Mathematical model of a reactor for solid chemisorption refrigeration systems

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Abstract. The formulation of a mathematical model that allows simulating the operation of chemisorption refrigeration systems that use medium and low temperature thermal sources such as waste heat and have the purpose of increasing the energy efficiency of industrial and/or residential applications, is a prerequisite to design and facilitate the use of these systems. Such model is described here and is intended to evaluate the heat transfer inside of chemisorption reactor for refrigeration system that can operate with a metallic salt (sorbent) mixed with expanded graphite and NH3 as refrigerant fluid (adsorbate). The effectiveness of the model is validated through experimental results obtained for a SrCl2/NH3 pair allowing to postulate, a kinetic and thermal model that can be adapted to sorbent/adsorbate pairs of the same type operating under various conditions and thus quantify how operational variables affect the performance parameters of these systems. To this end, the impact of the cycle time and reactor radius on the specific cooling power (SCP) and the coefficient of performance (COP) is measured, concluding that these operational variables exert effects of an opposite nature on the SCP and COP of the system.

Keywords: Refrigeration, Chemisorption, Mathematical model, Composite sorbent.

1. Introduction

Energy consumption is estimated to grow at an annual rate of 1.2% between the years 2008-2035 [1]. This growing increase and the strong dependence on non-renewable energy sources are encouraging the study of alternative applications that use renewable or underutilized energy sources. Under this scenario, in recent decades there has been a growing increase in studies on sorption cooling systems [2]. Sorption refrigeration systems produce the cooling effect using mainly thermal energy. Therefore, they have the ability to reduce electricity consumption if they are powered with waste heat, especially those at low temperature levels, or with solar energy.
In particular, solid sorption refrigeration systems can be divided into physical adsorption and solid chemisorption [3-4]. Compared to physical adsorption, the solid chemisorption systems have a higher sorption capacity, which is beneficial for increasing the specific cooling power per kilogram of sorbent (SCP) and decreasing the volume of the reaction bed. In addition, these systems use working pairs with zero ODP and GWP and are less sensitive to shock and installation position [5].

Despite the advantages of solid chemisorption systems, they have the disadvantage of having a low coefficient of performance (COP) and a low cooling power [6-7]. To overcome these problems, the alternatives include the improvement of the heat and mass transfer properties in the sorbent bed, the improvement of the sorbent properties, the development of sorbents for specific applications and a better management of the heat supplied to the system [6, 8-9]. These improvements can be applied with greater possibility to the system's reactor, which is basically a solid-liquid heat exchanger and performs a similar operation to the one that makes the compressor in traditional steam refrigeration systems.

In this scenario, several papers have addressed the reactors modelling for solid chemisorption systems employing a variety of mathematical models being a large number of them one-dimensional and transient [10-14]. For instance, Huang et al. [15] proposed a 1D model coupled to heat transfer chemical kinetics to simulate the dynamic behaviour of the gas-solid fixed-bed reactors used in CHP. Also, the performance of solid–gas reaction heat transformer system using MnCl₂ and CaCl₂ with the consideration of multistep reactions between CaCl₂ and NH₃ was investigated by Wang et al. [16]. This literature review indicates that there is limited information on the physics of transfer processes associated with sorbent beds, in particular, with surfaces extended to the interior of these systems in order to increase the thermal contact area and reduce the contact resistance between the bed and the metallic surface of the reactor.

In this context, this paper addresses the modelling and simulation of a reactor for a chemisorption refrigeration system that allows evaluating how the type of sorbent (consolidated and in powder), the use of extended surfaces (fins) in the sorbent and variables related to the construction and operation of the system influence the cooling power and coefficient of performance (COP) of the proposed reactor configuration. The paper is divided as follows: in section 2 is presented the two-dimensional heat transfer model of the chemisorption reactor as well as the boundary conditions and the numerical method required to solve the discretised equations. Subsequently, the main results that expose the transient operating dynamics of the reactor and system performance parameters as a function of the sorbent type are indicated in section 3.

