1	A NEW METHOD FOR CALCULATING CONDUCTION RESPONSE FACTORS FOR
2	MULTILAYER CONSTRUCTIONS BASED ON FREQUENCY-DOMAIN SPLINE
3	INTERPOLATION (FDSI) AND ASYMPTOTIC ANALYSIS
4	Javier SANZA PÉREZ ª, Manuel ANDRÉS CHICOTE ª,♭, Fernando VARELA DÍEZ º, Eloy VELASCO
5	GÓMEZ ª
6	^a University of Valladolid, School of Engineering, Department of Energy Engineering and Fluidmechanics.
7	Paseo del Cauce n.59, 47011, Valladolid, Spain
8	^b CARTIF Technology Center, Parque Tecnológico de Boecillo, 205, 47151 Boecillo, Valladolid, Spain
9	^c Universidad Nacional de Educación a Distancia (UNED), School of Industrial Engineering, Department
10	of Energy Engineering. Juan del Rosal n.12, 28040, Madrid, Spain
11	Abstract
12	Conduction heat transfer through building construction elements is one of the main components of space
13	heating and cooling loads, and, thus, one of the key aspects when planning sustainable energy designs in
14	the building sector. The Response Factors (RF) method sets the base for related dynamic calculations
15	implemented by most well-known Building Energy Simulation (BES) software, and it represents a
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1 1 16 research topic of present interest. In this regard, this work introduces a new method for calculating 17 conduction Response Factors in building multilayer constructions, based on the definition of an 18 approximated wall model through Frequency-Domain Spline Interpolation (FDSI) and asymptotic 19 analysis. Its conceptual development as well as first validations comparing with existing methods from 20 previous literature are presented. Finally, as a result of applying a table-lookup approach and the 21 possibility of pre-calculating most of the involved operations, an accurate, fast and easy-to-code algorithm 22 is obtained, which constitutes a promising alternative to improve the current state-of-art calculation 23 procedures.

Keywords: Building transient heat transfer, Thermal Response Factors, spline interpolation, frequency domain, asymptotic analysis.

26 Nomenclature

27 <u>General</u>

- 28 a, b, c, d coefficients of the piecewise polynomial approximation
- 29 A_k, B_k, C_k, D_k transmission matrix elements of the kth construction layer

30	At, Bt, Ct, Dt	transmission matrix elements of the total multilayer construction
31	Cp	specific heat capacity [J·kg ⁻¹ ·K ⁻¹]
32	E	Error estimate (%)
33	f _k	cubic spline approximation functions [W·m ⁻² ·K ⁻¹]
34	F[]	Fourier transform
35	F ⁻¹ []	inverse Fourier transform
36	G	transfer function
37	hĸ	amplitude of the intervals between frequency evaluation points (ω_k) [rad·s ⁻¹]
38	L	layer thickness [m]
39	j	complex variable
40	MFF	Modified Frequency Function [W·m ⁻² ·K ⁻¹]
41	q	heat flux [W·m ⁻²]
42	R	thermal resistance [m ² ·K·W ⁻¹]
43	۲ _k	slope of the MFFs at selected frequency evaluation points (ω_k)
44	S	independent variable in the Laplace domain
45	t	time [s]
46	т	temperature [C]
47	Ť	first derivative of the temperature variable $[C \cdot s^{-1}]$
48	T_Δ	shaping function [-]
49	Δt	timestep [s]
50	U	wall's thermal transmittance [W·m ⁻² ·K ⁻¹]
51	X_{RF}, Y_{RF}, Z_{RF}	internal, cross and external terms for the Response Factor method [W \cdot m $^{-2} \cdot$ K $^{-1}$]
52	XCTF, YCTF, ZCTF	internal, cross and external terms for the CTF method [W \cdot m ⁻² ·K ⁻¹]
53	Ук	Value of the MFFs at selected frequency evaluation points (ω_k) [W·m ⁻² ·K ⁻¹]
54	<u>Greek symbols</u>	
55	α	hermal diffusivity [m ² ·s ⁻¹]
56	β _k	oots of the transfer function $B_T(s)$
57	λ	hermal conductivity [W·m ⁻¹ ·K ⁻¹]
58	Ψ	mplitude of the frequency characteristic
59	Γκ, φκ	uxiliary terms for the recursive calculation of the spline coefficients

60	Φ	weighting coefficients of the previous heat fluxes in the CTF method [-]
61	ρ	material density [kg·m ⁻³]
62	σ _k	second derivative of the MFFs at selected frequency evaluation points
63	ω	frequency [rad·s ⁻¹]
64	<u>Subscripts</u>	
65	a, b, c, d	relative to the corresponding coefficients of the piecewise polynomial approximation
66	i, k	integer counts
67	A / P	asymptotic / polynomial
68	C / S	cosine / sine
69	H / T	head / tail
70	int / ext	internal / external
71	m	number of timesteps
72	n	total number of elements of a given vector or identifier of a given element into a
73		Response Factor series (X, Y or Z)
74	Ν	total number of frequency points
75	X, Y, Z	relative to the corresponding term of the Response Factor method
76	<u>Acronyms</u>	
77	BES	Building Energy Simulation
78	CTF	Conductive Transfer Functions
79	DRF	Direct Root Finding
80	FDR	Frequency-Domain Regression
81	FDM	Finite Difference Method
82	FDSI	Frequency-Domain Spline Interpolation
83	FEM	Finite Element Method
84	HVAC	Heating, Ventilating and Air Conditioning
85	RF	Response Factors
86	SSM	State-Space Method
87	Specific notation	on for FDSI method constants and integration factors
88	AF	Asymptotic function
89	k	constant (construction-dependent)

90	К	integration factor (construction non-dependent) (¹ , ²)
91		(1) KAHC, KAHS, KATC, KATS, KPCa, KPCb, KPCc, KPCd, KPSa, KPSb, KPSc, KPSd are those
92		'integration factors' which can be interpreted according to the following criteria:
93		A/P: asymptotic/polynomial
94		H/T: head/tail
95		C/S: cosine/sine
96		a/b/c/d: associated to the corresponding spline coefficient
97		(²) KATC0, KATC(+), KATS(+), KATC (-), KATS(-) are particular definitions of the integration factors
98		to determine the tail asymptotic equivalents

99 1. Introduction

100 As energy and environmental sustainability in the building sector have become increasingly important in 101 these days, Building Energy Simulation (BES) software has attained a fundamental role in the design of 102 new constructions and the planning of energy retrofitting actions [1,2]. This software can estimate the 103 amount of energy required to assure indoor thermal comfort conditions throughout the year (that is to say, 104 space heating and cooling loads), which allows architects and engineers to better benefit from passive 105 energy techniques and design more efficient HVAC systems and strategies. In this sense, among other 106 capabilities, BES software involves methods to evaluate short-wave and long-wave radiative heat 107 transfer, convective heat flows, one-dimensional heat conduction through multi-layered walls, as well as 108 the dynamics of the energy facilities within the built environment.

In particular, the conduction heat transfer through building construction elements is one of the key components of space loads. Wang and Chen [3] present an exhaustive review of those methods available to determine its contribution. Despite the existence of numerical methods [4,5] and the so-called harmonic or periodic approaches [6,7], currently, the most widely used techniques are the Response Factors (RF) method and the Conductive Transfer Function (CTF) method, which set the base for the calculations implemented by well-known BES programs such as Energy-Plus [8] or TRNSYS [9]. These methods are generally considered to derive from the research conducted by Mitalas and Stephenson [10-12]

The Response Factors method calculates the heat flux at discrete times as a function of the previoustemperatures on both sides of the construction (Eqs.1).

118
$$q_{ext}(i \cdot \Delta t) = \sum_{k=0}^{\infty} X_{RF}[k] \cdot T_{ext}[(i-k) \cdot \Delta t] - \sum_{k=0}^{\infty} Y_{RF}[k] \cdot T_{int}[(i-k) \cdot \Delta t] \quad Eq. 1a$$

119
$$q_{int}(i \cdot \Delta t) = \sum_{k=0}^{\infty} Y_{RF}[k] \cdot T_{ext}[(i-k) \cdot \Delta t] - \sum_{k=0}^{\infty} Z_{RF}[k] \cdot T_{int}[(i-k) \cdot \Delta t] \quad Eq.1b$$

120 Tint and Text strictly are the internal and external surface temperatures. However, for general validation 121 purposes, numerous case studies from literature often consider them to represent ambient temperatures 122 including massless inner and outer layers with a thermal resistance value equivalent to that derived from 123 the corresponding convective heat transfer coefficient (see Tables 5 and 7). The terms X[k], Y[k] and Z[k] 124 for k ranging from zero to infinity are called response factors (RF). These factors tend to zero when k tend 125 to infinity so, in practice, a finite number of them is accurate enough to describe the construction 126 dynamics. However, the simulation of HVAC systems integrated in BES programs sometimes requires 127 time-steps shorter than 1 hour to reproduce realistic control strategies and equipment time responses. In 128 such situations, the required amount of RF to get good accuracy often becomes inconveniently large for 129 computer implementation [3, 13].

The Conductive Transfer Function method (CTF) [12] reduces the number of terms needed to describe the construction dynamics. This method expresses the internal and external heat flux values at a given time in a more convenient form as a function of a finite number of previous temperatures and previous heat fluxes (see Eqs.2).

134
$$q_{ext}(i \cdot \Delta t) = \sum_{k=0}^{N} X_{CTF}[k] \cdot T_{ext}[(i-k) \cdot \Delta t] - \sum_{k=0}^{N} Y_{CTF}[k] \cdot T_{int}[(i-k) \cdot \Delta t] + \sum_{k=1}^{M} \Phi[k] \cdot q_{ext}[(i-k) \cdot \Delta t] \quad Eq. 2a$$

135
$$q_{int}(i \cdot \Delta t) = \sum_{k=0}^{\infty} Y_{CTF}[k] \cdot T_{ext}[(i-k) \cdot \Delta t] - \sum_{k=0}^{\infty} Z_{CTF}[k] \cdot T_{int}[(i-k) \cdot \Delta t] + \sum_{k=1}^{M} \Phi[k] \cdot q_{int}[(i-k) \cdot \Delta t] \quad Eq. 2b$$

136 The series of terms $X_{RF}[k]$, $Y_{RF}[k]$ and $Z_{RF}[k]$ for the Response Factor Method (RF) as well as $X_{CTF}[k]$, 137 $Y_{CTF}[k]$ and $Z_{CTF}[k]$ for the Conductive Transfer Function Method (CTF), can be calculated by several 138 procedures.

