density of particles, assumed to be continuously spread. If we denote by $\psi(x, t)$ the position of a particle which starts at x at time t = 0, and by P(x, t) the particles density at (x, t), then

$$\frac{d^2\psi(x,t)}{dt^2} = -\Delta\varphi(\psi(x,t),t) \qquad \text{(Newton's law),} \Delta\varphi(x,t) = -P(x,t) \qquad \text{(from Maxwell's equations),} P(x,t) = P_0(\psi^{-1}(x,t)) J(\psi^{-1}(x,t))$$

where φ is the electric potential, $P_0(x)$ is the initial distribution of the density, $\psi^{-1}(x, t)$ is the inverse to $y = \psi(x, t)$, and J is the Jacobian; the last equation is simply the law of conservation of mass.

The above system is to be satisfied in a region bounded above by y = b (from which the paint particles emerge) and below by the surface of the workpiece

$$y = \varepsilon f(x) \quad -\infty < x < \infty, \quad \varepsilon > 0,$$

and

$$\varphi = M$$
 on $y = b$, $\varphi = 0$, on $y = \varepsilon f$.

Friedman and Huang [4] proved, under some conditions, that the above system has a unique solution. Moreover, they computed the thickness of the paint coat in cases of interest. In Figure 3 we see a profile of the workpiece and of the paint coat thickness (not drawn to scale).



We conclude that the convex top of the workpiece gets less paint than the ridge. This is another instance of the «edge effect» we saw earlier in Figure 2.

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