A CASE STUDY DEMONSTRATING THE UTILITY OF INTER-PROGRAM COMPARATIVE TESTING FOR DIAGNOSING ERRORS IN BUILDING SIMULATION PROGRAMS

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ABSTRACT

The validation of a building simulation program or model is a daunting task, and one that should receive as much attention as algorithm and code development. Previous research in this field has led to a well-accepted approach composed of analytical verification, empirical validation, and inter-program comparative testing to diagnose model deficiencies, mathematical solution errors, and coding errors. Through a case study, this paper demonstrates the utility of inter-program comparative testing. It shows that by comparing program-to-program results, solution problems, coding errors, and deficiencies in mathematical model descriptions can be efficiently identified, diagnosed, and subsequently repaired.

INTRODUCTION

Building simulation model validation

The validation of building simulation programs is a complex and challenging field that has existed almost as long as building simulation itself. Extensive efforts have been conducted under the auspices of the International Energy Agency (IEA), the American Society for Heating Refrigeration and Air-Conditioning Engineers (ASHRAE), the European Committee for Standardization (CEN) and others to create methodologies, tests, and standards to verify the accuracy and reliability of building simulation programs. Notable examples include Jensen (1993), Lomas et al (1994), Judkoff and Neymark (1995), ANSI/ASHRAE (2004), and CEN (2004).

In addition to providing consistent methods for comparing predicted results by simulation programs, these initiatives have proven effective at diagnosing *internal sources of errors*. Judkoff et al (1983) have provided a useful classification for these errors:

- Differences between the actual thermal transfer mechanisms taking place in the reality and the simplified model of those physical processes.
- Errors or inaccuracies in the mathematical solution of the models.
- Coding errors.

Judkoff and Neymark (1995) proposed a pragmatic approach composed of three primary validation constructs to check for these internal errors. These are:

- Analytical verification
- Empirical validation
- Comparative testing

With analytical verification, the program output is compared to a well known analytical solution for a problem that isolates a single heat transfer mechanism. Typically this necessitates very simple boundary conditions. Although analytical verification is limited to simple cases for which analytic solutions are known, it provides an exact standard for comparison.

Program outputs are compared to monitored data with empirical validation. The measurements can be made in real buildings, controlled test cells, or in a laboratory. The design and operation of experiments leading to high-quality data sets is complex and expensive, thus restricting this approach to a limited number of cases. The characterization of some of the more complex physical processes (such as heat transfer with the ground, infiltration, indoor air motion, and convection) is often excluded due to measurement difficulties and uncertainty.

A program is compared to itself or other programs with comparative testing. This includes both sensitivity testing and inter-model comparisons. This approach enables inexpensive comparisons at many levels of complexity. However, in practice the difficulties in equivalencing program inputs can lead to significant uncertainty in performing inter-model comparisons.

A general principle applies to all three validation constructs. The simpler and more controlled the test case, the easier it is to identify and diagnose sources of error. Realistic cases are suitable for testing the interactions between algorithms, but are less useful for identifying and diagnosing errors. Although the comparison of the actual long-term energy usage of a building with simulation results is perhaps the most convincing evidence of validity from the building designer's perspective, this is actually the least conclusive approach. This is because the simultaneous operation of all possible error sources combined with the possibility of offsetting errors means that good or bad agreement cannot be attributed to program validity.

This paper is focused upon the inter-program comparative testing validation construct. Specifically it demonstrates its effectiveness as a diagnostic tool to reveal and isolate internal sources of errors associated with the implementation of a common model into five separate simulation platforms.

Subject of case study

Annex 42 of the International Energy Agency's Energy Conservation in Buildings and Community Systems Programme (IEA/ECBCS) was formed in 2003 with the objective of developing, validating, and implementing models of residential-scale cogeneration devices for whole-building simulation programs. One of the models designed by Annex 42, that for treating solid-oxide fuel cell (SOFC) cogeneration devices, is the object of the current paper. This is a system-level model that considers the thermodynamic performance of all components that consume energy and produce the SOFC-cogeneration device's thermal and electrical output. This model is appropriate for use in whole-building simulation programs where it can be coupled to models of associated HVAC plant components (e.g. hot-water storage, hydronic heating systems) and models that predict the building's thermal and electrical demands. The motivation for and detailed description of this model is provided by Beausoleil-Morrison et al (2005).