2. Mathematical model and considerations
The production of cooling effect in adsorption machines is mainly due to the heat exchanges that occur between the system reactor and the heating and/or cooling fluid. Therefore, in order to know the dynamics of heat transfer in the reactor, a mathematical model was developed that represents this phenomenon in the different elements that constitute it, that is, the sorbent bed, the reactor internal tube that contains the sorbent, the annular fins and the thermal fluid that flows through the annular region, as shown in Figure 1. It should be noted that the annular fins inserted in the sorbent allow standardizing the internal temperature of the system and improving the thermal contact between the surface of the sorbent medium and the thermal fluid that exchanges heat with the reactor.
The necessary heat transfer equations were obtained by means of energy balances in the four elements that form the heat exchanger. Regarding the sorbent bed, the mathematical model allows reproducing the exothermic and endothermic reactions during the synthesis and decomposition phases, as well as the heat transfer in axial and radial directions. In addition, the bed is modelled as a porous medium that can be either consolidated or powder. From these assumptions, the heat diffusion in the sorbent bed is given by the following equation:

$$\frac{t}{x} \Delta H_{n} N_{r} T_{\lambda} r_{T} T_{\lambda} r_{T} \lambda_{T} r_{T} \lambda_{T} r_{T} T_{C}(x) r_{s}^{2} a_{e}, \quad (1)$$

where the first three terms on the right side of equality represent the heat conduction in the sorbent and the last one the thermal energy generation (which occurs during the synthesis and decomposition phases). Parameter $C(x)$ describes the sorbent volumetric heat capacity, which is a function of the local reaction conversion.

2.1 Volumetric heat capacity
The volumetric heat capacity of Equation (1) is evaluated considering the contributions of expanded graphite, salt and refrigerant, according to the following equation:

$$C(x) = \sum_{i=1}^{3} \left( \frac{mc_{p}}{pc_{p}} \right)_{i} = \frac{(mc_{p})_{\text{salt}} + (mc_{p})_{\text{ref}} + (c_{p} (m_{\text{initial}} + x \Delta m))_{\text{NH}_{3}}}{\text{bed}}, \quad (2)$$

where $\Delta m_{\text{NH}_{3}}$ is the maximum mass of refrigerant that can be adsorbed or desorbed and $x$ is the local reaction conversion.

2.2 Sorbent bed thermo-source
Several of the elements that make up the expression of the thermo-source in Equation (1) are constants inherent to the process, these being: $\Delta H_{r}$ the reaction enthalpy, $N_{s}$ the apparent molar density and $n$
the adsorbed or desorbed moles of the refrigerant. The term $\frac{\partial x}{\partial t}$ represents the conversion rate and is described by the following chemical kinetic models [17], during synthesis and decomposition phases, respectively:

$$\frac{\partial x}{\partial t} = Ar (1 - x)^M \left( \frac{P_{eq}}{P_{eq}} - 1 \right), \quad (3)$$

$$\frac{\partial x}{\partial t} = Ar x^{M_{eq}} \left( \frac{P_{eq}}{P_{eq}} - 1 \right), \quad (4)$$

where $Ar$ is called the Arrhenius factor that relates the chemical reaction rate to the temperature at which the reaction occurs. This factor can be expressed as $k_0 e^{\left(\frac{E}{RT(x)}\right)}$, where $k_0$ represents the pre-exponential factor of Arrhenius and $E$ the activation energy of the reaction. In turn, $P_{eq}$ is the equilibrium pressure corresponding to the bed temperature and can be calculated according to [18] by:

$$\ln P_{eq} = \frac{\Delta H}{RT} + \frac{\Delta s}{R}, \quad (5)$$

2.3 Effective thermal conductivity of the sorbent bed

Porosity has a great influence on the physical properties of a material, including specific mass and thermal conductivity – Note that the latter is known for porous solids as effective thermal conductivity ($\lambda_e$). The conductivity value of sorbent compound is also influenced by the graphite fraction ($f_g$) and by the number of refrigerant moles per mole of salt during the reaction [19-21]. This relationship is not fully defined due to the difficulty of measuring conductivity in the presence of chemical reactions.