The use of Laplace transform methods is probably the most extended one. Briefly, these methods obtain the heat flux response of the construction to a temperature shaping function (typically a triangle of height one) in the frequency domain, and then apply the inverse Laplace transform to get the corresponding solution in the time domain. Eqs.3 show the expressions for the Response Factors, where A_T(s), B_T(s), C_T(s) and D_T(s) are the terms of the characteristic matrix of the construction (see section 2), while β_k are the poles of the transfer function B_T(s).

145
$$X_{RF}(t) = t \cdot \left[\frac{D_T(s)}{B_T(s)}\right]_{s=0} + \frac{d}{ds} \left[\frac{D_T(s)}{B_T(s)}\right]_{s=0} + \sum_{k=1}^{\infty} \frac{1}{\beta_k^2} \cdot \left[\frac{D_T(s)}{B_T(s)}\right]_{s=0} \cdot e^{-\beta_k \cdot t} \quad Eq.3a$$

146
$$Y_{RF}(t) = t \cdot \left[\frac{1}{B_T(s)}\right]_{s=0} + \frac{d}{ds} \left[\frac{1}{B_T(s)}\right]_{s=0} + \sum_{k=1}^{\infty} \frac{1}{\beta_k^2} \cdot \left[\frac{1}{B_T(s)}\right]_{s=0} \cdot e^{-\beta_k \cdot t} \quad Eq. \, 3b$$

147
$$Z_{RF}(t) = t \cdot \left[\frac{A_T(s)}{B_T(s)}\right]_{s=0} + \frac{d}{ds} \left[\frac{A_T(s)}{B_T(s)}\right]_{s=0} + \sum_{k=1}^{\infty} \frac{1}{\beta_k^2} \cdot \left[\frac{A_T(s)}{B_T(s)}\right]_{s=0} \cdot e^{-\beta_k \cdot t} \quad Eq.3c$$

This approach was first developed by Stephenson and Mitalas [10-12] and later improved by other authors [13, 14] in order to avoid pole skipping and enhance calculation efficiency. These methods are often referred as Direct Root-Finding (DRF) methods, as the inversion process (based on the residue theorem) involves iterative root finding, which is computationally expensive. In addition, the number of poles is infinite, so one must settle for a limited number of them. Varela et al. [15] proposed the Direct Numerical Integration (DNI) of the inversion formula as a viable option.

Moreover, other alternatives not based on the Laplace transform have been developed to obtain the RF or CTF coefficients. Davies [16] evaluated them using elementary time domain solutions for wall heat flow. Similarly, State-Space Methods (SSM) [17] are also based on a time-domain formulation. As shown in Figure 1, a temperature node is set for each construction layer. Then, a numeric algorithm (Finite Element Method - FEM, or Finite Differences Method - FDM) is applied to obtain the terms of the matrices A, B, C and D of the equivalent space-state model. Once the terms of these matrices are calculated, the coefficients of the conduction transfer function (CTF) can be deduced by Leverrier's algorithm [18].

161
162

$$\begin{bmatrix}
T_1 \\
T_2 \\
\vdots \\
T_n
\end{bmatrix} = A \cdot \begin{bmatrix}
T_1 \\
T_2 \\
\vdots \\
T_n
\end{bmatrix} + B \cdot \begin{bmatrix}
T_{int} \\
T_{ext}
\end{bmatrix} = Eq. 4a$$

$$\begin{bmatrix}
q_{int} \\
q_{ext}
\end{bmatrix} = C \cdot \begin{bmatrix}
T_1 \\
T_2 \\
\vdots \\
T_n
\end{bmatrix} + D \cdot \begin{bmatrix}
T_{int} \\
T_{ext}
\end{bmatrix} = Eq. 4b$$

164

Figure 1. General approach of the space-state methods

165 Seem et al. [19] demonstrated that this approach can also be used to calculate transfer functions for walls 166 that require two-dimensional models, which could be applied to overcome the limitations of the one-167 dimensional approach when dealing with hollow blocks or relevant thermal bridge effects into wall 168 constructions. In this sense, Kossecka et al. [20] also described a method to derive conduction z-transfer 169 function coefficients from response factors for 3D wall assemblies. Moreover, Kosny et al. [21] contributed 170 to the accuracy improvement in whole building thermal modeling tools, through the definition of an 171 'equivalent wall' concept and the proposal of additional thermal structure factors to account for building 172 envelope components containing high thermal mass and/or 2D and 3D heat transfer effects.

However, state-space formulations for multi-dimensional heat conduction problems often rely on linear models with high-order matrices involving important computation times. Gao et al. [22] proposed a solution based on the application of model reduction techniques to decrease computation costs with no significant accuracy losses.

177 Returning to the Response Factor method for 1D transient heat transfer, another more recent 178 methodology consists of the Frequency-Domain Regression (FDR) methods developed by Wang et al. [3, 179 23-26]. They set out a general transfer function whose parameters are estimated by a regression 180 algorithm (Eq. 5). Starting from several frequency evaluations of the construction dynamics, these 181 methods find the set of coefficients that minimize the quadratic error between those evaluations and the 182 ones given by the approximate model.

183
$$G(s) = \frac{\beta_0 + \beta_1 \cdot s + \beta_2 \cdot s^2 + \dots + \beta_{r-1} \cdot s^{r-1} + \beta_r \cdot s^r}{1 + \alpha_1 \cdot s + \alpha_2 \cdot s^2 + \dots + \alpha_{m-1} \cdot s^{m-1} + \alpha_m \cdot s^m} \quad Eq.5$$

184 It is a fast and accurate method. In addition, it allows a direct calculation of the coefficients for the CTF
185 method instead of the sequence of response factors (RF).

Finally, it should be remarked that research on this field is of present interest, what can be supported by additional improved or innovative approaches contributed in recent years [27-34].

Along these lines, this work introduces a new method for calculating conduction response factors (RF) of 188 189 building multilayer constructions. It is based on the definition of an approximated wall model through 190 Frequency–Domain Spline Interpolation (FDSI) and asymptotic analysis. First, temperature evolutions are 191 expressed as sums of harmonics by means of Fourier transform methods. Then, the FDSI model is 192 applied to obtain the heat flux solution in the frequency domain. Nevertheless, the particular definition of 193 such wall model enables to rearrange the Fourier transform inversion integrals so that each response 194 factor is obtained as the sum of several simple terms. In addition, those terms depending on the 195 construction thermo-physical properties can be separated and pre-calculated, making it possible to use 196 an efficient table-lookup approach. Therefore, the FDSI method provides an accurate, fast and easy-to-197 code alternative to the current RF calculation methodologies.

198 2. Frequency response in multilayer constructions

Given the Laplace model of a construction, it is easy to evaluate the gain and the phase shift associated
to each frequency. For a particular layer (k), its mathematical expression is the following [3]:

201
$$\begin{bmatrix} T_{ext} \\ q_{ext} \end{bmatrix} = \begin{bmatrix} A_k(s) & B_k(s) \\ C_k(s) & D_k(s) \end{bmatrix} \cdot \begin{bmatrix} T_{int} \\ q_{int} \end{bmatrix} \xrightarrow{s=j\omega} \begin{bmatrix} T_{ext} \\ q_{ext} \end{bmatrix} = \begin{bmatrix} A_k(j\omega) & B_k(j\omega) \\ C_k(j\omega) & D_k(j\omega) \end{bmatrix} \cdot \begin{bmatrix} T_{int} \\ q_{int} \end{bmatrix} \quad Eq.6$$

202
$$\begin{bmatrix} A_{k}(j\omega) & B_{k}(j\omega) \\ C_{k}(j\omega) & D_{k}(j\omega) \end{bmatrix} = \begin{bmatrix} \cosh\left(L_{k} \cdot \sqrt{\frac{j\omega}{\alpha_{k}}}\right) & \frac{\sinh\left(L_{k} \cdot \sqrt{\frac{j\omega}{\alpha_{k}}}\right)}{\lambda_{k} \cdot \sqrt{\frac{j\omega}{\alpha_{k}}}} \\ \lambda_{k} \cdot \sqrt{\frac{j\omega}{\alpha_{k}}} \cdot \sinh\left(L_{k} \cdot \sqrt{\frac{j\omega}{\alpha_{k}}}\right) & \cosh\left(L_{k} \cdot \sqrt{\frac{j\omega}{\alpha_{k}}}\right) \end{bmatrix} \quad Eq.7$$

Numeric evaluation of the matrix above for each frequency yields four complex numbers that describe the gain and phase shift of the layer thermal response associated to these frequencies. Besides, the characteristic matrix of the whole construction can be expressed as the product of the matrices for each individual layer:

$$207 \qquad \begin{bmatrix} A_T(j\omega) & B_T(j\omega) \\ C_T(j\omega) & D_T(j\omega) \end{bmatrix} = \begin{bmatrix} A_1(j\omega) & B_1(j\omega) \\ C_1(j\omega) & D_1(j\omega) \end{bmatrix} \cdot \begin{bmatrix} A_2(j\omega) & B_2(j\omega) \\ C_2(j\omega) & D_2(j\omega) \end{bmatrix} \cdots \begin{bmatrix} A_{n-1}(j\omega) & B_{n-1}(j\omega) \\ C_{n-1}(j\omega) & D_{n-1}(j\omega) \end{bmatrix} \cdot \begin{bmatrix} A_n(j\omega) & B_n(j\omega) \\ C_n(j\omega) & D_n(j\omega) \end{bmatrix} \quad Eq.8$$

208 If heat fluxes are written down as a function of temperatures, the following formulation (Eq.9) is obtained.

209
$$\begin{bmatrix} q_{int} \\ q_{ext} \end{bmatrix} = \begin{bmatrix} \frac{D_T(j\omega)}{B_T(j\omega)} & -\frac{1}{B_T(j\omega)} \\ \frac{1}{B_T(j\omega)} & -\frac{A_T(j\omega)}{B_T(j\omega)} \end{bmatrix} \cdot \begin{bmatrix} T_{ext} \\ T_{int} \end{bmatrix} = \begin{bmatrix} X(\omega) & -Y(\omega) \\ Y(\omega) & -Z(\omega) \end{bmatrix} \cdot \begin{bmatrix} T_{ext} \\ T_{int} \end{bmatrix}$$
 Eq. 9

210 Therefore:

211
$$X(\omega) = \frac{D_T(j\omega)}{B_T(j\omega)}; \quad Y(\omega) = \frac{1}{B_T(j\omega)}; \quad Z(\omega) = \frac{A_T(j\omega)}{B_T(j\omega)} \quad Eqs. 10$$

3. Description of the Frequency-Domain Spline Interpolation (FDSI) algorithm

The basic idea of the FDSI method is to split the temperature evolution into a sum of harmonics using the Fourier transform. Then, by means of an approximated model for the construction, the gain and phase shift for each frequency are calculated. Finally, this method gets the heat fluxes in time domain using the inverse Fourier transform.