The mathematical model developed by Annex 42 for simulating SOFC-cogeneration devices is extensively documented in (at least by intention) an unambiguous fashion. It discretizes the SOFC-cogeneration device into nine control volumes (e.g. the fuel cell power module, the gas-to-water heat exchanger) and provides energy balances for each. Detailed methods and equations are provided to calculate the terms of these energy balances, such as the air and fuel supply rates, the electrical conversion efficiency, and the heat exchange between the hot product gases and the water stream that delivers the thermal output.

This mathematical model has been independently implemented into five simulation platforms. This provides a unique opportunity to apply inter-model comparison testing to diagnose the internal sources of errors outlined above. The opportunity is unique because the same mathematical model has been implemented into all five programs. As such, all ambiguity in equivalencing program inputs can be eliminated and all predictive differences can be attributed to either errors in the mathematical solution of the models or to coding errors (bugs).

Outline of paper

The next section briefly describes how the Annex 42 SOFC-cogeneration model has been implemented into the five simulation platforms. The suite of test cases that has been created for conducting inter-model comparisons is then described. Example results are then provided and some of the errors that were identified and repaired through this process are revealed. Finally, conclusions are drawn and recommendations made for future work.

FIVE SIMULATION PROGRAMS

ESP-r

The model has been implemented into the explicit plant domain of the ESP-r building simulation program (ESRU 2002). ESP-r's explicit plant modelling domain is based upon a component-level approach whereby users assemble components (e.g. water tank, pump) and subject them to control (e.g. sense a room air temperature and actuate a pump) to represent a coherent HVAC system.

Each component is represented by one of more control volumes and each control volume is characterized by mathematical models that describe the control volume's energy and mass exchanges with connected components and the environment. The energy balances are expressed in the following form,

$$\begin{Bmatrix} storage\ of \\ heat\ in\ CV \end{Bmatrix} = \begin{Bmatrix} energy\ \ flows \\ into\ CV \end{Bmatrix} - \begin{Bmatrix} energy\ \ flows \\ out\ of\ CV \end{Bmatrix} \qquad (1)$$

Depending upon the component under consideration, the terms on the right side of this equation might be a convective flux from the skin of the component to the containing room, an energy release due to combustion, or advection resulting from water or air flow through the control volume. These energy flows can be expressed with simple or complex models and can be based upon first-principle or empirical approaches, as the situation dictates.

The evaluation of equation 1 for each control volume of each component leads to a matrix of equations that describe the plant network's thermal state for the given time-step wherein temperature defines the state point. A direct solution approach is used to solve this matrix to yield the temperature of each control volume. As the equation set is highly non-linear, iteration is used to reform and resolve the matrix until convergence is achieved for the given time-step. The results of the solved plant state for the given time-step are communicated to the modelling domains that treat the thermal state of the building fabric, the electrical systems, etc., and then the process elaborated above is repeated for each subsequent time-step of the simulation.

EnergyPlus

The SOFC model was also implemented in the EnergyPlus simulation program (Crawley et al. 2001). Sequential substitution and iteration procedure are used to solve energy balances for the nine control volumes. This is demonstrated by focusing on the energy balance that represents the fuel cell power module's (FCPM) control volume[1],

$$\dot{H}_{fuel} + \dot{H}_{air} + \dot{H}_{liq-water} + P_{el,anc-AC} \tag{2}$$

$$= P_{el} + \dot{H}_{FCPM-cg} + q_{skin-loss}$$

The first three terms on the left side of the equation represent the enthalpy flow rates of the fuel, air, and liquid water entering the control volume. P_{el} is the net DC electric power production while $P_{el,anc-AC}$ is the power draw of ancillaries. $q_{skin-loss}$ are the parasitic thermal losses by radiation and convection to the containing room.

The second term on the right side of equation 2 ($\dot{H}_{FCPM-cg}$) is the enthalpy flow rate of the hot gases produced by electrochemical and combustion reactions that exit the control volume. (The thermal energy of these gases is transferred to a water stream in a subsequent control volume to produce the SOFC-cogeneration device's thermal output.) In the Annex 42 model this term is established by summing the contributions of each product gas constituent (e.g. CO_2, H_2O), where the molar enthalpy of each gas constituent is written as a polynomial function of temperature,

$$\hat{h}_i = A \cdot \left(\frac{T_{FCPM-cg}}{1\,000}\right) + \frac{B}{2} \cdot \left(\frac{T_{FCPM-cg}}{1\,000}\right)^2 \tag{3}$$

$$+ \frac{C}{3} \cdot \left(\frac{T_{FCPM-cg}}{1\,000}\right)^3 + \frac{D}{4} \cdot \left(\frac{T_{FCPM-cg}}{1\,000}\right)^4 - \frac{E}{\left(\frac{T_{FCPM-cg}}{1\,000}\right)} + F$$

Where the coefficients A, B, C, D, E, and F are tabulated.