In this sense, Han et al. [19] evaluated the effective thermal conductivity of sorbent beds in blocks mixed with GE, formed by CaCl2, MnCl2, and BaCl2, using NH3 as working refrigerant. The results presented by these authors indicate that the effective thermal conductivity of the sorbents evaluated is a function of the sorbent's apparent specific mass, the graphite fraction in the mixture and the number of NH3 mols in the compound, thus, the effective thermal conductivity does not undergo a significant change when the type of salt is changed as long as its apparent specific mass, graphite fraction and the number of adsorbed refrigerant moles are maintained.

From this premise, in the present study was established an equation that relates the effective thermal conductivity to the number of refrigerant moles per salt mol of the sorbent, keeping constant the apparent specific mass and the graphite fraction, that is:

$$\lambda_{e, syn} = C_1 \frac{n_{NH_3}}{n_{sorbent}} + C_2, \quad (6)$$

$$\lambda_{e, dec} = C_1 \frac{n_{NH_3}}{n_{sorbent}} + C_2 \varphi, \quad (7)$$
Constants $C_1$ and $C_2$ can be adjusted minimizing the absolute error (AAD) using as reference the conductivity data published by Han et al. [19] as a function of the salt (sorbent) and the number of NH$_3$ moles adsorbed. Likewise, the constant $\varphi$ in Equation (7) weighs the material anisotropy that can be determined for adsorbents of consolidated type from the Equation (8) [22].

$$\varphi = 1 + \frac{3.247 \times 10^{-7} \rho_b^3}{1.863 \times 10^6 + \rho_b}, \quad (8)$$

A similar procedure can be performed to obtain an expression of the effective thermal conductivity for adsorbent powder beds as follows:

$$\lambda_v = C_{1,\rho} \frac{n_{NH_3}}{n_{sorbent}} + C_{2,\rho}, \quad (9)$$

2.4 Sorbent bed boundary conditions

The following boundary conditions were defined to solve the Equation (1) of the sorbent bed which considers axial and radial temperature gradients. Firstly, as initial conditions of temperature and local conversion it was considered that:

$$T(0,r,z) = T_{amb}, \quad (10)$$
$$x(0,r,z) = 0, \quad (11)$$

As the refrigerant vapour flows through the interior of the reactor, it was considered that the temperature of the refrigerant vapour is that of the sorbent surface. In addition, the heat transfer by convection between the sorbent and the refrigerant vapor was neglected, considering that the latter flows at low speed inside the gas channel. On the other hand, it was considered that the thermal contact between the sorbent and the reactor wall is not uniform and therefore there is a contact thermal resistance between these materials. From these assumptions, the boundary conditions in radial direction can be expressed as:

$$\frac{\partial T}{\partial r} \bigg|_{r=r_{gas,channel}} = 0, \quad (12)$$

$$-\lambda \frac{\partial T}{\partial r} \bigg|_{r=r_{gas}} = \frac{(T_{bed} - T_{w})}{R_{cont}}, \quad (13)$$

Considering the space between two consecutive fins along the adsorbent in the axial direction, the boundary conditions in this direction can be defined as:

$$-\lambda \frac{\partial T}{\partial z} \bigg|_{z=0} = \frac{(T_{bed} - T_{bed})}{R_{cont}}, \quad (14)$$
where $\delta$ represents the spacing between two consecutive fins. The contact thermal resistance ($R_{\text{cont}}$) in Equations (14) - (15) was considered the same value as that adopted between the sorbent bed and the reactor tube wall. The boundary conditions of Equations (12) - (15) are shown in Figure 2.

Figure 2. Section of the reactor for boundary conditions, (a) boundary conditions in radial direction of Equation (12) – (13), and (b) boundary conditions in axial direction of Equation (14) – (15).

