The object of this column is to enhance our readers' collection of interesting and novel problems in chemical engineering. Problems of the type that can be used to motivate the student by presenting a particular principle in class, or in a new light, or that can be assigned as a novel home problem, are requested as well as those that are more traditional in nature, which elucidate difficult concepts. Please submit them to Professor H. Scott Fogler, ChE Department, University of Michigan, Ann Arbor, MI 48109.

MODELING OF HEAT TRANSFER WITH CHEMICAL REACTION

Cooking a Potato

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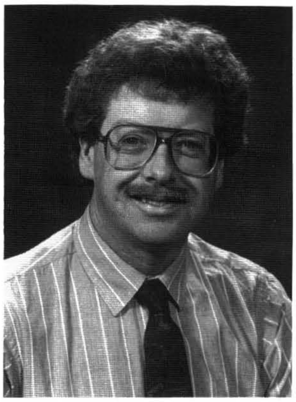
PROBLEM

The cooking of a potato in a hot water bath may be readily described by combining a model of transient heat transfer in a sphere (with convective boundary conditions) and kinetic data given by Personius and Sharp [1] for the rate of change in tensile strength in potato tubers as a function of temperature. A computer program may be written which uses finite difference methods to solve the transient heat transfer equation. When these results are combined with kinetic data, transient tensile strength profiles may be generated. The cooking of the potato can therefore be simulated. The model is readily verified with a minimum of laboratory time and equipment.



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CHEMICAL BASIS: COOKING A POTATO

Roughly 60-80% of the dry matter of a potato tuber is starch. Potato starch is a mixture of two polymers of α-D-glucose, amylose and amylopectin. Amylose (20% of potato starch) is a linear unbranched chain of α-D-glucose units joined by $\alpha(1 \rightarrow 4)$ acetal linkages. Amylopectin is a branched polysaccharide with $\alpha(1 \rightarrow 6)$ branch points. Native amylose and amylopectin polymers have molecular weights in the millions.

Within the potato tuber, starch occurs as microscopically visible granules which are 15-100 microns in diameter and oval in shape. Thin sections of starch granules reveal them to be highly organized consisting of concentric layers. Within these layers, starch molecules associate through extensive hydrogen bonding between parallel linear segments.

The microscopic appearance of starch granules changes markedly upon heating. In cold water, isolated starch granules will take up 20-30% of their weight in water. This association is reversible *i.e.*, the granule can be recovered in its original state upon drying. At about 65°C, starch granules will swell rapidly, taking up large amounts of water (up to 25 times the original weight of the granule). This swelling process, termed gelatinization, is irreversible. Heating disrupts regional hydrogen bonding between adjacent starch segments, replacing starch-starch association with starch-water association. Upon cooling, the hydrated segments are no longer free to hydrogen bond to other starch segments. Starch granules in plant tissue undergo gelatinization upon heating by taking up cellular water and/or water from their environment if heated by steam or hot water.

The individual potato cell is surrounded by a rigid cell wall consisting principally of cellulose interwoven with pectins. Cellulose is a high molecular weight polysaccharide in which the repeating unit is β-D-glucose. Pectins are a complex mixture of polysaccharides of galacturonic acid or its methyl ester. These pectic substances are regarded as the cementing substances which hold plant cells together.

The softening that occurs upon cooking of fruits and vegetables is partially the result of depolymerization of pectic substances. Depolymerization of pectins occurs in all types of cooking processes. The common observation that potatoes cook faster when immersed in water than if steamed or baked is attributed to diffusion of pectin degradation products out of the tissue and their solubilization in the cooking water.

When potatoes are cooked, the starch they contain is gelatinized and the water contained within the cell is adsorbed in the process. The cells become filled by swollen starch granules, applying pressure to the cell wall if sufficient starch granules are present. The cell walls of individual cells normally remain intact; however, weakening of the cell walls by depolymerization of pectins makes the cell wall somewhat flexible. Therefore, if sufficient starch is present, the cell (which is normally box-like in shape) becomes roughly spherical. The change in shape further weakens the cementing forces which bind cells together by limiting surface-surface contact.

