F_{AO} = input flow rate of ammonia kmol/h
(i) = surface concentration of ith component
k = rate constant for dissociation reaction, kmol/m^3·h·(Pa)$^{-0.5}$
k_o = preexponential factor, k mol/m^3·h·(Pa)$^{-0.5}$
P = total pressure, Pa
r_A = rate of reaction, kmol ammonia dissociated/h·kg catalyst
R = gas constant, kJ/kmol·K
T = temperature of reaction, K
W = weight of catalyst, kg
X_A = kmol ammonia dissociated/kmol ammonia feed
y_i = mole fraction of component i

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A Lagrangian Finite Element Method for the Simulation of Flow of Newtonian Liquids

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INTRODUCTION

In the Lagrangian description, the fluid mechanical equations are formulated as an initial value problem. Thus, at an initial instant the location and velocity of all fluid particles are considered known, and the subsequent motion of the particles is then followed. An advantage of this description is that the transient motion of a free surface is described in a particularly simple fashion. Another possible advantage is that the nonlinear convective terms are absent, which means that it is simple to construct a stable implicit forward integration method.

The method described here is related to that of Hirt, Cook and Butler (1970) who used a Lagrangian method to solve the Navier Stokes equations. These authors, however, used a finite difference method; as a result their method for the application of boundary conditions is somewhat complicated. By contrast the finite element method enables a particularly simple application of the boundary conditions, both no-slip and slip conditions as well as free surface conditions. Thus Frederiksen and Watts (1981) have formulated a finite-element method for time-dependent incompressible flow, but these authors use the Eulerian formulation of the Navier Stokes equations. In the following it will be demonstrated how a simple Lagrangian finite element method may be implemented for an incompressible Newtonian liquid.

FLUID MECHANICAL EQUATIONS

At an initial time, t_0, the space coordinates of all fluid particles to be considered are denoted x_i^0 $(i = 1,2,3)$. The set of numbers (x^0,t_0) therefore denotes a particular fluid particle. Now for each fluid particle (x^0,t_0), we wish to solve for the space coordinates $x_i = x_i(x^0,t_0,t)$, the Lagrangian velocity field $u_i = u_i(x^0,t_0,t)$ and the pressure field $p = p(x^0,t_0,t)$ as a function of time t for $t \geq t_0$. These variables are determined from the solution of the following initial value problem:

$$\frac{\partial}{\partial t} x_i(x^0,t_0,t) = u_i \qquad (i = 1,2,3) \tag{1}$$

$$\rho \frac{\partial}{\partial t} u_i(x^0,t_0,t) = -\frac{\partial}{\partial x_i} p + \mu \sum_{m=1}^{3} \frac{\partial^2}{\partial x_m \partial x_m} u_i + \rho g_i \qquad (i=1,2,3) \tag{2}$$

$$0 = \sum_{m=1}^{3} \frac{\partial}{\partial x_m} u_m \tag{3}$$

with

$$(x_i,u_i) = (x_i^0,u_i^0) \text{ at } t = t_0 \tag{4}$$

Equation 1 is the definition of the Lagrangian velocity field. Equations 2 and 3 are the conservation equations for incompressible Newtonian liquids. To prove the latter statement introduce the Eulerian velocity field $v_i(x,t) = u_i(x^0,t_0,t)$ for $x_i = x_i(x^0,t_0,t)$ where v_i is a function of the independent variables x_i and t. As a result of the change of independent variables when going from u_i to v_i their time derivatives must be related through the use of the chain rule for partial differentiation, which yields:

$$\frac{\partial}{\partial t} u_i(x^0,t_0,t) = \frac{\partial}{\partial t} v_i(x,t) + \sum_{m=1}^{3} v_m(x,t) \frac{\partial}{\partial x_m} v_i(x,t) \qquad (5)$$

When v_i is substituted for u_i and the expression in Eq. 5 is substituted for $(\partial/\partial t)\, u_i$ in Eqs. 2 and 3 these equations are then recognized as the familiar equations of conservation of momentum and mass for an incompressible Newtonian liquid (Bird, Stewart and Lightfoot, 1960). Notice that the terms to the right of the equality signs in Eqs. 2 and 3 have been formulated for convenience in terms of derivatives with respect to the dependent variables x_i.