217 218

Figure 2. Block diagram for the FDSI fundamental conception

In order to simplify this method, the temperature evolution between sampling points is often considered as linear. This is a reasonable assumption when such evolution is sufficiently slow compared to the time interval between these points, but not when there are abrupt temperature changes.

- 222 Considering this hypothesis, the interpolated time-domain function can be split into a set of triangular
- 223 pulses, as it is represented in Figure 3.



Figure 3. Breakdown of a linearly interpolated temperature evolution into unitary triangles

Therefore, the temperature function (for both the external or the internal temperature variables) can be expressed as the sum of a set of scaled and shifted unitary triangles (T_{Δ}) which constitute the so-called 'shaping function'. Figure 4 describes in detail the characteristics of such function.

229
$$T(t) = \sum_{k=-\infty}^{m} T(k \cdot \Delta t) \cdot T_{\Delta}(t - k \cdot \Delta t) \quad \text{with} \quad m \cdot \Delta t \ge t \quad Eq. 11$$

Temperature (Celsius)

230

231

$$T_{\Delta}(t) = \begin{cases} 0 & if \ t < -\Delta t \\ \frac{t + \Delta t}{\Delta t} & if \ t \in [-\Delta t, 0] \\ \frac{-t + \Delta t}{\Delta t} & if \ t \in [0, \Delta t] \\ 0 & if \ t > \Delta t \end{cases} Eq. 12$$
232

233

Figure 4. Description of a triangular shaping function

Shaping functions might also adopt expressions other than triangular, thus describing different types of interpolation [34]. In this case, starting from the temperature as a linear combination of shaping functions, the Fourier transforms yields an equivalent sum of harmonics. For the external temperature evolution this can be expressed through the equation Eq.13a.

238
$$T_{ext}(\omega) = F[T_{ext}(t)] = F\left[\sum_{k=-\infty}^{m} T_{ext}(k \cdot \Delta t) \cdot T_{\Delta}(t-k \cdot \Delta t)\right] = \sum_{k=-\infty}^{m} T_{ext}(k \cdot \Delta t) \cdot F[T_{\Delta}(t-k \cdot \Delta t)]$$

239
$$= \sum_{k=-\infty}^{\infty} T_{ext}(k \cdot \Delta t) \cdot e^{-k \cdot \Delta t \cdot j\omega} \cdot F[T_{\Delta}(t)] \quad with \quad m \cdot \Delta t \ge t \qquad Eq. 13a$$

240 Similarly, Eq.13b can be derived for the internal temperature evolution:

241
$$T_{int}(\omega) = F[T_{int}(t)] = \sum_{k=-\infty}^{m} T_{int}(k \cdot \Delta t) \cdot e^{-k \cdot \Delta t \cdot j\omega} \cdot F[T_{\Delta}(t)] \quad with \quad m \cdot \Delta t \ge t \qquad Eq. 13b$$

According to this formulation, the heat flux solutions in the frequency domain are obtained as follows:

243
$$q_{ext}(\omega) = X(\omega) \cdot T_{ext}(\omega) - Y(\omega) \cdot T_{int}(\omega) =$$

244
$$= X(\omega) \cdot \sum_{k=-\infty}^{m} T_{ext}(k \cdot \Delta t) \cdot e^{-k \cdot \Delta t \cdot j\omega} \cdot F[T_{\Delta}(t)] - Y(\omega) \cdot \sum_{k=-\infty}^{m} T_{int}(k \cdot \Delta t) \cdot e^{-k \cdot \Delta t \cdot j\omega} \cdot F[T_{\Delta}(t)] \quad Eq. 14a$$

245 $q_{int}(\omega) = Y(\omega) \cdot T_{ext}(\omega) - Z(\omega) \cdot T_{int}(\omega) =$

246
$$= Y(\omega) \cdot \sum_{k=-\infty}^{m} T_{ext}(k \cdot \Delta t) \cdot e^{-k \cdot \Delta t \cdot j\omega} \cdot F[T_{\Delta}(t)] - Z(\omega) \cdot \sum_{k=-\infty}^{m} T_{int}(k \cdot \Delta t) \cdot e^{-k \cdot \Delta t \cdot j\omega} \cdot F[T_{\Delta}(t)] \quad Eq. 14b$$

At this point, heat fluxes in time domain can be calculated via the inverse Fourier transform.

248
$$q_{ext}(t) = F^{-1}[q_{ext}(\omega)]; \quad q_{int}(t) = F^{-1}[q_{int}(\omega)] \quad Eq. 15$$

$$249 \qquad q_{ext}(t) = \sum_{k=-\infty}^{m} T_{ext}(k \cdot \Delta t) \cdot F^{-1} \left[X(\omega) \cdot e^{-k \cdot \Delta t \cdot j\omega} \cdot F[T_{\Delta}(t)] \right] - \sum_{k=-\infty}^{m} T_{int}(k \cdot \Delta t) \cdot F^{-1} \left[Y(\omega) \cdot e^{-k \cdot \Delta t \cdot j\omega} \cdot F[T_{\Delta}(t)] \right] = \frac{1}{2} \sum_{k=-\infty}^{m} T_{ext}(k \cdot \Delta t) \cdot F^{-1} \left[Y(\omega) \cdot e^{-k \cdot \Delta t \cdot j\omega} \cdot F[T_{\Delta}(t)] \right]$$

$$250 \qquad \qquad = \sum_{k=-\infty}^{m} T_{ext}(k \cdot \Delta t) \cdot F^{-1}[X(\omega) \cdot F[T_{\Delta}(t)]](t - k \cdot \Delta t) - \sum_{k=-\infty}^{m} T_{int}(k \cdot \Delta t) \cdot F^{-1}[Y(\omega) \cdot F[T_{\Delta}(t)]](t - k \cdot \Delta t) \quad Eq. 16a$$

$$251 \qquad q_{int}(t) = \sum_{k=-\infty}^{m} T_{ext}(k \cdot \Delta t) \cdot F^{-1}[Y(\omega) \cdot F[T_{\Delta}(t)]](t - k \cdot \Delta t) - \sum_{k=-\infty}^{m} T_{int}(k \cdot \Delta t) \cdot F^{-1}[Z(\omega) \cdot F[T_{\Delta}(t)]](t - k \cdot \Delta t) \ Eq.16b$$

In the formulation above, the following expression yields the response factors by conveniently substituting
in Eq.17 the term RF (Response Factor) by each corresponding series of factors (X, Y or Z).

254
$$RF(t) = F^{-1}[RF(\omega) \cdot F[T_{\Delta}(t)]] =$$

$$255 \qquad \qquad = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} |RF(\omega)| \cdot e^{j \cdot arg[RF(\omega)]} \cdot F[T_{\Delta}(t)] \cdot e^{j\omega t} \, d\omega = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} |RF(\omega)| \cdot e^{(\omega t + arg[RF(\omega)]) \cdot j} \cdot F[T_{\Delta}(t)] \, d\omega \qquad Eq. 17$$

256 If the shaping function is even (as it happens to be when linear interpolation is applied to the temperature257 evolution) the above integral can be rewritten in a much simpler way.

258
$$RF(t) = F^{-1}[RF(\omega) \cdot F[T_{\Delta}(t)]] = \sqrt{\frac{2}{\pi}} \int_{-\infty}^{\infty} |RF(\omega)| \cdot F[T_{\Delta}(t)] \cdot cos(\omega t + arg[RF(\omega)]) \cdot d\omega \qquad Eq. 18$$

259 $RF(t) = F^{-1}[RF(\omega) \cdot F[T_{\Delta}(t)]] =$

260
$$= \sqrt{\frac{2}{\pi}} \int_{-\infty}^{\infty} |RF(\omega)| \cdot F[T_{\Delta}(t)] \cdot [\cos(\omega t) \cdot \cos(\arg[RF(\omega)]) - \sin(\omega t) \cdot \sin(\arg[RF(\omega)])] \cdot d\omega \quad Eq.19$$

These expressions could be solved analytically if the exact phase shift and the amplitude gain functions were used for each frequency. However, this becomes exceedingly complex, so $X(\omega)$, $Y(\omega)$ and $Z(\omega)$ will be substituted by an approximate description inferred from a limited number of frequency evaluations. With this idea in perspective, it results useful to group all the terms that depend on the construction into separate functions which, from now on, will be called "Modified Frequency Functions" or MFFs. Eqs.20 develop this approach for each response factor.