A potato which is regarded as being of high quality for cooking will have a mealy texture upon being baked, boiled, steamed or fried. Mealiness is that quality of being soft, dry, and easily crumbled. Mealiness in a cooked potato results from an ease of separation of individual cells. A good cooking quality potato will therefore be one which contains a high proportion of cells which possess sufficient starch content to cause cellular and interstitial water to be adsorbed and to cause distortion of the cell shape to something more spherical when gelatinization takes place. The absence of sufficient starch leads to a hard, soggy texture even after cooking. In addition, a high quality cooking potato will have a high proportion of cells which are small enough to resist rupturing when the cooked tuber is mashed. Rupturing of cells results in release of swollen starch granules which gives the cooked potato a sticky, waxy texture.

The cooking of a potato in a hot water bath may be readily described by combining a model of transient heat transfer in a sphere (with convective boundary conditions) and kinetic data for the rate of change in tensile strength in potato tubers as a function of temperature.

KINETICS OF COOKING A POTATO

Personius and Sharp [1] have examined the adhesion of potato tuber cells as influenced by temperature. In their experiments, whole potato tubers were coated with a thin layer of rubber paint and held in a constant temperature water bath. The rubber paint prevented the exchange of water and salts between the tuber and water bath. Thermocouples measured the temperature of the potato centers. After the potato centers reached the temperature of the water bath, potato tubers were removed at various times and the tensile strength of sections was obtained.

From data reported by Personius and Sharp, the rates of decrease in tensile strength as a function of incubation temperature were determined in order to prepare an Arrhenius plot (see Figure 1). The primary assumption made here was that these rates are roughly equivalent to those which would have been

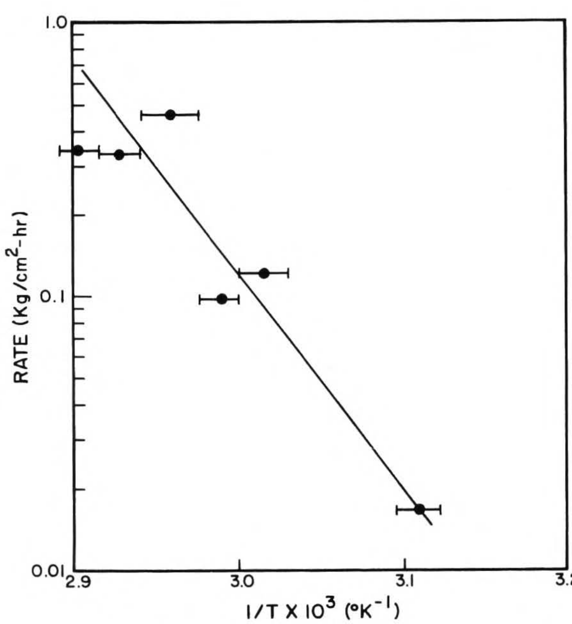


FIGURE. 1. Arrhenius plot of data of Personius and Sharp [1]

observed if the potatoes warmed to the incubation temperatures instantly. The effect of heat during warming time on these rates is unknown.

The rate equation for the cooking process may be expressed as follows

$$-\frac{d(TS)}{dt} = k\ f(x) = k_o\ e^{-E_a/RT}\ f(x) \qquad (1)$$

where
- TS = tensile strength (kg/cm^2)
- k = a rate constant
- k_o = frequency factor
- E_a = energy of activation
- R = universal gas constant
- T = temperature (°K)
- $f(x)$ = some function of the condition of the potato, assumed to be constant during the cooking process

In logarithmic form the rate equation becomes

$$\ell n \left(-\frac{d(TS)}{dt}\right) = \frac{-E_a}{RT} + \ell n \left(k_o\ f(x)\right) \qquad (2)$$

