TREATING MULTIPHASE CHANNELFLOW WITH THERMOSIM

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ABSTRACT

This paper introduces a new bond graph element, named CIS (for Compliance, Inertance and Entropy), to the THERMOSIM package that replaces a complex method. The CIS element is directed at the modeling and dynamic simulation of the many engineering systems that contain tubes with flowing compressible fluid and thermal communication with the environment. It includes the effects of wall shear, fluid inertance, fluid compressibility and heat interaction with a containing wall having its own thermal compliance with its environment. A prior element also is upgraded to serve a needed ancillary purpose.   Convergence of simulations is achieved through the conventional use of upwinding. Application is illustrated for the case of a copper tube containing nitrogen at cryogenic temperatures undergoing a transient within an atmospheric environment. The development is detailed in version 5 of the Users' Manual [1].

key words: dynamic simulation, bond graphs, convection bonds, thermodynamic systems

1. INTRODUCTION

The promise of bond graphs, to treat all kinds of dynamic physical systems based only on the properties of the substances employed in these systems and a straight-forward application of conservation principles generally understood by engineers and physicists, faces its most daunting task when it comes to thermodynamic systems, since they exhibit relatively complex properties. Files of the properties of many common substances have been assembled in a form that does not employ interpolation. Also introduced are convection bonds, which have three variables instead of the usual two, adding entropy to the conventional mass flow rate and stagnation enthalpy.

The THERMOSIM package handles non-thermodynamic systems based on mechanical, electrical, hydraulic, thermal   and magnetic energies with aplomb.   Its unique capability relative to other bond graph packages, however, is to address in a simple and direct way a wide variety of engineering and other systems involving thermodynamic systems and components. Since bond graphs were created

based largely on concepts of energy and power, and thermodynamics is the science of energy, these systems should be included as an integral part of the package. The package is intended for use not only by those who are grounded in elementary thermodynamics, but by engineers and scientists whose knowledge of this subject is modest. Further, it includes models in which elements are based on explicit analytic expressions for energy, which are particularly helpful in dealing with electromagnetic systems. Also, hydraulic systems can be treated with greater attention to thermodynamic consequences than is traditional.

Learning how to use THERMOSIM requires some effort as ought to be expected.   An extensive opening tutorial of the freely available Users' Manual instructs the user by having him or her inspect and run simulations for up to nine selected system models. A graphical interface called BondGrapher, written by Scott A. Brown who is a computer engineer, makes entering bond graph models extremely easy. The balance of the roughly 120 page manual gives a compendium of subject-oriented descriptions of the bond-graph elements and procedures plus several more detailed examples.

Traditional bond:
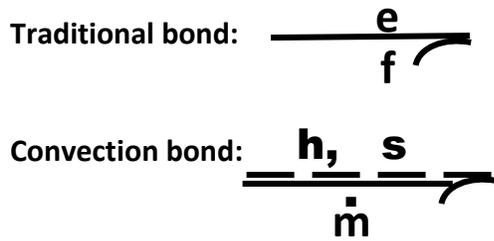

Convection bond:

Fig. 1 Traditional and convection bonds

THERMOSIM is a bond graph package that employs 10 elements with traditional bonds only, and 11 elements that *sometimes* employ convection bonds and one short-hand macro element. As shown in Fig.1, traditional bonds have one effort (e) and one flow (f) with their product being the power transmitted through the bond (or in the case of the R element, dissipated by it). Convection bonds, which are used for flowing fluids, have one flow (the mass flow rate m) and *two* efforts. h is the stagnation enthalpy; the product $h\dot{m}$ is the power transmitted. s is the entropy; $s\dot{m}$ is the entropy transmitted. Thermodynamics requires the bookkeeping of entropy as well as energy so as to satisfy the second low of thermodynamics.

The author presented a preliminary stab at modeling multiphase channel flow through a channel in a 2016 paper[2]. This employed a newly segmented IRS element similar to the new CIS element but without the fluid volumetric compliance. The special case of the segmented IRS element for liquids is presented, with an example, in Chapter 8 of a book edited by W. Borutzky[3]. The author subsequently applied this model to compressible flow by alternating this element with lumped fluid compliance elements (CS elements). Although this worked, the author concluded that the approach was unnecessarily complicated and too slow computationally. He decided to restrict the use of the IRS element to cases with essentially incompressible liquid flow, and to create the new comprehensive segmented CIS element as described below. The software for the restricted IRS element has also been updated.

2. THE *CIS* ELEMENT

The *CIS* element along with its companion *Ct* element is entered into the graphical interface

BondGrapher in the form shown on the left in Fig. 2. The fluid flow enters and leaves over the convection bonds. BondGrapher actually interprets this model as being segmented, as suggested in the form shown on the right in the figure.

