A3606LS - Improved-Lumped Formulations for Heat and Mass Transfer in Adsorbed Gas Storage

L. A. Sphaier, D. S. Jurumenha
Department of Mechanical Engineering, Universidade Federal Fluminense, Rua Passo da Pátria 156, sl. 216, bl. E. Niterói, RJ, 24210-240, Brazil.
E-mail: lasphaier@id.uff.br

Abstract. The purpose of this study is to provide an improved-lumped formulation for simulating adsorbed gas storage operations. The approach is shown to reduce the original spatial-dependent PDEs to two time-dependent ODEs, as similar to the ones obtained using classical lumped-system analyses (CLSA), the main differences being an additional equation that is required for calculating the reservoir wall temperature, and modified Biot numbers. The average reservoir temperature is then calculated with the improved lumped formulation, using two different approximation schemes, and compared with the results of the CLSA and the one-dimensional formulation that originated all approximate lumped models. A case of slow discharge with negligible wall heat capacity is analyzed, and the results show that, even for a large Biot number, one of the proposed approximation schemes can reproduce the 1D results with reasonable accuracy, while the CLSA yields very different results.

Nomenclature

| Symbol | Description                  |
|--------|------------------------------|
| Bi     | Biot number                  |
| $c_p$  | constant pressure specific heat |
| $c_{tg}$ | specific heat ratio     |
| $C^*$  | thermal capacity ratio       |
| $F_0$  | Fourier number               |
| $i_{sor}$ | heat of sorption          |
| $\dot{j}$ | mass flux vector         |
| $k$    | thermal conductivity        |
| $h$    | convective heat transfer coefficient |
| $H_{\alpha,\beta}$ | Hermite approximation |
| $H$    | dimensionless heat transfer coefficient |
| $\bar{m}$ | mass flow rate            |
| $M^*$  | maximum stored gas fraction |
| $p$    | pressure                     |
| $\dot{q}$ | heat flux vector        |
| $t$    | time                         |
| $T$    | temperature                  |

Greek symbols

| Symbol | Description                  |
|--------|------------------------------|
| $\alpha$, $\beta$ | Hermite approximation parameters |
| $\epsilon$ | porosity                    |
| $\kappa$ | specific heat ratio         |
| $\rho$  | specific mass                |
| $\sigma$ | Darcy equation coefficient   |

Subscripts and superscripts

| Symbol | Description                  |
|--------|------------------------------|
| $e$    | effective or apparent        |
| $g$    | gas phase                    |
| $in$   | inlet/outlet condition       |
| $ex$   | external condition            |
| $i$    | at inner reservoir radius    |
| $w$    | at outer reservoir radius (wall) |
| $l$    | adsorbed phase               |
| $s$    | solid phase (adsorbent)      |
| *      | dimensionless quantity        |
| *      | modified quantity             |
1. Introduction

Adsorbed gas (AG) storage has been considered as a potential alternative to compressed gas (CG) or liquified gas (LG) storage due to a number of factors, such as high pressures required for CG and low temperatures associated with LG. In spite of the advantages associated with this storage mode, AG requires efficient thermal designs for their storage vessels, in order to properly minimize the limitations brought in by the heating and cooling effects inherent to the adsorption process. As a result, a number of mathematical models and computational simulations have been proposed as design tools for adsorbed gas reservoirs [1–9]. A common agreement among previous studies is that typical discharge operations for fuel consumption applications involve lower gradients and can hence be simulated using one-dimensional, and in some cases, even lumped-capacitance formulations. Naturally, whenever possible, lumped formulations are preferred, due to their simplicity and consequently a lower required computational time. Very recently, the suitability of using a lumped-capacitance formulation for describing adsorbed gas discharge operations was analyzed [10], showing that, in some circumstances, the usage of lumped models can lead to a considerable error. These critical situations involve cases under which the classical lumped analysis simplification, in which small gradients are assumed, cannot be made. This problem may be circumvented by employing the so-called improved-lumped formulations, which remain simple, due to their independence on spatial coordinates, while retaining some information regarding gradients and boundary conditions through additional relations. One such methodology for obtaining improved-lumped formulations is based on the Coupled Integral Equations Approach (CIEA). The approach is based on the approximation of integrals in terms of a linear combination of the integrand values and its derivatives at the integration limits, an idea originally developed by Hermite [11] and first presented by Menning et al. [12]. The CIEA was successfully utilized in a variety of problems. Among recent applications, one should mention radiative cooling [13], ablation [14], drying [15], thermal analysis of nuclear fuel rods [16], heat conduction with temperature-dependent conductivity [17], and combined convection-radiation cooling [18]. In this context, the purpose of this study is to provide an improved-lumped formulation, using the CIEA, for simulating adsorbed gas storage operations. The text will focus on discharge operations and different levels of approximation will be presented and comparatively analyzed. A more comprehensive version of this work can be found in [19]. Nevertheless, the results herein presented consider cases not analyzed in [19].