From the Arrhenius plot the energy of activation and the factor $[k_o f(x)]$ were determined to be 32500 cal/mole and 2.85×10^{20} kg/cm^2-hr, respectively. Substituting these values into the rate equation and integrating we have

$$TS_o - TS_t = \left[2.85 \times 10^{20} \exp\left(\frac{-1.64 \times 10^4}{T}\right)\right] t \qquad (3)$$

where
- TS_o = tensile strength at t = 0
- TS_t = tensile strength at time t
- T = temperature (°K)
- t = time (hrs)

Based on data presented by Personius and Sharp, a value of 6.8 kg/cm^2 may be taken as the average tensile strength of a raw potato tuber (TS_o).

Personius and Sharp noted that the limiting value of the tensile strength of a potato heated in a constant temperature water bath was somewhat dependent upon the incubation temperature. Above 73°C the limiting tensile strength was 0.4 kg/cm^2. Below 49°C relatively little change in tensile strength occurred over long periods of incubation. Between 49°C and 73°C there was observed to be a linear relationship between incubation temperature and limiting tensile strength. In this range the limiting tensile strength can be given by Eq. (4), derived from the data given by Personius and Sharp

$$TS_l = -0.24\ T_i + 17.8 \qquad (4)$$

where
- TS_l = limiting tensile strength (kg/cm^2)
- T_i = incubation temperature (°C)

SOLUTION

Modeling the Cooking of a Potato

The process to be modeled is the cooking of a potato in a hot water bath under conditions of forced convection. Transient temperature profiles in the potato may be produced by numerical solution of Eq. (A1) (see Appendix) which describes unsteady-state heat conduction in a sphere of constant thermal conductivity, heat capacity and density, heated by a surrounding fluid. The numerical solution of this equation is detailed in the Appendix utilizing the Crank-Nicolson finite difference method. Coupling this solution with the integrated form of the rate equation describing the change in tensile strength in a potato tuber as a function of time and temperature (Eq. 3) allows transient tensile strength profiles to be generated.

A FORTRAN program which produces transient tensile strength profiles in a cooking potato is available from the author. The program incorporates the following assumptions:

- **The potato is spherical with a diameter of 3 inches.**
- **The heat capacity and thermal conductivity of the potato are assumed to be approximately that of water (the potato is roughly 80% water).**
- **The specific gravity of the potato is approximately 1.08.**
- **The potato is coated with a thin layer of rubber paint or rubber cement to prevent loss of salts or exchange of water with its environment (a requirement for validity of Personius and Sharp's data).**

The basic sequence of calculations in this program is as follows (see appendix):

1. The cooking temperature and value of the parameter hR_o/k are assigned. Under conditions of forced convection the heat transfer coefficient, h, is estimated to be 700-2000 W/m^2-°C using the correlation given by Vliet and Leppert [2]. These values correspond to a relative fluid velocity over the sphere of 0.1-1.0 ft/s. It may be readily demonstrated that temperature profiles in the cooking potato are relatively insensitive to hR_o/k when $hR_o/k > 40$. For