DISCRETIZATION METHOD

In order to implement a numerical solution procedure for the Lagrangian formulation we need to discretize time and *material*. This is in contrast to a numerical solution of an Eulerian formulation, where one would discretize time and *space*. At the initial instant, t_0, we introduce a finite element grid which spans the liquid that we wish to include in the simulation. In the particular program we use linear quadrilateral elements (Cook (1974)). This means that each nodal point represents a fluid particle, and the motion of the liquid is simulated by following the motion of each nodal point. The motion of an arbitrary fluid particle initially in a given element is determined by the specification that the particle remains in the same element at all times with unchanged element coordinates. The result of this interpolation is that the x_i and u_i change linearly along the element boundaries and bilinearly inside each element. The pressure field must be chosen one order lower than the velocity field and is therefore constant in each element in this approximation. A Galerkin principle similar to that of Tanner, Nickell and Bilger (1975) is used to convert the differential expressions on the right sides of Eqs. 2 and 3 into a set of algebraic expressions. If we collect the nodal velocities in the vector U and the element pressures in the vector P and collect all these variables in the global vector $Y = (U,P)$ then the result of the application of the Galerkin principle can be written in the form:

$$A\dot{Y} = -SY - B \qquad (6)$$

where the dot denotes a time derivative. The elements of the matrices A and S and of the vector B depend on the nodal coordinates collected in the vector X. Equation 1 is converted into

$$\dot{X} = U \qquad (7)$$

Equations 6 and 7 together with an initial condition on (X,Y) may now be solved by any forward integration method. For reasons of numerical stability we have chosen simple implicit or semiimplicit Euler integration methods. Since the elements of A, S and B are functions of the nodal coordinates, the solution in each time step will usually involve an iteration, which however has been found to be rapidly convergent in all test examples considered. The creeping motion solutions correspond to $\rho = 0$, and with the use of a fully implicit method these solutions are obtained in a single iteration.

SOLUTION OF TWO PLANE FLOW PROBLEMS

Solitary Waves

Consider a channel of length 60 L initially filled with liquid to a depth of 6 L, where L is a unit of length. A rectangular coordinate system with x-axis in the direction of the channel and y-axis in the vertical direction is defined with an origin such that initially the liquid is contained in the space $0 \le x \le 60\,L$, $0 \le y \le 6\,L$. No-slip conditions are imposed at the bottom ($y = 0$). Free slip conditions are imposed at the left constraint (initially at $x = 0$) and the right constraint (at $x = 60\,L$). A free surface condition is imposed at the top (initially at $y = 6\,L$). The liquid has viscosity 1 M/LT and density 1 M/L^3 where M and T are units of mass and time respectively. A gravitational acceleration of $2\,L/T^2$ is imposed in the negative y-direction. A solitary wave (Miles, 1980) is generated by moving the left constraint in the positive x-direction with velocity $2\,L/T$ from time $t = 0$ to $t = 3T$ at which time the motion of the constraint is stopped. The displaced hump of fluid then moves as a solitary wave through the channel, and is seen at time $t = 12.6\,T$ in Figure 1. The velocity of the wave, c, at this instant as calculated from successive time steps is $3.50\,L/T$. This differs only about 1.7% from the value $3.56\,L/T$ computed from the wave height H, the liquid depth h and the gravitational acceleration g according to the Boussinesq theory (Miles, 1980):

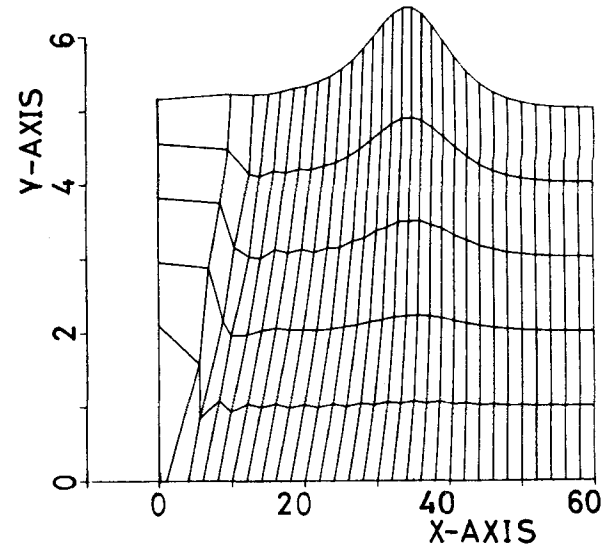

Figure 1. Propagating solitary wave. Liquid viscosity 1 *M/LT* and density 1 *M/L*^{3}. Gravitational acceleration 2 *L/T*^{2}. Note that the figure has been drawn with unequal scales in the two coordinate directions.

$$c = \sqrt{g(h + H)} \qquad (8)$$

The Boussinesq theory applies to an inviscid liquid, and the good agreement with the present computations therefore demonstrates the ability of the program to simulate flow situations with large inertial terms. The Boussinesq theory predicts a wave shape symmetrical around the plane of maximum height, whereas this simulation shows a wave that is steeper on the front than on the back in agreement with the experimental observations of Goring (1978).