The Ct element is a macro shorthand for one of the combinations of primitive elements shown in Fig. 3. If one wishes to keep the environment but drop the compliance of the wall, replace the Ct element with an RSh heat-conduction element. To keep the compliance but drop the heat conduction, set the thermal conductance to zero. Three aspects of the channel represented by the CIS –Ct combination are depicted in parallel in Fig. 4, along with associated state variable vectors. There are N segments for the wall and the fluid energy. There are N+1 segments for the fluid momentum, staggard relative to the segments for the fluid energy and for the wall; those at the two ends have half the length of the
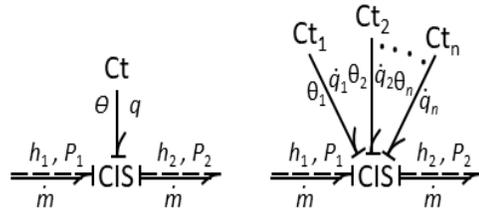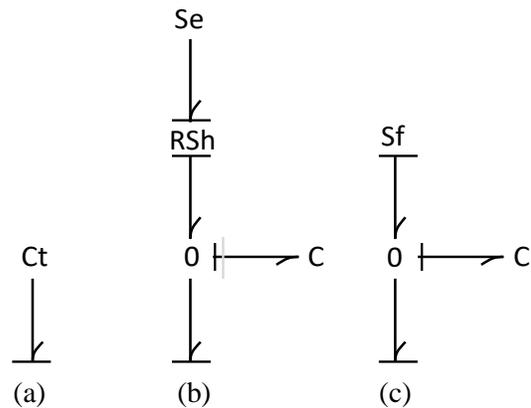

Fig. 2 The combination of the *CIS* and *Ct* elements

(a) generic symbol; (b) option used herein; (c) alternate option
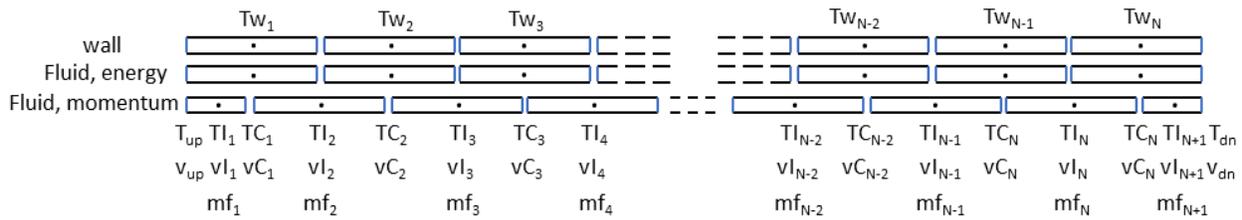
Fig. 3 Decomposition of a Ct element

Fig. 4 Segments for the IRCS-Ct combination

others. The state variables for the wall fluid temperatures are $Tw(1). \ldots Tw(N)$ and $CT((1). \ldots CT(N))$, respectively. The state variables for the fluid masses and mass flow rates are $Cm((1). \ldots .Cm(N))$ and $mf(1) \ldots mf(N\text{i}+1)$, respectively. The specific volume of the fluid in the kth segment is related to $Cm(k)$, the cross-sectional are of the channel, A, the length of the channel, L, and N by $vC(\text{k}) = L\,A/N/Cm(k)$.

3. EXAMPLE OF A TUBE WITH FLOWING CRYOGENIC NITROGEN IN AN ATMOSPHERIC ENVIRONMENT

The upper part of the main page of BondGrapher with the bond graph for this system and the left side of the screen with the CIS element and "initial values" clicked is shown in Fig. 5. The upstream and downstream sources (*Sec*) represent effectively infinite volume chambers filled with nitrogen at a specified temperatures and specific volumes, chosen in the mixed liquid/vapor region. The other BondGrapher screen with *Custom* activated is shown in Fig. 6. Note that the *Custom* area gives the values of the various initial conditions introduced into the first screen by symbols. Note also that nitrogen is specified as the principal substance and the atmospheric air surrounding the tube as the secondary substance. The MATLAB integrator chosen is ode23, which seems to be particularly reliable when thermodynamic substances are involved.   For the given example, data is requested for a single interval of 0.1 seconds. In practice, the author frequently used [.001 1 200] for total of 200 intervals, giving a total simulation time of 0.2 seconds. This implies the *data reduction option,* which is appropriate for virtually all simulations with thermodynamic substances. The actual step size is much smaller,

and is adjusted automatically to satisfy accuracy requirements.   The simulation results given below were achieved without the use of BondGrapher, however, which wasn't ready at the time.

A single simulation was run with three sequential time stages. The first stage had the sole objective of establishing an interesting steady-state initial condition for the second time stage, which implies that all fluid segments have the same mass flow rates. The author guessed roughly at what the various variables would be, and just ran the simulation until an equilibrium was achieved. The data reduction option allows you to stop the simulation at any time and plot the mass flow (or any set of state variables) to see whether the equilibrium has been reached, and if not to resume the simulation. Since it was known that the thermal compliance of the tube walls was large enough to slow down the process, whereas the details of the transient were of little actual
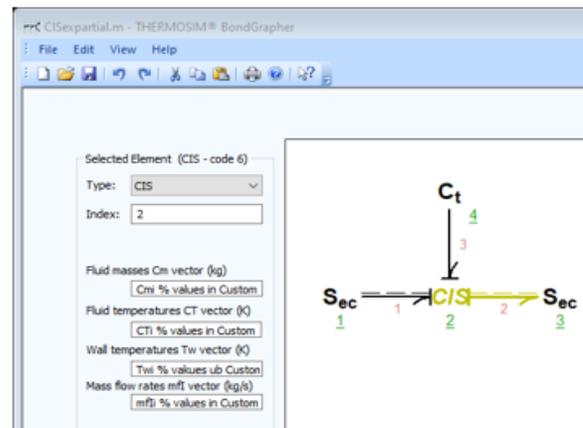