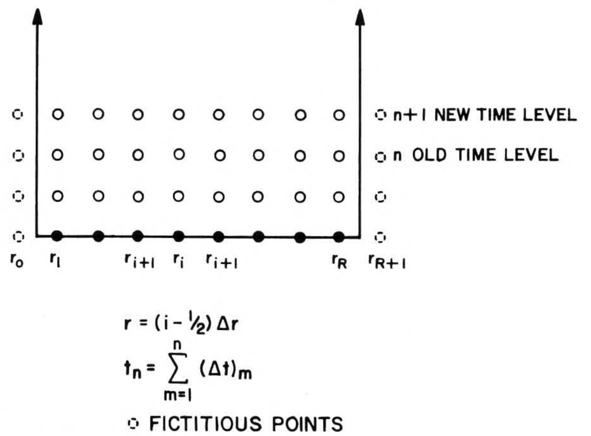


FIGURE 2. Grid points for finite difference calculations

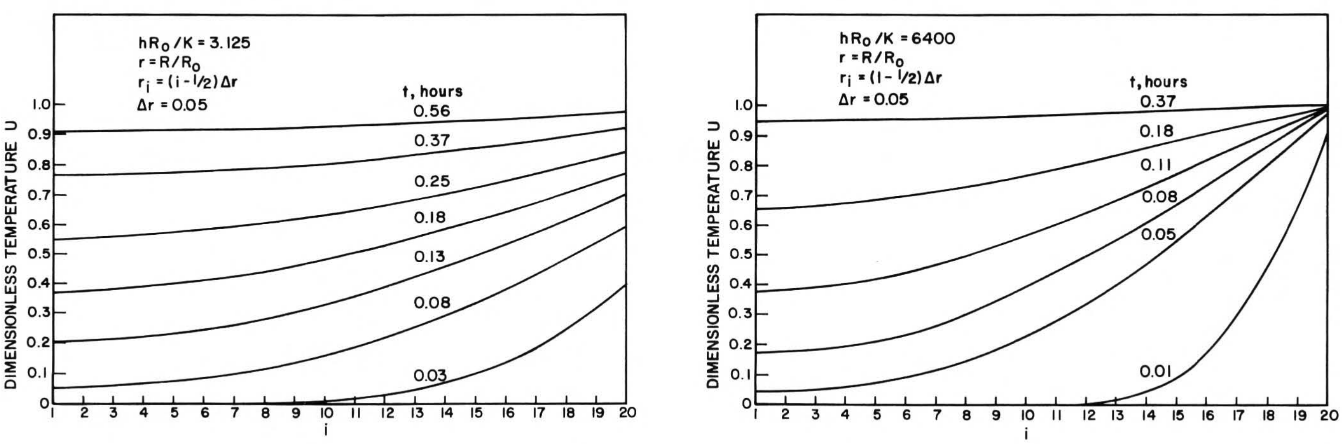
a 3 in. diameter potato with a thermal conductivity equal to that of water, this corresponds to a heat transfer coefficient of 540 W/m^2-°C.

2. As shown in Figure 2, n is the time level index and i the index of points in space where the dimensionless temperature u and the subsequent tensile strength are calculated by the program. Initially the dimensionless temperatures $u_{i,0}$ for i=1,20 are set to zero and tensile strengths set to 6.8 kg/cm^2, the average tensile strength of a raw potato. Each set of dimensionless temperatures $u_{i,n}$ are then calculated in turn (n=1,2,3,...) from the finite difference equation described in the Appendix. At all points i for each set of time levels n and n+1 the average temperature (TAVG) between the "old" and "new" time levels is calculated.
3. Utilizing Eq. (3) the change in tensile strength (ΔTS) at each point i which results from cooking at TAVG for a length of time equal to the Δt between the nth and (n+1)th time level is then calculated. At each point i these changes in tensile strength are added to all of those changes in tensile strength which took place between t=0 and the nth time level. These summations for all points i are then subtracted from 6.8 kg/cm^2, the tensile strength of a raw potato tuber. The result is then the tensile strength at all points i at the (n+1)th time level.
4. Next the lower limits are applied to the tensile strength at any point i at the (n+1)th time level according to the cooking temperature (TAVG) over the time interval of n to n+1. If TAVG < 49°C, the lower limit of TS is 6.8 kg/cm^2. If TAVG > 73°C, the lower limit is 0.4 kg/cm^2. If 49°C < TAVG < 73°C, the lower limit is given by Eq. (4).
5. The (n+1)th time level becomes the nth level and calculations are repeated giving tensile strength profiles as a function of radial distance from the center and time.

Sample outputs of dimensionless temperature and tensile strength profiles from this program are shown graphically in Figure 3(a-b) and Figure 4(a-b), respectively, for a 3 in. diameter potato cooking at 90°C with hR_o/k of 3.125 and 6400.

