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CTF vs FD based numerical methods: accuracy, stability and computational time's comparison

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Abstract

Conduction Transfer Function (CTF) and Finite Difference (FD) based numerical methods, are widely used to calculate transient heat conduction in Building Performance Simulation tools (BPSts). The first method is still preferred, when linear system are modelled, to the second one, thanks to the small computational time required during the simulation. However, current BPSts have not yet implemented effective warning messages to stop their "costumers" when these methods are misused. In this article, those methods are compared in terms of computational time and accuracy, with the aim of identifying selection criteria based on the specific addressed problem.

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1. Introduction

Today, buildings performance simulation tools (BPSts) users try to simulate even more than in the past the impact of the use of more complex control systems on the energy performance of the building. To characterize the system behavior, under such control's actions, short time steps (minutes) might be needed when performing numerical simulation. However, in such case, problems could arise in simulating low diffusive walls: very small time discretization might lead to unacceptable errors for the transient heat conduction problem's solution, depending on the used method. In this article, to address this problem, the periodic steady state heat conduction is solved for five different walls in 1D domain applying five different numerical methods. Two of the tested numerical methods belong to the family of the CTF methods, i.e. the State-Space method (SS), implemented in EnergyPlus, and the Direct Root

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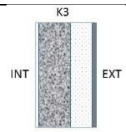
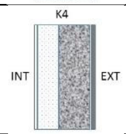
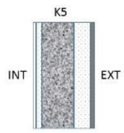
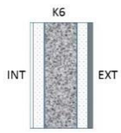
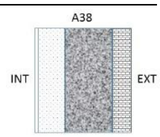
Finding method (DRF), implemented in TRNSYS. The other three methods are Explicit, Implicit and Crank-Nicolson Finite Difference schemes. Two different time periods have been used for the boundary condition (BC), and the results in terms of superficial temperatures and fluxes have been compared with analytical exact solutions. Three different time steps have been investigated for the numerical solutions. The dependence of solution's accuracy upon the wall average diffusivity and upon the relative position of low thermal diffusive and high thermal diffusive layers with respect to the driving force has been investigated. For each of the studied numerical methods and schemes, considerations have been carried out regarding its complexity to understand differences among them with respect to their computational time.

2. Methodology

Five walls, as described in Table 1, have been chosen from existing literature. The first four, numbered with 3, 4, 5 and 6 by Kossecka [1], are characterized by the same overall thermal capacity and transmittance, but different mass-insulation distribution. The last wall is the ASHRAE Wall Group 38, as described in the ASHRAE Handbook of 1997 [2]. Wall A38 has instead the lowest average diffusivity among all the tested walls.

Table 1. Tested walls description (*values changed in the modified version of the wall)

wall type	layer (from **inside** to **outside**)	thickness [m]	conductivity [W/(mK)]	density [kg/m³]	cp [kJ/(kg K)]	picture
K3	gypsum board	0.0127	0.160	800	1.089	
	concrete	0.1524	1.440	2240	0.838	
	insulation foam	0.1016	0.036	16	1.215	
	stucco	0.0191	0.720	1856	0.838	
K4	gypsum board	0.0127	0.160	800	1.089	
	insulation foam	0.1016	0.036	16	1.215	
	concrete	0.1524	1.440	2240	0.838	
	stucco	0.0191	0.720	1856	0.838	
K5	gypsum board	0.0127 (0.019*)	0.160	800	1.089	
	insulation foam	0.0254 (0.058*)	0.036	16	1.215	
	concrete	0.1524	1.440	2240	0.838	
	insulation foam	0.0762	0.036	16	1.215	
	stucco	0.0191 (0.029*)	0.720	1856	0.838	
K6	gypsum board	0.0127	0.160	800	1.089	
	insulation foam	0.0508	0.036	16	1.215	
	concrete	0.1524	1.440	2240	0.838	
	insulation foam	0.0508	0.036	16	1.215	
	stucco	0.0191	0.720	1856	0.838	
A38	E1: 20 mm Plaster or gypsum	0.0200	0.727	1602	0.8368	
	B15: 150 mm Insulation	0.1500	0.043	91	0.8368	
	C20: 300 mm high density concrete block	0.3000	0.675	897	0.8368	
	A2: 100 mm Face brick	0.1000	1.333	2002	0.920	

The numerical simulations have been carried out for three time steps: 60 minutes, 15 minutes and 3 minutes.