Transient Entrainment

In the transient entrainment problem we consider the withdrawal of a vertical plate from a long fluid bath of finite depth. Initially the fluid is a rest and occupies the region $0 < x < D$, $0 < y < d$ where $D \gg d$. The boundary at $y = d$ is a free surface, and the boundaries at $y = 0$ and at $x = D$ are stationary with no-slip conditions. No-slip conditions are also imposed on the boundary at $x = 0$ and this boundary is moved in the positive y-direction with speed u for times $t > 0$. Figure 2 shows the location of the free surface in a simulation for a liquid of viscosity 1 M/LT and density 1 M/L^3. The gravitational accleration is $0.5{\cdot}10^{-2}\,L/T^2$, the bath has dimensions $d = 1\,L$ and $D = 10\,L$ and the left boundary is

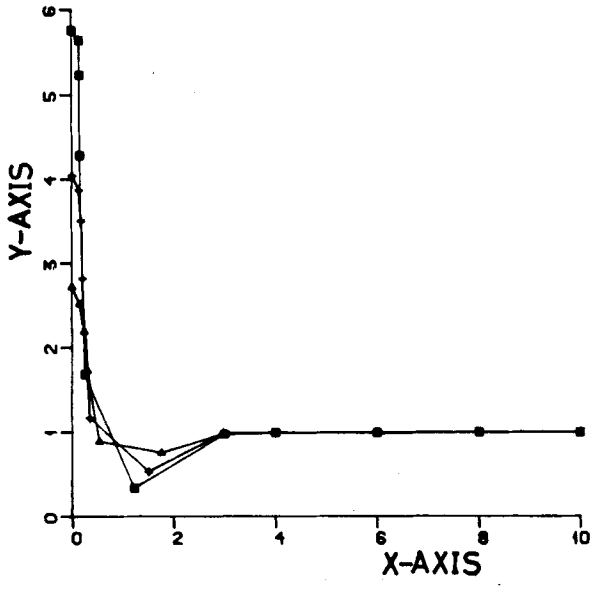

Figure 2. Shape of free surface in transient entrainment after onset at time $t = 0$ of motion of left boundary in the positive y-direction with speed 0.1 L/T. The surface is indicated by the location of the surface nodal points at three times (Δ: $t/T = 17.1$, + $t/T = 30.4$, □ $t/T = 47.6$). Liquid viscosity 1 M/LT and density 1 M/L^3. Gravitational acceleration $0.5 \cdot 10^{-2}$ L/T^2, no interfacial tension.

moving with speed $u = 0.1\ L/T$. The surface is shown at times t/T = 17.1, 30.4, 47.6. The simulation shows that a film of constant thickness approximately 0.15 L is rapidly formed. The general shape of the surface is in agreement with Frederiksen and Watts (1981). Notice in particular the growing indentation of the liquid close to the film surface, which indicates that the vertical surface in this situation is withdrawn too rapidly for a steady state to be established.

DISCUSSION

A Lagrangian finite element method for the solution of initial value flow problems with Newtonian liquids has been described. Although the two particular flow problems considered have a relatively simple geometry, it would be very simple to simulate the flow in much more complicated geometries.

In many chemical engineering flow situations it is important to know whether a steady state flow solution is stable or even possible. An advantage of the Lagrangian, initial value formulation is that no separate stability analysis is necessary. If a steady-state solution is reached through a transient process, then this solution is stable. For example in the transient entrainment simulation performed above it appears from the growing indentation that no steady-state solution is reached with the high entrainment velocity used. Other simulations have been performed which show an approach to steady-state entrainment, and these steady-state solutions are stable solutions.

The element program has been extended to include surface tension and higher order elements, and promising simulations of the wavy interface of a liquid film falling on a vertical wall are currently being performed.

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NOTATION

A = global "mass" matrix
B = global "load" vector
c = celerity of solitary wave
d = initial depth of liquid bath (entrainment)
D = length of liquid bath (entrainment)
g_i = component of gravitational acceleration vector
H = solitary wave height
h = depth of liquid in solitary wave tank
L = unit of length
M = unit of mass
P = global vector of element pressures
p = hydrostatic pressure
S = global "stiffness" matrix
t = time
t_0 = initial time
T = unit of time
u_i = component of Lagrangian velocity
U = global vector of node velocities
v_i = component of Eulerian velocity
x = set of coordinates x_i, (i = 1,2,3)
x_i = coordinate of particle at time t
x^0 = set of coordinates x_i^0, (i = 1,2,3)
x_i^0 = coordinate of particle at time t_0
X = global vector of node coordinates
Y = global element vector

Greek Letters

μ = viscosity
ρ = density

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