MODELING HEAT, MOISTURE AND CONTAMINANT TRANSPORT IN BUILDINGS: TOWARD A NEW GENERATION SOFTWARE

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ABSTRACT

This paper describes a general purpose software, Florida Software for Engineering Calculations (FSEC 1.1), that is capable of solving various transport equations used in building science (e.g., combined heat and moisture transfer, fluid flow, contaminant dispersion equations, etc.). The governing equations are solved by finite element methods. General capabilities and an overview of the software structure are given. Results are presented for several types of combined heat and moisture transfer simulations: 1) in buildings; 2) in the presence of natural convection; 3) in attics 4) in a typical wall.

INTRODUCTION

The advent of computers has provided a tremendous impetus to the development of computational analyses. High-speed computers have made it possible for us to solve ever more complex problems and, as a result to gain much better insight into complex processes. It is quite accurate to say that modern technological achievements in such areas as space, automotive and atomic energy would have been impossible without high-speed computers and advances in numerical techniques. For instance, automakers are coming to rely on supercomputers for computational analyses that complement, and someday may even replace physical experiments. When applied early in the cycle of development, computational methods enable researchers and designers to bypass several cycles of time-consuming and expensive prototype tests. In the last few years computers have become so fast, so inexpensive, and so accessible that now for the first time in history, man and computer are rapidly forming a symbiosis that can be of enormous benefit to mankind. Neither the new computational techniques nor the power of computers have been used to capacity in building science.

In 1982 the Florida Solar Energy Center (FSEC) began a study on the interaction of moisture and dehumidification systems in southern buildings [1]. It quickly became apparent that both the available physical data and computational tools were insufficient for the task. No existing public domain building energy analysis software was capable of modeling combined heat and moisture transport. In order to study the problem, an existing software developed at the National Bureau of Standards (now called NIST) [2] was modified to allow moisture modeling using a single lumped moisture capacitance. This revised software was called Moisture Adsorption and Desorption Thermal Analysis Research Program (MADTARP) [1]. The code was preliminary and unable to fully couple the heat and moisture transport in buildings. Nonetheless, it provided significant insight on the significance of moisture sorption in buildings [3].

During the same period a more detailed, general modeling capability was also under development by FSEC researchers [4]. This software, known as FEMALP (Finite Element Method Application Language Program), provided the general capabilities to accurately solve many problems, including combined heat and moisture transport. Since its development, this software has been used in FSEC research and student theses to study thermal, moisture, fluid flow, structural and many other problems.

The software introduced by this paper is called the Florida Software for Engineering Calculations (FSEC 1.1). It builds on the capabilities of the preceding software as applied to the study of complex building science problems. Examples include combined heat and moisture transport, thermal bridges, cavity radiation, air pollutant disbursement, convective air flows, etc.

Interested researchers may obtain copies of a main frame version (VAX/VMS) of the software and users manual by written request to the Florida Solar Energy Center, 300 State Road 401, Cape Canaveral, Florida 32920, Attn: Dr. A. Kerestecioglu.

The remainder of this paper describes the structure and capabilities of the software and gives selected examples of results from a variety of simulations using this capability.

SOFTWARE STRUCTURE

Many of the capabilities of FSEC 1.1 derive from the software structure itself. This section discusses the structural capabilities, whereas the next section discusses the technical or problem solving capabilities.

The general architecture of the software is given in Figure 1. The Computational Processor Segment (CPS) and the segments above it are from the original FEMALP. The CPS is the heart of the software. It performs the following major operations:

- o Computes the capacitance, stiffness and Jacobian matrices and force vectors on an element basis, using numerical volume and surface integrations.
- o Assembles the element matrices and force vectors.
- o Solves the resulting linear or nonlinear algebraic equations.

This portion of the software can be independently executed without interfacing with User Defined Programs (UDP). The buildings simulator is connected to the CPS through a common interface. Similarly, other UDPs can be connected to the CPS through this interface. UDPs are stand-alone software elements (subroutines); they may get some inputs from the CPS and return some outputs to the CPS. For instance, the building simulator gets surface temperatures and moisture conditions from the CPS and returns the zone air temperatures and moisture conditions to the CPS through the interface.