The driving forces, located once at the internal and once at the external side of the walls, are:

- a sinusoidal ambient temperature with amplitude 1°C and period 24 hours;
- a sinusoidal ambient temperature with amplitude 1°C and period 1 hour;

Little and non-relevant differences in the errors have been noticed changing the BCs amplitude to 10 °C, respectively for the CTF and FD methods.

In all the tests, the internal and external superficial heat transfer coefficients have been chosen equal to 10 W/(m² K) to preserve symmetry in the BCs on both sides. To compare the numerical solutions with the analytical exact solution, all cases have been run over a sufficient number of periods until they reached the periodic steady state. The solution accuracy has then been evaluated over the last period through the following errors definition:

- the amplitude percentage error on the inner surface peak flux, calculated as: $(\varphi_{num}^{max} - \varphi_{exact}^{max})/\varphi_{exact}^{max}$
- the percentage phase shift of the inner surface peak flux: $(t_{num}^{si,max} - t_{exact}^{si,max})/T$, with T as the period of the driving force;
- the internal and external normalized error on the maximum surface temperature, calculated as: $(\vartheta_{num}^{max,sx} - \vartheta_{exact}^{max,sx})/\Delta\vartheta$, with $\Delta\vartheta$ as the amplitude of the driving force and the superscript *sx*, for *si* or *se*.

In the majority of the cases, the attention has been focused on the internal surface of the wall, since its temperature and heat flux are of great importance for the control strategy.

3. Tested Numerical methods: starting considerations

The tested numerical methods are:

- the State-Space Conduction Transfer Function (SS), as implemented in EnergyPlus 8.1 [3];
- the Direct Root Finding Conduction Transfer Function (DRF), as implemented in TRANSYS 17 [4];
- Explicit (EE), Implicit (IE) and Crank-Nicolson (CN) Finite Difference methods [5].

For each tested walls the CTF coefficients have been taken from EnergyPlus for the SS method and from TRNSYS 17 for the DRF method. Since both tools provide a reduced precision printout of these coefficients, which led to poor results with short time steps, direct extraction of such coefficients has been performed. Coefficients with 12 significant digits are provided by TRNSYS in its non-formatted file in input to Type 56, despite they are calculated in double precision (15–17 significant decimal digits precision); consequently this precision has been taken. To get the full precision coefficients in EnergyPlus, instead, we had modified its source code in order to print out more digits, in particular from 8 to 15. If the 15 digit are truncated instead of rounded, relevant differences arise with short time step (3 min) for some of the tested wall. This means that the number of digits used for the CTF coefficients or their rounding at the 16th digit might have an impact on the results when dealing with short time steps. With time steps of 60 min and 15 min 12 digits were enough for both DRF and SS methods. Another important difference between the two software concerned the rules implemented to prevent the use of inaccurate coefficients. In all the tested cases, EnergyPlus has always provided a set of coefficients even if they led to poor results. TRNSYS implements more stringent internal stability criteria, which do not allow coefficients determination if not satisfied. These criteria, as implemented in the last open BID file (TRNSYS 14), are the well-known “transmittance” check and an empirical check on the coefficients sums which have to be greater than 0.0005. With a 3 min time base, TRNSYS 17 had never provided the CTF coefficients for the tested walls. In these cases, using TRNSYS 14 BID source code, the coefficients sums resulted to be very low (i.e. less than 0.0005) while the “transmittance” check was fulfilled, except for wall A38. If these coefficients are used, they give on the internal flux even lower or comparable errors with respect to those obtained with the SS method, whose sums was below the TRNSYS limits too (**bold values** in Table 1). A higher number of coefficients provided by TRNSYS explains this better performance. Stability problems also arose for the Explicit FD method, given the exiguous thickness of some walls layers; stability criteria have not been met with any of the investigated time step, even with the smallest one of 3 minutes.

4. Results

4.1. Sinusoidal temperature BC

In most of the cases, the FD methods gave better results than the CTF ones at shorter time steps, and the CN method gave smaller or comparable errors at bigger time steps, with some exceptions (ref. Table 2). In general, among the FD methods, the CN one gave better results, even if high frequency boundary conditions might cause instabilities during the startup period (the pure transient), which are more evident on flux or superficial temperature on the same side of applied BC.

