

ANALYTICAL EXPRESSION FOR THE NON-ISOTHERMAL EFFECTIVENESS FACTOR: The n^{th} -order reaction in a slab geometry

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Abstract

The problem of calculating the effectiveness factor, for a porous slab of catalyst pellet under non-isothermal conditions, was revisited. An exact formal analytical solution was obtained for an n^{th} -order, exothermic and irreversible chemical reaction. A closed analytical formula was obtained (Muñoz Tavera, 2005) for the very fast reaction limit, and its applicability was numerically tested for a significant range of values of the parameters involved in the model, i.e the thermicity group β and the Arrhenius group γ .

1. Introduction

A wide variety of chemical processes involve the use of heterogeneous catalytic reactors as a core unit operation. Traditional chemical engineering applications (Lee, 1985; Satterfield, 1970), like hydrogenation of organic compounds, oxidation, dehydrogenation, polymerization and catalytic cracking, among many others, are performed by contacting a fluid (gas or liquid) reacting phase with solid porous particles, which possess a high surface-volume ratio to enhance contact between the fluid phase and the actual catalytic agent, typically a metal (Ni, Pd, Fe, Cu, Pt) or metal oxide. Analogous situation arises in some biochemical engineering processes (Bucholz, 1982; Engasser and Horvath, 1976), in particular in immobilized enzyme reactors, where enzymes are fixed to a porous matrix, such as agarose.

From a chemical engineering perspective, only macroscopic variables in the reactor are accessible for both measurement and control. However, in the processes described above, chemical or biochemical catalytic reactions take place at the surface of solid particles, usually at the pore surfaces in the particle interior, and consequently they depend on microscopic distributed parameters, such as concentration and temperature, which are related to the macroscopic values through a combination of mass and heat transfer resistances, in addition to the chemical reaction itself. A simplified analysis of the real situation is to consider two resistances in series (Lee, 1985; Satterfield, 1970), the first one for transport through the external boundary layer which surrounds the particle, and the second one due to the combination of diffusion and reaction at the interior of the pores. At steady state, the over all reaction rate will be controlled by the higher resistance, i.e. the slowest step. For the case in which reaction and diffusion at the interior of the pores controls, the theory of effectiveness factors can be applied. Originally developed independently by Damköhler (1935), Thiele

(1939) and Zeldovich (1939), this theory has become an important and useful concept in heterogeneous reactor analysis, design and control for many years.

Extensive theoretical studies have been performed for the calculation of effectiveness factors by assuming isothermal conditions and different reaction rates (Bischoff, 1965), and analytical expressions can be obtained for typical cases: simple n^{th} -order, Langmuir isotherm (Chu and Hougen, 1962) assuming simple slab one-dimensional geometries. Other shapes (spheres, cylinders) have been studied (Amundson and Luss, 1967) in the context of the first-order reaction.

Under conditions when intra-particle thermal resistance becomes important, i.e. non-isothermal pellet, the analysis becomes more complicated due to the unavoidable coupling between heat and mass transfer equations. Much theoretical work has been performed to study questions related to uniqueness and stability of solutions (Aris, 1969; Drott and Aris, 1969; Hlaváček et al., 1969a,b; Luss, 1968)

Despite the inherent mathematical complexity of general solutions described above, in many practical cases the internal temperature gradients are comparatively small (Hlaváček et al., 1969a) (but not necessarily negligible), and for very fast irreversible reactions the concentration of reactant at the center of the pellet will be close to zero, so uniqueness of solutions in those cases is guaranteed even on physical grounds. In this context, simple empirical analytical expressions for the temperature dependence of the effectiveness factor in the first-order reaction have been reported (Liu, 1969).

An exact formal analytical solution was developed (Muñoz Tavera, 2005) for the non-isothermal effectiveness factor in a slab geometry, for the case of irreversible and exothermic n^{th} -order reaction rate. This general formal expression is specialized for the limit of a very fast chemical reaction, where the concentration at the center of the slab can be assumed to be close to zero, obtaining an analytical formula suitable for direct calculations.

2. Theory

2.1. Definition of the effectiveness factor

For a porous catalyst pellet, where the controlling resistance is assumed to be diffusion and chemical reaction occurring at the interior pores, the effectiveness factor is defined by the expression:

$$\eta \equiv \frac{R_{avg}}{R_{surf}} = \frac{\frac{1}{V_{pellet}} \iiint R dV}{R_{surf}} \quad (1)$$

where R represents the volumetric reaction rate inside the pellet pores, and V_{pellet} is the total volume of the catalyst pellet.