During each iteration or time step, certain parameters can be modified through User Defined Routines (UDR). These modifications can be local or global (see Figure 1). Local modifications are performed on an element level i.e. field variable dependent material properties and/or boundary conditions. Global modifications are performed at the beginning of an iteration or time step. Examples of global modifications are time dependent material properties or boundary conditions, variable time-step simulations, numerical solution schemes (direct iteration versus Newton type iterations) etc.

The software utilizes a single vector array to store all information. The array is dimensioned to the maximum capacity of the hardware being used. Depending on user input, the array is a priori partitioned to separate the different data segments. This vector is conceptually divided into static and dynamic portions. The static portion contains the data that are stationary during execution, such as nodal coordinates, nodal connectivity, material and boundary condition flags, etc. The dynamic portion contains the data that are calculated during execution, such as global capacitance and stiffness matrices, force vectors and nodal unknowns at various time steps and iterations, etc.

Vector-array storage offers several advantages (see also [5]). One of them is the reduction of the storage requirement of the coefficient matrix (product of capacitance and stiffness matrices). For instance, one-dimensional calculations using n number of nodes will require n^2 storage locations for nonvectorized arrays but only 2n-1 for vectorized arrays. (If used properly, finite element analysis results in a banded matrix.)

A second and very powerful advantage of single vector array storage is that it allows access to software variables for UDRs or UDPs. This obviates the need to alter program common blocks or subroutine call statements in the main body of the software.

MAJOR CAPABILITIES

FSEC 1.1 has a wide variety of problem solving capabilities that can be used to study building science problems at many levels of detail [6]. The major capabilities are as follows:

- o One-, two- or three-dimensional simulations using distorted or undistorted elements.
- o Automatic mesh generation with automatic bandwidth minimization for minimizing storage and computation time.
- o Ability to select from a library of built-in governing equations or to define additional equations.
- o Ability to modify time steps, boundary conditions, numerical solution schemes, material properties, and other variables on a run-time basis.
- o Utilities that include: detailed, inter-element thermal radiation modelling, psychometric algorithms, and matrix and vector manipulation algorithms.
- o Provisions for interfacing user defined routines and programs.
- o A building simulator.

Due to its ability to use a wide variety of numerical solution schemes the computational speed is highly user dependent. We have run the software for pure conduction problems where it was as fast as a conduction transfer model. The remainder of this section provides a detailed discussion of some of these capabilities and the philosophy behind their inclusion.

The software is designed to solve up to 25 coupled linear or nonlinear, spatially-distributed, steady-state or transient partial differential equations. The equations with their boundary conditions can be either selected from an equation library or defined by the user. The following equations are available to the user directly from the equation library and they are invoked through the input data file:

- o Energy equation.
- o Various moisture transport equations.
- o Fluid flow equations (in primitive variables for one-, two- or three-dimensional problems or using vorticity-stream function equations for two-dimensional problems).
- o Turbulent kinetic energy equation and dissipation rate equations (k-ϵ model).
- o Contaminant diffusion equation.

Additionally, the user is allowed to modify any of the governing equations that are in the library. This feature can be best explained with the following example. Let's assume that the user wants to solve a three-dimensional advection-conduction problem defined by the following equation.

$$\rho C_p \, DT/D\tau = (k \, T_{,i})_{,i} + Q \quad \text{in } \Omega \tag{1}$$

If Eq. (1) did not exist in the library then the user must apply the standard finite element techniques to arrive to the following algebraic statement [4].

$$(C+\theta K\Delta\tau)a^{\tau+\Delta\tau}=[C-(1-\theta)K\Delta\tau)a^{\tau}+\theta\Delta\tau f^{\tau+\Delta\tau}+(1-\theta)\Delta\tau f^{\tau} \tag{2}$$