Despite all walls are characterized by the same transmittance and thermal capacity, at short time steps, the position of the lowest diffusive layers inside the wall affects the results accuracy and led to errors on the amplitude of the internal flux up to 90% with a time step of 3 min for wall K3 using the SS method.

Table 2. Amplitude and time shift inner flux percentage errors due to a sinusoidal external and internal temperature with period of 24 h and 1 h.

varBC_Period		Tout_24h						Tin_24h						Tin_1h	
Timestep		60 min		15 min		3 min		60 min		15 min		3 min		3 min	
Interior Error		Flux	Shift	Flux	Shift	Flux	Shift	Flux	Shift	Flux	Shift	Flux	Shift	Flux	Shift
NM	wall	%	%	%	%	%	%	%	%	%	%	%	%	%	%
CTF SS	K3	-3.43	1.2	-0.55	0.2	**90.78**	-8.8	0.31	0.0	0.13	0.0	**-7.62**	-2.7	**-9.27**	-1.4
	K4	-2.38	-0.5	-0.47	0.5	**-0.55**	0.1	2.35	0.6	0.39	0.6	**0.02**	-0.1	**-1.71**	1.3
	K5	-4.24	-2.1	**-0.60**	0.0	**-13.64**	0.0	3.46	-0.2	**0.55**	-0.2	**-0.18**	0.0	**-1.81**	1.4
	K6	-4.12	1.9	**-0.51**	-0.1	**18.26**	0.1	3.79	0.2	**0.60**	0.2	**0.38**	0.0	**-1.79**	1.3
	A38	-6.34	-2.0	**175.62**	-19.7	**625.85**	-38.0	-0.77	2.2	**-46.65**	0.2	**-74.35**	3.1	**-29.04**	-6.9
CTF DRF	K3	-3.33	1.2	-0.43	0.2	n.d.	n.d.	0.23	0.0	0.04	0.0	n.d.	n.d.	n.d.	n.d.
	K4	-2.23	-0.5	-0.33	-0.5	n.d.	n.d.	2.34	0.6	0.37	0.6	n.d.	n.d.	n.d.	n.d.
	K5	-2.55	-2.1	1.11	0.0	n.d.	n.d.	4.83	-0.2	1.87	-0.2	n.d.	n.d.	n.d.	n.d.
	K6	-4.04	1.9	-0.33	-0.1	n.d.	n.d.	3.84	0.2	0.63	0.2	n.d.	n.d.	n.d.	n.d.
	A38	-4.42	-2.0	n.d.	n.d.	n.d.	n.d.	-0.90	2.2	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
FD IE	K3	-11.45	-3.0	-3.82	-0.9	-1.54	0.0	-0.90	0.0	0.63	0.0	1.05	-0.2	1.42	-1.4
	K4	-11.37	-0.5	-3.71	-0.5	-1.58	-0.1	3.01	0.6	1.30	0.6	0.71	0.1	-3.37	1.3
	K5	-10.84	-2.1	-4.03	0.0	-2.01	0.4	3.91	-0.2	1.32	-0.2	0.56	0.0	-3.64	1.4
	K6	-10.64	-2.2	-3.94	-0.1	-1.96	0.3	4.49	0.2	1.47	0.2	0.53	0.0	-3.69	1.3
	A38	-30.70	-6.2	-17.96	-4.1	-13.99	-3.7	-0.18	2.2	1.14	0.2	1.46	0.0	-2.72	-1.9
FD CN	K3	-1.77	1.2	-1.00	0.2	-0.97	0.2	1.20	0.0	1.15	0.0	1.16	-0.2	0.94	-1.4
	K4	-1.69	-0.5	-1.11	0.5	-1.04	0.1	0.97	0.6	0.55	-0.5	0.56	-0.1	0.85	1.3
	K5	-2.61	2.1	-1.57	0.0	-1.49	0.4	0.52	-0.2	0.37	-0.2	0.37	0.0	0.52	1.4
	K6	-2.46	1.9	-1.52	0.9	-1.45	0.5	0.60	0.2	0.30	0.2	0.29	0.0	0.59	1.3
	A38	-14.24	-2.0	-13.05	-3.0	-12.96	-3.5	1.39	-1.9	1.56	0.2	1.54	0.0	-0.24	-1.9
	A38'	-2.24	2.2	-0.44	0.1	-0.37	-0.1	-0.13	-1.9	0.10	0.2	0.08	0.0	-0.10	-1.9

To analyze such position effect, we have defined a "thermal inertia" index, calculated as the integral of the square of the distance from each surface over the inverse of the diffusivity, reported in Table 3.