Fig 5.   Upper part of the main page of BondGrapher, with the CIS element clicked
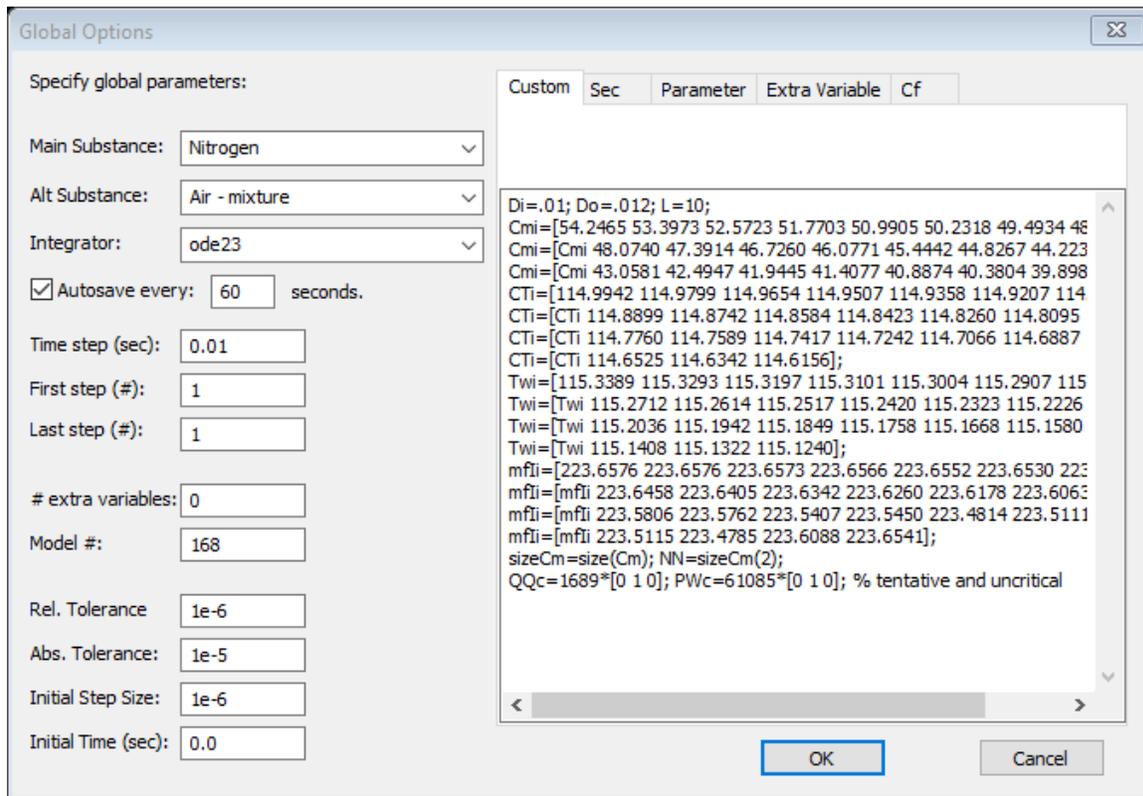
Fig. 6 The other BondGrapher screen with *Custom* activated

interest (and is not documented herein), the author set this compliance 100 times larger than it actually was supposed to be. He reset the compliance for the subsequent time segments to the proper value.

Selected results from the second time stage are shown in Fig. 7. At its beginning, the downstream source was suddenly switched to one having a smaller pressure which, since the upstream source remained in the mixed state, meant only raising the downstream temperature, although keeping it below the temperature of the upstream source in order to keep the flow traveling in the same direction. This meant a new equilibrium would result after a complex transient of interest. The mass flow rate of the last segment (segment 24) drops first, and that of the first segment (k=1) drops last. Note carefully the two different time scales. The changes for the first 0.25 seconds of both the second and the third time stages occur very rapidly due to wave propagation at about 80 to 95m/s, dictating the short 0.001 second reporting intervals. Thereafter, the changes were at a relatively glacial pace but of at least as much consequence; data storage intervals there were increased by a factor of 100, to 0.1 second. The primary changes here were an increase in the specific volumes (or decease in the fluid masses) in the more downstream segments. During the second time stage, the states in all the segments remained in the mixed liquid/vapor domain, nevertheless; the quality of the mixture in the farthest downstream segment rose from 66 percent vapor by mass to 82 percent Most of the wall temperatures rose significantly higher, however. The wall temperatures, on the other hand, rose above the temperatures that would have caused the fluid itself to become a vapor, starting at about 0.02 seconds.

