DYNAMIC MODELS
FOR
INSTRUCTION AND EXPLORATION
IN
CHEMISTRY

COOLING CUP OF COFFEE II

BY

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EDITOR' NOTES (January 2002): Al Powers was one of the earliest high school teachers to embrace system dynamics as a valuable tool with which to stimulate students' thinking and analysis. His contributed curricular units are typically marvelous guides that provide a wealth of opportunities, suggestions, and support for other teachers and their students without pushing those folks into a lock-step progression of activities. In reviewing this unit, we made conscious effort to change as little as possible, restricting ourselves largely to:

1. Provide models of the scenarios he describes. We provide those models in both STELLA5 and STELLA7 versions, in separate folders.
2. We also, in hindsight, have questioned one equation in the final model. That is documented toward the end of the unit and our suggested modification is utilized in the final model of the packets.

Dynamic Models for Instruction and Exploration in Chemistry is a collection of interactive computer models intended for use in introductory chemistry programs. Each model clarifies fundamental chemical concepts and encourages their exploration by simulating the dynamic behavior of carefully selected systems.

These models have been developed using STELLA II v. 2.2.2 software[1] and contain

- structural diagrams that identify essential system components and their interrelationships.
- equations needed to define the quantitative behavior of each component and its impact on the entire system.
- animated, graphical, and tabular representations of system behavior with interpretive material.
- suggestions for instruction and for enrichment activities.

They are unique in their ability to enhance student understanding and appreciation of chemical systems. Features which contribute to this uniqueness include

- spatial relationships of system components that will have appeal for students who find it difficult to contemplate systems that they cannot observe directly.
- quantitative relationships that are clearly defined and are accompanied by documentation intended to facilitate fundamental understanding and to encourage manipulation of variables.
- dynamic simulations of the behavior of all parameters that may be selected individually or in combination and viewed graphically or in tabular format as desired by the learner.

The intuitive qualities of STELLA II are truly empowering and provide a platform for learner–directed learning that not only effectively generates insight and mastery, but is also grand fun! Although you may choose to have your students simply view and interpret the behavior generated by these models, you will likely encounter an irresistible urge to modify and explore the models further. This activity should always be encouraged. Of course, backup the models and graphs first!

Computer simulations make it no longer necessary to rely solely upon discrete, initial and final state observations and calculations to generate understanding. However, <u>they must never be implemented as a substitute for direct observations of chemical interactions in the laboratory</u>. Such experiences offer excitement, relevance, insights, and skills unattainable by other means.

Use these models as part of a balanced program to provide a dynamic introduction to chemistry that promises to reach many who might otherwise find it too abstract, elusive and, therefore, perhaps uninteresting. Then share your experiences and those of your students with others by communicating them to the author directly or through the Creative Learning Exchange.[2]

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[1] High Performance Systems, Inc., 45 Lyme Rd., Hanover, NH 03755

[2] Creative Learning Exchange, 1 Keefe Rd., Acton, MA 01720

Table of Contents

I. Introduction

The cooling behavior of a cup of coffee was first introduced as a subject for computer modeling and systems education by Roberts, et al.[3] More recently, Chung[4] used this system as a tool for differentiating and clarifying the behaviors of constant flow and flow influenced by negative feedback. After incorporating much of Chung's work, *Cooling Cup of Coffee II* transforms the model into an investigative tool that guides students through a careful, stepwise analysis of the structure and behavior of a physical system and provides a stimulus for learner–directed study in the laboratory.

When students are asked what will happen to a hot cup of coffee if it sits for an extended time at room temperature, they will normally respond, "It'll get cold." If pushed a bit further, they may state that heat will flow out into the room. Part II (Linear Heat Loss) includes a model and simulation results for a system so described.

If students follow the construction and simulation of this model with an experimental determination of the actual cooling behavior of a real cup of coffee, they will find that their real–world results do not conform to those generated by the simulation. Having exposed the incomplete nature of their model and, therefore, their thinking, they are confronted with a need for a more precise articulation of system structure.

Part III (Nonlinear Heat Loss Due to Decreasing Heat Content) includes a feedback structure that might evolve if the students concentrate on the fact that a decreasing level of heat in the coffee will be accompanied by a decreasing rate of heat loss. This second model generates a behavior that reflects the laboratory data more closely but still possesses a serious flaw. It fails to stabilize at room temperature!

Finally, analysis and group discussion should eventually lead to the incorporation of the gap between the coffee and room temperatures as a regulator for the outflow of energy from the coffee as shown in Part IV (Nonlinear Heat Loss Regulated by the Temperature Gap). This modification generates cooling behavior that resembles student laboratory observations quite closely.

Part V (A Model for Exploration) contains modifications to the model that are intended to encourage explorations of the system's dependence upon parameters such as coffee mass, specific heat, varying starting temperatures, and even ambient cooling breezes! These activities can be easily designed and conducted by students on the computer and in the laboratory and are implemented best in an open—ended format. In addition to clarifying fundamental concepts, they provide a unique introduction to the mutually supportive roles of theoretical modeling and laboratory investigation.

This paper does not contain detailed, step–by–step, lessons because such detail discourages creative thinking and exploration. Study this resource carefully and then use your own professional abilities to generate an approach that is effective for your program and your students. Modifications such as providing students with preconstructed models, are easy to accomplish and can make this activity appropriate for a wide range of grade levels, student abilities, and scheduling parameters.

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[3] Roberts, N., Anderson, D., Deal, R., Garet, M., Shaffer, W., Introduction to Computer Simulations, Addison Wesley, Reading, MA 1983.

[4] Chung, C., A Cooling Cup of Coffee: An Introduction to Constant Outflow and Negative Feedback, MIT System Dynamics in Education Project, D-4292-1, MIT, Cambridge, MA 1993.

