The Iterative Transformation Method and Length Estimation for Tubular Flow Reactors*

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ABSTRACT

In this note we apply an iterative transformation method in order to find the numerical solution and, more important, to provide the numerical evidence of the existence and uniqueness for the free boundary value problem describing the optimal length determination for tubular flow reactors. The main idea is to introduce in the mathematical model a nonphysical parameter and then require partial invariance under an extended stretching group. The solution of the original problem can be obtained by requiring that the parameter transforms in the unity. Finally we report numerical results that show the existence and uniqueness of the solution and give us an approximation to the free boundary value involved.

1. INTRODUCTION

This note is devoted to testing a possible way to investigate numerically the existence and uniqueness of solutions of free boundary value problems.

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The present approach can be used with problems of the type [5]

$$\frac{d^2u}{dx^2} = f\left(x, u, \frac{du}{dx}\right), \qquad x \in (0, s), \tag{1.1a}$$

$$g\left(u(0), \frac{du}{dx}(0)\right) = 0, \qquad u(s) = \beta, \quad \frac{du}{dx}(s) = l(u(s), s), \tag{1.1b}$$

where $f(\cdot, \cdot, \cdot)$, $g(\cdot, \cdot)$, and $l(\cdot, \cdot)$ satisfy appropriate smoothness conditions and s is the unknown free boundary, while

$$u(s) = \beta \quad \text{and} \quad \frac{du}{dx}(s) = l(u(s), s)$$

define the value of s. The interest in numerical investigation of the existence and uniqueness of solutions of the problem (1.1) arises because there are no general theorems about this question.

In this note we will reconsider the engineering problem of determining the optimal length for tubular flow chemical reactors with axial missing [6]. The mathematical model describing an isothermal nth-order reaction in a homogeneous tubular flow reactor is given by

$$\frac{d^2u}{dx^2} = N_{\mathrm{Pe}}\left(\frac{du}{dx} + Ru^n\right), \qquad x \in (0, s), \quad u \in [0, 1],$$

$$u(0) - \frac{1}{N_{\mathrm{Pe}}}\frac{du}{dx}(0) = 1, \qquad u(s) = \tau_1 \quad \frac{du}{dx}(s) = 0. \tag{1.2}$$

In (1.2) x represents the dimensional length $0 \leqslant x \leqslant s$, and $u(x)$ is the ratio of the concentration of reactant at the point x to its concentration at the inlet $x = 0$. N_{Pe} and R are respectively the dimensionless Peclet group and the reaction rate group. The boundary condition at $x = 0$ is due to the axial missing hypothesis [7], τ represents the feed material of reactant at s, $(0 < \tau < 1)$, and the derivative condition at $x = s$ physically means that the reactor is long enough for the reactant to react to form the product [9].

Recently [2, 3], noniterative and iterative numerical transformation methods based on invariance properties were introduced for free boundary value problems. Moreover, interesting applications to real world problems have

been already considered in [2–6]. In [6] it was pointed out that the noniterative transformation method can be used in order to obtain an upper bound for the value of s in (1.2).

In the next section we explain how it is possible to solve the above problem numerically by the iterative transformation method. Moreover, within the numerical process we are able to test, by producing computational evidence, the existence and uniqueness question.

2. ITERATIVE TRANSFORMATION METHOD AND NUMERICAL RESULTS

The iterative transformation method we are going to use was applied first in [2] and formalized in [5]. Essentially we have to introduce a parameter in the mathematical model and to require partial invariance under an extended stretching group. For instance, instead of (1.2) we could consider

$$\frac{d^2u}{dx^2} = \frac{N_{\mathrm{Pe}}}{h}\left(\frac{du}{dx} + Ru^n\right),$$

$$u(0) - \frac{h}{N_{\mathrm{Pe}}}\frac{du}{dx}(0) = 1, \quad u(s) = h^{1/(1-n)}\tau, \quad \frac{du}{dx}(s) = 0, \tag{2.1}$$

where h is the parameter introduced. Then the differential equation and the two boundary conditions at $x = s$ are invariant under the following stretching group:

$$x^* = \lambda^{1-n}x, \qquad u^* = \lambda u, \qquad h^* = \lambda^{1-n}h. \tag{2.2}$$

This means that problems (2.1) with different values of $u(0)$, $du/dx(0)$, and h will transform one into another [1].