EnergyPlus solves equation 2 by grouping all terms to the right hand side and by calculating the magnitude of the energy imbalance for the value of $T_{FCPM-cg}$ from the previous solver iteration. The value of $\dot{H}_{FCPM-cg}$ from the previous solver iteration is then incremented by this imbalance and an updated $T_{FCPM-cg}$ determined by inverting equation 3 using the numerical method of regula falsi. The solution is accepted as converged when the imbalance becomes less than $P_{el} \cdot 10^{-5}$. Typically, the sequential substitution loop requires three iterations and the regula falsi search requires two.

[1] The energy balance includes other terms that are omitted here for the sake of clarity.

EES

The model has also been implemented into the Engineering Equation Solver (Klein 2005). Unlike the other platforms employed in this study, EES is a generic algebraic equation solver rather than a building simulation program.

EES allows equations to be entered in any order with unknown variables placed anywhere in the equations. EES automatically identifies and groups equations that must be solved simultaneously and provides many built-in mathematical and physical functions useful for engineering calculations.

The energy balances representing the nine control volumes of the Annex 42 model were implemented into EES with user-written functions. EES's built-in functions were used to calculate enthalpies rather than employing equation 3.

IDA-ICE

The Annex 42 model has also been implemented into the IDA Indoor Climate and Energy (ICE) building simulation program (Sahlin & Sowell 1989). IDA-ICE employs the Neutral Model Format (NMF) modelling language. With NMF, algorithms for new component models are not created but rather simply described with equations, variables, and parameters. The various components comprising a coherent system are then linked. The NMF compiler then orders, arranges, and solves the resulting equation set.

The Annex 42 model has been coded in NMF and linked to IDA-ICE's built-in library components to represent a complete building and energy generation system.

TRNSYS

TRNSYS is a modular software environment for the transient simulation of systems (Klein et al 2004). Components from a library (referred to as *TYPEs*) can be parameterized and connected to each other in order to define a coherent system. The library includes components commonly found in thermal and electrical energy systems, as well as component routines to handle input of weather data or other time-dependent forcing functions and output of simulation results. A thermal multi-zone building model and many HVAC system components can be used for building simulations.

A new TRNSYS TYPE was created to represent the Annex 42 model. This was accomplished through the creation of a *wrapper routine* that encapsulates the ESP-r FORTRAN plant component source code. Essentially, this wrapper acts as an interface between TRNSYS's solution procedure and the ESP-r plant component source code. The wrapper passes all input data required by the ESP-r source code and then solves the set of returned energy balances (in the form

simulation period	0h00 to 24h00 on January 9
time-step	less than or equal to 15 minutes
weather data	inconsequential
FCPM electrical efficiency	$\varepsilon_{el} = 0.3 + (1.1 \cdot 10^{-4}) \cdot P_{el} - (2 \cdot 10^{-8}) \cdot P_{el}^2$ no degradation associated with stop-start cycles or with operating time
Electrical demand	The DC electrical output of the FCPM is made to follow an electrical demand which varies from 1 000 W to 3 300 W, with 100 W step increments at the top of each hour.
FCPM transient response	$(dP_{el}/dt)_{max}$ = 10 (W/s) for both increasing and decreasing power (this is sufficiently high to enable the FCPM to follow the electrical demand pattern above)
fuel molar fractions	$\chi_{H_2} = 0;$ $\chi_{CH_4} = 1.0;$ $\chi_{C_2H_6} = 0;$ $\chi_{C_3H_8} = 0;$ $\chi_{C_4H_{10}} = 0;$ $\chi_{C_5H_{12}} = 0;$ $\chi_{C_6H_{14}} = 0;$ $\chi_{CH_3OH} = 0;$ $\chi_{C_2H_5OH} = 0;$ $\chi_{CO_2} = 0;$ $\chi_{N_2} = 0;$ $\chi_{O_2} = 0$
air molar fractions	$\chi_{N_2} = 0.7728;$ $\chi_{O_2} = 0.2073;$ $\chi_{H_2O} = 0.0104;$ $\chi_{Ar} = 0.0092;$ $\chi_{CO_2} = 0.0003;$
air supply to FCPM	$\dot{N}_{air} = \left[5 \cdot 10^{-5} + (1.5 \cdot 10^{-7}) \cdot P_{el} + (1.1 \cdot 10^{-12}) \cdot P_{el}^2\right] \cdot \left[1 + 0 \cdot T_{air}\right]$
air supply blower	$T_{blower-in} = 20^oC$
	$\alpha_{blower-heat-loss} = 1.0$
fuel compressor	$T_{comp-in} = 20^oC$
	$\alpha_{comp-heat-loss} = 1.0$