2. One-dimensional formulation

The problem of adsorbed gas discharge at constant mass flow rate, as usual for fuel consumption applications, is commonly treated as a long circular cylindrical reservoir with inner and outer radii given by \( r_i \) and \( r_w \). At \( r = r_w \) there is an impermeable wall that exchanges heat with the surroundings, whereas at the inner radius mass flows out of the reservoir. The governing equations for this problem, in dimensionless form are given by [20]:

\[
\begin{align*}
  M_g^* \frac{\partial \rho_g^*}{\partial r^*} + M_l^* \frac{\partial \rho_l^*}{\partial r^*} &= -\frac{1}{\hat{r}^*} \frac{\partial}{\partial \hat{r}^*} \left( \hat{r}^* j_{g,r}^* \right), \tag{1a} \\
  C_e^* \frac{\partial T^*}{\partial t^*} + j_{g,r}^* \frac{\partial T^*}{\partial r^*} &= -\frac{\hat{C}_s^*}{\hat{r}^*} \frac{\partial}{\partial \hat{r}^*} \left( \hat{r}^* q_r^* \right) + M_l^* i_{sor}^* \frac{\partial \rho_l^*}{\partial t^*} + M_g^* \phi \frac{\partial p^*}{\partial t^*}, \tag{1b}
\end{align*}
\]

for \( 0 \leq r^* \leq 1 \), where \( \hat{r}^* = r^* + r_i^* \) and the dimensionless thermal capacity \( C_e^* \) is given by:

\[
C_e^* = C_s^* + M_g^* \rho_g^* + c_l^* M_l^* \rho_l^*, \tag{2}
\]

where \( T^* \) is the dimensionless reservoir temperature and \( \rho_g^* \) and \( \rho_l^* \) are the dimensionless concentrations in the gaseous and adsorbed phases. The dimensionless heat and mass fluxes
The first step in the lumping process is defining the dimensionless volume average:

\[ j_{g,r}^* = -M_g^* \rho_g^* \phi^* \frac{\partial p^*}{\partial r^*}, \quad q_r^* = -\frac{\partial T^*}{\partial r^*}, \]  

(3)

and the dimensionless initial and boundary conditions are given by:

\[ T^*(r^*,0) = 1, \quad p^*(r^*,0) = 0, \]  

(4a)

\[ j_{g,r}^* = 0 \quad \text{and} \quad -\frac{\partial T^*}{\partial r^*} = Bi(T^* - 1) + C_w^* \frac{1}{C_s^* F_0^*} \frac{\partial T^*}{\partial t^*}, \quad \text{at} \quad r^* = 1, \]  

(4b)

\[ j_{g,r}^* = j_{in}^* \quad \text{and} \quad -\frac{\partial T^*}{\partial r^*} = Bi_{in}(T^* - 1), \quad \text{at} \quad r^* = 0, \]  