Since a second equilibrium had been reached, it was desired that the transient for the third stage would result with a third equilibrium having a lower mass flow rate and higher specific

volumes downstream of the unchanged upstream source. Accordingly, the temperature of the third downstream source was raised yet further, but ough 24, starting with the downstream segment 24, reached the pure vapor stage before equilibrium was established. The fluid temperatures in each segment remained within a narrow band when the fluid was a saturated mixture, but breaks upward dramatically the moment it became a vapor. In segments 22 to 24

still below that of the upstream source. This time, as shown in the plots of Fig. 8, segments 16

the temperature exceeded the critical value of 126K (only temporarily for segment 22). Most of the wall temperatures rose significantly higher, however, reaching 135K for the downstream segment. The time for an equilibrium to be reached was almost twice that for the second stage.
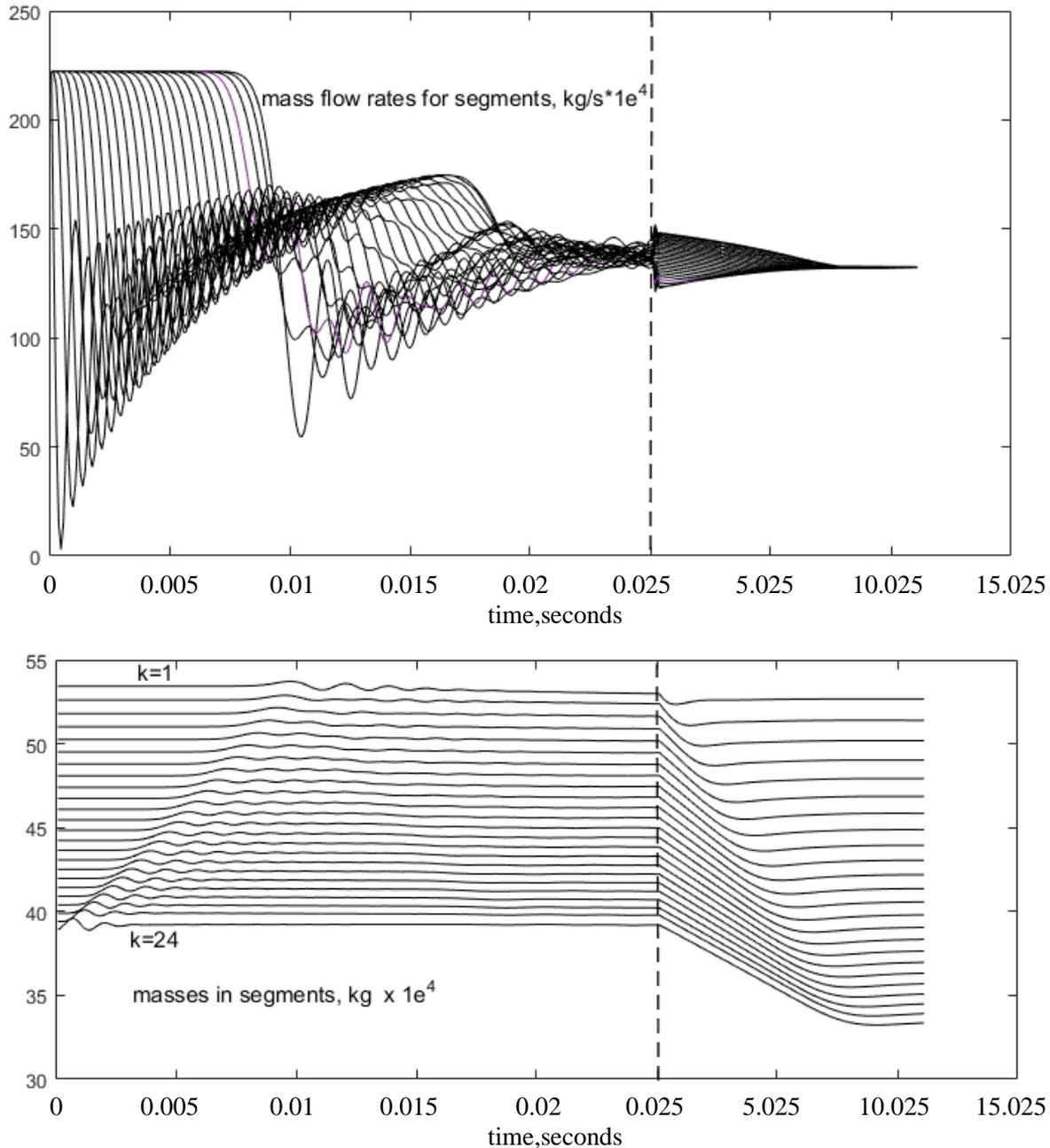
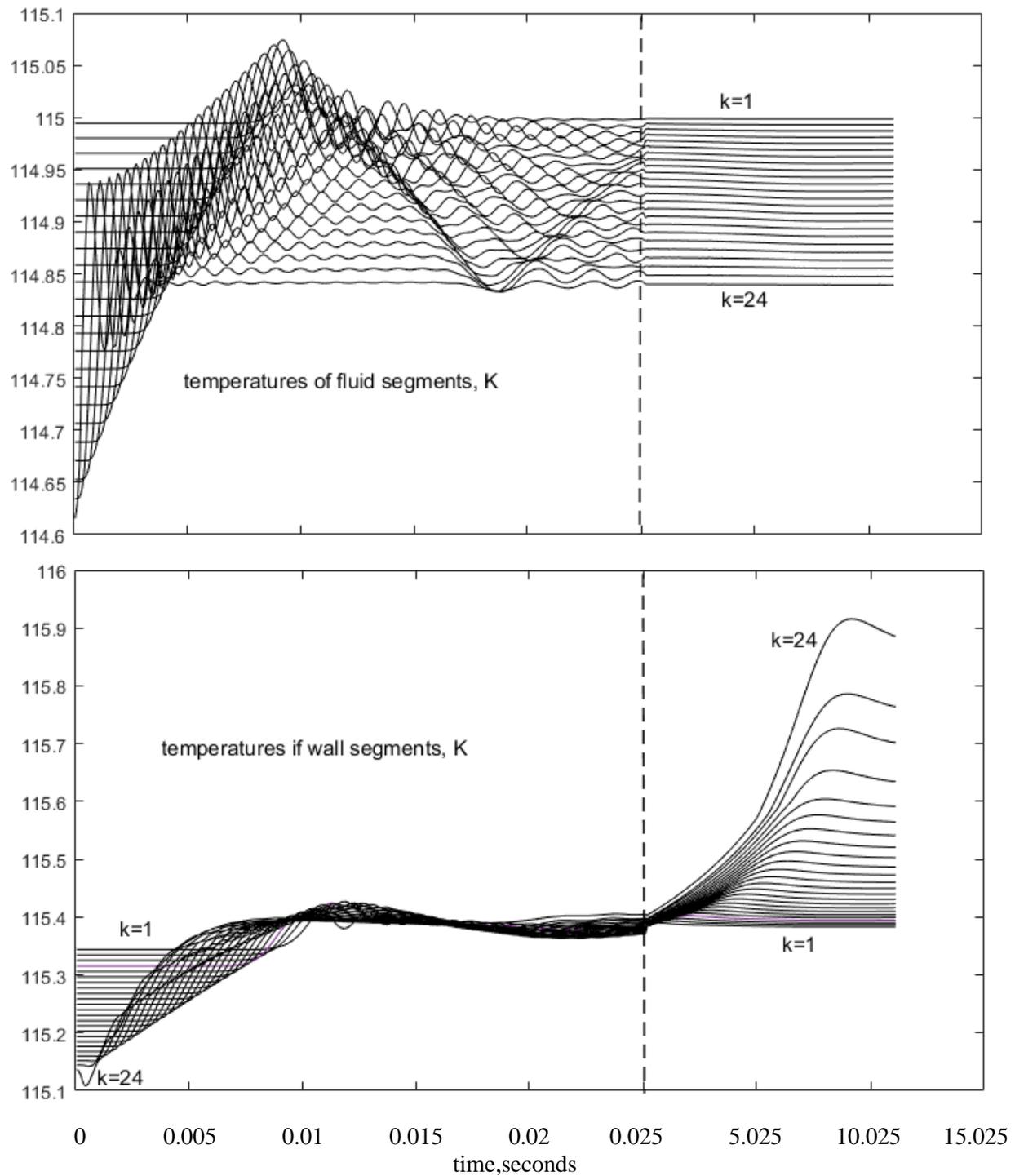Fig. 7 Selected simulation results for the second time stage