In what follows, we shall assume that C is the reactant concentration at the interior of the pellet pores. We shall also consider effective transport properties inside the pores: D_{eff} and k_{eff} will be the effective diffusion coefficient and thermal conductivity. The reaction enthalpy will be ΔH_R , and the stoichiometric coefficient (negative) for the reactant will be ν_c .

Under steady-state conditions, the mass and energy balance equations are:

$$\text{Mass Balance:} \quad -D_{\text{eff}} \nabla^2 C = \nu_c R \quad (2)$$

$$\text{Energy Balance:} \quad -k_{\text{eff}} \nabla^2 T = (-\Delta H_R) R \quad (3)$$

Substituting the reaction rate from equation (2) into the effectiveness factor definition (1), and after applying Gauss' Theorem:

$$\eta = \frac{D_{\text{eff}}}{(-\nu_c) V_{\text{pellet}} R_{\text{surf}}} \iint_{S_{\text{pellet}}} \nabla C \cdot \hat{n} dS \quad (4)$$

Expression (4) is in general valid for any geometry. However, in many applications the interesting cases are simple geometries (slabs, cylinders, spheres) whose symmetry allows us to assume that the concentration gradient is independent of the position over the surface. Under this last assumption, equation (4) can be reduced to:

$$\eta = \frac{D_{\text{eff}} S_{\text{pellet}}}{(-\nu_c) V_{\text{pellet}} R_{\text{surf}}} \hat{n} \cdot \nabla C_{\text{surf}} \quad (5)$$

2.2. Pellet with the shape of a slab

Consider a catalyst pellet with the shape of a slab, of thickness $2L$, with $L^2 \ll S_{\text{pellet}}$. For this geometry, the mass and energy balance equations (2,3) reduce to the following expressions:

$$\text{Mass Balance} \quad -D_{\text{eff}} \frac{d^2 C}{dx^2} = \nu_c R \quad (6)$$

$$\text{Energy Balance} \quad -k_{\text{eff}} \frac{d^2 T}{dx^2} = (-\Delta H_R) R \quad (7)$$

The boundary conditions for this system of differential equations are:

$$I) \quad T(x = \pm L) = T_s, \quad C(x = \pm L) = C_s$$

$$II) \quad \frac{dT}{dx}(x = 0) = 0, \quad \frac{dC}{dx}(x = 0) = 0$$

From equations (6) and (7), it is possible to eliminate the reaction rate. After integration subjected to boundary conditions (I) and (II), in dimensionless form one obtains:

$$\theta = 1 - \beta(f - 1) \quad (8)$$

$$\zeta = \frac{x}{L}, \quad f = \frac{C}{C_s}, \quad \theta = \frac{T}{T_s}, \quad \beta = \frac{(-\Delta H_R)D_{eff}C_s}{(-v_c)k_{eff}T_s}$$

Note that for an exothermic reaction $\beta > 0$.

The non-dimensional group β has been referred in the literature (Satterfield, 1970) as *thermicity* or *heat generation function*. It represents the ratio between the rate of heat generation due to the chemical reaction, and the rate at which heat is transported by thermal conduction mechanisms. The *thermicity* is then a direct measure of non-isothermal effects, and it follows from (8) that, for a very fast reaction $f_{center} \approx 0$:

$$\beta \approx \theta_{center} - 1 = \frac{T_{center} - T_s}{T_s} = \frac{\Delta T_{max}}{T_s} \quad (9)$$

It can be concluded from (9) that the limit $\beta \rightarrow 0$ represents the isothermal pellet case, while non-isothermal effects becomes more important as the *thermicity* value increases. However, even for highly exothermic reactions (Hlaváček, 1969a ; Satterfield, 1970), the *thermicity* rarely exceeds 0.2.