II. Linear Heat Loss

A. Model Structure

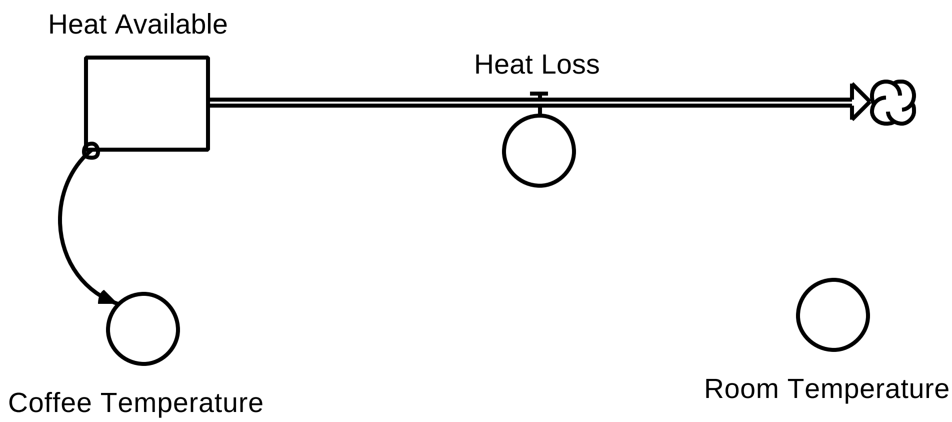

Figure 1. Linear heat flow model

The heat energy available is included in Figure 1 as the stock because Joules of energy flow into and out of systems rather than degrees Celsius. The coffee temperature is calculated within the converter. Neither temperature values have impact on the behavior of this system as modeled. The distinction between heat energy available and temperature is important and frequently confuses students. Hopefully, this model structure will help them grasp this concept more fully.

B. Equations

Heat_Available(t) = Heat_Available(t - dt) + (- Heat_Loss) * dt
INIT Heat_Available = 210000
DOCUMENT: The energy supply is initialized at 210,000 Joules to be consistent with the needs of the final model (Part IV).

Heat_Loss = 3000
DOCUMENT: This factor is selected to give a cooling period of approximately 1 hour. The final flow units are Joules/minute.

Coffee_Temperature = (Heat_Available -105400)/(4.184*250)
DOCUMENT: This provides 104,600 J of energy which, when divided by the specific heat of water ($4.184 \frac{J}{g°C}$) and the mass of 1 cup of water (250 g), gives a starting temperature of 100°C.

Room_Temperature = 25
DOCUMENT: The room temperature is set at 25°C by convention.

C. Simulation and Interpretation

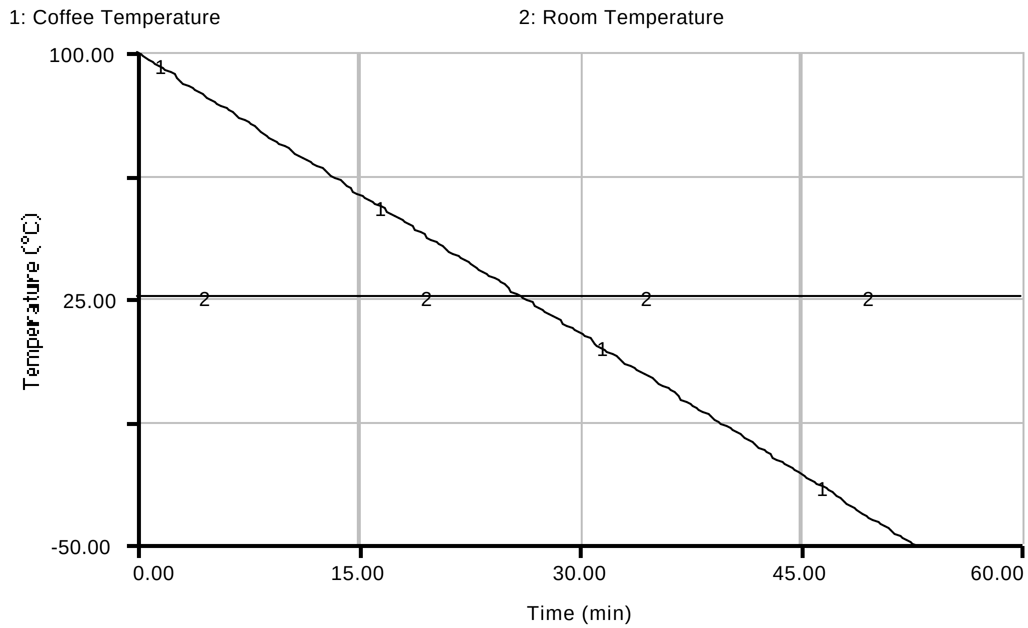

Figure 2. Simulation of temperature change as a result of a linear heat loss.

Figure 2 illustrates the linear outflow of energy that results from the absence of a feedback process. Clearly, this pattern will conflict with student laboratory data not only with respect to its linearity, but also in its extension to values well below room temperature. The presence of both behaviors should compel students to re–evaluate the original model. A possible revision is depicted in Part III.

III. Nonlinear Heat Loss Due to Decreasing Heat Content

A. Model Structure

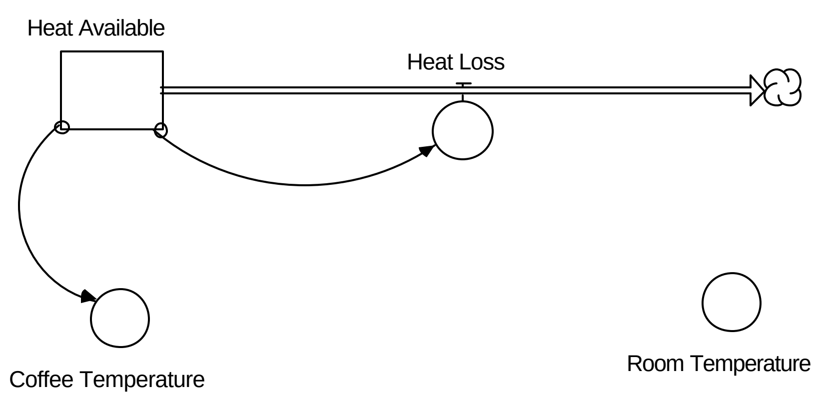

Figure 3. Model for nonlinear heat loss dependent upon heat available.

In Figure 3, the connector between Heat Available and Heat Loss establishes the negative feedback loop that would result if heat loss were controlled by the decreasing availability of energy.

B. Equations

Heat_Available(t) = Heat_Available(t - dt) + (- Heat_Loss) * dt
INIT Heat_Available = 210000
DOCUMENT: This is initialized at 210,000 Joules to be consistent with the model in Part IV.

Heat_Loss = Heat_Available*.1
DOCUMENT: This includes a feedback structure reflecting the decreasing energy of the stock. The multiplying factor functions as a proportionality constant and is selected to permit cooling and stabilization within a 60 minute time period. The final units are Joules/min.