267
$$X_{RF}(t) = \sqrt{\frac{2}{\pi}} \int_{-\infty}^{\infty} MFF_{XC}(\omega) \cdot F[T_{\Delta}(t)] \cdot \cos(\omega t) \cdot d\omega - \sqrt{\frac{2}{\pi}} \int_{-\infty}^{\infty} MFF_{XS}(\omega) \cdot F[T_{\Delta}(t)] \cdot \sin(\omega t) \cdot d\omega \qquad Eq. 20a$$

268
$$Y_{RF}(t) = \sqrt{\frac{2}{\pi}} \int_{-\infty}^{\infty} MFF_{YC}(\omega) \cdot F[T_{\Delta}(t)] \cdot \cos(\omega t) \cdot d\omega - \sqrt{\frac{2}{\pi}} \int_{-\infty}^{\infty} MFF_{YS}(\omega) \cdot F[T_{\Delta}(t)] \cdot \sin(\omega t) \cdot d\omega \qquad Eq. 20b$$

269
$$Z_{RF}(t) = \sqrt{\frac{2}{\pi}} \int_{-\infty}^{\infty} MFF_{ZC}(\omega) \cdot F[T_{\Delta}(t)] \cdot \cos(\omega t) \cdot d\omega - \sqrt{\frac{2}{\pi}} \int_{-\infty}^{\infty} MFF_{ZS}(\omega) \cdot F[T_{\Delta}(t)] \cdot \sin(\omega t) \cdot d\omega \qquad Eq. 20c$$

270 where:

271
$$MFF_{XC}(\omega) = |X(\omega)| \cdot cos[arg[X(\omega)]] \quad Eq. 21a$$

272
$$MFF_{XS}(\omega) = |X(\omega)| \cdot sin[arg[X(\omega)]] \quad Eq. 21b$$

273
$$MFF_{YC}(\omega) = |Y(\omega)| \cdot cos[arg[Y(\omega)]] \quad Eq.21c$$

274
$$MFF_{YS}(\omega) = |Y(\omega)| \cdot sin[arg[Y(\omega)]] \quad Eq. 21d$$

275
$$MFF_{ZC}(\omega) = |Z(\omega)| \cdot cos[arg[Z(\omega)]] \quad Eq.21e$$

276
$$MFF_{ZS}(\omega) = |Z(\omega)| \cdot sin[arg[Z(\omega)]] \quad Eq.21f$$

277 If MFFs are replaced by third order piecewise polynomials inside a given frequency range $[\omega_1, \omega_2]$ and by 278 asymptotic functions outside this range, the following general expression (Eq.22) for the X response 279 factor is obtained.

$$280 \qquad X_{RF}(n \cdot \Delta t) = \sqrt{\frac{2}{\pi}} \cdot \begin{cases} \int_{0}^{\omega_{1}} [k_{XHC1} \cdot AF_{HC1}(\omega) + k_{XHC2} \cdot AF_{HC2}(\omega)] \cdot F[T_{\Delta}(t)] \cdot \cos(\omega \cdot n \cdot \Delta t) \cdot d\omega + \\ + \sum_{k=1}^{N-1} \left[\int_{\omega_{k}}^{\omega_{k+1}} (a_{XC(k)} \cdot \omega^{3} + b_{XC(k)} \cdot \omega^{2} + c_{XC(k)} \cdot \omega + d_{XC(k)}) \cdot F[T_{\Delta}(t)] \cdot \cos(\omega \cdot n \cdot \Delta t) \cdot d\omega \right] + \\ + \int_{k=1}^{\infty} [k_{XTC1} \cdot AF_{TC1}(\omega) + k_{XTC2} \cdot AF_{TC2}(\omega)] \cdot F[T_{\Delta}(t)] \cdot \cos(\omega \cdot n \cdot \Delta t) \cdot d\omega - \\ - \int_{0}^{-1} [k_{XHS1} \cdot AF_{HS1}(\omega) + k_{XHS2} \cdot AF_{HS2}(\omega)] \cdot F[T_{\Delta}(t)] \cdot \sin(\omega \cdot n \cdot \Delta t) \cdot d\omega - \\ - \sum_{k=1}^{N-1} \left[\int_{\omega_{k}}^{\omega_{k+1}} (a_{XS(k)} \cdot \omega^{3} + b_{XS(k)} \cdot \omega^{2} + c_{XS(k)} \cdot \omega + d_{XS(k)}) \cdot F[T_{\Delta}(t)] \cdot \sin(\omega \cdot n \cdot \Delta t) \cdot d\omega \right] - \\ - \int_{0}^{-1} [k_{XTS1} \cdot AF_{TS1}(\omega) + k_{XTS2} \cdot AF_{TS2}(\omega)] \cdot F[T_{\Delta}(t)] \cdot \sin(\omega \cdot n \cdot \Delta t) \cdot d\omega - \\ - \int_{0}^{-1} [k_{XTS1} \cdot AF_{TS1}(\omega) + k_{XTS2} \cdot AF_{TS2}(\omega)] \cdot F[T_{\Delta}(t)] \cdot \sin(\omega \cdot n \cdot \Delta t) \cdot d\omega - \\ - \int_{0}^{-1} [k_{XTS1} \cdot AF_{TS1}(\omega) + k_{XTS2} \cdot AF_{TS2}(\omega)] \cdot F[T_{\Delta}(t)] \cdot \sin(\omega \cdot n \cdot \Delta t) \cdot d\omega - \\ - \int_{0}^{-1} [k_{XTS1} \cdot AF_{TS1}(\omega) + k_{XTS2} \cdot AF_{TS2}(\omega)] \cdot F[T_{\Delta}(t)] \cdot \sin(\omega \cdot n \cdot \Delta t) \cdot d\omega - \\ - \int_{0}^{-1} [k_{XTS1} \cdot AF_{TS1}(\omega) + k_{XTS2} \cdot AF_{TS2}(\omega)] \cdot F[T_{\Delta}(t)] \cdot \sin(\omega \cdot n \cdot \Delta t) \cdot d\omega - \\ - \int_{0}^{-1} [k_{XTS1} \cdot AF_{TS1}(\omega) + k_{XTS2} \cdot AF_{TS2}(\omega)] \cdot F[T_{\Delta}(t)] \cdot \sin(\omega \cdot n \cdot \Delta t) \cdot d\omega - \\ + \int_{0}^{-1} [k_{XTS1} \cdot AF_{TS1}(\omega) + k_{XTS2} \cdot AF_{TS2}(\omega)] \cdot F[T_{\Delta}(t)] \cdot \sin(\omega \cdot n \cdot \Delta t) \cdot d\omega + \\ + \int_{0}^{-1} [k_{XTS1} \cdot AF_{TS1}(\omega) + k_{XTS2} \cdot AF_{TS2}(\omega)] \cdot F[T_{\Delta}(t)] \cdot \sin(\omega \cdot n \cdot \Delta t) \cdot d\omega + \\ + \int_{0}^{-1} [k_{XTS1} \cdot AF_{TS1}(\omega) + k_{XTS2} \cdot AF_{TS2}(\omega)] \cdot F[T_{\Delta}(t)] \cdot \sin(\omega \cdot n \cdot \Delta t) \cdot d\omega + \\ + \int_{0}^{-1} [k_{XTS1} \cdot AF_{TS1}(\omega) + k_{XTS2} \cdot AF_{TS2}(\omega)] \cdot F[T_{\Delta}(t)] \cdot \sin(\omega \cdot n \cdot \Delta t) \cdot d\omega + \\ + \int_{0}^{-1} [k_{XTS1} \cdot AF_{TS1}(\omega) + k_{XTS2} \cdot AF_{TS2}(\omega)] \cdot F[T_{\Delta}(t)] \cdot \sin(\omega \cdot n \cdot \Delta t) \cdot d\omega + \\ + \int_{0}^{-1} [k_{XTS1} \cdot AF_{TS1}(\omega) + k_{XTS2} \cdot AF_{TS2}(\omega)] \cdot F[T_{\Delta}(t)] \cdot \sin(\omega \cdot n \cdot \Delta t) \cdot d\omega + \\ + \int_{0}^{-1} [k_{XTS1} \cdot AF_{TS1}(\omega) + k_{XTS2} \cdot AF_{TS2}(\omega)] \cdot F[T_{\Delta}(t)] \cdot \sin(\omega \cdot n \cdot \Delta t) \cdot d\omega + \\ + \int_{0}^{-1} [k_{XTS1} \cdot AF_{TS1}(\omega) + k_{XTS2} \cdot AF_{T$$

Eq.22 can be adapted in the same way for Y and Z response factors, but they are not presented here for the sake of simplicity.

283 It should be noted that the asymptotic approximations of the MFFs out of the selected frequency range284 have been defined through the following general expression:

285 $MFF(\omega) \approx k_1 \cdot AF_1(\omega) + k_2 \cdot AF_2(\omega) \quad Eq. 23$

where k_1 and k_2 are constants, and $AF_1(\omega)$ and $AF_2(\omega)$ are functions that describe the asymptotic behavior of the MFFs along the 'head' $[0, \omega_1]$ and 'tail' $[\omega_2, \infty)$ frequency intervals. Sections 4 and 6 describe in detail the particular expressions of these constants and functions that should be applied on the calculation of each response factor (X, Y, or Z) along the head or tail intervals.

Finally, Eq.22 can be rearranged so that each response factor is simply obtained as the sum of several terms. Each addend will be the product of a factor that depends on the construction characteristics (lowercase constants) by another factor that can be pre-calculated (uppercase constants). Next, Eq.24 shows the expression of the X response factor as an example, but, again, similar expressions can be derived in the same way for Y and Z factors.

295
$$X_{RF}(n \cdot \Delta t) =$$

$$296 \qquad = \sqrt{\frac{2}{\pi}} \cdot \left\{ k_{XHC1} \cdot KAHC1_n + k_{XHC2} \cdot KAHC2_n + \sum_{k=1}^{N-1} [a_{XC(k)} \cdot KPCa_{n,k} + b_{XC(k)} \cdot KPCb_{n,k} + c_{XC(k)} \cdot KPCc_{n,k} + d_{XC(k)} \cdot KPCd_{n,k}] + k_{XHS1} \cdot KAHS1_n + k_{XHS2} \cdot KAHS2_n - k_{XTC1} \cdot KATC1_n - k_{XTC2} \cdot KATC2_n - \sum_{k=1}^{N-1} [a_{XS(k)} \cdot KPSa_{n,k} + b_{XS(k)} \cdot KPSb_{n,k} + c_{XS(k)} \cdot KPSc_{n,k} + d_{XS(k)} \cdot KPSd_{n,k}] - k_{XTS1} \cdot KATS1_n - k_{XTS2} \cdot KATS2_n \right\} Eq. 24$$

The uppercase constants (which from now on will be named as "integration factors") do not depend on the construction and can be obtained analytically. Therefore, they need to be calculated only once and then can be embedded as part of the FDSI main algorithm developed to obtain the response factors. Section 4 presents the detailed expressions of these integration factors.