2.5 Heat transfer models in the remaining reactor components

To complete the heat transfer analysis in the reactor it is necessary to consider the heat diffusion in the remaining components of the system. In the internal tube of the reactor the temperature distribution was modelled in a two-dimensional way, considering the temperature gradients in the direction of thermal fluid flow and the radial temperature gradients along the tube thickness. Thus, the heat diffusion equation in the tube is given by:

$$
\left(pc_{\text{p.w}}\right) \frac{\partial T}{\partial t} = \lambda_w \frac{\partial^2 T}{\partial r^2} + \frac{\lambda_w}{r} \frac{\partial T}{\partial r} + \lambda_w \frac{\partial^2 T}{\partial z^2},
$$

subjected to the following boundary conditions:

$$
\left. \frac{\partial T_w}{\partial z} \right|_{z=0} = 0,
$$

$$
\left. \frac{\partial T_w}{\partial z} \right|_{z=L} = 0,
$$

$$
- \lambda_w \frac{\partial T_w}{\partial r} \Bigg|_{r=r_s} = \left( T_w - T_{\text{bed}} \right) R_{r,\text{cont}},
$$
\[- \lambda_w \frac{\partial T_w}{\partial r} \bigg|_{r=r_{in}} = h_t (T_w - T_r), \tag{20}\]

where \( L \) is the length of the reactor tube, \( T_r \) represents the temperature of the thermal fluid and \( h_t \) is the heat transfer coefficient by convection in the fluid that depends on the Nusselt number and this at the same time depends on the type of fluid, the type of flow and the relationship between the internal and external diameters of the annular region.

In the aluminium fins, heat transfer by radial conduction and heat transfer by contact between the fins and the bed in the axial direction were considered. The transverse gradients were neglected due to the negligible thickness of the fin (~ 0.25 - 0.45 mm), so that the heat diffusion equation was:

\[
\left( \rho c_p \right)_{\text{fin}} \frac{\partial T}{\partial t} = \lambda_{\text{fin}} \frac{\partial^2 T}{\partial r^2} + \frac{\lambda_{\text{fin}}}{r} \frac{\partial T}{\partial r} - \frac{1}{R_{\text{cont-fin}}} \left( T_{\text{fin}} - T_{\text{bed}} \right), \tag{21}\]

subjected to the following boundary conditions:

\[
\left. \frac{\partial T}{\partial r} \right|_{r=r_{\text{fin,chanl}}} = 0, \tag{22}\]

\[
- \lambda_{\text{fin}} \left. \frac{\partial T}{\partial r} \right|_{r=r_{\text{fin}}} = \frac{\left( T_w - T_{\text{fin}} \right)}{R'_{\text{cont-fin}}}, \tag{23}\]

where \( R'_{\text{cont-fin}} \) is the contact resistance between the fin and reactor tube wall and \( \epsilon \) the fin thickness.

For the thermal fluid, it was considered that the outer wall of the heat exchanger shell is thermally insulated. Therefore, the energy losses between the thermal fluid and the environment were neglected. Furthermore, the temperature gradients in the radial direction were neglected, since the annular space in which the thermal fluid flows (Figure 2) is much smaller than the reactor tube length. Thus, the heat transfer equation is given by:

\[
\left( \rho c_p \right)_{f} \frac{\partial T_f}{\partial t} + \left( \rho c_p \right)_{f} V \frac{\partial T_f}{\partial z} - \left( \frac{2 \pi r_{\text{ext}}}{A_{\text{anul}}} \right) h_f \left( T_w - T_f \right), \tag{24}\]

Being \( V \) the flow velocity and \( A_{\text{anul}} \) the annular region area. The Equation (24) is subjected to \( T_{z=0} = T_{\text{in}} \).

### 2.6 Performance Indicators

The results of the numerical simulation make it possible to determine the most important performance parameters of sorption cooling systems, this is, the specific cooling power (SCP) and the COP. SCP is related to the machine cooling power per sorbent mass unit while the COP is a measure of the energy utilization that is supplied to the system. Each of these parameters can be calculated according to the following equations:
\[ \text{SCP} = \frac{Q_{\text{ref}}}{t_{\text{sys}} m_{\text{bed}}} = \frac{\sum_{i=1}^{m_{\text{NH}_3}} \left( h_{\text{f, NH}_3} - c_{P, \text{NH}_3} (T_{\text{cond}} - T_{\text{evap}}) \right)}{t_{\text{sys}} m_{\text{bed}}}, \quad (25) \]

\[ \text{COP} = \frac{Q_{\text{ref}}}{Q_{\text{lat,bed}} + \sum_{j=1}^{N_{\text{ele}}} Q_{\text{sen},j}}, \quad (26) \]

where \( Q_{\text{lat,bed}} \) and \( Q_{\text{sen}} \) represent the latent heat of the sorbent bed and the sensible heat of the different elements that compose the reactor, respectively.