Table 1: Input data for case 100

of equation 1). Consequently, inter-program comparisons between ESP-r and TRNSYS would reveal the impact of different mathematical solution procedures, although any coding bugs could not be identified.

COMPARATIVE TEST CASES

A suite of inter-program comparative tests has been created to examine the five (and future) implementations of the Annex 42 SOFC-cogeneration model. Each test case is carefully constructed to isolate specific aspects of the model and is described in sufficient detail to avoid any ambiguity in equivalencing program inputs. Since all programs have implemented the same mathematical model they should produce identical or near-identical results. The result is a diagnostic tool that can efficiently isolate internal sources of error through the comparison of program-to-program predictions.

The suite is organized into a number of series, each of which includes tests designed to exercise a certain grouping of models:

- The *100 series* cases exercise the portions of code that calculate the flow rates and enthalpies of the fuel and air supplied to the FCPM.
- The *200 series* cases exercise the portions of code that calculate the flow rates and enthalpies of the product gases exiting the FCPM. They also examine the impact that each term has upon the energy balance represented by equation 2.
- The *300 series* cases exercise the portions of code that treat the FCPM's transient response characteristics as well as its start-up and cool-down cycles.
- The *400 series* cases exercise the models that treat the air supply blower, fuel supply compressor, and water pump that supply air, fuel, and liquid water to the FCPM.
- The *500 series* cases exercise the portions of the code that model the auxiliary burner.
- The *600 series* cases exercise the portions of the code that model the exhaust-gas-to-water heat exchanger.
- The *700 series* cases exercise the portions of the code that model the dilution air system and heat recovery ventilator (HRV).
- The *800 series* cases exercise the portions of the code that model the battery and power conditioning unit.

The level of detail provided for each test case is illustrated by focusing on case 100, the base case. The input data are listed in Table 1.

CODING ERRORS DETECTED

As trivial as case 100 seems, it proved highly effective at diagnosing some coding errors. The initial ESP-r and EnergyPlus predictions of the enthalpy flow rates of the fuel and air supplied to the FCPM (the first two terms in equation 2) are compared in Figure 2. Since this test case isolates two terms in the FCPM energy balance, the clear differences revealed in this comparison allowed the code developers to confine their search for the error to relatively small sections of source code. This search quickly revealed an elusive bug in the ESP-r implementation of equation 3. The

erroneous code	corrected code

`Shomate = A(gas) * tempK/1000.`
`& + B(gas) / 2. * (tempK/1000.)**2.`
`& + C(gas) / 3. * (tempK/1000.)**3.`
`& + D(gas) / 4. * (tempK/1000.)**4.`
`& - E(gas) * (tempK/1000.)`
`& + F(gas)`
`& - H(gas)`
	`Shomate = A(gas) * tempK/1000.`
	`& + B(gas) / 2. * (tempK/1000.)**2.`
	`& + C(gas) / 3. * (tempK/1000.)**3.`
	`& + D(gas) / 4. * (tempK/1000.)**4.`
	`& - E(gas) / (tempK/1000.)`
	`& + F(gas)`
	`& - H(gas)`

Figure 1: ESP-r coding error detected with case 100

"E" coefficient was multiplied rather than divided by $T_{FCPM-cg}/1000$, as shown in Figure 1 which displays the erroneous and corrected code. Despite source code reviews and comparisons to hand calculations, this error went undetected until the inter-program comparative testing was performed due to the small impact it had upon the absolute value of predictions. Near-perfect agreement between the five programs was achieved once this coding error was detected, as shown in Figure 3. (The slight disagreement between EES and the other programs is a result of the use of EES's built-in functions to calculate enthalpies, as discussed earlier.)