(4c)

where \( j_{in}^* \) is calculated so that at \( t^* = 1 \) the average pressure reaches its minimal value. The dependent and independent variables were normalized by the following dimensionless forms:

\[ r^* = \frac{t}{t_f}, \quad T^* = \frac{T}{T_0}, \quad p^* = \frac{p - p_{\text{min}}}{p_{\text{max}} - p_{\text{min}}}, \quad r_s^* = \frac{r - r_i}{r_w - r_i}, \quad r_i^* = \frac{r_i}{r_w - r_i}, \]  

(5a)

and the dimensionless parameters involved in the employed formulation are given by:

\[ j_{in}^* = \frac{\nu_{in}^*}{\rho_c^* \Delta r^*}, \quad M_g^* = \frac{\rho_{g,\text{max}} \epsilon}{\rho_{\text{max}}}, \quad M_i^* = \frac{\rho_{\text{max}}}{\rho_{\text{max}}}, \quad \omega = \frac{\kappa - 1}{\kappa} \frac{\Delta p}{p_{\text{max}}}, \]  

(6a)

\[ C_s^* = \frac{c_s \rho_b}{c_p^* \rho_{\text{max}}}, \quad C_w^* = \frac{\rho_w c_w}{c_p^* \rho_{\text{max}} \Delta r}, \quad c_i^* = \frac{c_l}{c_p^*}, \quad \hat{i}_{\text{so}} = \frac{i_{\text{so}}}{T_0 c_p^*}, \]  

(6b)

\[ Bi_{in} = \frac{h_{\text{in}}}{k_b^*}, \quad Bi = \frac{h \Delta r}{k_b}, \quad Fo = \frac{k_b t_f}{\rho_b c_s \Delta r^*}, \]  

(6c)

where \( \kappa = c_p^*/c_{vg}^* \), \( \rho_{\text{max}} = \rho_{g,\text{max}} \epsilon + \rho_{\text{max}} \), \( \Delta p = p_{\text{max}} - p_{\text{min}} \) and \( \Delta r = r_w - r_i \).

### 3. Lumping procedure

The first step in the lumping process is defining the dimensionless volume average:

\[ \bar{\phi} = \frac{2}{2 r_i^* + 1} \int_0^{1} \phi(r^* + r_i^*) \, dr^*, \]  

(7)

where \( \phi \) is an arbitrary quantity. Then, the energy equation is written in conservative form:

\[ \frac{\partial (C_e^* T^*)}{\partial t^*} + (1 - c_i^*) M_i^* T^* \frac{\partial \rho_t^*}{\partial t^*} + \frac{1}{r^*} \frac{\partial}{\partial r^*} \left( \hat{i}_{\text{so}}^* j_{g,r}^* T^* \right) = \]  

\[ \frac{-Fo C_s^*}{r^*} \frac{\partial }{\partial r^*} \left( \hat{i}_{\text{so}}^* q_{r}^* \right) + M_i^* \hat{i}_{\text{so}}^* \frac{\partial \rho_t^*}{\partial t^*} + M_g^* \omega \frac{\partial p^*}{\partial t^*}. \]  

(8)

Integrating equations (1a) and (8) with the operator \( \int_0^{1} \hat{i}^* \, dr^* \), substituting boundary conditions, and rearranging, yields:

\[ M_g^* \frac{dp_t^*}{dt^*} + M_i^* \frac{dp_t^*}{dt^*} = -K_i j_{in}^*, \]  

(9)

\[ \frac{2}{1 + 2 r_i^*} \int_0^{1} \left( C_e^* \frac{\partial T^*}{\partial t^*} + \left( M_g^* \frac{\partial p_t^*}{\partial t^*} + M_i^* \frac{\partial \rho_t^*}{\partial t^*} \right) T^* \right) \hat{i}^* \, dr^* - \left( M_g^* \frac{dp_t^*}{dt^*} + M_i^* \frac{dp_t^*}{dt^*} \right) T_i^* = \]  

\[ = Fo C_s^* \left[ \frac{\rho_w c_w}{c_p^* F_0^*} (1 - T_w^*)^* - K_i (Bi_{in} (1 - T_i^*)) \right] + \left( M_i^* \frac{dp_t^*}{dt^*} + M_g^* \frac{dp_t^*}{dt^*} \right), \]  