Table 1: Experimental values (Hlaváček et al., 1969a) for the parameters involved in the model in some industrial chemical reactions

Reaction	β	γ	$\gamma\beta$	ϕ_0
NH ₃ synthesis	0.000061	29.4	0.0018	1.2
Oxidation of CH ₃ OH to CH ₂ O	0.0109	16	0.175	1.1
Synthesis of vinylchloride	0.25	6.5	1.65	0.27
Hydrogenation of ethylene	0.066	23-27	1-2.7	0.2-2.8
Oxidation of ethylene	0.13	13.4	1.76	0.08
Dissociation of N ₂ O	0.64	22	1.0-2.0	1.0-5.0
Hydrogenation of benzene	0.12	14-16	1.7-2	0.05-1.9
Oxidation of SO ₂	0.012	14.8	0.175	0.9

2.3. Reaction rate of arbitrary integer order

Let's restrict the analysis to a n^{th} -order reaction kinetics, where $n \geq 0$ is an integer

$$R = \kappa_s e^{-\frac{E}{R_g} \left(\frac{1}{T} - \frac{1}{T_s} \right)} C^n \quad (10)$$

and κ_s is the value for the kinetic constant at surface temperature T_s . It can be shown (Muñoz Tavera, 2005) that for this reaction rate, an exact expression for the effectiveness factor is

$$\eta = \frac{1}{\phi_0} \left[(n+1) \int_{f_{\text{center}}}^1 e^{-\frac{\gamma\beta(f-1)}{1-\beta(f-1)}} f^n df \right]^{1/2} \quad (11)$$

By defining the functional $H[f, f_{\text{center}}]$ as:

$$H[f, f_{\text{center}}] = \int_{f_{\text{center}}}^f e^{-\frac{\gamma\beta(w-1)}{1-\beta(w-1)}} w^n dw \quad (12)$$

it can be shown (Muñoz Tavera, 2005) that it satisfies the identity

$$\int_{f_{\text{center}}}^1 \frac{df}{\sqrt{H[f, f_{\text{center}}]}} = \frac{2\phi_0}{\sqrt{n+1}} \quad (13)$$

Note that by means of eq.(13), the non-dimensional concentration at the center of the slab f_{center} , is defined as a function of the generalized Thiele modulus at isothermal conditions ϕ_0 .

Using the same notation, the effectiveness factor in (13) can be expressed as:

$$\eta = \frac{\sqrt{n+1}}{\phi_0} \sqrt{H[1, f_{\text{center}}]} \quad (14)$$

2.4. Exact Analytical Expression

As is demonstrated in detail in the Appendix, a novel closed analytical expression for the integral (20) has been developed (Muñoz Tavera, 2005), in terms of well-known special functions, the exponential integrals E_k (Abramowitz and Stegun, 1970a).

$$H[f, f_{center}] = e^{\gamma} \sum_{k=0}^n \frac{n!(-1)^k}{k!(n-k)!} \frac{(1+\beta)^{n-k}}{\beta^{n+1}} \left\{ [1+\beta(1-f_{center})]^{k+1} E_{k+2} \left(\frac{\gamma}{1+\beta(1-f_{center})} \right) - [1+\beta(1-f)]^{k+1} E_{k+2} \left(\frac{\gamma}{1+\beta(1-f)} \right) \right\} \quad (15)$$

If a very rigorous calculation is desired, expression (15) can be substituted into (13), and performing a numerical integration, the exact value of the non-dimensional concentration at the center of the catalyst pellet f_{center} can be obtained, for any integer reaction order $n \geq 0$ and generalized Thiele modulus ϕ_0 . The calculation requires an iterative procedure, due to the non-linear dependence between both parameters. Once f_{center} is obtained, it is substituted in (14) to obtain the exact value of the non-isothermal effectiveness factor.

In the present work, a more practical approach is proposed, by assuming the case of a very fast reaction, where the approximate limiting condition $f_{center} \approx 0$ can be applied. Under this assumption, from the exact expression (14), the corresponding approximation for the effectiveness factor becomes

$$\eta = \frac{\sqrt{n+1}}{\phi_0} \sqrt{H[1, f_{center} \rightarrow 0]} \quad (16)$$

Taking the corresponding limit in the exact analytical expression (15)

$$\eta = \frac{\sqrt{n+1}}{\phi_0} e^{\gamma/2} \sqrt{\sum_{k=0}^n \frac{n!(-1)^k}{k!(n-k)!} \frac{(1+\beta)^{n-k}}{\beta^{n+1}} \left\{ (1+\beta)^{k+1} E_{k+2} \left(\frac{\gamma}{1+\beta} \right) - E_{k+2}(\gamma) \right\}} \quad (17)$$

To test the accuracy and validity of the limit (17), numerical calculations were performed to obtain the exact solutions $\phi_0(f_{center})$ from equation (13), for small values of f_{center} .