301 On the other hand, the constants that depend on the construction characteristics are the spline 302 coefficients for each frequency interval and the constants associated to the definition of the asymptotic 303 equivalents. All of them can be easily calculated by evaluating the MFFs at several frequency points, as it 304 is described in sections 5 and 6.

In conclusion, once all the integrals are pre-calculated and stored inside a large table, the operations tobe performed by the FDSI method are reduced to the following:

Evaluation of the Modified Frequency Functions (MFFs) at several frequency points, logarithmically
 spaced.

• Spline interpolation of the MFFs.

• Calculation of the coefficients associated to the asymptotic equivalents.

Sum of the products of the spline coefficients by the integration terms to calculate each response
 factor.

314

4. Generation of the integration factors

In order to generate the table of terms to be embedded within the method as pre-calculated factors, it is
necessary to solve a certain number of definite integrals. As it has been previously mentioned, there are

317 two types of integration factors, which can be referred as polynomial and asymptotic integration factors.

The polynomial factors are those derived from the piecewise polynomial interpolation that approximate MFFs at middle frequencies. The asymptotic factors derive from the definition of equivalent asymptotic functions that approximate MFFs at high and low frequencies.

321 4.1. Integration factors for the spline coefficients that approximate MFFs at middle frequencies.

322 Table 1 gathers the integration factors that multiply the spline coefficients at each frequency interval (see

323 Eq.24). There are $8 \cdot (k-1)$ terms of this kind for each response factor, being k the number of frequency 324 points where the MFFs are evaluated.

325

Table 1: Integration factors for the spline interpolation

Cosine factors	Sine factors
$KPCa_{n,k} = \int_{\omega(k-1)}^{\omega(k)} \omega^3 \cdot F[T_{\Delta}(t)] \cdot \cos(\omega \cdot n \cdot \Delta t) \cdot d\omega$	$KPSa_{n,k} = \int_{\omega(k-1)}^{\omega(k)} \omega^3 \cdot F[T_{\Delta}(t)] \cdot sin(\omega \cdot n \cdot \Delta t) \cdot d\omega$
$KPCb_{n,k} = \int_{\omega(k-1)}^{\omega(k)} \omega^2 \cdot F[T_{\Delta}(t)] \cdot \cos(\omega \cdot n \cdot \Delta t) \cdot d\omega$	$KPSb_{n,k} = \int_{\omega(k-1)}^{\omega(k)} \omega^2 \cdot F[T_{\Delta}(t)] \cdot sin(\omega \cdot n \cdot \Delta t) \cdot d\omega$
$KPCc_{n,k} = \int_{\omega(k-1)}^{\omega(k)} \omega \cdot F[T_{\Delta}(t)] \cdot \cos(\omega \cdot n \cdot \Delta t) \cdot d\omega$	$KPSc_{n,k} = \int_{\omega(k-1)}^{\omega(k)} \omega \cdot F[T_{\Delta}(t)] \cdot sin(\omega \cdot n \cdot \Delta t) \cdot d\omega$
$KPCd_{n,k} = \int_{\omega(k-1)}^{\omega(k)} F[T_{\Delta}(t)] \cdot cos(\omega \cdot n \cdot \Delta t) \cdot d\omega$	$KPSd_{n,k} = \int_{\omega(k-1)}^{\omega(k)} F[T_{\Delta}(t)] \cdot sin(\omega \cdot n \cdot \Delta t) \cdot d\omega$

326

(*) $F[T_{\Delta}(t)] = \frac{1 - \cos(\omega \cdot \Delta t)}{\omega^2 \cdot \Delta t}$ for linear interpolation.

4.2. Integration factors for the asymptotic functions that approximate MFFs at low and high frequencies.

So far, eight different terms of this kind have been proposed in a general description of the asymptotic equivalents (see Eq.24): KAHC1, KAHC2, KAHS1 and KAHS2 for the low-frequency or head interval, and KATC1, KATC2, KATS1 and KATS2 for the high-frequency or tail interval.

The low-frequency asymptotic behavior can be described by the same four head functions for any series of response factors (X, Y and Z) and in any particular case. However, that is not the case for the tail terms. Fortunately, it can be proved that proper combinations of only 5 different integration factors are needed to characterize this high-frequency behavior in any situation. From now on, these tail integration factors are named as KATC0, KATC(+), KATC(-), KATS(+) and KATS(-). The relation between them and the general asymptotic tail terms showed in Eq.24 depends on the response factor being calculated, as well as on the existence or inexistence of a zero-inertia outermost or innermost wall layer.

The rearrangement of these integration factors is a consequence of the particular form of the MFFs. Further considerations for practical implementation of the FDSI method are given in Appendix A. Nevertheless, a complete derivation of the asymptotic analysis that leads to these terms would be too long to be presented on this paper and has been intentionally omitted here.

Next, Table 2 compiles the aforementioned integration factors, which multiply the construction-dependent constants associated to the definition of the asymptotic equivalents. In conclusion, one can observe that 8 integration asymptotic factors need to be calculated.

346

Table 2: Integration factors for the approximate asymptotic functions

Head asymptotic equivalents (low frequency)	Tail asymptotic equivalents (high frequency)
$KAHC1_n = \int_0^{\omega_1} F[T_{\Delta}(t)] \cdot cos(\omega \cdot n \cdot \Delta t) \cdot d\omega$	$KATCO_n = \int_{\omega_N}^{\infty} F[T_{\Delta}(t)] \cdot \cos(\omega \cdot n \cdot \Delta t) \cdot d\omega$
$KAHC2_n = \int_0^{\omega_1} \omega \cdot (e^{\omega} - 1) \cdot F[T_{\Delta}(t)] \cdot \cos(\omega \cdot n \cdot \Delta t) \cdot d\omega$	$KATC(+)_n = \int_{\omega_N}^{\infty} \omega^{0.5} \cdot F[T_{\Delta}(t)] \cdot \cos(\omega \cdot n \cdot \Delta t) \cdot d\omega$
$KAHS1_n = \int_{0}^{\omega_1} (e^{\omega} - 1) \cdot F[T_{\Delta}(t)] \cdot sin(\omega \cdot n \cdot \Delta t) \cdot d\omega$	$KATS(+)_n = \int_{\omega_N}^{\infty} \omega^{0.5} \cdot F[T_{\Delta}(t)] \cdot sin(\omega \cdot n \cdot \Delta t) \cdot d\omega$
$KAHS2_n = 0$	$KATC(-)_n = \int_{\omega_N}^{\infty} \omega^{-0.5} \cdot F[T_{\Delta}(t)] \cdot \cos(\omega \cdot n \cdot \Delta t) \cdot d\omega$
	$KATS(-)_n = \int_{\omega_N}^{\infty} \omega^{-0.5} \cdot F[T_{\Delta}(t)] \cdot sin(\omega \cdot n \cdot \Delta t) \cdot d\omega$

347

Finally, it should be noted that both types of integration factors must be stored into a large table. However, this is not an issue for modern computers in order to handle the FDSI method easily. For example, if the number of intervals between frequency evaluations (k-1) is 1024 and the number of response factors is 300, the total number of terms to be handled is the following:

Eq.25

352 m = 8 · (k-1) · n + 8 · n ≈ 8 · 1024 · 300 = 2457600 terms

If each element of the table is stored as a double precision floating point number (8 bytes), the total size of the table would be 19660800 bytes, that is to say, 18.75 MB. Modern computers can easily hold tables this size and larger in RAM memory. Similar results can be obtained with less frequency evaluations and, therefore, with a smaller factor table, as it will be shown in the validation section.

358 **5. Spline interpolation of the Modified Frequency Functions (MFFs)**

An approximate model for the Modified Frequency Functions (MFFs) at middle frequencies can be performed by piecewise polynomials (see Figure 5). The target is to have an ensemble of simple expressions that describes the MFFs between the frequency evaluation points with sufficient accuracy.



362 363

Figure 5. Piecewise polynomial interpolation approach

In order to achieve this goal, the FDSI method turns to cubic splines, as they are suitable for continuous smooth functions. Starting from a set of n evaluations of the MFFs at logarithmically-spaced frequencies within the selected range [ω_1 , ω_n], (n-1) cubic polynomials (f_k) are defined, and their corresponding coefficients a_k , b_k , c_k and d_k (Eq.26) are calculated.

368

$$f_k(\omega) = a_k \cdot \omega^3 + b_k \cdot \omega^2 + c_k \cdot \omega + d_k \quad Eq.26$$

This calculation can be performed by a linear-time complexity algorithm. Particularly, based on the application of not-a-knot boundary conditions, Appendix B presents a detailed description of the recursive calculation procedure to get the spline coefficients in global coordinates.

372

373 6. Asymptotic analysis of the Modified Frequency Functions (MFFs)

374 Spline interpolation is able to reproduce with excellent precision the so-called Modified Frequency 375 Functions (MFFs) inside a given frequency range. However, outside this range the error becomes 376 unacceptably large since splines are not suitable for extrapolation. Luckily, when the frequency is 377 sufficiently low or sufficiently high, it is possible to replace the complex dynamics of the construction by 378 simple asymptotic equivalents that can be easily integrated into the method.

379 Given a general one-layer construction, the corresponding asymptotic equivalents can be expressed as 380 follows in Table 3.