Fig. 7 Selected simulation results for the second time stage, continued

The bond graph of a more significant application of the CIS element to a heat-pump system is shown in Fig. 9. CIS2 represents the condenser, and CIS7 the evaporator; neither may require many segments for a fair representation. The author hopes to work on this in the future.
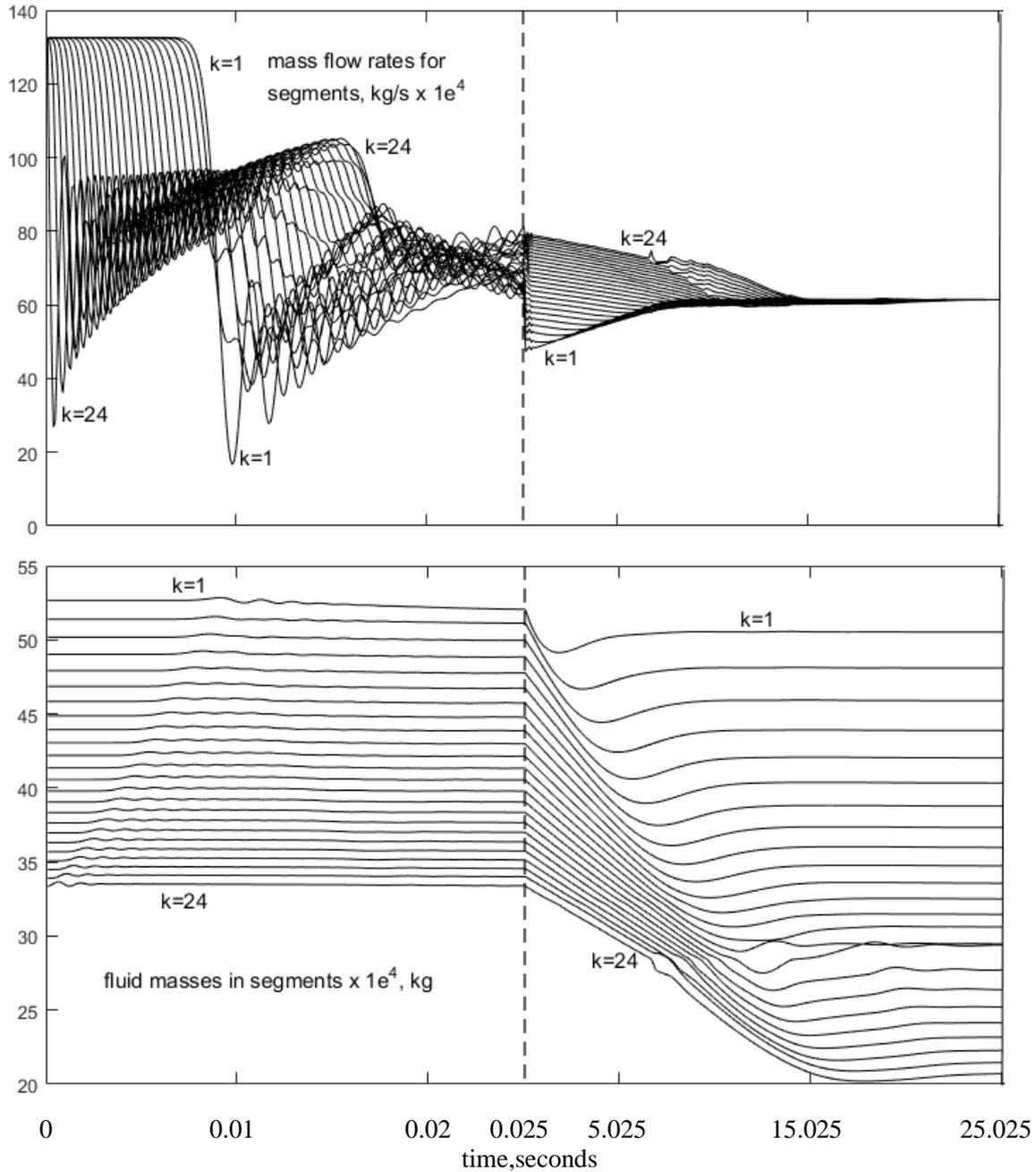
Fig. 8 Selected simulation results for the third time stage