Coffee_Temperature = (Heat_Available-105400)/(4.184*250)
DOCUMENT: This provides 104,600 Joules of energy which will give a starting temperature of 100°C for 250 g of coffee with a specific heat of 4.184 $\frac{J}{g°C}$.

Room_Temperature = 25
DOCUMENT: Room temperature is set at 25°C by convention.

C. Simulation and Interpretation

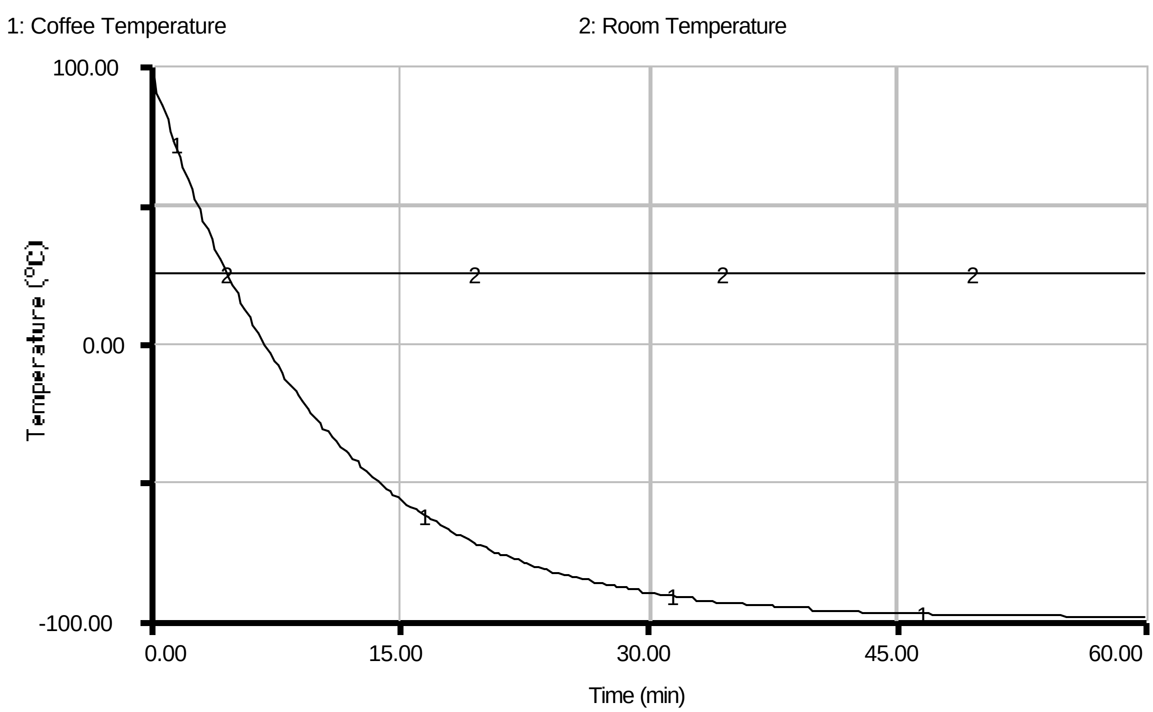

Figure 4. Temperature change due to heat loss dependent upon heat available.

Figure 4. illustrates the exponential temperature decline that results from the negative feedback connection between heat available and heat loss within the model (Figure 3.) This brings the simulation behavior one step closer to the behavior students should experience in the laboratory. However, the temperature still does not stabilize at the room value. Instead, it continues to drop to values well below room temperature. (The stabilization at -100°C occurs because of the depletion of the energy arbitrarily provided within the stock.) This behavior is corrected in Part IV.

IV. <u>Nonlinear Heat Loss Regulated by the Temperature Gap</u>

A. Model Structure

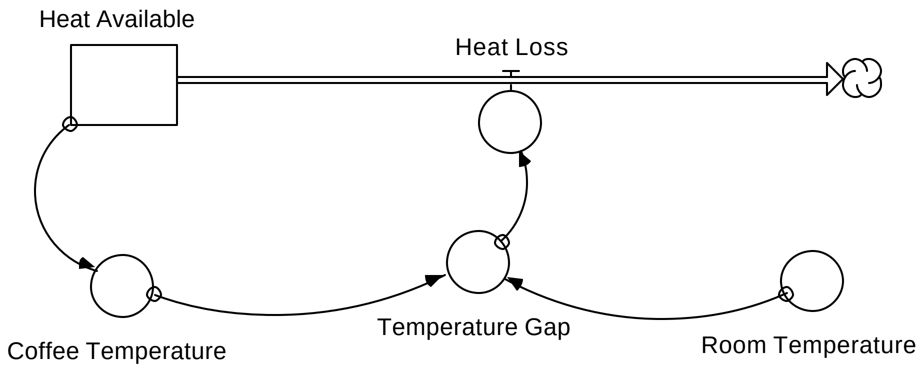

Figure 5. Model for nonlinear heat loss dependent upon the temperature gap.

In Figure 5, the feedback loop has been modified to include the controlling influence of the temperature differential existing between coffee and room temperature values. This is the first model of the series that incorporates temperature as anything other than a calculation of convenience.

B. Equations

Heat_Available(t) = Heat_Available(t - dt) + (- Heat_Loss) * dt
INIT Heat_Available = 210000
DOCUMENT: This stock is initialized with 210,000 Joules to be consistent with the value in Part IV.

Heat_Loss = Temperature_Gap*100
DOCUMENT: The heat loss is proportional to the temperature gap. The figure of 100 serves as a proportionality constant and has the units of J/°C.

Coffee_Temperature = (Heat_Available - 105400)/(4.184*250)
DOCUMENT: This calculation provides 104,600 Joules of energy which will start the simulation at 100°C for 250 g of coffee.

Room_Temperature = 25
DOCUMENT: The room temperature is set at 25°C by convention.

Temperature_Gap = Coffee_Temperature-Room_Temperature
DOCUMENT: The temperature gap is the difference between the coffee temperature and the room temperature. The flow will be reduced as this value approaches zero.