Testing the Model

Figure 4(b) may be taken as the predicted tensile strength profiles in a 3 in. potato cooking at 90°C in a hot water bath under conditions of forced convection (hR_o/k > 40). To test the model, ten Idaho baking



(a) ***(b)***

FIGURE 3. Transient dimensionless temperature profiles in a potato cooking at 90°C. hR_o/K = (a) 3.125, (b) 6400

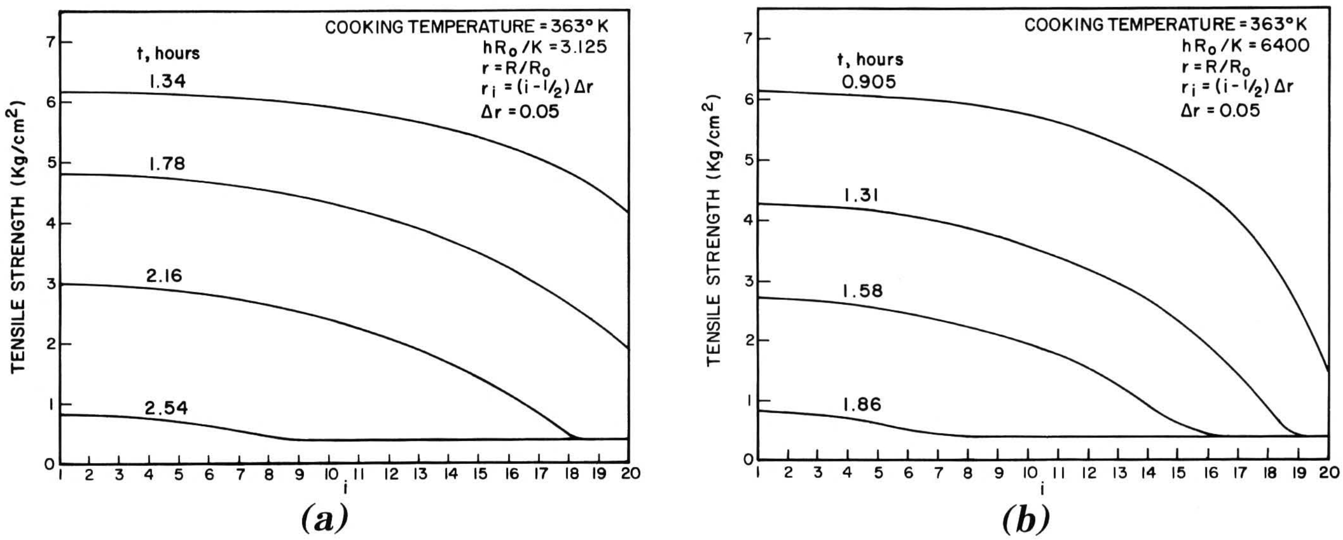


FIGURE 4. Transient tensile strength profiles in a potato cooking at 90°C. hR_o/K = (a) 3.125 (b) 6400

potatoes were coated with a thin layer of rubber cement and heated in a water bath at 90°C. Water was circulated by means of a propeller stirrer. Potatoes were chosen to be as nearly spherical as possible and approximately 3 in. in diameter. The potatoes chosen were more accurately described as oblong measuring two by three inches. Potatoes were removed periodically, cut in half and an assessment made of the texture at various locations. The following observations are typical

Time (hours)	Observation
0	cooking started
0.25	outmost 0.1-0.3 cm cooking
0.50	outmost 0.5 cm mealy
0.75	outmost 0.8 cm mealy
1.00	cooking throughout but outmost 1-1.2 cm mealy
1.25	outmost 2 cm mealy
1.50	outmost 2.6 cm mealy
1.67	mostly cooked, still hard in center
1.75	potato cooked and mealy throughout

These results are in good agreement with the predictions of the model as given by Figure 4(b).

CONCLUSION

In the proposed problem/experiment students couple transient heat transfer with reaction kinetics to predict the course of the gelatinization of starch in a cooking potato. Students are introduced to numerical methods for the solution of partial differential equations and computer simulation of a chemical reaction under nonisothermal, unsteady-state conditions. Students can readily use the model to make predictions and test the validity of those predictions in the laboratory with a minimum of time and equipment.