381

Table 3: Expression of the asymptotic equivalents for a one-layer construction

Term	Exact Modified Frequency Functions (one-layer construction)	Approximated functions
	$ X(\omega) \cdot \cos\varphi(\omega) = \left \frac{D_T(j\omega)}{B_T(j\omega)}\right \cdot \cos\left(\arg\left(\frac{D_T(j\omega)}{B_T(j\omega)}\right)\right) = \\ = \left \lambda \cdot \sqrt{\frac{j\omega}{\alpha}} \cdot \coth\left(L \cdot \sqrt{\frac{j\omega}{\alpha}}\right)\right \cdot \cos\left(\arg\left[\lambda \cdot \sqrt{\frac{j\omega}{\alpha}} \cdot \coth\left(L \cdot \sqrt{\frac{j\omega}{\alpha}}\right)\right]\right)$	At high frequencies $ X(\omega) \cdot \cos\varphi(\omega) \approx \frac{\lambda}{\sqrt{2\alpha}} \cdot \omega^{0.5}$ At low frequencies $ X(\omega) \cdot \cos\varphi(\omega) \approx \frac{\lambda}{L} + \frac{\lambda \cdot L^3 \cdot \omega \cdot (e^{\omega} - 1)}{45 \cdot \alpha^2}$
X	$ X(\omega) \cdot \sin\varphi(\omega) = \left \frac{D_T(j\omega)}{B_T(j\omega)} \right \cdot \sin\left(\arg\left(\frac{D_T(j\omega)}{B_T(j\omega)}\right)\right) = \\ = \left \lambda \cdot \sqrt{\frac{j\omega}{\alpha}} \cdot \coth\left(L \cdot \sqrt{\frac{j\omega}{\alpha}}\right) \right \cdot \sin\left(\arg\left[\lambda \cdot \sqrt{\frac{j\omega}{\alpha}} \cdot \coth\left(L \cdot \sqrt{\frac{j\omega}{\alpha}}\right)\right]\right)$	At high frequencies $ X(\omega) \cdot \sin\varphi(\omega) \approx \frac{\lambda}{\sqrt{2\alpha}} \cdot \omega^{0.5}$ At low frequencies $ X(\omega) \cdot \sin\varphi(\omega) \approx \frac{\lambda \cdot L \cdot (e^{\omega} - 1)}{3\alpha}$
Y	$ Y(\omega) \cdot \cos\varphi(\omega) = \left \frac{1}{B_T(j\omega)}\right \cdot \cos\left(\arg\left(\frac{1}{B_T(j\omega)}\right)\right) = \\ = \left \frac{\lambda \cdot \sqrt{j\omega}}{\sinh\left(L \cdot \sqrt{j\omega}\right)}\right \cdot \cos\left(\arg\left(\frac{\lambda \cdot \sqrt{j\omega}}{\sinh\left(L \cdot \sqrt{j\omega}\right)}\right)\right)$	At high frequencies $ Y(\omega) \cdot cos\varphi(\omega) \approx 0$ At low frequencies $ Y(\omega) \cdot cos\varphi(\omega) \approx \frac{\lambda}{L} + \frac{7k \cdot L^3 \cdot \omega \cdot (e^{\omega} - 1)}{360 \cdot \alpha^2}$
	$ Y(\omega) \cdot \sin\varphi(\omega) = \left \frac{1}{B_T(j\omega)}\right \cdot \sin\left(\arg\left(\frac{1}{B_T(j\omega)}\right)\right) = \\ = \left \frac{\lambda \cdot \sqrt{j\omega}}{\sinh\left(L \cdot \sqrt{j\omega}\right)}\right \cdot \sin\left(\arg\left(\frac{\lambda \cdot \sqrt{j\omega}}{\sinh\left(L \cdot \sqrt{j\omega}\right)}\right)\right)$	At high frequencies $ Y(\omega) \cdot \sin\varphi(\omega) \approx 0$ At low frequencies $ Y(\omega) \cdot \sin\varphi(\omega) \approx \frac{\lambda \cdot L \cdot (e^{\omega} - 1)}{6\alpha}$
z	$ Z(\omega) \cdot \cos\varphi(\omega) = \left -\frac{A_T(j\omega)}{B_T(j\omega)} \right \cdot \cos\left(\arg\left(-\frac{A_T(j\omega)}{B_T(j\omega)}\right)\right) = \\ = \left -\lambda \cdot \sqrt{\frac{j\omega}{\alpha}} \cdot \coth\left(L \cdot \sqrt{\frac{j\omega}{\alpha}}\right) \right \cdot \cos\left(\arg\left[-\lambda \cdot \sqrt{\frac{j\omega}{\alpha}} \cdot \coth\left(L \cdot \sqrt{\frac{j\omega}{\alpha}}\right)\right]\right)$	At high frequencies $ Z(\omega) \cdot \cos\varphi(\omega) \approx -\frac{\lambda}{\sqrt{2\alpha}} \cdot \omega^{0.5}$ At low frequencies $ Z(\omega) \cdot \cos\varphi(\omega) \approx -\frac{\lambda}{L} - \frac{\lambda \cdot L^3 \cdot \omega \cdot (e^{\omega} - 1)}{45 \cdot \alpha^2}$
	$ Z(\omega) \cdot \sin\varphi(\omega) = \left -\frac{A_T(j\omega)}{B_T(j\omega)} \right \cdot \sin\left(\arg\left(-\frac{A_T(j\omega)}{B_T(j\omega)}\right)\right) = \\ = \left -\lambda \cdot \sqrt{\frac{j\omega}{\alpha}} \cdot \coth\left(L \cdot \sqrt{\frac{j\omega}{\alpha}}\right) \right \cdot \sin\left(\arg\left[-\lambda \cdot \sqrt{\frac{j\omega}{\alpha}} \cdot \coth\left(L \cdot \sqrt{\frac{j\omega}{\alpha}}\right)\right]\right)$	At high frequencies $ Z(\omega) \cdot \sin\varphi(\omega) \approx -\frac{\lambda}{\sqrt{2\alpha}} \cdot \omega^{0.5}$ At low frequencies $ Z(\omega) \cdot \sin\varphi(\omega) \approx -\frac{\lambda \cdot L \cdot (e^{\omega} - 1)}{3\alpha}$

³⁸²

383 When the construction is made from more than one layer, approximate functions are similar to the ones 384 already shown in Table 3. They can be expressed, as well, in terms of several constants that depend on 385 the properties of the layers. However, it is more practical to estimate these constants by evaluating the 386 Modified Frequency Functions at the ends of the frequency vector used for spline interpolation; that is to 387 say, at ω_1 for the asymptotic heads and ω_2 for the asymptotic tails.

A particular case arises again when the innermost or the outermost layer in the construction has zero density or zero thermal capacity, which is a reasonable approximation when thermal diffusivity is high enough. This assumption implies a change in the asymptotic functions, as shown in Table 4.

391

Table 4: Expression of the asymptotic equivalents for a multilayer construction considering zero-inertia cases

Functions for response	Approximate functions
------------------------	-----------------------

factor calculation					
		Outermost layer without thermal inertia	Innermost layer without thermal inertia	All layers have thermal inertia	Low frequency
x	$ X(\omega) \cdot cos(arg(X(\omega)))$	$\frac{\lambda_1}{L_1} - k_{XTC2} \cdot \omega^{-0.5}$ $\left(k_{XTC1} = \frac{\lambda_1}{L_1}\right)$	$k_{XTC2} \cdot \omega^{0.5}$ $(k_{XTC1} = 0)$	$k_{XTC2} \cdot \omega^{0.5}$ $(k_{XTC1} = 0)$	$\frac{1}{\sum_{i=1}^{n} \frac{L_{i}}{\lambda_{i}}} + \lambda_{XHC2} \cdot \omega \cdot (e^{\omega} - 1)$ $\binom{k_{XHC1}}{\left(k_{XHC1} = \frac{1}{\sum_{i=1}^{n} \frac{L_{i}}{\lambda_{i}}}\right)}$
	$ X(\omega) \cdot sin(arg(X(\omega)))$	$k_{XTS2} \cdot \omega^{-0.5}$ $(k_{XTS1} = 0)$	$k_{XTS2} \cdot \omega^{0.5}$ $(k_{XTS1} = 0)$	$k_{XTS2} \cdot \omega^{0.5}$ $(k_{XTS1} = 0)$	$k_{XHS2} \cdot (e^{\omega} - 1)$ $(k_{XHS1} = 0)$
Y	$ Y(\omega) \cdot cos(arg(Y(\omega)))$	0	0	0	$\frac{\frac{1}{\sum_{i=1}^{n} \frac{L_{i}}{\lambda_{i}}} + k_{YHC2} \cdot \omega \cdot (e^{\omega} - 1)}{\left(k_{YHC1} = \frac{1}{\sum_{i=1}^{n} \frac{L_{i}}{\lambda_{i}}}\right)}$
	$ Y(\omega) \cdot sin(arg(Y(\omega)))$	0	0	0	$k_{YHS2} \cdot (e^{\omega} - 1)$ $(k_{YHS1} = 0)$
Z	$ Z(\omega) \cdot cos(arg(Z(\omega)))$	$k_{ZTC2} \cdot \omega^{0.5}$ $(k_{ZTC1} = 0)$	$\frac{\lambda_N}{L_N} - k_{ZTC2} \cdot \omega^{-0.5}$ $\left(k_{ZTC1} = \frac{\lambda_N}{L_N}\right)$	$k_{ZTC2} \cdot \omega^{0.5}$ $(k_{ZTC1} = 0)$	$-\frac{1}{\sum_{i=1}^{n} \frac{L_i}{\lambda_i}} + k_{ZHC2} \cdot \omega \cdot (e^{\omega} - 1)$ $\begin{pmatrix} k_{ZHC1} = -\frac{1}{\sum_{i=1}^{n} \frac{L_i}{\lambda_i}} \end{pmatrix}$
	$ Z(\omega) \cdot sin(arg(Z(\omega)))$	$k_{ZTS2} \cdot \omega^{0.5}$ $(k_{ZTS1} = 0)$	$k_{ZTS2} \cdot \omega^{-0.5}$ $(k_{ZTS1} = 0)$	$k_{ZTS2} \cdot \omega^{0.5}$ $(k_{ZTS1} = 0)$	$k_{ZHS2} \cdot (e^{\omega} - 1)$ $(k_{ZHS1} = 0)$

393 Once the constants kxtc1, kxtc2, kxts2, kxHc1, kxHc2, kxHs2, kyHc1, kyHc2, kyHs2, kztc1, kztc2, kzts2, kzHc1, 394 kzHc2 and kzHs2 are calculated, an accurate mathematical characterization of the MFFs for both low and 395 high frequencies is completed, which combined with the spline model for intermediate frequencies yields 396 a good approximation for the dynamics of the construction.