C. Simulation and Interpretation

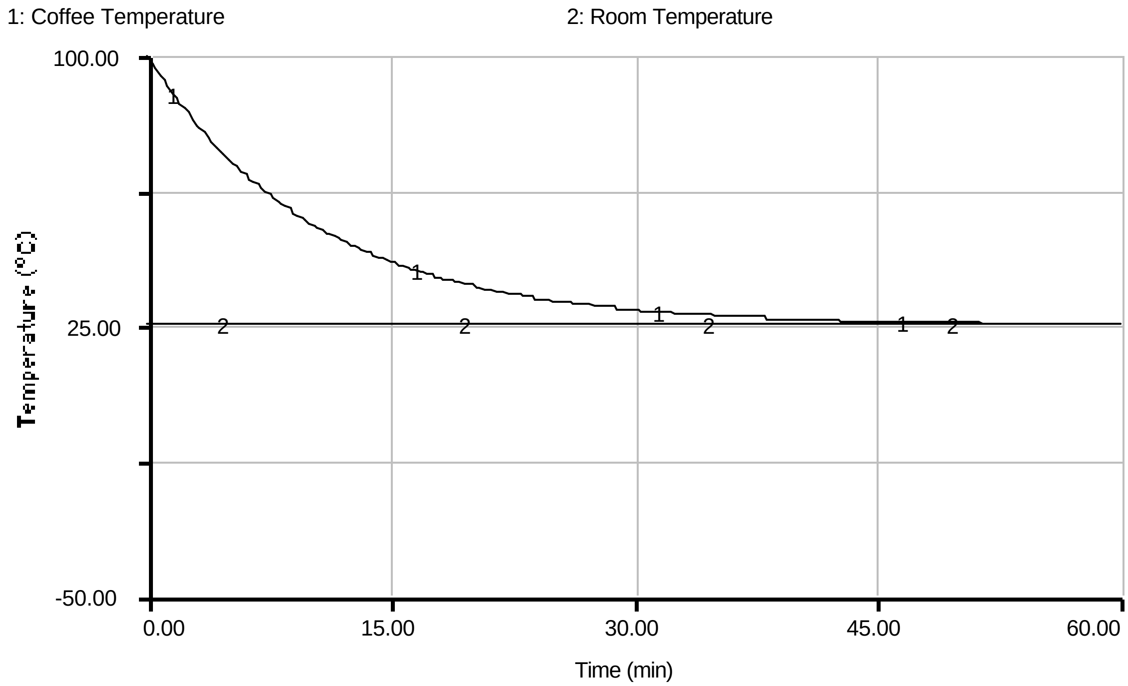

Figure 6. Temperature change due to heat loss dependent upon the temperature gap.

Finally, the simulation results depicted in Figure 6 conform quite well with the cooling behavior students should observe in the laboratory. The exponential temperature decline with stabilization at room temperature should be a consistent feature in all student laboratory work. The rate of change will, however, be dependent upon such factors as the insulating characteristics of their containers, mass of coffee, and air currents. Part V includes some model refinements that will encourage and facilitate student exploration of these influencing factors.

V. A Model for Exploration

A. Model Structure

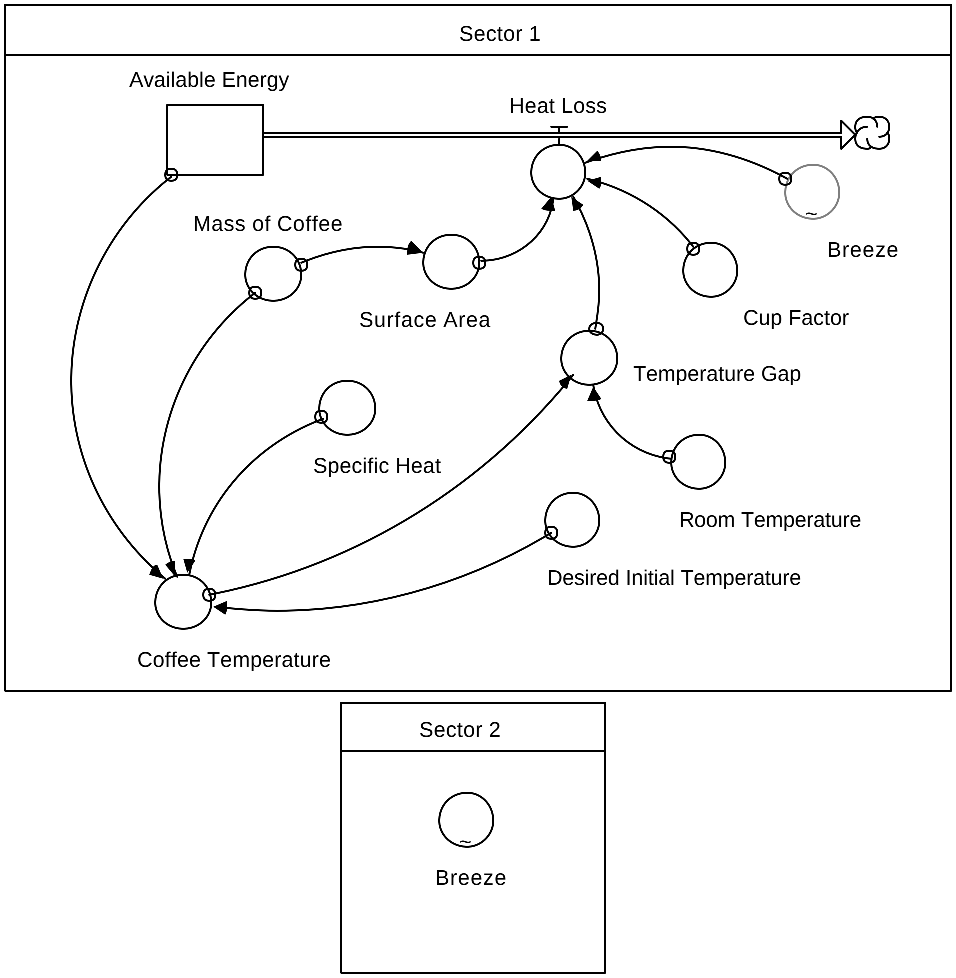

Figure 7. Exploratory model

The model depicted in Figure 7 has been created to encourage further exploration of cooling behavior. The mass, specific heat, desired starting temperature, surface area, cup factor, and breeze (activated only if Sector 2 is selected with Sector 1) converters facilitate the varying of these factors singly or in any combination. The sensitivity capability in the STELLA II application provides a convenient method for simulating the effect of changing values.

A cycle of prediction, simulation, laboratory study, and reconciliation of differences (including changing the model, if appropriate) will support the development of new insights, inquiry skills, and creative thinking skills.