Table 3. Wall's characterization.

	External inertia	Internal inertia	Ext inertia/Int inertia
k3 internal mass	13802	7704	1.79
k4 external mass	10348	11007	0.94
k5 sandwich ext insul	12713	8305	1.53
k6 simm sandwich	11775	9055	1.30
A38_heavy concrete	95811	77040	1.24

Table 4. Internal and external temperature errors due to a sinusoidal external and internal temperature with period of 24 h.

BC Period		Tout_24h						Tin_24h					
Time step		60 min		15 min		3 min		60 min		15 min		3 min	
Error		Tso	Tsi	Tso	Tsi	Tso	Tsi	Tso	Tsi	Tso	Tsi	Tso	Tsi
NM	wall	%	%	%	%	%	%	%	%	%	%	%	%
CTF SS	K3	-2.169	-0.023	-0.326	-0.004	1.829	0.615	-0.023	-0.260	-0.004	-0.057	0.615	7.241
	K4	-0.476	-0.020	-0.038	-0.004	0.000	-0.005	-0.020	-1.092	-0.004	-0.131	0.003	-0.023
	K5	-2.142	-0.009	-0.316	-0.001	-0.067	-0.029	-0.009	-0.858	-0.001	-0.105	-0.020	-0.047
	K6	-2.083	-0.007	-0.301	-0.001	-0.033	0.032	-0.007	-0.985	-0.001	-0.117	0.010	0.014
CTF DRF	K3	-2.169	-0.023	-0.319	-0.003	n.d.	n.d.	-0.023	-0.247	-0.003	-0.038	n.d.	n.d.
	K4	-0.496	-0.019	-0.056	-0.003	n.d.	n.d.	-0.019	-1.091	-0.003	-0.127	n.d.	n.d.
	K5	-2.140	-0.005	-0.307	0.002	n.d.	n.d.	-0.005	-0.998	0.002	-0.227	n.d.	n.d.
	K6	-2.083	-0.007	-0.295	-0.001	n.d.	n.d.	-0.007	-0.985	-0.001	-0.114	n.d.	n.d.

Considering the error on both side, walls with higher inertia towards the exterior got worst results on the external side with a sinusoidal BC on the same side and vice versa, except in one case, as can be seen in Table 4. This could not have been noticed looking to the outermost and innermost layers properties, which are equal among all the tested walls from Kossecka [1]. FD methods are less sensitive than the CTF ones to these aspects.

Using 1 h period for the sinusoidal internal BC instead of 24 h, to maintain similar relative time resolution, the equivalent time step for 60 min = 1/24 T_{24h} is 2.5 min (=60/24 T_{1h}). Thus, no investigations have been made for time steps larger than 3 min (for instance 15 min) because of lack of time resolution.

The most critical case is represented by Wall A38, which is characterized by quite similar external and internal inertia, but has the lowest average diffusivity. This low average diffusivity of wall 38 had caused problems to all the methods, when no optimization has been applied. For this wall, TRSNYS did not allow the calculation already with a time step of 15 min. Energy Plus calculated 12 CTF coefficients to represent this wall with a time base of 1h, but it gave worst results that DRF method that used 10 coefficients (-6.34 % vs. -4.42%). For FD methods, the use of three nodes per layer was not assuring good accuracy (even if FD accuracy, with time steps of 15 and 3 minutes, was better than the accuracy of the DRF one). On the contrary, for the shortest time step good results has been achieved for FD applying the criterion of similar local Fourier numbers, Fo_x, among all layers nearer as possible to 0.5 (in cases where the layers thickness is too thin). This criterion has led to an error of -0.37%, with the CN method and a time step of 3 min, instead of the -12.96% reached before, as can be seen from the last two rows of Table 1 (case A38' with respect to case A38).