(10)

where, for simplification purposes, the notation \( T_i^* = T^*(0, t^*) \) and \( T_w^* = T^*(1, t^*) \), is used. In addition, \( K_i \) and \( K_w \) are geometric ratios, given by:

\[ K_i = \frac{2 r_i^*}{1 + 2 r_i^*}, \quad K_w = \frac{(r_i^* + 1)}{1 + 2 r_i^*} = 2 - K_i. \]  

(11)
3.1. Classical Lumped System Analysis

The Classical Lumped System Analysis (CLSA) is based on the negligible gradient approximation, which leads to:

\[ T_w^* \approx T_i^* \approx \bar{T}(t^*), \quad \frac{2}{2 r_i^* + 1} \int_0^1 f g \, \hat{r}^* \, \text{d}r^* \approx \hat{f} \hat{g}, \]  

(12)

where \( f \) and \( g \) are arbitrary quantities. Using these relations, equation (10) is simplified to yield:

\[ (\bar{C}_e + K_w C_w^*) \frac{d\bar{T}}{d\bar{r}^*} = H_{ex} (1 - \bar{T}^*) + H_{in} (1 - \bar{T}^*) + \left( M_i^* \hat{i}_{\text{sof}} \frac{d\rho_i^*}{d\bar{r}^*} + M_g^* \omega \frac{d\rho^*}{d\bar{r}^*} \right), \]  

(13)

where \( H_{in} = K_i \text{Bi}_{in} \text{Fo} C_s^* \), \( H_{ex} = K_w \text{Bi}_{ex} C_s^* \) and \( \bar{C}_e = M_g^* \rho_{\text{sof}}^* + c_i^* M_i^* \rho_i^* + C_s^* \).

4. Coupled Integral Equations Approach (CIEA)

The basis for the CIEA is the Hermite approximation of an integral, denoted, \( H_{\alpha,\beta} \):

\[ \int_{x_0}^{x_1} f(x) \, \text{d}x = \sum_{\nu=0}^{\alpha} c_{\nu}(\alpha,\beta) \Delta x^{\nu+1} f^{(\nu)}(x_0) + \sum_{\nu=0}^{\beta} c_{\nu}(\beta,\alpha) (-1)^\nu \Delta x^{\nu+1} f^{(\nu)}(x_1) + E_{\alpha,\beta}, \]  

(14)

where \( \Delta x = x_1 - x_0 \) and \( c_{\nu} \) are coefficients, as described in [12]. In this paper, only the two different approximations below are considered:

\[ H_{0,0} \Rightarrow \int_{x_0}^{x_1} f(x) \, \text{d}x \approx \frac{1}{2} \Delta x \left( f(x_0) + f(x_1) \right), \]  

(15a)

\[ H_{1,1} \Rightarrow \int_{x_0}^{x_1} f(x) \, \text{d}x \approx \frac{1}{2} \Delta x \left( f(x_0) + f(x_1) \right) + \frac{1}{12} \Delta x^2 \left( f'(x_0) - f'(x_1) \right), \]  

(15b)

corresponding to the well-known trapezoidal and corrected trapezoidal integration rules.