In Eq. (2) θ and $\Delta\tau$ denote the time integration constant and time step, respectively. The C and K matrices and f vector for the problem are defined as:

$$C = \int_\Omega N^T \{\rho\} N \, d\Omega \tag{3}$$

$$K = \int_\Omega N^T \{\rho C_p\} N \, u_i \, N_{,i} \, d\Omega + \int_\Omega N^T_{,i} \{k\} N_{,i} \, d\Omega \tag{4}$$

$$f = \int_\Omega N^T \{Q\} \, d\Omega \tag{5}$$

In Eqs. (3-5) N denotes the shape function and $N_{,i}$ denotes the derivative of the shape function in the ith coordinate direction. Equations (3-5) consist of eight different types of integrations, they are applicable to any three-dimensional element. The software utilities offer an extensive volume and surface integration library. The integration library consists of several integral types that might be encountered in transport phenomena. The user invokes any desired integral by defining the magnitudes shown in {} in Eqs. (3-5). For user defined equations, the user must supply these values (material property and boundary condition data) in order to construct the C and K matrices and F vector. For instance, if the user supplies Q=0 then no force vector will exist. For user defined equations and modifications, the integral equations as shown in Eqs. (3-5) must be derived by the user.

The software uses several numerical solutions schemes. Solution can be obtained either by assembling and solving n number of equations simultaneously or successively assembling and solving the equations one by one. The latter, even for linear problems, requires an iterative scheme but uses less storage space. The second option is especially appropriate for personal computers. For nonlinear problems both options require iterative solutions. Both options impact stability and convergence rate.

COMBINED HEAT AND MOISTURE TRANSFER CALCULATIONS

The software allows the user to perform combined heat and moisture transfer simulations at different levels of detail. Conceptually, a building is composed of several solid and air interfaces. The solids may consist of the envelope, internal walls or furniture and the air can may be indoor or outdoor air. Spatially lumped or distributed equations may be used to define the characteristics of the solid and air domains. Based on this classification the following simulation options are available:

- o Distributed heat and moisture transfer calculations for solid and air domains. Both the solid and the air domains are discretized and the problem is solved as a continuum. This option requires either the solution of the flow equations (laminar or turbulent) or the specification of a flow field.
- o Distributed heat and moisture transfer calculations for solid domains exposed to user defined boundary conditions. This option requires that convective boundary conditions be specified by the user (e.g. time dependent UDR). With this option the performance of a stand-alone solid structure can be investigated in detail. For instance, the performance of a wall configuration (e.g. possible condensation, structural damage, impact of air penetration, etc.) can be studied in detail by using the ambient data at one boundary and scheduled indoor conditions at the other.
- o Distributed heat and moisture calculations for solids and lumped heat and moisture calculations for air. This option is particularly appropriate for whole-building simulations where bulk indoor conditions and associated mechanical system loads are desired.
- o Distributed heat transfer calculations for solids, lumped moisture transfer calculations for solids and lumped heat and moisture calculations for air. Similar to the third option, this option allows the calculation of indoor conditions and associated loads. The lumped moisture transfer calculations for the solids are performed by the building simulator.

<u>Distributed combined heat and mass transfer calculations for solids</u>: Mathematical description of heat transfer (pure conduction) in building solids is straightforward and well known. However, combined heat and moisture transfer in building solids is very complex. The complexities are due to definition of the driving potentials and transport coefficients. Moisture can migrate in liquid and/or vapor form and its transport is governed by diverse forces (air pressures, liquid or capillary pressures, vapor pressures, thermal gradients, etc.). Detailed theoretical and computational investigation of various combined heat and moisture transfer theories are given in [6]. The major differences between theories result from manipulation of the driving potentials and transport coefficients. A recent study [10] relates all these theories to each other through chemical potentials. The various potentials are related to each other through the definition of the transport coefficients. FSEC 1.1 allows users to define their own chemical potentials and equations. Additionally, most well known theories are available from the equation library.

<u>Lumped moisture transfer calculations for solids</u>: The concept and mathematical formulation of lumped transfer calculations are also straightforward and well known for heat transfer problems. Their use in moisture transport problems is discussed in detail in [6,7,8]. The theory assumes that a very thin surface layer is actively participating in moisture exchange. The thickness of this surface layer is called the Effective Moisture Penetration Depth (EMPD). In this layer, the moisture content is assumed to be uniform. Simulations using the EMPD theory compare favorably with experimental data, under specific circumstances [7]. However, proper selection of the EMPD value is problematic [7,8]. Different materials and building operating conditions require different EMPD values (e.g., a change in operating or initial conditions will require a change in EMPD values). This theory has recently been implemented in the public domain computer program TRNSYS [8].