Let us explain how it is possible to obtain, for instance, the condition $u(s) = h^{1/(1-n)}\tau$. It is evident that $u(s) = \tau$ was not invariant with respect to (2.2). We would like to have

$$\lambda u(s) = \lambda h^{\theta}\tau \quad \text{and} \quad u^*(s^*) = h^{*\theta}\tau. \tag{2.3}$$

We know that

$$h^* = \lambda^{1-n}h, \qquad \text{and from (2.3)} \quad h^{*\theta} = \lambda h^{\theta}. \tag{2.4}$$

Then from (2.4) it follows that

$$\theta(1-n)=1. \tag{2.5}$$

Now, in order to solve the problem (2.1), we can set and fix a value of $s^*>0$ and we can choose a value of $h^*\neq 0$. Therefore we have the boundary conditions we need at s^* in order to integrate numerically inwards in $[0, s^*]$ and to compute

$$\lambda = u^*(0) - \frac{h^*}{N_{\mathrm{Pe}}}\frac{du^*}{dx^*}(0). \tag{2.6}$$

Then from (2.2) it follows that

$$s=\lambda^{n-1}s^*. \tag{2.7}$$

Naturally, in order to obtain the numerical solution of (1.2), we have to find a zero of the function

$$\Gamma(h^*)=\lambda^{n-1}h^*-1. \tag{2.8}$$

We note here that if we fix the value of s^*, as we have to do, then λ will be a function of h^* only; i.e., $\lambda=\lambda(h^*)$. So we don't know the functional form of $\Gamma(\cdot)$.

The existence and uniqueness of the solution of the problem (1.2) will correspond to having only one root of (2.7). No root means nonexistence, and more than one root nonuniqueness. Therefore we can also use a root finder like the secant method [10].

Let us report an application of the ideas developed in the above text. We will consider values of the parameters involved in (1.2) as follows:

$$N_{\mathrm{Pe}}=6, \qquad R=2, \qquad \tau=0.1, \qquad n=2. \tag{2.9}$$

Table 1 lists a selected range of values that confirm the existence and uniqueness of the solution.

When h^* is small compared with unity, numerical instability was observed on reducing the constant step size to $-1\text{D}-05$ and $-1\text{D}-06$. However, $\Gamma(h^*)$ seems to be monotone decreasing for both $s^*=0.5$ and

TABLE 1[a]

h^*	$\Gamma(h^*)$	h^*	$\Gamma(h^*)$
−0.75	−5984.613063	0.16	1058.154587
−0.76	−1368.9906	0.161	255.721316
−0.77	−503.795863	0.1625	74.200431
−0.78	−235.621159	0.165	22.313065
−0.79	−127.433666	0.17	5.859518
−0.795	−97.422061	0.175	2.476156
−0.8	−76.021749	0.18	1.214805
−0.85	−12.843959	0.19	0.238909
−0.9	−4.425216	0.2	−0.144528
−0.95	−2.300024	0.3	−0.742239
−1.0	−1.567991	0.5	−0.840414
−2.0	−0.913088	1.0	−0.876699
−5.0	−0.90409	5.0	−0.895951
−1.D01	−0.902009	1.D01	−0.897993
−1.D03	−0.90002	1.D03	−0.89998

[a]Here we used $s^* = 1.0$. The step size was $\Delta x = -1\text{D}-04$.

$s^* = 1.0$ (see Table 1). Moreover, Table 1 shows that the function (2.7) has only one root. More integrations were made in order to exclude any other possible root of $\Gamma(h^*)$.

Tables 2 and 3 report iterations computed with a secant method. The values of s and of $du/dx(0)$ reported are in agreement respectively within two and three decimal places with that obtained in [6].

TABLE 2[a]

k	h_k^*	$\Gamma(h_k^*)$	$u(0)$	$\frac{du}{dx}(0)$	s
0	0.09	1.188592			
1	0.08	609.404812			
2	9.0D−02	1.182214	0.745998	−0.698378	12.120779
3	9.0D−02	1.175891	0.746341	−0.699462	12.083047
4	0.093661	0.397904	0.796571	−0.873146	7.462572
5	9.55D−02	0.177273	0.814778	−0.943989	6.162865
6	9.7D−02	4.45D−02	0.826964	−0.993969	5.383979
7	9.75D−02	6.51D−03	0.830652	−1.009514	5.161555
8	9.76D−02	2.81D−04	0.831266	−1.012121	5.125101
9	9.76D−02	1.86D−06	0.831293	−1.012238	5.123469
10	9.76D−02	5.32D−10	0.831293	−1.012239	5.123458
11	9.76D−02	1.03D−15	0.831293	−1.012239	5.123458

[a]$s^* = 0.5$; $\Delta x = -1\text{D}-03$.

TABLE 3[a]

k	h_k^*	$\Gamma(h_k^*)$	$u(0)$	$\frac{du}{dx}(0)$	s
0	0.18	1.202268			
1	0.19	0.235257			
5	0.195249	4.02D−05	0.83128	−1.012281	5.121882
6	0.19525	8.29D−08	0.83128	−1.012298	5.121648
7	0.19525	3.41D−12	0.83128	−1.012298	5.121648

[a] $s^* = 1$; $\Delta x = -1\text{D}-03$.

In all numerical integration we used the classical Runge–Kutta method of fourth order with constant step size. Moreover, reduction of step size was utilized to check the accuracy of the numerical results; see [8].

Application of the present methodology to an ill-posed free boundary value problem describing a nonlinear dynamical context is given in [5].

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