5. MODEL DEFINING EQUATIONS AND THEIR SOURCES

There is one differential equation for each of the $4*N(2)+1$ state variables given above (where $N(2)=24$) are $(Cm(2,1:N(i))$, $CT(2,1:N(2))$, $Tw(2,1:N(2))$ and $fmI(2,1:N(2)$. The CIS element is given as number 2 in the bond graph model.) There are in addition $N(2)$ other state variables

that appear in the coding but are suppressed because they are negligible in magnitude and practically serve only to slow down the simulation.   These are the dynamic heads (pressures) of the fluid in the $N(2)$ energy segments.   They are extremely small for the example cited because the fluid compressibility is so great throughout most of the mixed-state and vapor regimes.   This is not the case for the IRS
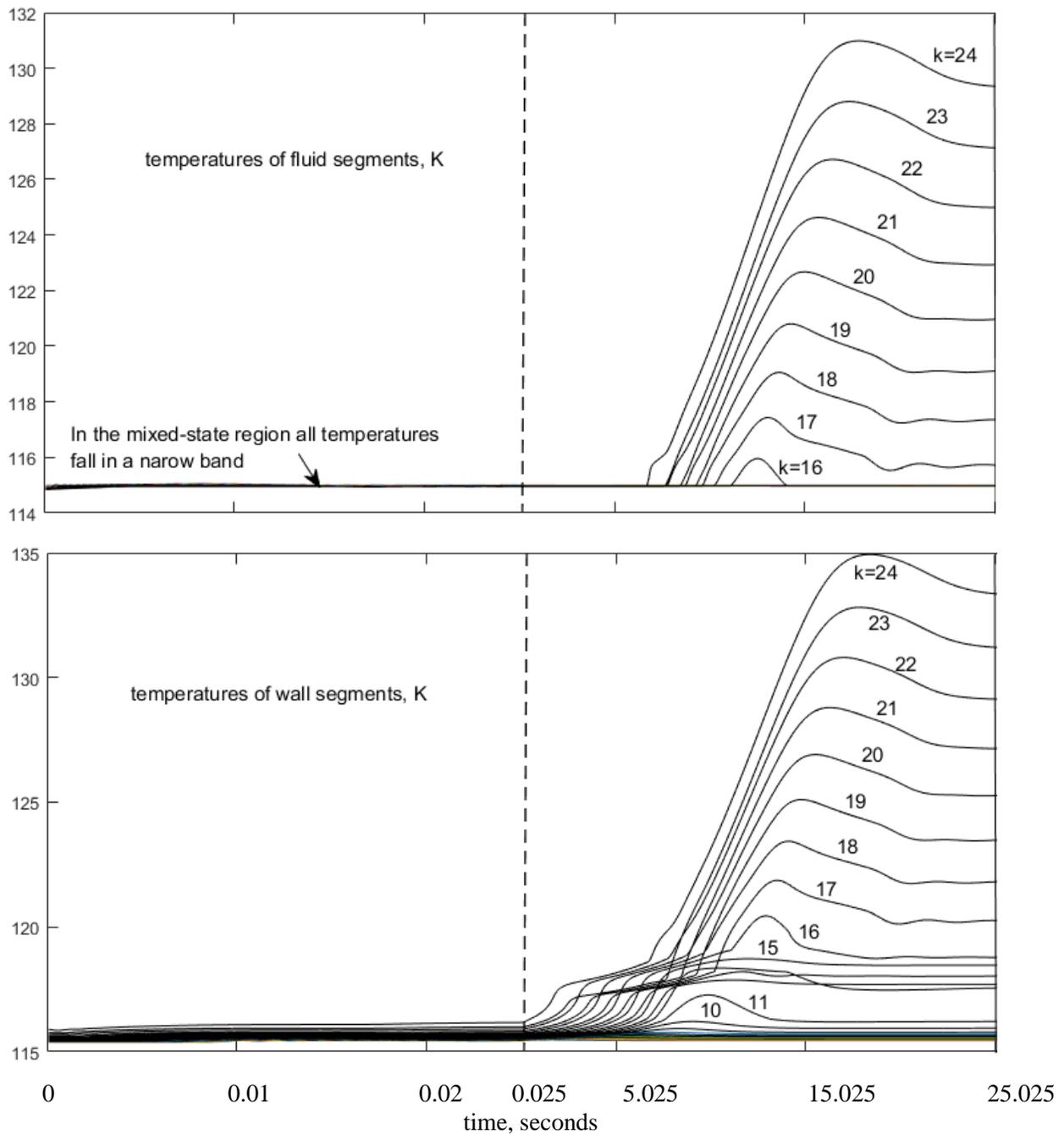
Fig. 8 Selected simulation results for the third time stage, continued