B. Equations

Available_Energy(t) = Available_Energy(t - dt) + (- Heat_Loss) * dt
INIT Available_Energy = 210000
DOCUMENT: The energy source has been initialized with 210,000 J. This will allow simulations containing up to 500 mL of water with a starting temperature of 100°C. Excess energy in this source will not impact the behavior of the runs.

Heat_Loss = Temperature_Gap*Cup_Factor*Surface_Area*Breeze
DOCUMENT: The rate of heat loss is proportinal to surface area, temperature gap, insulating characteristics of the mug, and breezes. The final units are J/min.

Coffee_Temperature = If (Mass_of_Coffee*Specific_Heat* Desired_Initial_Temperature)/(Specific_Heat*Mass_of_Coffee) = 210000 then (Available_Energy - (210000-(Mass_of_Coffee*Specific_Heat* Desired_Initial_Temperature)))/(Specific_Heat*Mass_of_Coffee) else 210000/(Specific_Heat*Mass_of_Coffee)
DOCUMENT: This calculation determines the number of Joules remaining in the stock after providing the designated starting temperature for any mass of coffee = 500 g. It then subtracts this value from the total Joules available. This gives the actual number of Joules contained in the liquid at the start of the simulation. The temperature is calculated by dividing the Joules in the liquid by both the specific heat and the mass of the liquid.

> *EDITORS' NOTE: The first expression of this equation:*
> *"(Mass_of_Coffee * Specific_Heat * Desired_Initial_Temperature)/(Specific_Heat * Mass_of_Coffee)" simplifies to: "Desired_Initial_Temperature," which is certainly not what Powers intended.*
> *A more useful expression is provided and used in the final model we provided in this package:*
> *(Mass_of_Coffee * Specific_Heat * Desired_Initial_Temperature)*

Cup_Factor = .15
DOCUMENT: The cup factor incorporatates the insulating characteristics of the hypothetical coffee mug and a proportionality constant. These are a function of exposed surface area and temperature. The units for this term are $\frac{J}{cm^2 °C}$.

Desired_Initial_Temperature = 100
DOCUMENT: This is set at 100°C but may be varied between 25°C and 100°C.

Mass_of_Coffee = 250
DOCUMENT: 1 cup of coffee is approximately 250 mL or 250 g. The energy source contains sufficient energy to warm 500 g of coffee to 100°C. Using larger masses of coffee will result in lower starting temperatures.

Room_Temperature = 25
DOCUMENT: The room temperature has been set at 25°C by convention.

Specific_Heat = 4.184
DOCUMENT: The specific heat of water (4.184 $\frac{J}{g°C}$) is used. The behavior of substances with specific heats other than this value can be simulated simply by inserting the desired figure in place of the value for water.

Surface_Area = ((Mass_of_Coffee/250)*193)+44)
DOCUMENT: 250 g of coffee will fill a 3.75 cm radius mug to a 8.2 cm depth. The lateral surface area (2prh) will be approximately 193 cm^2 and the top surface area (pr^2) will be approximately 44 cm^2. The surface area calculation used in this model will be reasonably good for no more than 300 g of coffee. After that, the mug proportions will change.

Temperature_Gap = Coffee_Temperature-Room_Temperature
Breeze = GRAPH(time)(0.00, 1.00), (10.0, 1.00), (20.0, 1.91), (30.0, 1.00), (40.0, 1.00), (50.0, 1.00), (60.0, 1.00), (70.0, 1.00), (80.0, 1.00), (90.0, 1.00), (100, 1.00), (110, 1.00), (120, 1.00)
DOCUMENT: This is a graphical input that enables the simulation of an ambient breeze effect upon the cooling pattern. The breeze behavior can be varied by modifying the graph. It is activated only upon running the entire model. It will not be activated if Sector 1 is run alone.

C. Simulation and Interpretation

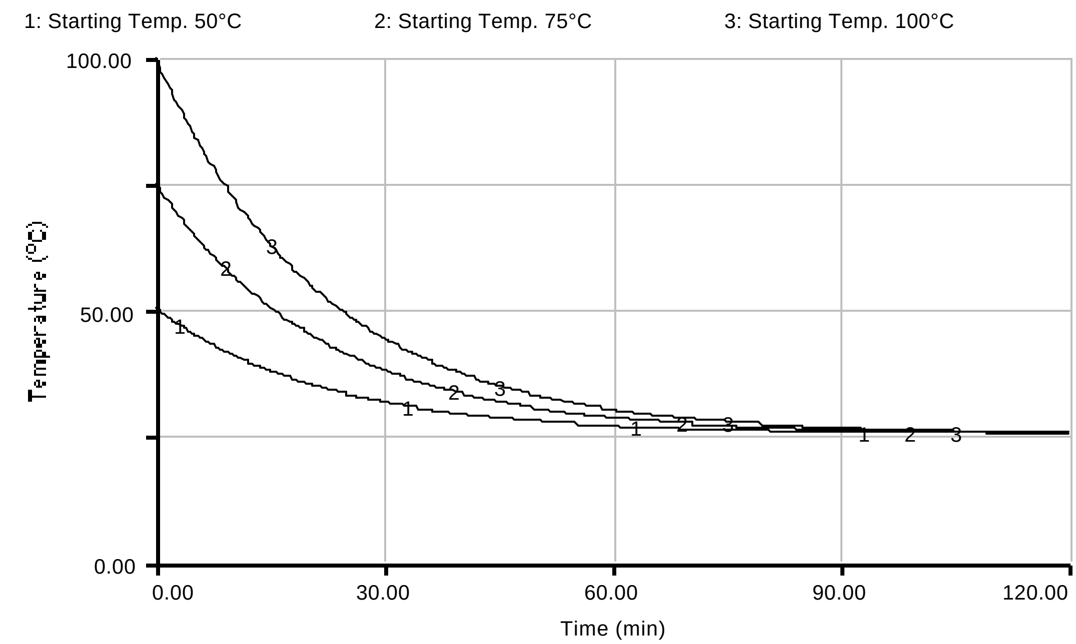

Figure 8. The variation in cooling rate relative to starting temperature.