Another coding error was diagnosed with the 603 test case. The 600 series of cases isolate sections of code modelling the heat exchanger which transfers heat from the hot FCPM product gases to a water stream that delivers the useful thermal output. The 603 case tested the model for condensing heat exchangers. Figure 4 compares results from the initial simulations performed with ESP-r and EnergyPlus. This clearly illustrates differences in the predicted temperatures for water leaving the heat exchanger. A coding error was diagnosed in the EnergyPlus implementation where the rate of condensation of water from the gas stream was being allowed to have negative values. This situation is physically impossible but had the mathematical effect of considerable evaporative cooling of the water stream that reduced the leaving water temperatures. The error was corrected by adding a single line of code to trap negative values for the rate of condensation and set them to zero. Once this was corrected, agreement between the programs was greatly improved as illustrated in Figure 5.

Another coding error was diagnosed with the 601 test case which tested the log mean temperature difference (LMTD) method of modelling the heat exchanger. The initial predictions of the temperature of the water stream exiting the heat exchanger for case 601 are compared in Figure 6. This comparison revealed a clear difference between the predictions of IDA-ICE and those of ESP-r and EnergyPlus. A subsequent examination of the IDA-ICE source code revealed a coding error. The heat capacity of the water stream had been expressed on a mass rather than a molar basis (J/kgK rather than J/kmolK). This error went

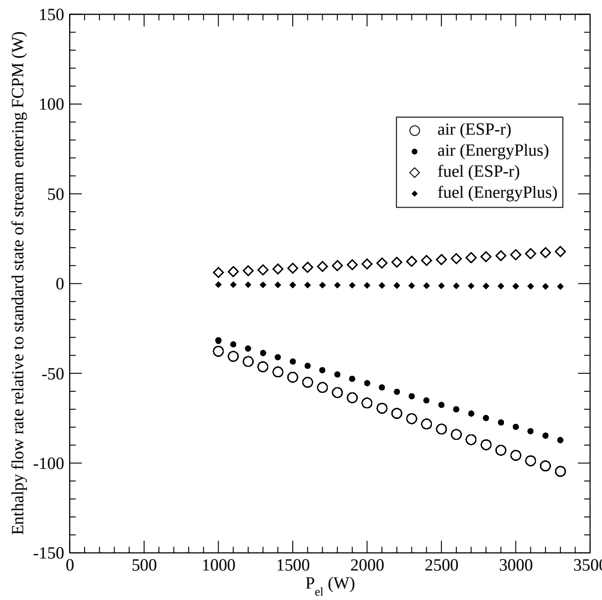

Figure 2: Case 100 reveals bug in ESP-r

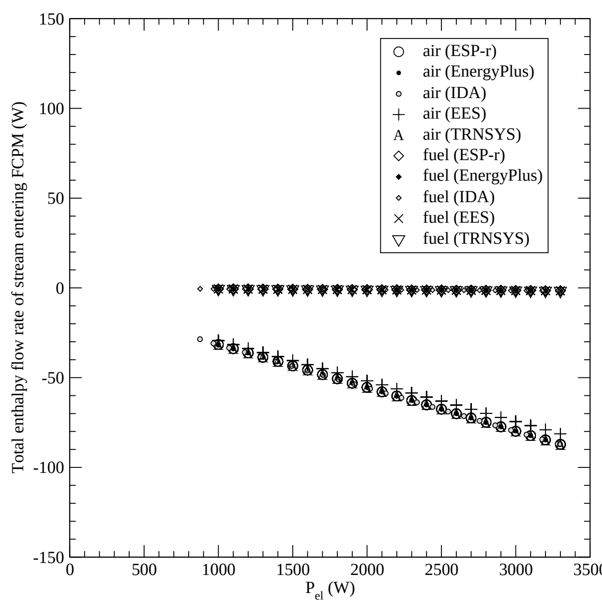

Figure 3: ESP-r bug fixed

undetected in initial testing because it only manifested itself under certain operating conditions and because detailed checking against hand calculations was too onerous due to the complexity of the model. Case 601