397

398 **7. Complexity considerations and validation analyses**

399 7.1. Algorithm complexity

The FDSI algorithm has a linear-time complexity. This means that increasing the number of response factors to be calculated (for instance in order to get accurate results with improved time resolution), multiplies the number of operations by the same scale factor.

This particular feature makes the FDSI method extremely fast compared to most of the previous alternatives. There is no need to solve systems of linear equations, to apply iterative pole finding or to use finite element algorithms, what would involve quadratic-time or even greater complexity and make the method much slower.

407 **7.2. Validations**

For the purpose of validation, the present FDSI method was tested in two different case studies, and the obtained results were compared with published data derived from previous existing methods. These case studies consist of two multilayered walls of different thermal inertia that have already served as test cases for other authors. Both are described in detail below.

Moreover, it should be noted that different criteria have been used for the comparison of the obtained results. In first place stationary thermal trasmittance (U-value) can be used as a checking parameter in the calculation of thermal response factors, as the sum of the infinite series of response factors for a given construction has to be equal to its U-value. Therefore, an error estimate can be expressed through Eq.27.

$$E_U(\%) = \left| \frac{U - \sum_{i=1}^{\infty} RF_i}{U} \right| \cdot 100 \qquad Eq. 27$$

418 However, obtaining low values for this estimate is a necessary but not sufficient condition. That is to say, 419 it does not guarantee itself the accuracy of the method, but having high E_{U} values always involves lack of 420 it. Then, this estimate is presented for the studied test cases as a first premise, but also further validations 421 are provided.

422 7.2.1. Case study I

The physical characteristics of the first test wall are presented in Table 5. It was chosen by Ouyang and Haghighat [17] to demonstrate the application of their SSM approach and then, it has been used by other authors to compare their own results, which derive from 3 other different methods, namely, DRF [35], FDR [3] and DNI [15].

427

417

Table 5: Detailed wall description of case study I

Description	L (mm)	λ (W·m⁻¹K⁻¹)	ρ (kg∙m⁻³)	c _p (J·kg ⁻¹ K ⁻¹)	R (m ² ·K·W ⁻¹)
Outside surface film					0.0500
Concrete	89	1.73	2235	1106	0.0514
Insulation	127	0.0744	24	992	1.7070
Concrete	89	1.73	2235	1106	0.0514
Inside surface film					0.16

428

Table 6 compiles the first 20 cross (Y) response factors obtained by those methods (these data are extracted from [15]) and adds the corresponding results from the present FDSI approach. It can be observed that the accuracy of the FDSI results is comparable to that of the methodologies used so far. Particularly, considering the reference of the FDR method as the most exact among them [15], the FDSI and the DNI alternatives clearly represent better approximations. Indeed, for this case study, it is noticeable that all the calculated response factors are identical for the FDSI and the DNI methods (at least considering the precision used in Table 6), when, however, they are based on completely different conceptual approaches.

	FDR	SSM	DRF	DNI	FDSI
0	0.00001521	0.00001771	0.00001549	0.00001531	0.00001531
1	0.00163441	0.00164078	0.00164541	0.00163463	0.00163463
2	0.00849218	0.00852682	0.00852884	0.00849216	0.00849216
3	0.01600825	0.01606351	0.01605804	0.01600833	0.01600833
4	0.02127237	0.02132861	0.02132482	0.02127245	0.02127245
5	0.02453370	0.02458189	0.02458376	0.02453375	0.02453375
6	0.02630043	0.02634117	0.02634535	0.02630044	0.02630044
7	0.02697839	0.02701426	0.02701681	0.02697837	0.02697837
8	0.02687682	0.02690951	0.02690827	0.02687681	0.02687681
9	0.02622975	0.02625774	0.02625429	0.02622975	0.02622975
10	0.02521328	0.02523350	0.02523131	0.02521329	0.02521329
11	0.02395904	0.02397017	0.02397118	0.02395907	0.02395907
12	0.02256462	0.02256861	0.02257155	0.02256466	0.02256466
13	0.02110158	0.02110207	0.02110402	0.02110163	0.02110163
14	0.01962166	0.01962103	0.01962030	0.01962172	0.01962172
15	0.01816159	0.01815949	0.01815708	0.01816165	0.01816165
16	0.01674674	0.01674130	0.01673967	0.01674679	0.01674679
17	0.01539396	0.01538425	0.01538486	0.01539401	0.01539401
18	0.01411377	0.01410104	0.01410310	0.01411382	0.01411382
19	0.01291201	0.01289871	0.01290017	0.01291206	0.01291206

437 Table 6: Comparison of thermal response factors for case study I obtained with different calculation methods

438

The twenty RF from Table 6 have been shown for comparison purposes, but it can be proved that they are insufficient to provide a complete representation of the transient thermal response of the selected wall. Actually, Table 7 presents the error estimate (E_U) when considering different number of thermal response factors calculated by the FDSI method.

443

Case study I	Case study II
Ouyang and Haghighat's wall	Chen's heavyweight wall

Number of RF (N)	$\sum_{i=1}^{N} RF_i$	Eu (%)	$\sum_{i=1}^{N} RF_i$	E∪ (%)
20	0,3681307	25,642%	0,1846084	76,380%
50	0,4888178	1,265%	0,5783250	26,006%
100	0,4950393	0,008%	0,7491220	4,153%
150	0,4950788	0,000%	0,7763976	0,663%
200			0,7807529	0,106%
300			0,7815595	0,003%
Actual U-value	0,4950791		0,7815806	

As expected, the error is drastically reduced when considering a higher number of response factors, proving an adequate fulfilment of the U-value premise. Particularly, for Case study I, 100 calculated factors provide an error lower than 0.01%.

448 **7.2.2. Case study II**

Table 8 reports the physical properties of the second test construction selected for validation. It consists of a heavyweight wall widely used in China and proposed by Chen et al. [36] to demonstrate the application of a verification methodology for transient heat flow calculations in multilayered walls. Moreover, results derived from the DNI method [15] are also available in literature for this wall, what justifies the present choice.

454

Table 8: Detailed wall description of case study II

Description	L (mm)	λ (W·m⁻¹K⁻¹)	ρ (kg·m⁻³)	$c_p(J\cdot kg^{-1}K^{-1})$	R (m ² ·K·W ⁻¹)
Outside surface film					0.0538
Common brick	370	0.814	1800	879	
Foam concrete	100	0.209	600	837	
Wood wool board	25	0.163	400	2093	
Stucco	20	0.814	1600	837	
Inside surface film					0.1147

455

In the first place, Table 7 should be referred again to check that the U-value premise is also fulfilled for Case study II. Indeed, the error estimate can be reduced to negligible values (lower than 0.005 %) when considering a properly high number of RF. However, in this case, approximately 300 factors are needed to get the aforementioned error values. This is consistent with the heavyweight characteristics of the present wall. Note that the number of response factors that are required to correctly model a given 461 construction depends on its physical properties (which determine its time constant), as well as on the462 considered timestep.

In the second place, results obtained through the FDSI method have been compared with literature values according to the verification procedure developed in [36]. This methodology proposes the comparison of the theoretical frequency characteristics of the wall (obtained from its transmission matrix) with the dynamic behavior data derived from the calculated RF. This can be done visually by representing a Bode diagram with the amplitude and phase lag of the wall's thermal response. As an example, Figure 6 shows the theoretical and calculated characteristics of cross heat conduction for Case study II considering 144 factors.



470

471 Figure 6. Comparison between the theoretical frequency response of the heavyweight wall (case study II) and
472 that obtained from the calculated response factors with the FDSI method

473 It can be observed that both frequency characteristics are almost indistinguishable, what is also generally
474 reported in literature for other test cases and calculation methods [3, 25, 36]. For this reason, the use of
475 the following error estimate (Eq.28) was proposed and recommended [36].

476
$$E_{\psi} = \frac{1}{U} \sqrt{\frac{1}{N} \sum_{k=1}^{N} \left[\psi(\omega_k) - \tilde{\psi}(\omega_k)\right]^2 \cdot 100} \qquad Eq.28$$

477 According to this criterion, results from the FDSI, DNI and FDR methods are compared in Table 9. The 478 first 72, 96, 120 and 144 cross (Y) factors were considered. Data from the existing methods were 479 extracted from [15].

480

Table 9: Compared accuracy for FDSI, DNI and FDR methods for 'Case study II' wall.

Number of RF	72	96	120	144
E _Ψ _FDSI (%)	9.15	3.76	1.55	0.64
Ε _ψ _DNI (%)	8.92	3.66	1.50	0.62
E _Ψ _FDR (%)	9.12	3.74	1.54	0.63

481

It can be seen that the obtained errors for the FDSI method, despite being slightly higher, are very close to those of the DNI and the FDR method. As pointed out in [15], the latter, by definition, minimizes the present error estimate E_{ψ} , so the observed small differences prove a very interesting behavior of the FDSI method.

486 **7.3. Accuracy dependence on the number of frequency points**

Figure 7 shows an estimation of the absolute difference between the actual U-value and the sum of 300 calculated X response factors as a function of the number of frequency points used by the FDSI method when applied to 'Case study I'. Similar results can be obtained for Y and Z response factor series.



490 491

Figure 7. Influence of the number of frequency points on the method's accuracy

492 As expected, Figure 7 reveals that the accuracy of the FDSI method improves as the number of 493 frequency points becomes larger, because the MFFs are better estimated. However, once the 494 mathematical approximation is good enough, there is no use in increasing the number of interpolation 495 points. With 512 frequency evaluations and a sufficient number of factors, the absolute error falls easily 496 under 10⁻⁸. Better estimates could be obtained by widening the frequency range or by calculating more 497 response factors. Nevertheless, here the conceptual development and first validations of the FDSI 498 method are presented, but further work needs to be done in this sense in the future.

Moreover, it should be noted that data in Figure 7 come from an indirect calculation procedure that provides approximated results. Only the pre-calculated integration factors for the case with 1024 frequency points were actually determined. For the other frequency sampling cases, the corresponding pre-calculated constants required by the FDSI method were estimated by a grouping routine. This aspect explains the scattering of the plot shown in Figure 7 and suggests not considering those exceptional accuracy values associated to certain singular frequencies.