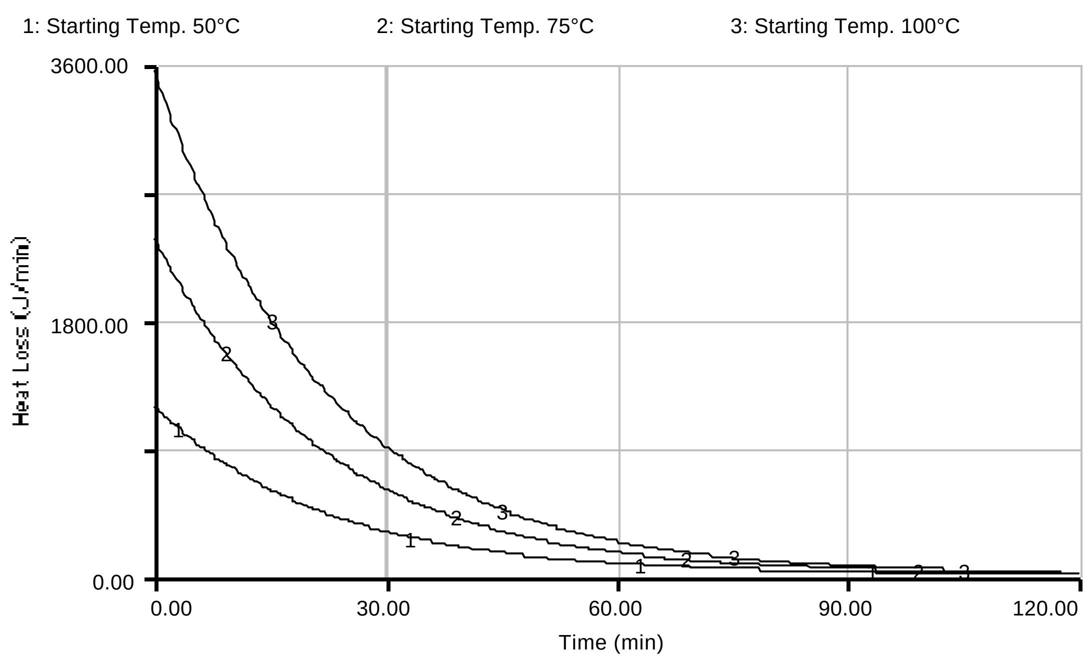

Figure 9. The variation in rate of energy loss relative to starting temperature.

Figures 8 and 9 (previous page) illustrate the simulated changes in temperature and heat loss commencing with three different starting temperatures (50°C, 75°C, and 100°C). A valuable lesson in energy conservation resides within these graphs. The warmer solution remains warmer through most of the cooling period but possesses a higher heat loss rate than a cooler solution. Clearly, a hot water heater set at 140°F will be cheaper to maintain than one set at 160°F!

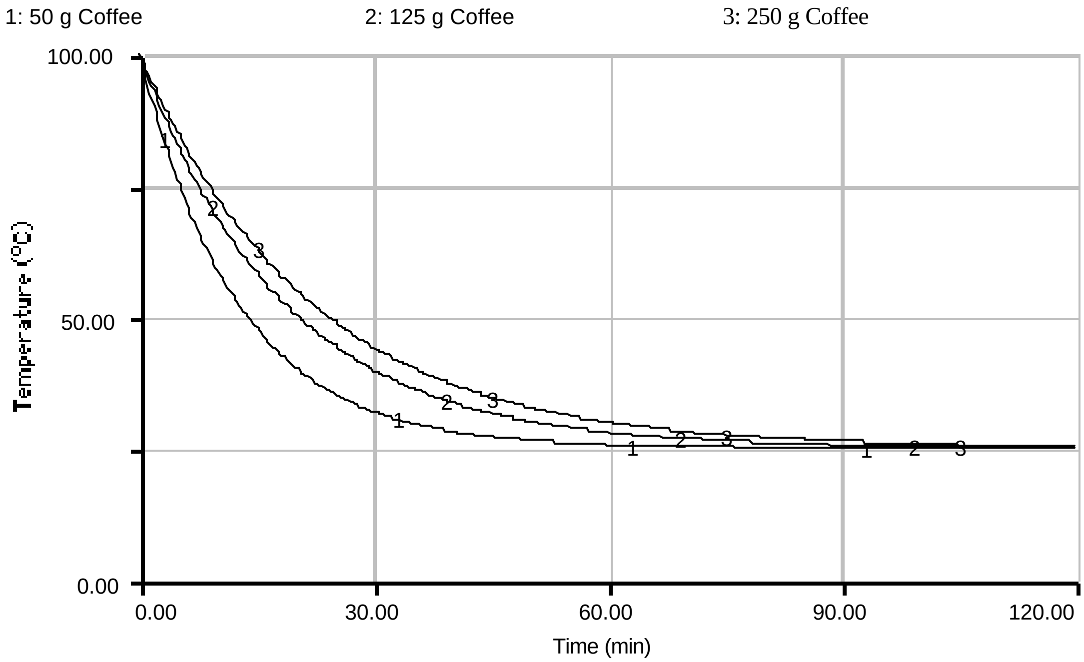

Figure 10. The variation in cooling rate for samples of varying masses.

Figure 10 illustrates the effect of mass upon the cooling pattern. The modeling of this relationship, in particular, requires very careful thought. Clearly, the cooling rate of the coffee depends upon mass and specific heat. But exactly <u>how</u> <u>does</u> it depend upon these parameters? Analyses of laboratory data and alternative model structures have resulted in the constructions used in this paper. The mass and specific heat influence the rate of change in coffee temperature through the coffee temperature converter. The coffee temperature is then used to calculate a temperature gap relative to the room temperature. It is this temperature differential that directly controls the rate of heat loss.

The quantity of coffee in the mug does, however, alter the surface area available for cooling. This influence has been incorporated by calculating the lateral and top surface area that 250 g of coffee would possess in an ordinary mug (see equations). The lateral component of this value is then multiplied by a ratio of the actual mass to the 250 g reference and combined with the top surface area to produce an area factor for the final heat loss determination.

The cup factor incorporates a proportionality constant as well as the mass and thermal characteristics of the cup. An interesting project might involve the study of the influence of various container materials and shapes upon cooling rate. Is there an ideal shape for minimizing heat loss? Perhaps, you know the answer already. However, students might find the results quite interesting.