The proposed modeling exercise combines skills in mathematics, computer programming, heat transfer, and kinetics. The problem is challenging but manageable by a senior chemical engineering student.

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3. von Rosenberg, D., "Methods for the Numerical Solution of Partial Differential Equations," Gerald L. Farrar & Associates, Tulsa OK (1969).

APPENDIX
Temperature Profiles in a Cooking Potato

The cooking of a potato in a water bath may be modeled after that of a sphere of constant thermal conductivity (k), density (ρ), and heat capacity (C_p) heated by a surrounding fluid. The differential equation for the temperature distribution, u(r,t), in the sphere is given by Eq. (A1)

$$\frac{\partial^2 u}{\partial r^2} + \frac{2}{r}\frac{\partial u}{\partial r} = \frac{\partial u}{\partial t} \qquad \text{(A1)}$$

The boundary and initial conditions are

$$u = 0 \qquad \text{for } t = 0, \text{ all } r$$

$$\frac{\partial u}{\partial r} = 0 \qquad \text{for } r = 0, \text{ all } t$$

$$\frac{hR_o}{k}(1 - u) - \frac{\partial u}{\partial r} = 0 \qquad \text{for } r = 1, \text{ all } t$$

h = coefficient of heat transfer between the surface of the sphere and the bulk fluid

u, r and t are all dimensionless parameters defined as follows

$u = \frac{T - T_i}{T_\infty - T_i}$ where T_∞ = bulk temperature of the fluid surrounding the sphere

T_i = initial temperature of the sphere

$r = \frac{R}{R_o}$ where R_o = radius of the sphere

R = distance from the center of the sphere

$t = \frac{k}{R_o^2 \rho C_p} \hat{t}$ where $\hat{t}$ = real time

Eq. (A1) with accompanying boundary conditions may be solved numerically utilizing the Crank-Nicolson finite difference method. The two independent continuous variables (r and t) are replaced by discrete variables (also called here r and t) defined at points located on the grid shown in Figure 2.

The following finite difference analogs may be written

$$\left(\frac{\partial u}{\partial t}\right)_{i,n+1/2} = \frac{u_{i,n+1} - u_{i,n}}{\Delta t}$$

$$\left(\frac{\partial^2 u}{\partial r^2}\right)_{i,n+1/2} = \frac{1}{2}\left(\frac{u_{i+1,n} - 2u_{i,n} + u_{i-1,n}}{(\Delta r)^2} + \frac{u_{i+1,n+1} - 2u_{i,n+1} + u_{i-1,n+1}}{(\Delta r)^2}\right)$$

$$\left(\frac{\partial u}{\partial r}\right)_{i,n+1/2} = \frac{1}{2}\left(\frac{u_{i+1,n} - u_{i-1,n}}{2(\Delta r)} + \frac{u_{i+1,n+1} - u_{i-1,n+1}}{2(\Delta r)}\right)$$

Making these substitutions in Eq. (A1) results in the following finite difference analog

$$u_{i-1,n+1} + u_{i,n+1}\left[\frac{-2(\Delta t) - 2(\Delta r)^2}{\Delta t}\left(\frac{i - 1/2}{i - 3/2}\right)\right] + u_{i+1,n+1}\left(\frac{i + 1/2}{i - 3/2}\right)$$

$$= - u_{i-1,n} + u_{i,n}\left[\frac{2(\Delta t) - 2(\Delta r)^2}{\Delta t}\left(\frac{i - 1/2}{i - 3/2}\right)\right]$$

$$+ u_{i+1,n}\left[-\left(\frac{i + 1/2}{i - 3/2}\right)\right]$$

This equation applies for $2 \le i \le (R\text{-}1)$. In writing this equation for i = 1 or i = R, terms involving fictitious points ($u_{0,n+1}$ and $u_{0,n}$ or $u_{R+1,n}$ and $u_{R+1,n+1}$, respectively) are produced. Writing finite difference analogs for the boundary equations allows these terms to be eliminated.