4.1. \( H_{0,0}/H_{0,0} \) approximation scheme

This scheme is based on using the \( H_{0,0} \) approximation for the integral involved in the average temperature definition, as well as for the integral of the temperature derivative:

\[ \int_0^1 T^* \hat{r}^* \, \text{d}r^* \approx \frac{1}{2} \left( r_i^* T_i^* + (1 + r_i^*) T_w^* \right), \]  

(16a)

\[ \int_0^1 \frac{\partial T^*}{\partial \bar{r}^*} \hat{r}^* \, \text{d}r^* \approx \frac{1}{2} \left( \left( \frac{\partial T^*}{\partial \bar{r}^*} \right)_{r^*=0} + \left( \frac{\partial T^*}{\partial \bar{r}^*} \right)_{r^*=1} \right). \]  

(16b)

Performing integration, using eq. (7), and substituting boundary conditions yields:

\[ \bar{T}^* \approx \frac{1}{2} \left( K_i T_i^* + K_w T_w^* \right), \]  

(17a)

\[ T_w^* - T_i^* \approx \frac{1}{2} \left( \left( \text{Bi}_{in} (T_i^* - 1) \right) - \left( \text{Bi} (T_w^* - 1) + \frac{C_w^*}{C_s^*} \text{Fo} \frac{dT_w^*}{dt^*} \right) \right). \]  

(17b)

These equations are algebraically solved for \( T_w^* \) and \( T_i^* \), and substituted into eq. (10), yielding:

\[ \frac{2}{1 + 2 r_i^*} \int_0^1 \left( C_e^* \frac{\partial T^*}{\partial t^*} + \left( M_g^* \frac{d\rho_i^*}{dt^*} + M_i^* \frac{d\rho_i^*}{dt^*} \right) \hat{T}_i^* \hat{r}^* \, \text{d}r^* - \left( M_g^* \frac{d\rho^*}{dt^*} + M_i^* \frac{d\rho_i^*}{dt^*} \right) \hat{T}_i^* \right) + K_w C_w^* \frac{dT_w^*}{dt^*} = \]

\[ = \text{Fo} C_s^* \text{Bi}_{in} K_i (1 - \bar{T}^*) + \text{Fo} C_s^* \text{Bi}_{ex} K_w (1 - \bar{T}^*) + \left( M_i^* \hat{i}_{\text{sof}} \frac{d\rho_i^*}{dt^*} + M_g^* \omega \frac{d\rho^*}{dt^*} \right), \]  

(18)
where $Bi_{ex}^*$, $Bi_{in}^*$, and $C_w^*$ are modified Biot numbers, and a modified $C_w^*$, defined as:

$$Bi_{ex}^* = \frac{2Bi (Bi_{in} + 2)}{4 + Bi_{in} K_w + Bi K_i}, \quad Bi_{in}^* = \frac{2(Bi + 2)Bi_{in}}{4 + Bi_{in} K_w + Bi K_i}, \quad C_w^* = C_w^* Bi_{ex}^*/Bi.$$ (19)

For discharge operations, the outlet temperature in the advective terms may be reasonably approximated by the average value:

$$\left(M_g^* \frac{d\hat{\rho}^*_i}{dt^*} + M_t^* \frac{d\hat{\rho}^*_w}{dt^*}\right) T_i^* = -K_i j_{in}^* T_i^* \approx -K_i j_{in}^* T^*.$$ (20)

Using equation (20) and approximating the remaining integral in (18) using eq. (12) yields:

$$C_w^* \frac{dT^*}{dt^*} + K_w C_w^* \frac{dT^*_w}{dt^*} = H_{ex}^* (1 - T^*) + H_{in}^* (1 - T^*) + \left(M_t^* i_{sor}^* \frac{d\hat{\rho}^*_i}{dt^*} + M_t^* \frac{dp^*}{dt^*}\right).$$ (21)

where $H_{in}^* = K_i Bi_{in}^* Fo C_w^*$ and $H_{ex}^* = K_w Bi_{ex}^* Fo C_w^*$. This equation must be solved together with an ODE for the reservoir wall temperature, obtained from combining equations (17a) and (17b):

$$\frac{C_w^*}{C_w^* Fo} \frac{dT^*_w}{dt^*} = -Bi (T^*_w - 1) + Bi_{in} (T^*_w - 1) + \frac{Bi_{in} K_w + 4}{K_i} (T^*_w - T^*_w)$$ (22)