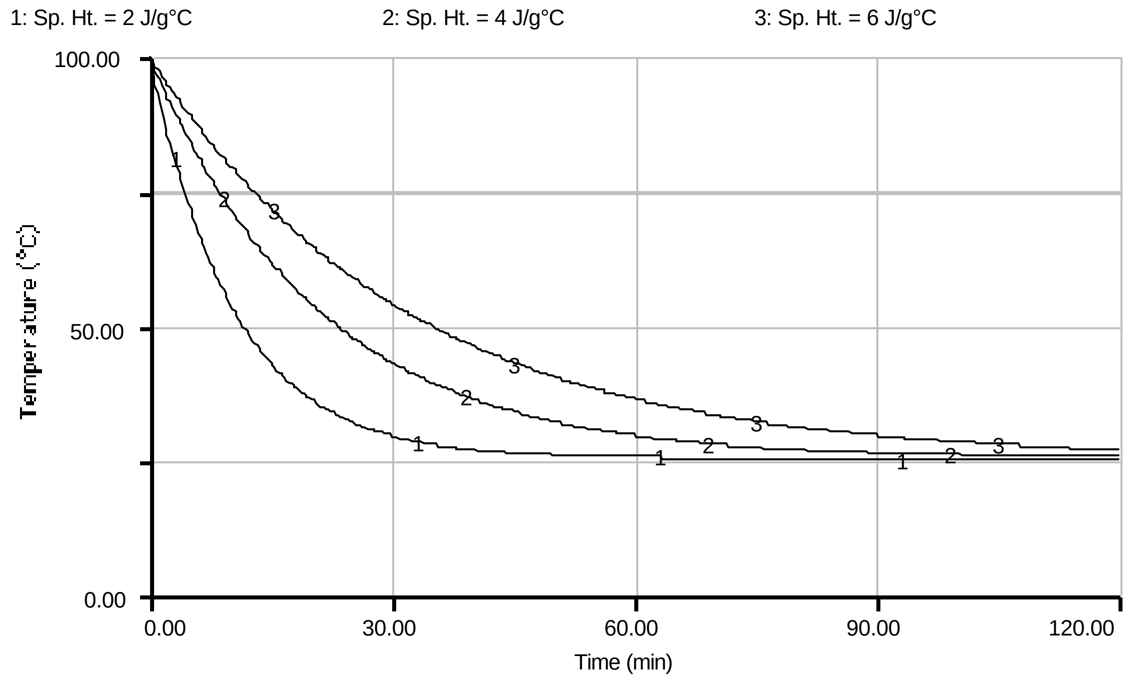

Figure 11. The cooling behaviors of solutions having different specific heat values.

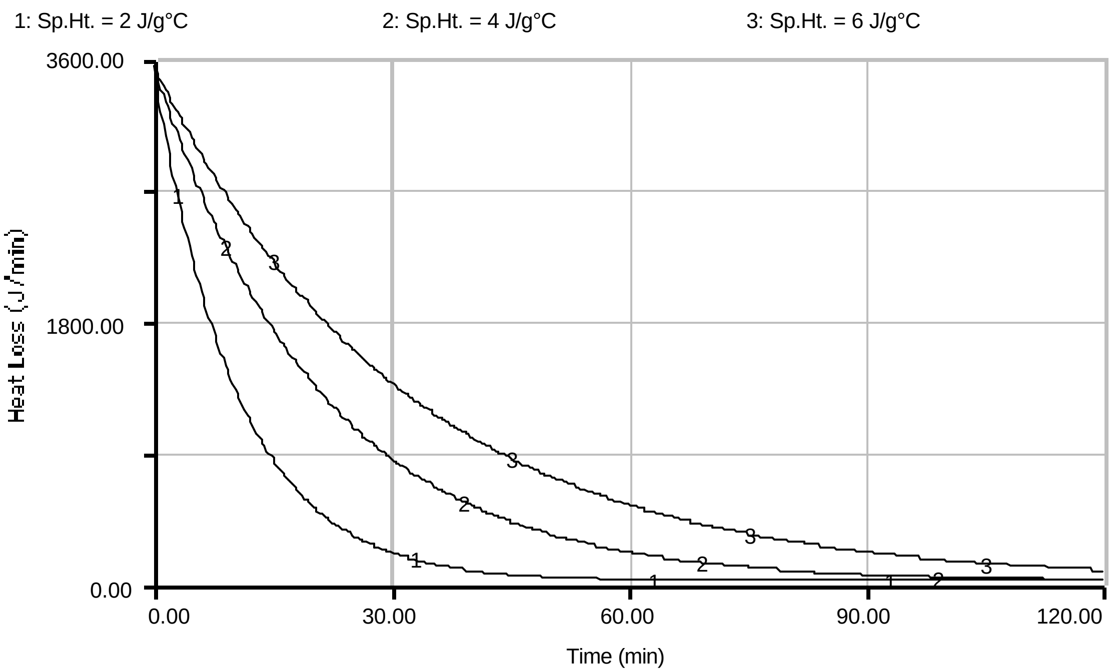

Figure 12. The variation in heat loss rates for solutions of varying specific heats.

The simulation results shown in Figure 11 reflects the impact of specific heat upon cooling behavior. The higher the specific heat value, the more gradual the temperature change. This results in a higher heat loss rate (Figure 12) throughout the transition period because of the maintenance of a larger temperature gap. The understanding of weather patterns and the identification of effective energy sinks for solar collectors are among the many areas for which this concept has great importance.