Table 2 displays the results for the cases $n = 1, 2$. Also shown is the relative error involved in the calculation of the effectiveness factor by using (17), compared with the exact expression (14), according to the formula:

$$\left| \frac{\eta(f_{center}) - \eta(f_{center} \rightarrow 0)}{\eta(f_{center})} \right| = \left| 1 - \frac{\sqrt{H[1, 0]}}{\sqrt{H[1, f_{center}]}} \right| \quad (18)$$

As expected on physical grounds, Table 2 reflects the fact that $f_{center} \rightarrow 0$ as $\phi_0 \rightarrow \infty$. However, even for finite values of the generalized Thiele modulus and $f_{center} \neq 0$, the relative

error involved in calculating the effectiveness factor by using the analytical approximation (17) does not exceed 5% for most cases shown in Table 2. As the product $\gamma\beta$ increases, the minimum threshold $\phi_{0,\min}$ in the Thiele modulus to achieve an acceptable precision decreases. Recommended threshold values for the applicability of equation (17) are shown in Table 3. Comparing the values of the calculated Thiele modulus for the different cases presented in Table 2, with the experimental values for common industrial reactions presented in Table 1, it is concluded that the approximation (17) is applicable for many real cases.

Table 2: Numerical solution of eq.(21) for $\phi_0(f_{\text{center}})$. Also shown is the relative error, as defined in eq.(27), involved in the calculation of the effectiveness factor by using (26), compared with the exact expression (22).

γ	β	f_{center}	n=1		n=2	
			ϕ_0	$ 1-\eta(0)/\eta(f_{\text{center}}) $	ϕ_0	$ 1-\eta(0)/\eta(f_{\text{center}}) $
5	0.1	10^{-3}	6.735	6.7E-7	8,116.5	6.9E-10
		10^{-2}	4.353	6.7E-5	122.23	1.1E-7
		0.1	2.511	6.56E-3	6.845	6.7E-4
	0.3	10^{-3}	4.506	9.8E-7	1,746.4	1.1E-9
		10^{-2}	3.172	9.8E-5	33.754	1.1E-6
		0.1	1.893	9.39E-3	5.296	1.03E-3
	0.6	10^{-3}	3.213	1.3E-6	717.537	1.6E-9
		10^{-2}	2.271	1.3E-4	15.0877	1.6E-6
		0.1	1.386	1.26E-2	3.87786	1.48E-3
10	0.1	10^{-3}	5.143	8.8E-7	5,223.8	9.6E-10
		10^{-2}	3.551	8.8E-5	55.484	9.5E-7
		0.1	2.108	8.45E-3	5.890	9.0E-4
	0.3	10^{-3}	2.608	1.8E-6	638.65	2.3E-6
		10^{-2}	1.904	1.8E-4	17.363	2.2E-6
		0.1	1.197	1.61E-2	3.329	1.98E-3
	0.6	10^{-3}	1.340	2.9E-6	200.791	4.3E-9
		10^{-2}	0.977	2.8E-4	5.777	4.2E-6
		0.1	0.641	2.54E-2	1.774	3.62E-3
30	0.1	10^{-3}	2.286	2.3E-6	1,504.1	3.1E-9
		10^{-2}	1.611	2.3E-4	17.040	3.1E-6
		0.1	1.047	2.05E-2	2.906	2.62E-3
	0.3	10^{-3}	0.322	8.9E-6	50.853	2.0E-8
		10^{-2}	0.247	8.7E-4	1.507	1.9E-5
		0.1	0.187	6.98E-2	0.520	1.37E-2
	0.6	10^{-3}	0.0417	1.6E-5	3.554	4.9E-8
		10^{-2}	0.0343	1.56E-3	1.736	4.7E-5
		0.1	0.0282	0.121	0.0774	3.05E-2

The other interesting feature that can be observed from the results presented in Table 3, is that non-isothermal effects are strongly dependent on the values of the Arrhenius group γ . As was pointed out previously, in the isothermal limit it is expected that $\eta\phi_0 \rightarrow 1$ for large ϕ_0 .

However, due to internal temperature gradients, $\eta\phi_0$ raises up to 100 for zero-order, up to 50 for first-order, and up to 30 for second-order kinetics, when large values of γ and β are attained. Those numbers represent correction factors to the isothermal limit $\eta \approx 1/\phi_0$. This fact has been reported in previous numerical studies (Aris, 1969; Drott and Aris, 1969; Hlaváček et al. 1969a,b; Liu, 1969; Luss, 1968), and a dependence related to the product $\gamma\beta$ as been proposed (Hlaváček et al. 1969a,b; Liu, 1969). Such a dependence also becomes explicit in a low beta approximation to eq. (17) (Muñoz Tavera, 2005), with a proportionality of the effectiveness factor to the expression $(\gamma\beta)^{-(n+1)/2}$. In agreement with this asymptotic result, a compensation tendency for non-isothermal effects is observed, according to the results in Table 3, for high values of the reaction order n .