4.2. Applicability of Fourier Stability's Criterion

Since for all the selected walls, the local Fourier stability criterion, i.e. $Fo_x < 0.5$, was not fulfilled even with the minimum time step chosen for the simulation, an additional wall has been created, starting from wall K5 and widening the thickness of its most critical layers, as shown in Table 1 by values signed with *. We have found that in order to get stable solutions, the Fo_x, should have been limited to 0.4. Since the modified wall was "good enough" for the explicit FD method, we have tried to see if this criterion could have been applied also to the CTF methods. For this modified wall TRNSYS did not provide any coefficients again; consequently, this criterion is not strong enough to fulfill TRNSYS internal stability criteria. Also using EnergyPlus (SS method), the solution did not show any improved accuracy.

4.3. Numerical methods' computational time

For all the tested numerical methods, a pre-calculation phase is mandatory before beginning the simulation (to determine the CTF coefficients or the FD matrix elements) and during the simulation, at each iteration or time step, a different number of calculations is needed according to the selected method.

Even if the pre-calculation is more complex for the case of the CTF methods than for the FD ones, since it is done only once, it will not be further analyzed and evaluated in assessing the time performance of the selected methods. To qualify these methods from the time performance point of view, time variable superficial heat transfer coefficient have been taken into account; that means two auxiliary equations for CFT and continuous matrix inversion in FD. If we quantify a computational time of 1 unit for sum and subtraction, 4 units for multiplication and 10 units for division, the used Calculation Time Units (CTUs) of the two methods at each time step or iteration are:

- *for the CTF methods*: 80 + 30 * N, CTUs (assuming the number of coefficients N is the same for exterior, cross, and interior CTF terms and it is equal to the number of flux history CTF terms plus one);
- *for the worst case of the FD methods, i.e. the CN one*: 8 + 50 * N (where N is the number of nodes).

If the number of elements (coefficients or nodes), i.e. N, is the same for both methods, the FD methods require more CTUs than the CTF ones, but for low values of N, the CTUs are not too different among each other. Indeed, the number of elements is normally different because N is strictly related to the method used. In the tests done, we have tried to use the minimum number of nodes for the FD methods, i.e. twice the number of the wall's layers plus one, to find out when this minimum space discretization fails. All the encountered cases has been summarized in Table 4. The CTUs for CTF are depending on the coefficients number that are growing with the time step reduction, while the CTUs for FD are depending on the space discretization. However, at short time steps, we have seen that, even with 18 coefficients, in most of the cases, the results obtained with the CTF methods have still poor accuracy. The same accuracy can be obtained using FD with few nodes and thus with a lower CTUs number. These considerations might help in weakening the belief that the CTF methods are, no matter what, faster than the FD ones.

Table 4. CTUs cases

Numerical method	Time step	Wall	N	CTUs
CTF SS	60 min	Kx	7	290
		A38	12	440
	15 min	Kx	12	440
		A38	15	530
	3 min	K3	16	560
		K4, K5, K6	19	650
		A38	18	620
FD CN	all	K3, K4, A38	9	475
		K5, K6	11	575
		A38'	32	1625

5. Conclusions

The need to perform simulation with short time steps required a new analysis of the CFT methods, still employed to reduce the computational time. However, we have found that, without any optimization of the space discretization, the FD-CN method gave comparable/lower errors with a time step of 15 minutes with respect to CTF ones, requiring comparable CTUs with respect to CTF methods. In general CTF gave better results with 1h time step, requiring less computational time, but in some critical applications, with specific walls, the CN methods gave better results also with this kind of time step. We have seen that in some cases the CN method might be more accurate and more fast than the CTF methods.

To further investigate the response of the different families of methods to the variation of the BC's frequency it will be interesting to test the third method of the CTF family, i.e. the Frequency Domain Regression (FDR) method [6]. Unfortunately this method is not implemented in any available tool, thus, in the next step of the analysis it will be implemented inside the tool used to test the FD methods, in order to evaluate its accuracy with respect to the other methods.

Other tests will be carried out with pure transient BCs, using step-type functions, to investigate the capability of CTFs and FD methods to emulate the behavior of a wall under generic time dependent boundary conditions.

Nomenclature

CTF	Conduction Transfer Function	FDR	Frequency Domain Regression
BCs	Boundary Conditions	Fo_x	Local Fourier Number
BPSts	Building Performance Simulation tools	n.d.	not defined
CTUs	Calculation Time Units	NM	Numerical Method
DRF	Direct Root Finding	SS	State Space
FD	Finite Difference		

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