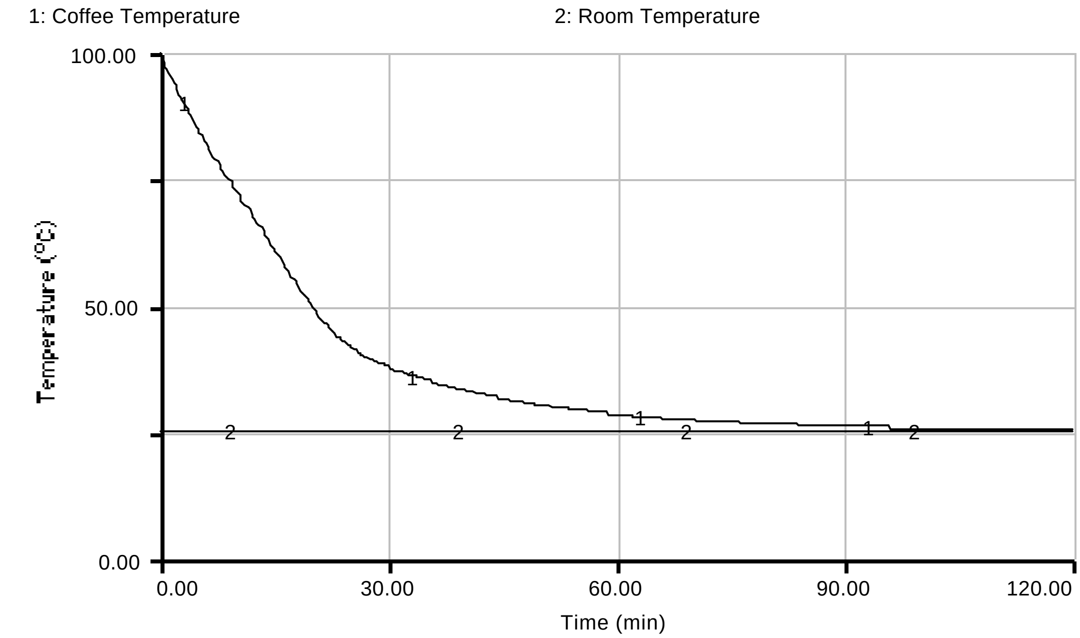

Figure 13. The influence of an ambient breeze upon cooling behavior.

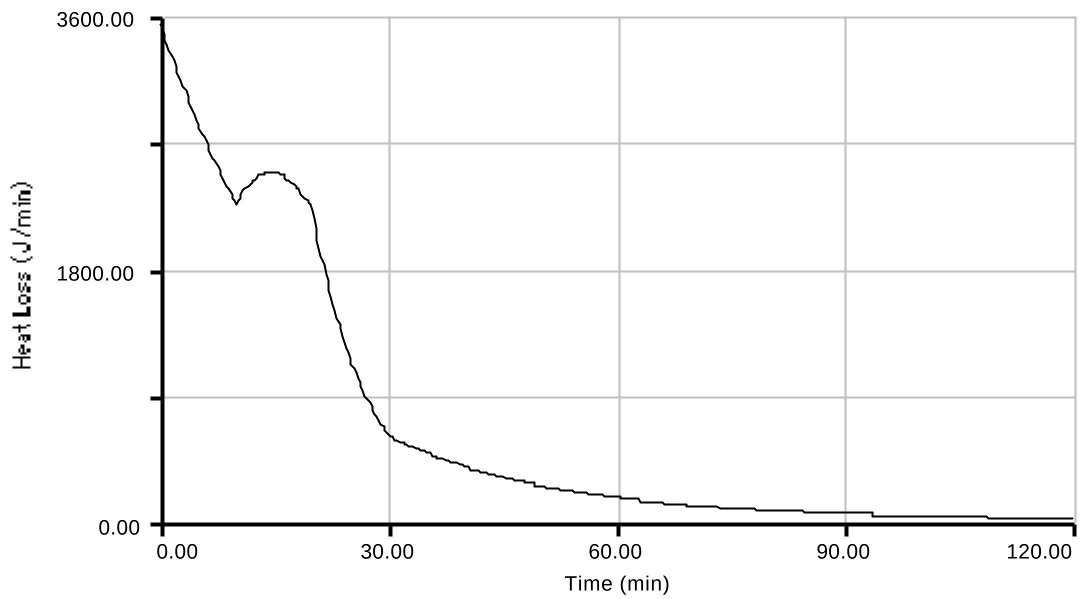

Figure 14. The influence of an ambient breeze upon the rate of heat loss.

The cooling irregularity illustrated in Figures 13 and 14 is often seen in student laboratory work. By selecting Sectors 1 and 2 together to allow the breeze converter to exert its influence… analogous to opening a window, it is possible to simulate the abnormal behavior and to explore its cause. This analysis is much better than ignoring or 'justifying' the deviation as observer error as many students are prone to do!

VI. Suggestions for Instruction and Exploration

Formal outcomes of *Cooling Cup of Coffee II* will vary with its audience and mode of implementation. However, general objectives might include (1) the enhancement of critical thinking skills and (2) the development of understanding of the cooling behavior of a liquid and the factors upon which this behavior depends. These can be accomplished by

- eliciting initial student predictions and explanations for the cooling behavior of a liquid.
- modeling and simulating these behaviors.
- evaluating the simulated behavior by conducting laboratory investigations.
- reconciling simulated behavior with laboratory observations.
- changing the model to reflect and account for observed behavior in the laboratory.
- using the model and simulations as a stimulus for learner–directed inquiry that includes the formulation of hypotheses, laboratory investigation, and reconciliation of the model and observed behaviors.

Upon the completion of a such an instructional sequence, students should be able to

- explain the difference between heat content and temperature of a substance.
- explain and perform calculations illustrating the dependency of temperature upon heat content, mass, and specific heat.
- explain and model the role of the temperature gap in determining cooling behavior as a negative feedback process.
- identify and explain relevant applications of these concepts.
- demonstrate improved critical thinking skills by modeling and investigating a second system such as cooling behavior through a phase transition.

Specific suggestions for the instructional use and exploration of these models are provided throughout *Cooling Cup of Coffee II.* They are listed below along with a few additional ideas.

- Bring a hot cup of coffee into class and ask students to describe fully their beliefs concerning its behavior over time. This might be best done with students collaborating in small groups. Encourage graphical predictions. Support this activity with both laboratory and modeling experiences.
- Modify the previous activity by bringing in several different liquids (hot chocolate, syrup, rubbing alcohol, etc.) and challenging them to predict, verify, and explain the cooling characteristics of each.
- Have students vary the mass of the liquid in the laboratory and on the computer and compare the behaviors. If differences exist, account for them and modify the model if appropriate.
- Does the specific heat impact the cooling pattern only at the point of the coffee temperature calculation? Change the model to reflect other possibilities and compare simulation outputs with real lab data.
- Experimentally determine the thermal characteristics of cup materials and use these values to refine the model structure.
- Modify the model to illustrate the effect of evaporation upon the cooling pattern. Conduct laboratory investigations to validate the new structure.
- Identify optimum dimensions for minimal heat loss from specific fluid volumes and compare these results with the dimensions of home hot water heaters, thermos bottles, etc.

- Have students modify the model to simulate the warming of cool solutions to room temperature.

The *Cooling Cup of Coffee II* should be viewed as a story with no end. Contributions to its further development are encouraged and will be appreciated and enjoyed. They may be sent to the author directly or through the Creative Learning Exchange.