EXAMPLE RESULTS

This section gives selected results from a number of simulations applied to buildings using the software. They are given to demonstrate the diverse capabilities of FSEC 1.1.

Combined Heat and Moisture Transfer in Buildings: In building applications, where yearly simulations are sought, it is not always feasible to use the detailed heat and moisture transfer equations. Some form of simplification is necessary. The EMPD concept is a viable choice for many of these applications. The theory, assumptions, limitations and results of the EMPD concept have been dealt with at great length in [6-8]. In the example given here, temperature distributions in the walls were obtained through distributed equations, and the lumped approach was used for the zone air and the moisture transport in the walls. Figure 2 compares indoor conditions (2.a) and loads (2.b) obtained from the simulation with experimental data [12].

Combined Heat and Mass Transfer in the Presence of Natural Convection: This example presents some results from a study of the combined heat and mass transfer in a square cavity in the presence of natural convection [11]. Both heat and mass transport, and fluid flow were modeled in detail. The geometry and boundary conditions for the square cavity are shown in Figure 3. Figure 4 shows the velocity (a), temperature (b) and vapor density distributions (c) for a combined Rayleigh number (due to temperature and moisture potentials) of 10^6, ratio of wall to air conductivity (k^*) 10, and ratio of wall to air water vapor diffusivity ratio (D^*) 0.01.

Combined Heat and Mass Transport in Attics: Combined heat and moisture transport in attics was analyzed in detail and compared to measured data [13]. Figure 5.a shows the layout of the attic. A multizone lumped model was used for the air and the attic envelope was simulated using detailed temperature and moisture equations. Figure 5.b shows the measured mass flux carried by the attic ventilation air and temperature prediction errors occurring at the attic floor for cases with and without moisture simulation.

Combined Heat and Moisture Transfer in a Typical Wall: A conventional wood frame wall has been studied using detailed temperature and moisture equations [10]. The wall analyzed is shown in Figure 6. The external surface of the wall is subjected to typical July, Miami ambient conditions. The internal surface was subjected to a constant convective temperature of 27°C and relative humidity of 55%. Wall temperature distribution for selected hours is shown in Figure 7. Figures 8 and 9 show the total moisture flux and partial water vapor pressure distributions within the wall, respectively.

CONCLUSIONS

FSEC 1.1 has been successfully used to simulate a variety of building science problems. The software offers extensive capabilities, but input file preparation is tedious. The current version is intended for users with an extensive numerical analysis background.

In the future, program FSEC 2.0 will be made available to a wider, less experienced audience. Before this can occur additional work on the input and output processors and an enhanced users manual are required. This work is in progress. The authors would welcome any suggestions or comments that may prove useful in completing this task.

ACKNOWLEDGEMENTS

Part of the work reported here is funded under GRI contract #5087-243-1515 with the Gas Research Institute, 860 West Bryn Mawr Ave., Chicago, Illinois, and DOE cooperative agreement #DE-FC03-865F16305 with the Department of Energy San Francisco Operations Office, 1333 Broadway Oakland, California. The authors thank Doug Kosar of GRI and David Pellish of DOE-Solar for their continued support of this research.