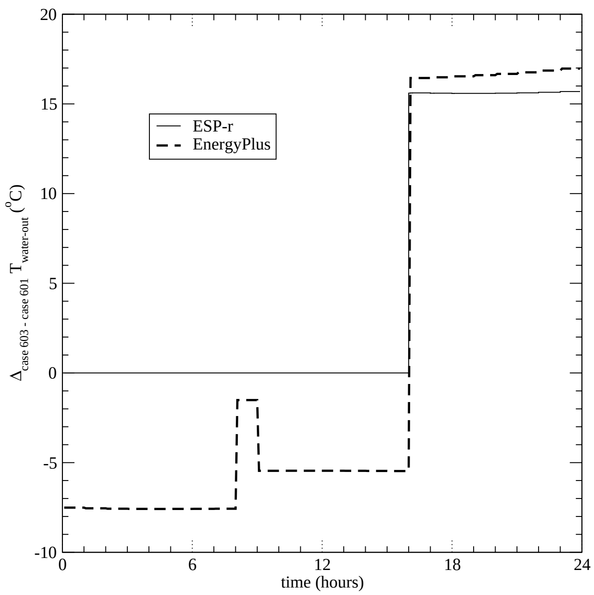

Figure 4: Case 603 reveals bug in EnergyPlus

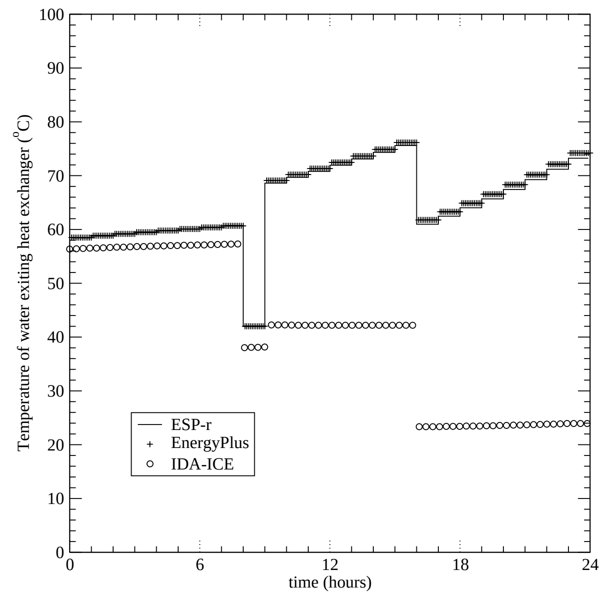

Figure 6: Case 601 reveals bug in IDA-ICE

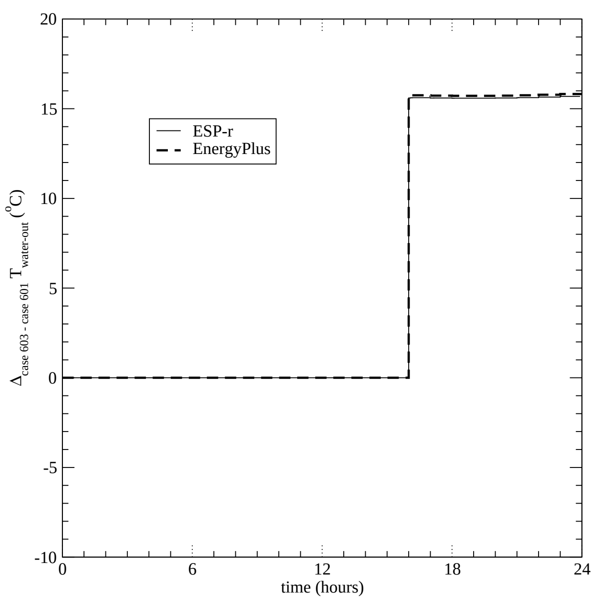

Figure 5: EnergyPlus bug fixed

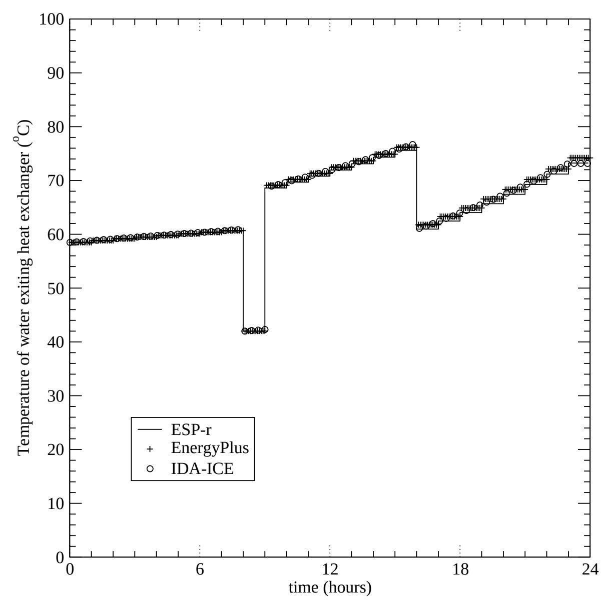

Figure 7: IDA-ICE bug repaired

was specifically designed to exercise the full range of operating conditions for the heat exchanger model and thus revealed the error. Following a simple correction to the code, IDA-ICE was seen to agree with ESP-r and EnergyPlus, as can be seen in Figure 7.