### 2.7 Numerical method of solving differential equations

Considering that the reactor analysed in this study has a well described geometry in cylindrical coordinates, the technique of central finite differences was adopted to discretize the partial differential equations of heat transfer obtained in the four elements of the reactor. The implicit scheme was used to solve the system of discretized equations with the exception of the energy generation term.

The generation term in the sorbent is a temperature function and is non-linear. Usually these terms are treated through a linearization [23]. However, for this specific problem, linearization has become complex due to the exponential type terms present in the reaction rate \( \left( \frac{\partial x}{\partial t} \right) \), which composes the generation term.

Another way to approach this difficulty is to make an explicit discretization about this term, that is to say, it is evaluated according to the property at time \( t \) [24]. However, this approach has the disadvantage of depending on the time step used to solve the system of equations, since if it is not properly chosen, it can cause instabilities and convergence problems. Therefore, a previous study is necessary to define the most appropriate time step for each type of problem.

Adopting this discretization for the reaction rate that composes the generation term, we have:

\[ \frac{\partial x}{\partial t} = k_0 e^{\left( \frac{E}{R T_{\text{ref}}} \right)} \left( 1 - x \right)^n \left( \frac{\Delta H}{R T_{\text{ref}}} \Delta \left( \frac{R}{T} \right) \right)^{\text{syn}} e^{\left( \frac{\Delta H}{R T_{\text{ref}}} \Delta \left( \frac{R}{T} \right) \right)^{\text{syn}}} - 1 \], \quad (27)

A similar discretization was used in Equation (4) during decomposition phase.

### 3 Results

This section presents the results generated by the mathematical model of the chemisorption reactor system. SrCl\(_2\) is used as a sorbent salt to verify the results of the model developed here since the chemical kinetic parameters \( (k_0, E \text{ and } M) \) necessary for the advancement rate in the Equation (3)-(4) are available in the literature. Table 1 shows the values of the different variables required by the mathematical model.

At the same time, the adjustment parameters of Equation (6)-(7) that describe the effective thermal conductivity of the sorbent were adjusted with the experimental data published by [19] for the consolidated and powder sorbents. In this sense, the values of \( C_1 \) and \( C_2 \) for the consolidated sorbent in Equation (3) were 1.217 and 18.566, however, \( C_{1,p} \) and \( C_{2,p} \) for the powder sorbent were 0.044 and
0.355. The AAD obtained through these adjustment parameters were 1.23 and 4.4e-04 for the consolidated bed and powder, respectively.

Table 1. Parameter values and operating conditions used in the model.

| Parameter                                  | Symbol      | Value             |
|--------------------------------------------|-------------|-------------------|
| Radius of the gas channel                  | $r_{\text{gas-channel}}$ | 5 mm              |
| Thermal fluid volumetric flow rate         | $\dot{V}$ | 0.0011 m$^3$ s$^{-1}$ |
| Enthalpy of reaction                       | $\Delta H_e$ | 41431 J mol$^{-1}$ |
| Number of moles                            | $n$         | 7                 |
| Arhenious factor during the syntesis reaction | $k_{0,\text{syn}}$ | 0.0190 s$^{-1}$ |
| Activation energy during the synthesis reaction | $E_{\text{syn}}$ | 6921 J mol$^{-1}$ |
| Adjustment Factor in the Synthesis Reaction | $M_{\text{syn}}$ | 2.96              |
| Evaporating pressure                       | $P_{\text{evap}}$ | 400 kPa           |
| Latent heat                                | $\Delta H$ | 41431 J mol$^{-1}$ |
| Entropy of Phase Changes                   | $\Delta s$ | J mol$^{-1}$ K$^{-1}$ |
| Condensing pressure                        | $P_{\text{cond}}$ | 1200 kPa          |
| Arhenious factor during the decomposition reaction | $k_{0,\text{dec}}$ | 0.125 s$^{-1}$ |
| Activation energy during the decomposition reaction | $E_{\text{dec}}$ | 9000 J mol$^{-1}$ |
| Adjustment factor in the decomposition reaction | $M_{\text{dec}}$ | 3.02              |
| Reactor length                             | $L$         | \leq 750 mm       |