4.2. $H_{1,1}/H_{0,0}$ approximation scheme

This scheme differs from the previous as the $H_{1,1}$ approximation is used for the average integral:

$$\int_0^1 T^* r^* dr^* \approx \frac{1}{2} \left(r_i^* T_i^* + (1 + r_i^*) T_w^*\right) + \frac{1}{12} \left(\left(\frac{\partial (\hat{\rho}^* T^*)}{\partial r^*}\right)_{r^*=0} - \left(\frac{\partial (\hat{\rho}^* T^*)}{\partial r^*}\right)_{r^*=1}\right).$$ (23)

Using the average definition, boundary conditions, and equation (16b) gives:

$$T^* \approx \frac{1}{2} \left(K_i T_i^* + K_w T_w^*\right) - \frac{1}{12} \left(Bi_{in} (T_i^* - 1) + (2 K_i - 3) \left(Bi (T^*_w - 1) + \frac{C_w^*}{C_w^* Fo} \frac{dT^*_w}{dt^*}\right)\right).$$ (24)

Then, as similarly carried-out for the $H_{0,0}/H_{0,0}$ scheme, equations (17b) and (24) are algebraically solved for $T_w^*$ and $T_i^*$, substituted in equation (10). The advective terms are approximated according to eq. (20) and the remaining integrals are approximated according to relation (12). The resulting equation is identical to (21) where $C_w^*$ is still given by eq. (19); however, the modified Biot numbers are now given by alternate expressions:

$$Bi_{ex}^* = \frac{Bi (32K_i K_w - 22) + 24 (2K_i - 1) K_w}{Bi Bi_{in} (4 K_i - 2) + Bi (2K_i (6 K_i + 1) - 5) + Bi_{in} (6 (3 - 2 K_w) K_w + 1) + 24 (2 K_i - 1)},$$ (25a)

$$Bi_{in}^* = \frac{Bi_{in} (16 K_i (2 K_i - 1) - 2) + 24 (2 K_i - 1)}{Bi Bi_{in} (4 K_i - 2) + Bi (2K_i (6 K_i + 1) - 5) + Bi_{in} (6 (3 - 2 K_w) K_w + 1) + 24 (2 K_i - 1)}.$$ (25b)

In addition, the equation that must be solved together with (21) for the wall temperature is:

$$\frac{C_w^*}{C_w^* Fo} \frac{dT^*_w}{dt^*} = -Bi (T^*_w - 1) + \frac{Bi_{in} (6 (1 - 2 K_i) K_i + 1)}{Bi_{in} (2 - 4 K_i) - 2K_i (6 K_i + 1) + 5} (T^*_w - 1) + \frac{Bi_{in} (6 (3 - 2 K_w) K_w + 1) - 48 K_w + 72}{Bi_{in} (2 - 4 K_i) - 2K_i (6 K_i + 1) + 5}.$$ (26)
| $p_{\text{min}}$ | 0.1 MPa | $p_{\text{max}}$ | 4 MPa |
|----------------|---------|-----------------|-------|
| $R$ | 518 J/(kg K) | $c_p/c_v$ | 1.3 |
| $T_0$ | 293.15 K | $c^*$ | 2 |
| $M^*$ | 0.8 | $C^*$ | 2 |
| $C_w^*$ | 0 | $t_{\text{sor}}^*$ | 1.5 |
| $\sigma^*$ | $10^{10}$ | $K_i$ | 0.1 |

5. Results and discussion

Table 1 displays the adopted input values for the simulations herein presented. The high value of $\sigma^*$ is chosen to reproduce the usual case of small pressure gradients found in discharge operations for fuel consumption applications [2; 7]. The values for the dimensionless parameters represent a common configuration found in adsorbed natural gas storage reservoir, as also demonstrated in [20]. Langmuir’s adsorption isotherm model was chosen, as similarly adopted in previous studies [1; 2; 7; 20]. Since a low pressure gradient situation is considered, both the CLSA and improved-lumped formulations yields average pressure histories equivalent to those calculated with the one-dimensional model, such that only temperature histories need be presented. As previously mentioned, the results shown in [19] focused on a case with $C_w^* = 5$ and $C_s^* = 2$, which showed that if the Fourier number is small, even for small Biot number the CLSA yields results with a significant error when compared to the one-dimensional solution. The results herein presented are aimed at investigating the situation of a negligible wall thermal capacity, i.e. $C_w^* = 0$.