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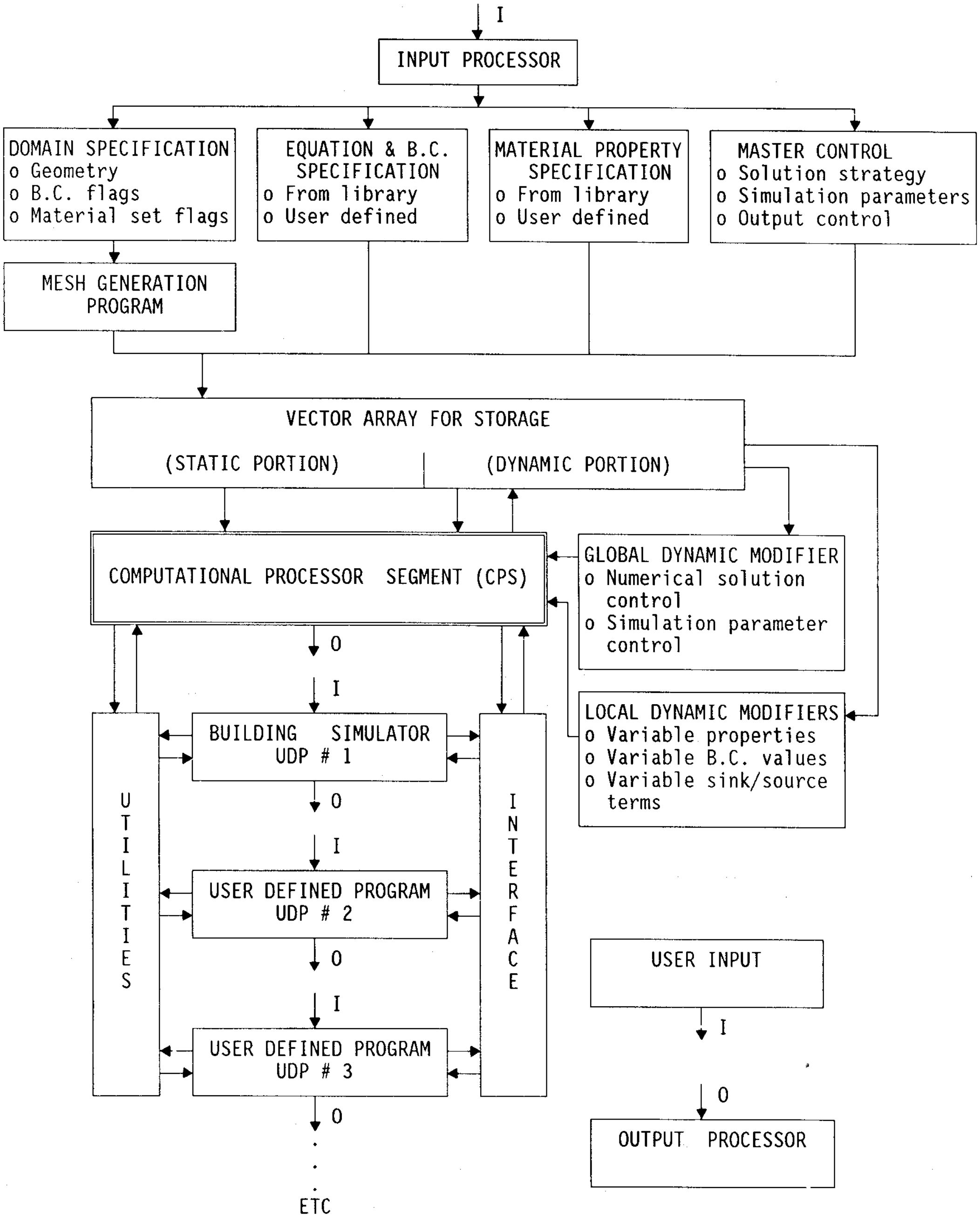
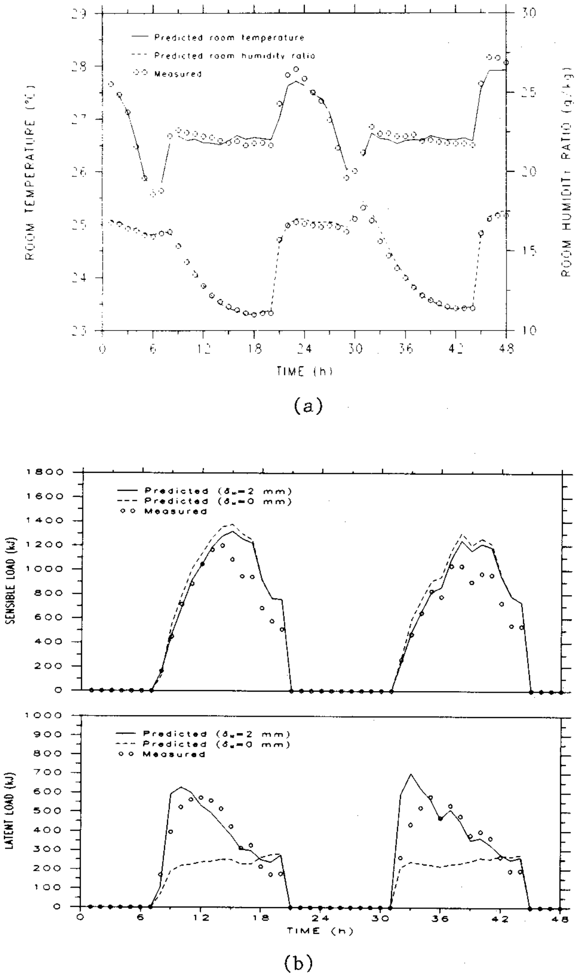


Figure 1. Software structure and interfaces.