CONVERGENCE PROBLEM DIAGNOSED

ESP-r's explicit plant modelling approach and its iterative solution procedure were previously described. To express the FCPM's energy balance, equation 2 had to be cast in the form of equation 1 such that $T_{FCPM-cg}$ could be explicitly solved. Recall that the $\dot{H}_{FCPM-cg}$ term of equation 2 is calculated as a polynomial function of $T_{FCPM-cg}$ (see equation 3). To achieve this arrangement, in the initial implementation of the model into ESP-r the $\dot{H}_{FCPM-cg}$ term was multiplied and divided by the temperature at two solver iterations,

$$\dot{H}^{j}_{FCPM-cg} = \dot{H}^{j-1}_{FCPM-cg} \cdot \frac{T^{j}_{FCPM-cg}}{T^{j-1}_{FCPM-cg}} \tag{4}$$

Where the superscript j represents the current solver iteration and the superscript $j-1$ represents the previous solver iteration.

In initial testing this technique lead to rapid and stable solutions. However, a problem was revealed by some of the 200 series test cases. Figure 8 plots the difference in $T_{FCPM-cg}$ predictions from one test case to another (202 versus 203) As the ESP-r simulations were conducted with a five-minute time-step and the electrical demand pattern given in Table 1 ramps hourly, there were in fact 12 simulation predictions for each unique value of P_{el}. Each of the 12 predictions for a given P_{el} should have produced identical results, as was the case for EnergyPlus (see Figure 8).

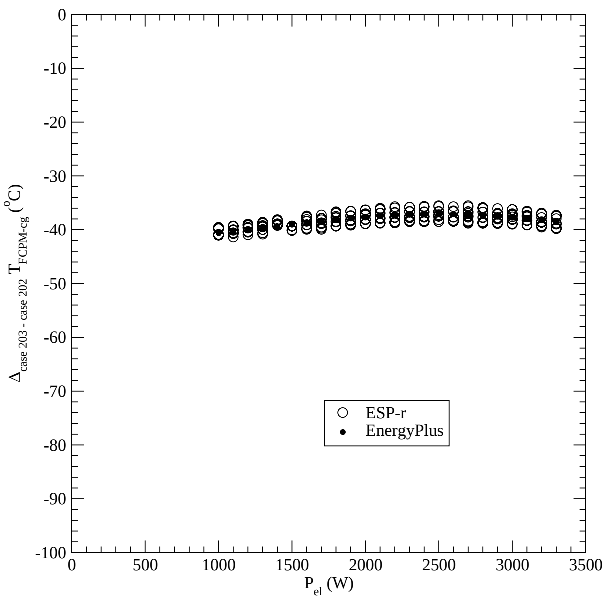

Figure 8: Case 203 reveals convergence problem in ESP-r

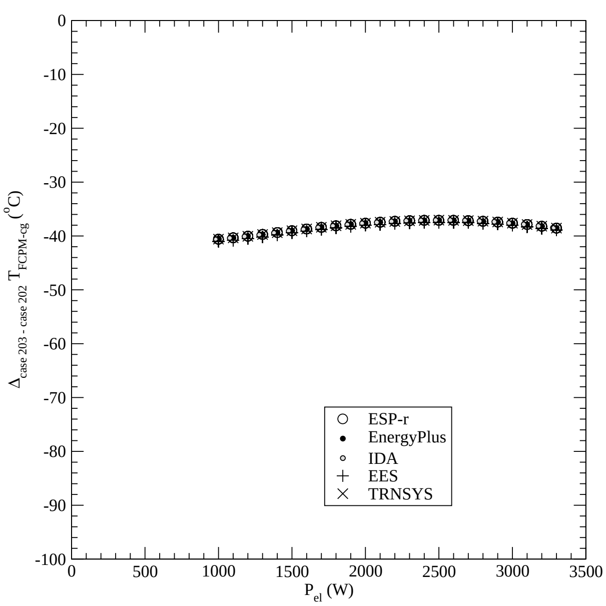

Figure 9: ESP-r convergence problem resolved

The only difference in input data between cases 202 and 203 was related to the method used to calculate the rate of supply air to the FCPM. This change itself was not the cause of the problem, but rather resulted in a particular combination of magnitudes of the terms in the energy balance that initiated the instability in the iterative solution. Figure 10 reveals the instability by plotting values of $T_{FCPM-cg}$ and $\dot{H}_{FCPM-cg}$ at each solver iteration. As can be seen, The under-prediction of $T_{FCPM-cg}$ at one solver iteration lead to an over-prediction at the next, and then to an under-prediction at the next.