$$\left(\frac{\partial u}{\partial r}\right)_{1/2,n} = \frac{u_{1,n} - u_{0,n}}{2} = 0$$

for all n. Therefore

$$u_{0,n} = u_{1,n} \quad \text{and} \quad u_{1,n+1} = u_{0,n+1}$$

For i = 1 we have then

$$u_{1,n+1}\left(\frac{3\Delta t + 2(\Delta r)^2}{\Delta t}\right) - 3u_{2,n+1} = u_{1,n}\left(\frac{2(\Delta r)^2 - 3\Delta t}{\Delta t}\right) + 3u_{2,n}$$

$$\frac{hR_o}{k}(1 - u) - \frac{\partial u}{\partial r} = 0$$

becomes

$$\frac{hR_o}{k}\left[1 - \frac{u_{R,n} + u_{R+1,n}}{2}\right] - \left[\frac{u_{R+1,n} - u_{R,n}}{\Delta r}\right] = 0$$

for all n. Replacing hR_o/k with $\hat{k}$ gives

$$u_{R+1,n} = u_{R,n}\left[\frac{\hat{k}\Delta r - 2}{-\hat{k}\Delta r - 2}\right] - \left[\hat{k} \Big/ \left(\frac{-\hat{k}\Delta r - 2}{2\Delta r}\right)\right]$$

for all n.

Therefore for i = R we have

$$u_{R-1,n+1} + u_{R,n+1}\left[\frac{-2\Delta t - 2(\Delta r)^2}{\Delta t}\left(\frac{R - 1/2}{R - 3/2}\right) + \frac{\hat{k}\Delta r - 2}{(-\hat{k}\Delta r - 2)}\left(\frac{R + 1/2}{R - 3/2}\right)\right]$$

$$= - u_{R-1,n} + u_{R,n}\left[\frac{2\Delta t - 2(\Delta r)^2}{\Delta t}\left(\frac{R - 1/2}{R - 3/2}\right) + \frac{\hat{k}\Delta r - 2}{(-\hat{k}\Delta r - 2)}\left(-\frac{R + 1/2}{R - 3/2}\right)\right]$$

$$+ 2\left(\frac{R + 1/2}{R - 3/2}\right)\frac{2\Delta r\,\hat{k}}{(-\hat{k}\Delta r - 2)}$$

At each time level (where t > 0) R equations may be written containing R unknowns. Furthermore these equations constitute a tridiagonal matrix. Equations of this form are readily solved for u as a function of r and t by the Thomas algorithm [3]. □

REVIEW: Multiphase Science

Continued from page 197.

Chapter Four is a review of a reboiler. The authors struck a balance between practical application and scientific analysis by discussing both the design strategy and the appropriate correlations used for thermal-hydraulic analysis. The authors recommend that a set of several design equations be presented and a comparison be made of the relative merit of each for particular design applications.

Chapter Five covers flow of gas-solid mixtures through standpipes and valves. In this chapter, most attention was devoted to the flow regimes of solid-gas in standpipes, which include four basic types: type I fluidized flow and type II fluidized flow, PACFLO and TRANPACFLO, and the combination thereof.

The gas-solid flow in a standpipe is still a subject with incomplete knowledge. The authors made an effort to introduce the subject in a rational manner. The readers can use this review as a good start to understand not only gas-solid flow in standpipes but may also find it inspirational in trying to understand other multi-phase flow systems.

Chapter Six deals with core-annular flow of oil and water through a pipeline. The motivation of such special flow is to find a reduction of pressure drop for pumping heavy, viscous oil through a pipe using water in annular as a "lubricant." Thus, the authors proposed their lubricating-film model. In this model, the main features are the inclusion of core eccentricity and the ripple lubricating film. The validity range of core-velocities for the lubricating-film model was given. The authors also proposed some possible ways of improving the models and predictions. □