(a)

(b)

Figure 2. Predicted versus measured (a) indoor conditions and (b) loads [7].

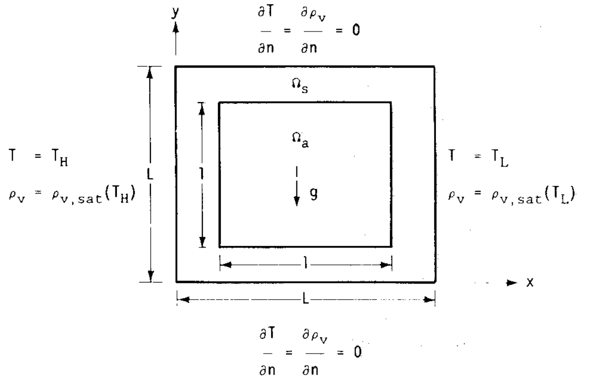
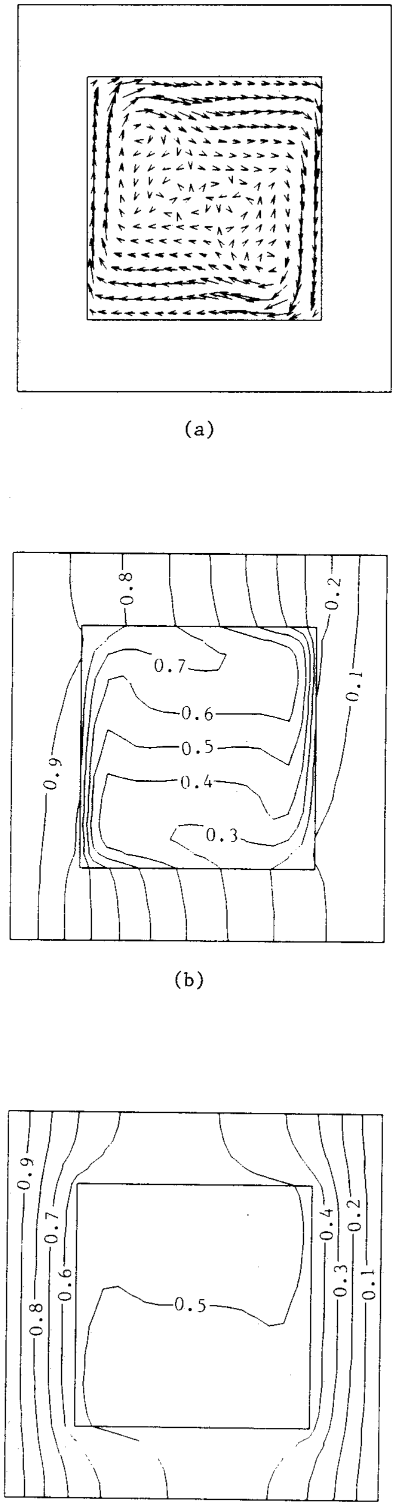


Figure 3. Natural convection in a square cavity: problem geometry.