$\gamma\beta$	n = 1	n = 2
	$\phi_{0,\min}$	$\phi_{0,\min}$
0.5	2	6
1.5	1.5	4
3	1	2
6	0.8	1.5
9	0.2	0.6
18	0.03	0.09

Table 3: Recommended threshold values for the generalized Thiele modulus, $\phi_0 \geq \phi_{0,\min}$, to apply the formula (26) with a relative error not exceeding 1%, for first and second order kinetics.

4. Conclusions

According to the standard theory for effectiveness factors, a novel rigorous mathematical result was derived for the case of a non-isothermal catalyst pellet, with the shape of a slab, for an exothermic irreversible reaction of n^{th} -order. After this result is specialized for the case in which the reaction is very fast, and the concentration in the center of the slab is close to zero, an analytical expression was derived for this limit. This approximation was compared with numerical integration results, for different realistic values of the parameters involved in the model, showing good agreement for finite values of the generalized Thiele modulus. This analytical formula is relatively simple, involving well known special functions, and therefore is suitable for computational applications, like simulation and design.

Notation

C	Reactant concentration, mol m ⁻³
C _s	Reactant concentration at pellet surface, mol m ⁻³
D _{eff}	Effective diffusion coefficient inside the pellet pores, m ² s ⁻¹

E	Activation energy of the chemical reaction, J mol ⁻¹
f	Dimensionless concentration
f _{center}	Dimensionless concentration at the center of the slab
ΔH _R	Reaction enthalpy, J mol ⁻¹
k _{eff}	Effective thermal conductivity inside the pellet pores, W m ⁻¹ K ⁻¹
R	Volumetric reaction rate, mol m ⁻³ s ⁻¹
R _{avg}	Average reaction rate, mol m ⁻³ s ⁻¹
R _g	Universal constant of gases, J mol ⁻¹ K ⁻¹
R _{surf}	Reaction rate at external surface conditions, mol m ⁻³ s ⁻¹
S _{pellet}	External surface of the pellet, m ²
T	Temperature, K
T _{center}	Temperature at the center of the slab, K
ΔT _{max}	Maximum temperature difference, K
T _s	Temperature at the pellet surface, K
V _{pellet}	Total volume of the catalyst pellet, m ³
L	Characteristic half thickness of the slab, m
β	Thermicity group, dimensionless
φ ₀	Generalized Thiele modulus, dimensionless
γ	Arrhenius group, dimensionless
η	Effectiveness factor, dimensionless
κ _s	Kinetic constant for n th -order reaction at surface conditions, mol ¹⁻ⁿ m ⁻³⁽¹⁻ⁿ⁾ s ⁻¹
v _c	Stoichiometric coefficient, negative for reactant, dimensionless
θ	Dimensionless temperature
θ _{center}	Dimensionless temperature at the center of the slab

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Appendix

The exact analytical integration for the function $H[f, f_{center}]$ was performed through the following steps

$$H[f, f_{center}] = \int_{f_{center}}^f e^{-\frac{\gamma\beta(w-1)}{1-\beta(w-1)}} w^n dw \quad (A1)$$

1. Rearrange the terms in the numerator:

$$\frac{-\gamma\beta}{1-\beta(w-1)} = \gamma - \frac{\gamma/(1+\beta)}{1-\frac{\beta}{1+\beta}w}$$

$$H[f, f_{center}] = e^\gamma \int_{f_{center}}^f e^{-\frac{\gamma/(1+\beta)}{1+\beta} w} w^n dw \quad (A2)$$

2. Change of variable:

$$z = 1 - \frac{\beta}{1+\beta} w$$

$$H[f, f_{center}] = \left(\frac{1+\beta}{\beta} \right)^{n+1} e^\gamma \int_{1-\frac{\beta}{1+\beta} f}^{1-\frac{\beta}{1+\beta} f_{center}} e^{-\frac{\gamma/(1+\beta)}{z}} (1-z)^n dz \quad (A3)$$