3.1 Spatial and temporal mesh analysis

To obtain a good numerical approximation of the discretized equations it is necessary to study the mesh in both the spatial and temporal components. For this purpose, a base or reference case was defined, which is characterized by having very well refined spacing in time and space, that is, $\Delta r = \Delta z = 0.25$ mm and $\Delta t = 0.5$ s, respectively. – Note that this analysis is made in the adsorbent layer, since it is there where the most significant gradients of temperature and advancement rate occur.

Starting from the values of $\Delta t$, $\Delta r$ and $\Delta z$ of the base case, simulations were carried out changing proportionally the values of $\Delta r$ and $\Delta z$ while the value of $\Delta t$ was kept constant. The reverse procedure was also performed. According to the results presented in Figure 3a and 3b for the consolidated and powder sorbent, respectively, it is noticed that the temperature profiles are remarkably influenced by time steps greater than 2 seconds. This is consistent because the source term in Equation (1) is being explicitly evaluated. Therefore, high values of $\Delta t$ provide instability in these profiles, which become more significant during the beginning of each reaction. After this analysis, it was concluded that values of $\Delta t < 2$ s and spacing of $\Delta r$ and $\Delta z$ lower than 3 mm are adequate to solve the Equation (1) considering the term of generation being discretized explicitly for both the consolidated and powder bed.
Figure 3. Analysis of temporal and spatial mesh for (a) consolidated and (b) powder sorbents, during the first seconds of the beginning of the synthesis phase.

3.2 Experimental model validation

The experimental results of Huang et al. [15] were used as reference in order to validate the mathematical model of the chemisorption reactor proposed in the present study. It is important to highlight that the large number of systems with circular geometry proposed in the literature consider temperature gradients in radial direction. However, temperature gradients in axial direction become significant as the length of the system increases. According to the results presented in Figure 4, it could be concluded that the present model can reproduce with good precision the experimental results of the global reaction conversion of Huang et al. [15] work. The AAD between the experimental and model values was 6.096 and 5.388 for the synthesis and decomposition phases, respectively. This validation also intends to corroborate the consideration adopted at the time of discretization of the local reaction conversion of Equations (3)-(4) – Note that, consolidated sorbent and a time and spacing step of 1 s and 3 mm were used for the validation.

Figure 4. Comparison between the experimental values of the global reaction conversion and those obtained through the present mathematical model during the synthesis and decomposition phases.
3.3 Temperature profiles and adsorption rate

Figure 5 shows the average temperature and global conversion profiles during the synthesis and decomposition stages of the system operating with a consolidated sorbent bed of apparent density ($\rho_b$) equal to 230 kg m$^{-3}$. The heat transfer fluid that flows through the reactor annular region is a thermal oil that during the previous stages had a temperature of 30 °C and 140 °C, respectively. As shown in Figure 5a, it is observed that the temperature difference between the thermal fluid and this adsorbent bed is of 5°C, approximately. At the same time, with powder sorbent bed, this value was of 10°C. The manufacturing process of the powder sorbent is much simpler when compared to consolidated sorbents, however, the heat transfer resistance of the latter is lower and, consequently, the differences in temperatures are less noticeable.