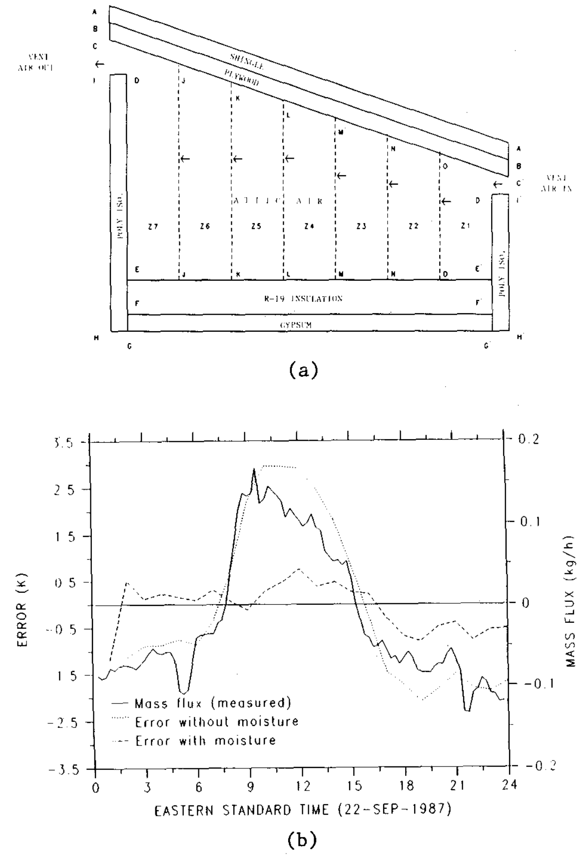


(a)

(b)

(c)

Figure 4. Natural convection in a square cavity: (a) Velocity, (b) Temperature and (c) Vapor density distributions [11].



(a)

(b)

Figure 5. Combined heat and moisture transfer in attics: (a) problem geometry (b) mass flux and prediction errors [13].

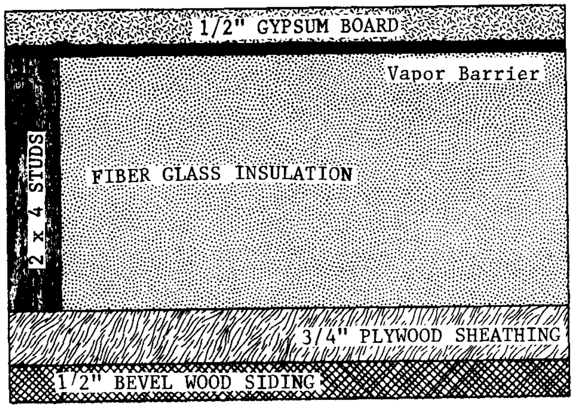
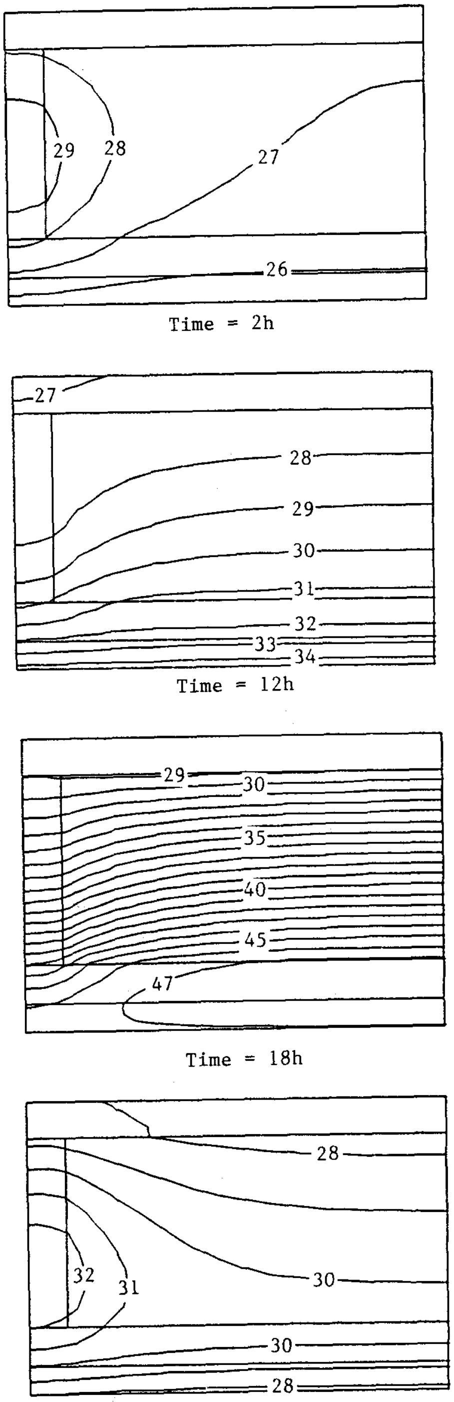


Figure 6. Schematic of a conventional wood frame wall.