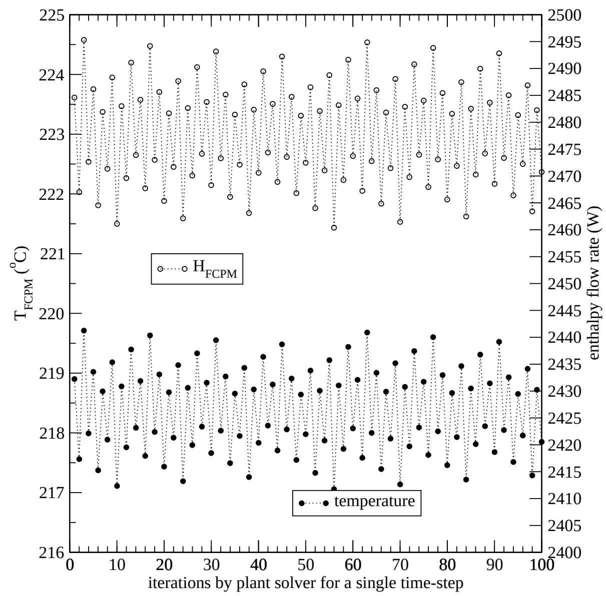

Figure 10: ESP-r solver not converging for case 203

Once this problem was detected an alternate method was found to arrange equation 2 to explicitly solve for $T_{FCPM-cg}$. This was accomplished by grouping all terms but $\dot{H}_{FCPM-cg}$ to the right side of equation 2 and by recognizing that the heat capacity of a gas constituents is defined as,

$$\hat{c}_P = \left. \frac{\partial \hat{h}}{\partial T} \right|_P \tag{5}$$

The enthalpy difference between a gas at any two states can be determined through integration of equation 5. $\hat{c}_P$ can be treated as constant if the two state points are sufficiently close for its variation to be negligible. In this context the two state points are taken to be the solutions at two successive solver iterations within the time-step ($j-1$ and j).

The introduction of equation 5 into the FCPM energy balance leads to a form that explicitly solves for $T_{FCPM-cg}$ as a function of the difference between $\dot{H}_{FCPM-cg}$ at two solver iterations. This alternate approach was found to produce rapid and stable solutions for all test cases. The ESP-r results for the previously plotted case are shown in Figure 9 along with those of the other four programs.

CONCLUSIONS

This paper set out to demonstrate the effectiveness of inter-program comparative testing for diagnosing errors and improving the validity of building simulation programs. This has been accomplished through a case study using a model developed by IEA/ECBCS Annex 42 for the simulation of SOFC-cogeneration systems. The methods used to implement this model into five simulation environments (by five developers) were briefly described.

The suite of test cases that has been created for conducting inter-model comparisons was then described. Each test case is carefully constructed to isolate specific aspects of the model and is described in sufficient detail to avoid ambiguity in equivalencing program inputs. It is worth noting that eliminating this ambiguity is non-trivial and that the first versions of some of the test cases did not achieve this objective. Some revision and re-testing was required to actualize test case descriptions that could be interpreted identically by all five program developers. Since all programs have implemented the same mathematical model they should produce identical or near-identical results. As a result this test suite provides a diagnostic tool that can efficiently isolate internal sources of error through the comparison of program-to-program predictions.

Although space limitations prevented a detailed enumeration, the paper provided three examples of coding errors (bugs) and one mathematical solution problem that were diagnosed and subsequently repaired as a result of the inter-program comparative testing. Without this kind of rigorous testing some of these errors would have gone undetected, perhaps for a significant period of time. In addition to revealing errors in the programs, the comparative testing also revealed deficiencies and ambiguities in the mathematical model. Some of the initial predictive disagreements between programs (not shown here) were a result of differing interpretations of aspects of the mathematical model, which were substantially clarified.

This case study demonstrates the utility of inter-program comparative testing nto improve the validity of building simulation models. In this context the inter-program comparative testing has validated the implementation of the mathematical model into five building simulation programs. The next step is the validation of the mathematical model itself through empirical testing, which will be the subject of future papers.

ACKNOWLEDGEMENTS

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