Figure 1 displays simulation results calculated with different formulations for $\text{Fo} = 0.1$ and different values of the Biot numbers. As can be seen, when comparing the cases with $\text{Bi} = 1$ and $\text{Bi} = 10$, one notices a small difference between the results, which indicates, for this low Fourier value, that the results of all formulations are weakly dependent on the external surface condition. For $\text{Bi} = 1$, all formulations yield the same results, but when $\text{Bi}$ is increased to 10 the results from the different formulations start deviating from the 1D solution. The one that seems to better represent the 1D model is the $H_{0,0}/H_{0,0}$ scheme.

![Figure 1](image-url)
However, when the Fourier number is increased to 1, as presented in figure 2, the observed behavior is very different. Although for $\text{Bi} = 1$ the different approximation schemes yield similar results, one can notice that the $H_{0,0}/H_{0,0}$ formulation has a tendency to follow the CLSA results, while the $H_{1,1}/H_{0,0}$ approximation follows the 1D solution. This behavior is greatly amplified when the Biot number is increased to 10, which clearly shows that the $H_{0,0}/H_{0,0}$ scheme deviates from the 1D solution and tends to follow the CLSA solution. In spite of this deviation, the $H_{1,1}/H_{0,0}$ scheme yields a reasonable representation for the average temperature calculated with the 1D model.

Finally, figure 3 shows the average temperature evolution calculated with the different formulations for $\text{Fo} = 10$. As can be seen from this figure, there is a greater difference between the solutions obtained with different formulations for $\text{Bi} = 1$ than that observed for $\text{Fo} = 0.1$ and 1. Again, it is seen that the $H_{0,0}/H_{0,0}$ scheme also tends to follow the CLSA behavior, and becomes unsuitable for representing the 1D behavior for higher Biot numbers. Nevertheless, the $H_{1,1}/H_{0,0}$ scheme provides, once more, a very good representation of the 1D behavior.

**Figure 2.** Average temperature for $\text{Fo} = 1$ calculated with different formulations.

**Figure 3.** Average temperature for $\text{Fo} = 10$ calculated with different formulations.

6. **Conclusions**

This paper presented an improved-lumped formulation for heat and mass transfer in adsorbed gas storage operations. The improved-lumped model was based on averaging the transport equations
of a one-dimensional formulation and employing the CIEA for obtaining relations between space-
averaged quantities and boundary conditions. Two approximation schemes were employed, based
on different formulas for approximating the integrals. The resulting equations are similar to those
obtained in classical lumped-capacitance analyses, the main difference being an additional ODE
that is required for evaluating the vessel wall temperature. Besides that, modified Biot numbers
arise from the application of the CIEA, which are given in terms of the actual Biot numbers and
geometric parameters. After presenting the methodology, a comparative analysis was carried-
out for investigating the behavior of the proposed approximation schemes for different Fourier
and Biot values. A case of slow discharge at a constant mass flow rate with a negligible wall
heat capacity was analyzed. The comparisons showed that the $H_{1,1}/H_{0,0}$ approximation scheme
yielded much better results than the $H_{0,0}/H_{0,0}$ scheme. The $H_{0,0}/H_{0,0}$ results presented a trend
to follow the CLSA solution, which was shown to lead to notable discrepancies when compared to
the actual 1D solution. On the other hand, the $H_{1,1}/H_{0,0}$ approximation yielded very reasonable
results for all Fo values.

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Acknowledgments
The authors would like to acknowledge the financial support provided by the Brazilian funding
agencies CNPq, CAPES and FAPERJ.