505 8. Conclusions

506 This work has introduced a new method for the calculation of conduction response factors in multilayer 507 constructions, based on frequency–domain spline interpolation (FDSI) and asymptotic analysis. Its 508 conceptual development as well as first validations comparing with existing methods from previous 509 literature have been presented.

510 The FDSI method enables the calculation of thermal response factors with great accuracy and speed, 511 which constitutes a promising alternative to improve those procedures implemented in Building Energy 512 Simulation programs so far. Particularly, it can make BES tools able to efficiently calculate with small 513 timesteps (1-5 min) which is of special interest in energy simulations combining buildings and HVAC 514 systems that often have much shorter time responses. In order to run simulations with small timesteps 515 (keeping the level of accuracy), the only requirement is to calculate more response factors, but thanks to 516 the lookup table approach most of the involved calculations will be done only once and stored, so the 517 'small timestep' condition will not increase a lot the computational effort and make such simulations 518 affordable.

519 In summary, the following features characterize the new proposed method:

Precision: As integration factors can be pre-calculated beforehand with excellent precision, error
 depends only on the number of frequency evaluations, the number of factors and the width of the
 frequency range. With 512 frequency evaluations and a sufficient number of factors, the estimate for
 this variable falls easily under 10⁻⁸.

- Speed: This algorithm has linear-time complexity, which makes it extremely fast compared to other
 methods. There is no need to solve linear systems, iterative pole finding or the use of finite element
 algorithms. It just requires N frequency evaluations, the calculation of spline coefficients and 8·N
 multiplications for each response factor.
- Stability: FDSI method is inherently stable. Convergence is always guaranteed because there are no
 iterative numeric algorithms involved.
- As a drawback, this method requires several megabyte of RAM to store the pre-calculated integration factors. However, since modern computers are able to handle up to several gigabytes of main memory, this is not a relevant issue.
- 533

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625 Appendix A. Summary of coefficients for the FDSI method

626

Table 1: Summary of different coefficients relevant for the FDSI method

		T1								
		Integration factors		Coefficients that depend on the construction						
Type of factor			Integration factors (pre-calculated factors)			MFF _x response factors	MFF _Y response factors	MFF _z response factors		
		MFF cos	x	Outermost layer without thermal inertia	$KATC1_n = KATC0_n$ $KATC2_n = KATC(+)_n$	$k_{XTC1} = \frac{\lambda_1}{L_1}$ k_{XTC2}				
				Other cases	$KATC1_n = 0$ $KATC2_n = KATC(+)_n$	$k_{XTC1} = 0$ k_{XTC2}				
			Y		No coefficients us	nealiaible)	· · · · · · · · · · · · · · · · · · ·			
	Asymptotic tail terms		7	Innermost layer without thermal inertia	$KATC1_n = KATC0_n$ $KATC2_n = KATC(-)_n$			$k_{XTC1} = \frac{\lambda_N}{L_N}$ k_{XTC2}		
ctor)				Other cases	$KATC1_n = 0$ $KATC2_n = KATC(+)_n$			$k_{XTC1} = 0$ k_{XTC2}		
ach response fa symptotic terms		MFF sin	x	Outermost layer without thermal inertia	$KATS1_n = 0$ $KATS2_n = KATS(-)_n$	$k_{XTS1} = 0$ k_{XTS2}				
				Other cases	$KATS1_n = 0$ $KATS2_n = KATS(+)_n$	$k_{XTS1} = 0$ k_{XTS2}				
or e (a			Y	Y No coefficients used (its contribution is negligible)						
Fc			z	Innermost layer without thermal inertia	$KATS1_n = 0$ $KATS2_n = KATS(-)_n$			$k_{ZTS1} = 0$ k_{ZTS2}		
				Other cases	$KATS1_n = 0$ $KATS2_n = KATS(+)_n$			$k_{ZTS1} = 0$ k_{ZTS2}		
	MFF cos			KAHC1 _n KAHC2 _n		$k_{XHC1} = \frac{1}{\sum_{i=1}^{n} \frac{L_i}{\lambda_i}}$	$k_{YHC1} = \frac{1}{\sum_{i=1}^{n} \frac{L_i}{\lambda_i}}$	$k_{ZHC1} = \frac{-1}{\sum_{i=1}^{n} \frac{L_i}{\lambda_i}}$		
	Asymp	MFF sin		KA KAHS	$HS1_n$ $S2_n = 0$	k_{XHS1} $k_{XHS2} = 0$	k_{YHS1} $k_{YHS2} = 0$	k_{ZHS1} $k_{ZHS2} = 0$		
r	le ω ³	MFF cos		KPCa _{n,k} KPSa _{n,k}		$a_{XC(k)}$	$a_{YC(k)}$	$a_{ZC(k)}$		
For each interval and response facto (polynomial terms)	Splir	MFF sin				$a_{XS(k)}$	$a_{YS(k)}$	$a_{ZS(k)}$		
	ne ω^2	MFF cos		$KPCb_{n,k}$		KPCb _{n,k}		b _{XC(k)}	$b_{YC(k)}$	$b_{ZC(k)}$
	ାର୍ଚ୍ଚ MFF sin			KPSb _{n,k}		$b_{XS(k)}$	$b_{YS(k)}$	$b_{ZS(k)}$		
	ine ω	MFF cos		$KPCc_{n,k}$		$KPCc_{n,k}$		C _{XC(k)}	$\mathcal{C}_{YC(k)}$	$C_{ZC(k)}$
	Spli	MFF sin		$KPSc_{n,k}$		$C_{XS(k)}$	$C_{YS(k)}$	$C_{ZS(k)}$		
	ne ω^0	MFF cos		KP	$Cd_{n,k}$	$d_{XC(k)}$	$d_{YC(k)}$	$d_{ZC(k)}$		
	Spli	MFF sin		$KPSd_{n,k}$		$d_{XS(k)}$	$d_{YS(k)}$	$d_{ZS(k)}$		

627

628 Appendix B. Calculation of the spline coefficients

629 The coefficients of each cubic polynomial for the MFFs spline interpolation can be easily expressed in 630 terms of the evaluated frequencies (ω_k), the MFF values at those frequencies (y_k) and the corresponding

631 second derivatives (y_k " = σ_k), as it is shown in Eqs. B.5.

As ω_k and y_k are known, the proposed calculation of the spline coefficients is focused on determining the second derivatives. This can be done through the recursive procedure described in Table B.1. For the sake of clarity, the following quantities have been defined:

635
$$h_k = \omega_{k+1} - \omega_k$$
 $0 < k < n$ $Eq. B. 1a$

636
$$r_k = \frac{y_{k+1} - y_k}{\omega_{k+1} - \omega_k} \qquad 0 < k < n \qquad Eq. B. \, 1b$$

637 Then, φ_k and Γ_k auxiliary terms are obtained in intermediate steps to finally calculate the MFF second

638 derivatives and the spline coefficients.

639

Table B.1.: Recursive calculation procedure to get the spline coefficients in a global coordinate system

1.- First, φ_k terms are calculated. It requires n-1 iterations, where n is the number of frequency evaluations. Eqs. B.2. $\begin{cases} \varphi_1 = \frac{h_2 \cdot (2h_2 - h_1)}{(h_2 - h_1)} \\ \varphi_k = 2 \cdot (h_{k+1} + h_k) - \frac{h_k^2}{\varphi_{k-1}} \\ \varphi_{n-1} = \left(h_{n-2} - \frac{h_{n-2}^2}{h_{n-2}}\right) + \frac{h_{n-1}}{\varphi_{n-2}} \cdot \left(3h_{n-1} + h_{n-2} + 2\frac{h_{n-1}^2}{h_{n-2}}\right) \end{cases}$ 2.- Once φ_k terms are stored, we can obtain a sequence of Γ_k terms, using the recurrence formulae shown below. Again, it requires n-1 iterations. Eqs. B.3. $\begin{cases} \Gamma_1 = \frac{6h_2^2}{(h_2^2 - h_1^2)} \cdot (r_2 - r_1) \\ \Gamma_k = 6 \cdot (r_{k+1} - r_k) - \frac{h_k \cdot \Gamma_{k-1}}{\varphi_{k-1}} \\ \Gamma_{n-1} = -\frac{6h_{n-1}}{h_{n-2}} \cdot (r_{n-1} - r_{n-2}) + \frac{\Gamma_{n-2}}{\varphi_{n-2}} \left(3h_{n-1} + h_{n-2} + 2\frac{h_{n-1}^2}{h_{n-2}}\right) \end{cases}$ 3.- Given φ_k and Γ_k terms, we can get the second derivatives of the splines σ_k for each evaluation point. Then, note that n σ_k -terms will be needed.

$$\begin{cases} \sigma_n = \frac{\Gamma_{n-1}}{\varphi_{n-1}} \\ \sigma_k = \frac{\Gamma_{k-1} - h_k \cdot \sigma_{k+1}}{\varphi_{k-1}} \\ \sigma_1 = \frac{\frac{-6h_1}{h_2} \cdot (r_2 - r_1) + \left(3h_1 + h_2 + 2\frac{h_1^2}{h_2}\right)\sigma_2}{h_2 - \frac{h_1^2}{h_2}} \end{cases} \quad 1 < k < n$$

Eqs. B.5. $a_{k} = \frac{\sigma_{k+1} - \sigma_{k}}{6h_{k}}$ $b_{k} = \frac{\sigma_{k}\omega_{k+1} - \sigma_{k+1}\omega_{k}}{2h_{k}}$ $c_{k} = \frac{\sigma_{k+1}\left(\frac{3 \cdot \omega_{k}^{2}}{h_{k}} - h_{k}\right) - \sigma_{k}\left(\frac{3 \cdot \omega_{k+1}^{2}}{h_{k}} - h_{k}\right)}{6} + \frac{y_{k+1} - y_{k}}{h_{k}}$

$$d_k = \frac{\sigma_k \left(\frac{\omega_{k+1}^3}{h_k} - h_k \omega_{k+1}\right) - \sigma_{k+1} \left(\frac{\omega_k^3}{h_k} - h_k \omega_k\right)}{6} - \frac{y_{k+1} \omega_k - y_k \omega_{k+1}}{h_k}$$
$$0 < k < n$$

640