element for liquids, however, cited in Ref[3]. The theoretically correct effort for the kth energy bond in the bond graph, defined as $e(2,k)$, is the stagnation enthalpy which is the sum of the actual enthalpy $hf(2,k)$ plus the dynamic head

The simplest of the two differential equations ascribable to each of the energy segments represents the conservation of mass). These are given in terms of the $N(2)+1$ interfacial mass flowrates, $mfIi(2,k$, which for all except the two ends are given by
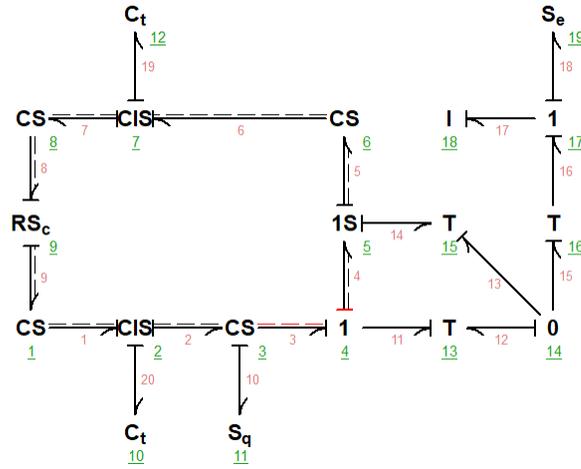
Fig. 9 Application of the CIS element to a heat-pump system.

$$\frac{dCm(2,k)}{dt} = \frac{mfIi(2,k-1) - mfIi(2,k)}{2}; \qquad k = 2:N(2) \qquad (1)$$

(Differential equations for the first and last segments are generally omitted here because they are a somewhat complicated special case that could serve to distract; they can readily be found in the coding, however.)

Many key variables for the energy segments, including most notably the pressure $PC(2,k)$, the enthalpy $hfC(2,k)$ and the quality $XC(2,k)$, are computed from the fluid property command *therprop2(vC(2,k) CT(2,k))*. Similarly, the associated variables for the energy segments are computed from the command *therprop2(vI(2,k) CI(2,k))*.

The differential equations for the accelerations of each of the $N(2)+1$ momentum segments are expressed as a function of the pressure difference $DPa(2,k)$ which drives the acceleration. The interfacial pressure for the momentum segment k+1 can be seen to equal the pressure for the energy segment k (for k=1:N(2)). This

establishes the rate of change of the flow for the kth segment as

$$\frac{dmfI(2,k)}{dt} = \frac{DPa(2,k)}{Cm(2,K)/1e4}. \qquad (2)$$

The rate of change of the temperature of the copper wall equals the difference between the heat rate it receives from the environment, Qe(2,k), and the heat rate it exports to the fluid within the tube, QC(2,k). divided by the thermal compliance of the stube wall:

$$\frac{dTw(2,k)}{dt} = \frac{Qe(2,k) - QC(2,k)}{C}, \qquad (3)$$

$$Qe(2,k) = \big(T_e - CT(2,k)\big)H. \qquad (4)$$

Perhaps the most complicated set of differential equations is for the rate of change of the fluid temperatures $CT(2,k)$. The conservation of energy principle for the segment k is

$$\frac{d\big(Cm(i,k) * u(i,k)\big)}{dt} = hfin(2,k) * mfIi(2,k-1) - hfout(2,k) * hfIi(2,k) + QC(i,k) \qquad (5)$$

in which *hfin(2,k)* and *hfout(2,k)* are the enthalpies of the flows entering and leaving the segment, neglecting the dynamic heads as discussed above, and u(2,k) is the specific internal energy of the fluid in the segment and therefore equal to *hC(2,k) – PC(2,k)*vC(2,k)*. Carrying out the algebra, there results

$$\frac{du(2.k)}{dt} = (mfin(2,k) * mfIi(2,k-1) - mfout(2,k) * mfIi(2,k) + QC(2,k) - u(2,k) * \frac{dCm(2,k)}{dt})/Cm(2,k) \qquad (6)$$