3. Change of variable:

$$x = 1/z$$

$$H[f, f_{center}] = \left(\frac{1+\beta}{\beta} \right)^{n+1} e^\gamma \int_{\frac{1+\beta}{1+\beta(1-f_{center})}}^{\frac{1+\beta}{1+\beta(1-f)}} e^{-\frac{\gamma}{1+\beta} x} (x-1)^n x^{-(n+2)} dx \quad (A4)$$

4. Binomial expansion:

$$(x-1)^n = \sum_{k=0}^n \frac{n!}{k!(n-k)!} (-1)^k x^{n-k} \quad (A5)$$

5. Substitute (A5) into (A4):

$$H[f, f_{center}] = \left(\frac{1+\beta}{\beta} \right)^{n+1} e^\gamma \sum_{k=0}^n \frac{n!(-1)^k}{k!(n-k)!} \int_{\frac{1+\beta}{1+\beta(1-f_{center})}}^{\frac{1+\beta}{1+\beta(1-f)}} e^{-\frac{\gamma}{1+\beta} x} x^{-(k+2)} dx \quad (A6)$$

6. Decompose the integrals in (A6) into two terms:

$$\frac{\int_{\frac{1+\beta}{1+\beta(1-f_{center})}}^{\frac{1+\beta}{1+\beta(1-f)}} e^{-\frac{\gamma}{1+\beta} x} x^{-(k+2)} dx}{\frac{1+\beta}{1+\beta(1-f_{center})}} = \frac{\int_{\frac{1+\beta}{1+\beta(1-f_{center})}}^{\infty} e^{-\frac{\gamma}{1+\beta} x} x^{-(k+2)} dx}{\frac{1+\beta}{1+\beta(1-f_{center})}} - \frac{\int_{\frac{1+\beta}{1+\beta(1-f)}}^{\infty} e^{-\frac{\gamma}{1+\beta} x} x^{-(k+2)} dx}{\frac{1+\beta}{1+\beta(1-f)}} \quad (A7)$$

7. Apply the following change of variables to the first and second integrals in (A7), respectively:

$$t = \frac{x}{(1+\beta)/(1+\beta(1-f_{center}))} \quad t = \frac{x}{(1+\beta)/(1+\beta(1-f))}$$

$$\frac{\frac{1+\beta}{1+\beta(1-f)}}{\frac{1+\beta}{1+\beta(1-f_{center})}} \int e^{-\frac{\gamma}{1+\beta}x} x^{-(k+2)} dx = \left[\frac{1+\beta}{1+\beta(1-f_{center})} \right]^{-(k+1)} \int_1^{\infty} e^{-\frac{\gamma}{1+\beta(1-f_{center})}t} t^{-(k+2)} dt$$

$$- \left[\frac{1+\beta}{1+\beta(1-f)} \right]^{-(k+1)} \int_1^{\infty} e^{-\frac{\gamma}{1+\beta(1-f)}t} t^{-(k+2)} dt$$
(A8)

From the definition of the Exponential Integral function (Abramowitz and Stegun, 1970a):

$$E_n(x) = \int_1^{\infty} \frac{e^{-xt}}{t^n} dt$$
(A9)

$$\frac{\frac{1+\beta}{1+\beta(1-f)}}{\frac{1+\beta}{1+\beta(1-f_{center})}} \int e^{-\frac{\gamma}{1+\beta}x} x^{-(k+2)} dx = \left[\frac{1+\beta}{1+\beta(1-f_{center})} \right]^{-(k+1)} E_{k+2} \left(\frac{\gamma}{1+\beta(1-f_{center})} \right)$$

$$- \left[\frac{1+\beta}{1+\beta(1-f)} \right]^{-(k+1)} E_{k+2} \left(\frac{\gamma}{1+\beta(1-f)} \right)$$
(A10)

8. Substituting the result (A10) into (A5), the final expression is obtained:

$$H[f, f_{center}] = e^{\gamma} \sum_{k=0}^n \frac{n!(-1)^k}{k!(n-k)!} \frac{(1+\beta)^{n-k}}{\beta^{n+1}} \left\{ \left[1+\beta(1-f_{center}) \right]^{k+1} E_{k+2} \left(\frac{\gamma}{1+\beta(1-f_{center})} \right) \right.$$

$$\left. - \left[1+\beta(1-f) \right]^{k+1} E_{k+2} \left(\frac{\gamma}{1+\beta(1-f)} \right) \right\}$$
(A11)

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