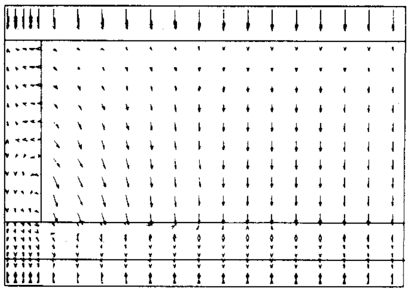
Time = 2h

Time = 12h

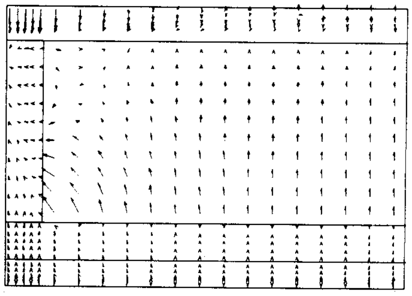
Time = 18h

Time = 23h

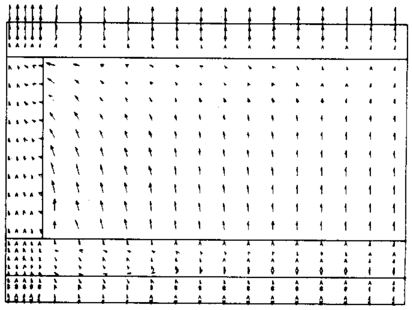
Figure 7. Temperature (°C) distribution history for a conventional wood frame wall [10].



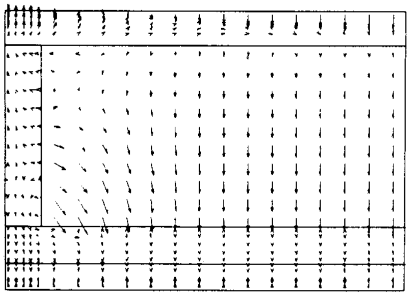
Time= 2h; $q''_{max}=0.8\ g/m^2.h$



Time= 12h; $q''_{max}=0.4\ g/m^2.h$

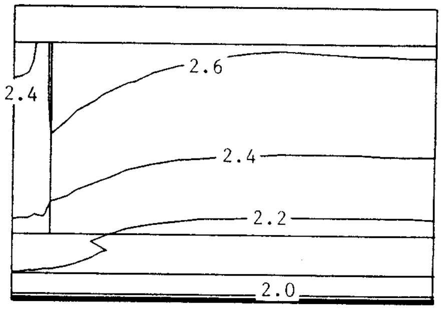


Time= 18h; $q''_{max}=1.5\ g/m^2.h$

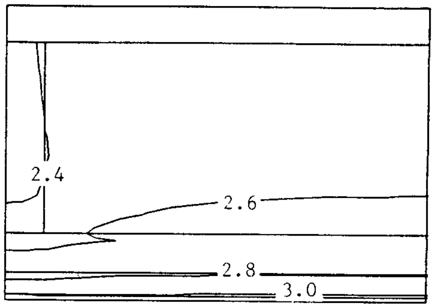


Time= 23h; $q''_{max}=0.7\ g/m^2.h$

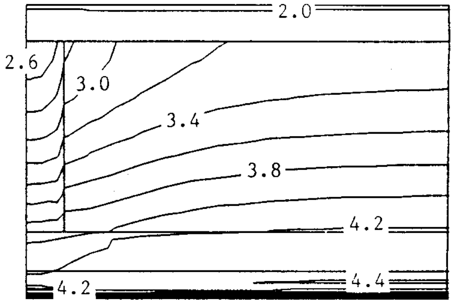
Figure 8. Total moisture flux ($g/m^2.h$) distribution history for a conventional wood frame wall [10].



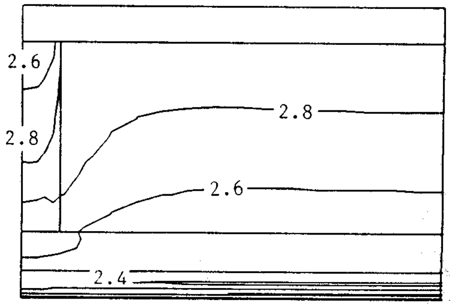
Time= 2h



Time=12h



Time=18h



Time=23h

Figure 9. Partial (kPa) vapor pressure distribution history for a conventional wood frame wall [10].