The specific internal energy **u** is a function of the states $vC(2,k)$ and $CT(2,k)$, giving

$$\frac{du(2,k)}{dt} = \frac{\partial u(2,k)}{\partial vC(2,k)} * \frac{dvC(2,k)}{dt} + \frac{\partial u(2,k)}{\partial t} * \frac{dCT(2,k)}{dt} = -\frac{\partial u(2,k)}{\partial vC(2,k)} * \frac{N(2)*DL(2,k)}{\frac{dCm(2,k)}{dt}} + \frac{\partial u(2,k)}{\partial t} * \frac{dCT(2,k)}{dt} \qquad (7)$$

so finally the desired state differential equation is

$$\frac{dCT(2,k)}{dt} = \frac{{du(2,k)}/{dt} + {\frac{\partial u(2,k)}{\partial vC(2,k)}} * {N(2)*DL(2,k)}/{dCm(2,k)/dt}}{\partial u(2,k)/\partial t}$$

$$= \frac{\frac{du(2,k)}{dt} + \left(\frac{\partial u(2,k)}{\partial vC(2,k)}\right) * N(2)*DL(2,k)/(\frac{dCm(2,k)}{dt})}{\partial u(2,k)/\partial t} \qquad (8)$$

6. EMPIRICAL RELATIONS USED FOR WALL FRICTION AND HEAT TRANSFER

The wall shear correlations assume fully developed flow in a circular tube; the hydraulic analogy may be used for simple alternative cross sections. The classical analytical result is used for laminar flow. Analytic models for heat transfer and wall shear in single-phase flow and condensing flow with two phases are adapted from Holman[5]. Smoothing between the laminar and turbulent relations is imposed, based on the Reynolds number, since sudden discontinuities would disrupt the simulation. Models for boiling heat transfer are adapted largely from Kandlikar[6].

These numerous and complex relations predate the CIS element but are critical to its operation. Their adaptation is the primary enduring contribution of the 2016 paper cited earlier[2]. Special attention is employed to avoid the possibility that boiling can be so intense that the assumption that it persists uniformly over an entire segment leads to a mistakenly exaggerated result.

7. COMPUTATION STABILITY AND UPWINDING

Digital simulation of one-dimensional models of a flowing fluid are notorious for exhibiting instabilities, although they may not appear near the outset. The author experienced this problem, and solved it in a conventional manner called *upwinding*. In full upwinding, the fluid in each segment is taken to be fully mixed, so its efflux has its mean properties. The author introduced an upwinding coefficient *up* such that *up* = 0 represents no upwinding and up = 1 represents full upwinding. He chose to use *up* = 0.5, which worked quite well.

As an example of the application of upwinding, the nominal relations

vCin(i,k)=(vC(i,k-1)+vC(i,k))/2 k=2:N(i);   (9)

TCin(I,k)=CT(I,k-1)+CT(I,k))/2k=2:N(i).   (10)

are respectively replaced by

vCin(i,k)=(1+up(i))/2*vC(i,k-1)+(1-up(i))/2*vC(i,k) k=2:N(i);   (11)

TCin(i,k)=(1+up(i))/2*CT(i,k-1)+(1-up(i))/2*CT(i,k k=2:N(i)).   (12)

Equations (11) and (12) apply only for positive flow; they are changed in the coding when the flow reverses direction, which can happen in the middle of the tube as well as everywhere.

8. FILE STRUCTURE

In THERMOSIM one directs the execution of a simulation simply by entering the name of its system file as generated by BondGrapher. For the simulations herein the system file is IRCSex28.m. It its helpful, however, to have some idea of other files that are automatically called up, for example if you want to examine or change an equation that is used. The system file calls the file THERMOSIM.m, which organizes

the simulation and how results are to be saved. This in turn calls the proper main simulation file convec4.m or convec7, (the latter is used here), which in turn calls other files as needed. In our case, most of the critical modeling equations are given in the file IRCS34. Other files which must be available for this case are therprop2.m, vapor3.m, nitrogen.dat, airmix.dat, oxygen.dat, nitrogen.dat, argon.dat, viscosity1.m, and CtH.m. You may contact the author with any questions or comments.

9. MAJOR OVERHAUL OF THE USERS' MANUAL

The fifth edition of the extensive *THERMOSIM Users' Manual* is planned to become downloadable without cost from the author's website [1] before this paper is presented in San Diego.

10. CONCLUSIONS

The simulation of physical and engineering systems with unsteady flowing compressible flow is dauntingly complicated for one who does not devote much of his or her career to the subject. This paper demonstrates that the basic well understood concepts of conservation of mass, momentum and energy along with a practical codification of the thermodynamic properties of a significant number of substances have been marshalled to simulate the dynamics of flow through a nominally one-dimensional channel with a minimum of expertise and effort

by an analyst. The principal limitation is that information of the viscous and heat transfer properties of the user's particular fluid of interest may not yet be assembled in the needed form, opening possibilities for significant further development. The principal irritation to the author has been the simulations in the present case, carried out on a conventional and not-so modern laptop computer, were slow to execute, as a result of the enormous amount of computation involved.

The author is interested in passing on the baton of THERMOSIM to a younger researcher, and would appreciate any related inquiries.

11. REFERENCES

1. http://www.lehigh.edu/~ftb0/index.html. Considerable other information about bond graphs and simulation is there also, including a slideshow shown in the plenary session of the 2007 of the International Conference on Bond Graph Modeling (ICBGM 2007) entitled "Bond Graph Modeling and Simulation of Thermodynamic Systems", which explains convection bonds and bond graphs from the more complex perspective that was pre-THERMOSIM.

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