Additionally, Figure 5b shows the global reaction conversion for the two phases of the cycle. In the case of SrCl$_2$, $x=1$ implies that 1 mol of SrCl$_2$ reacted with 7 moles of NH$_3$ according to Equation (27). During the first seconds of the synthesis phase ($t<20$ min) there is a marked increase of the reaction conversion that accompanies the increase of the adsorbent temperature. However, as the time of the synthesis phase increases, the temperature gradient decreases and the reaction becomes slower in that period. On the other hand, the decrease of $x$ after 20 min is a consequence of the beginning of the decomposition phase of NH$_3$ by the sorbent.

\[
\text{SrCl}_2\text{NH}_3 + 7\text{NH}_3 \leftrightarrow \text{SrCl}_2\text{8NH}_3 + 7\text{H}_2, \tag{28}
\]

As a function of the global conversion for this sorbent/adsorbate pair (SrCl$_2$/NH$_3$), the mathematical model indicates that after 6 cycles the system enters in a periodically developed regime and the simulation of additional cycles becomes unnecessary.

3.4 Specific cooling power and COP

From the mathematical model it is possible to identify how operational parameters affect the performance parameters of the modelled chemisorption reactor, for such purpose, Figure 6 describes the impact of the cycle time and the reactor tube radius on the specific cooling power (SCP) and the coefficient of performance (COP) for the two types of sorbents considered. In this sense, the impact of these parameters on the SCP of the system operating with consolidated and powder sorbent is presented in Figures 6a and 6b, respectively. The negative influence of this parameter on the power is
due to the fact that as time increases, the conversion capacity is reduced, since the conversion rate is not linear (see Equation (3)-(4)).

In addition, the power reduction as a function of the increase of sorbent bed thickness (increase of the tube radius) is related to the increase of the internal resistance to the heat transfer that it relates, the sorbent bed thickness with its effective thermal conductivity. This resistance becomes even more relevant due to the low thermal conductivity values of the sorbent powder. The negative effect of the radius increase on the consolidated sorbent system indicates that, even with the high thermal conductivity of this sorbent, the radius increase causes a sufficient temperature gradient to decrease the overall reaction rate and, therefore, cause a reduction in cooling power.

![Figure 6. Variation of SCP and COP for the chemisorption system operating with consolidated (Figures 6a and 6b) and powder (Figures 6c and 6d) sorbents as a function of the cycle time and the radius of reactor tube.](image)

Regarding the impact of the cycle time and the reactor radius on the COP, it can be observed in Figures 6b and 6d that the increase from 15 to 75 minutes in the cycle time produced a notoriously positive increase in the COP, reaching up to five times this parameter for the two types of systems, this comes from the fact that the cooling capacity of the refrigerant presents a proportionally higher growth than the energy consumption as the time of reaction of synthesis increases. Likewise, the positive effect of the increase of the reactor radius on the COP can be analyzed considering the heat portions involved in the computation of this parameter in Equation (26), thus, as the reactor radius increases,
the relationship between sorbent and metal mass also increases and, therefore, the increase of the sorbent mass reduces the impact of the sensible heat load of the metal on the COP.

4 Conclusions

In the present work was proposed a mathematical model that allows simulating the operation of a reactor to solid chemisorption refrigeration system that can operate with consolidated and powder sorbent beds. SrCl₂ impregnated with expanded graphite, was the salt sorbent considered to validate the mathematical model and to explore the behaviour of the main performance parameters of the system since the reaction kinetic constants between this salt and NH₃ are available in the literature.

Among the main results, it is noteworthy that regardless of the type of adsorbent considered, the cycle time and the reactor radius influence the SCP and the COP in the opposite way, and therefore, these performance parameters cannot be simultaneously optimized in relation to these variables. On the other hand, in a scenario where the heat source is different from the waste heat, the working conditions could be those that maximize the COP, so the system operating with consolidated sorbent is the best choice.

Although the internal temperature gradients in the powder adsorbent are higher when compared to the consolidated sorbent, the model allowed to verify that reactors that operate with sorbent/adsorbate pairs of the type analysed in this work, can be projected with a length of up to 750 mm without this considerably influencing the performance of the system.

Finally, assess the impact of a larger number of geometric and operational variables on the SCP and the COP through Multi-Objective Optimization so that optimal design values of these parameters can be identified could be included in future work. On the other hand, a thermo-economic analysis of reactors with similar configuration to that studied, and that use other metallic salts can be approached from this model, for instance, NaBr is a metallic salt that requires a low activation temperature (~65 °C) and, consequently, can be projected for systems powered by solar energy, among others.

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