Semi-Analytical Solution for a Lumped Model of a Co-Current Moving Bed Reactor

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Abstract

Several industrial processes are carried out on moving bed reactors (MBRs), and the development of mathematical models plays a fundamental role in designing, optimizing, and controlling these processes. Thus, this work initially develops a local solution for a linearized vertical MBR model to lumped parameters in the solid and fluid phases. Then, a semi-analytical solution (SAS) of the original nonlinear problem is obtained from the local solution. The SAS is easy to implement, stable, accurate, and performs fast, making it an efficient tool for MBR simulations. Excellent agreement was found comparing the SAS results with those of traditional numerical methods. SAS is capable of fast

integration of model equations for systems with stiffness ratio SR = 10^{33}. A numerical analysis was also carried out, indicating optimal refining parameters in relation to linearization error and machine error. The developments carried out can be easily extended to systems with multiple first-order reactions.

Keywords: Analytical solution, Heat transfer, Chemical reactor, Numerical solution, Numerical analysis, Stiffness

1. Introduction

There are several technological applications for the heat and/or mass transfer between a particulate solid phase and one or more fluid phases. We can highlight, for example, the pyrolysis of shale oil fines in moving beds (Lisbôa, 1987; Bertoli 1989, 2000), the waste tire pyrolysis in moving and fluidized beds (Aylón et al., 2010; Martinez et al., 2013), the flash kaolinite calcination in moving and fluidized bed (Teklay et al., 2014, 2015, 2016) as well as others industrial processes described in Shirzad et al. (2019).

However, these applications require high equipment efficiency levels, making it essential to model the phenomena involved for scaling up and process optimization. Therefore, several studies in MBR modeling with analytical and/or numerical solutions have been carried out, such as: Munro and Amundson (1950), Leung and Quon (1965), Lisbôa (1987), Bertoli (1989, 2000), Bertoli and Hackenberg (1990), Fan and Zhu (1998), Saastamoinen (2004), Meier et al. (2009), Almendros-Ibáñez et al. (2011), Bertoli et al. (2012, 2015a, 2015b, 2017, 2019, 2020, 2022, 2023, 2024), Yang et al. (2015), Isaza et al. (2016), Medeiros et al. (2018, 2021), Tribess et al. (2022).

Among these studies, the work of Bertoli et al. (2015a) is directly related to this investigation. The authors developed a semi-analytical solution of a lumped parameter model (Walas, 1965; Leung and Quon, 1965) to the butane pyrolysis process, with the assumed conditions: first-order chemical reaction in gas phase, reactor with adiabatic walls, particles considered as spheres and inert. The model solution was developed using the concepts of the finite-analytic method (FAM) (Chen and Li, 1980) – with the difference that first, through the use of integrating factors, an integral representation of the model equations is developed; then, by linearization and discretization of the resulting coupled system of integral equations, the interval solution is obtained – and presented a very good agreement with the numerical solution by the Runge-Kutta-Felhberg method.

Furthermore, the work of Medeiros et al. (2018, 2021) is also directly related to the study presented herein. The authors developed a semi-analytical solution for an isothermal wall MBR model to distributed parameters in the particles and to lumped parameters in the fluid phase, assuming - among other simplifications - irreversible chemical reaction occurring uniformly within spherical particles, and constant radiative heat transfer coefficient h_r - this hypothesis was mitigated by means of a corrective step, in which h_r is taken equal to the arithmetic mean between its value at the reactor inlet and its value at the discretization point -.

The solution was developed from the analytical solution of the associated homogeneous (linear) problem (Meier et al., 2009) and the spectral expansion of the non-homogeneous vector. The simulations accurately predicted kaolinite flash calcination's temperature and conversion profiles Teklay et al., 2016).

The main differences between the MBR model studied by Medeiros et al. (2018, 2021) and this work, is that, in the latter, the particle is modeled to lumped parameters - which

makes the model simpler -, and h_r is calculated only with local values, i.e., from the discretization interval - in better correspondence to physical reality -.

SAS will be developed using FAM concepts (Chen and Li, 1980): decomposition of the problem region into small intervals; maintaining terms as linear and evaluated under the conditions at the beginning of each interval; obtaining local analytical solutions in these intervals. Although there are studies/applications aiming to generalize the FAM (e.g., Civan, 1995, 2009; de Almeida Jr., 2016; de Almeida Jr. et al., 2016; Lemos et al., 2016), one of the difficulties in applying of the original finite analytical solution method is due to the fact that for each case there is a solution. Several applications of the method - see, Chen and Li, 1980 - demonstrate this difficulty. Among the applications of FAM for chemically reactive systems is the work of Ardestani et al. (2015), who used the practical FAM proposed by Civan (1995, 2009) to solve a model to describe the transport of contaminants dissolved in groundwater.

2. Mathematical modeling

The heat transfer model of a moving bed reactor was developed based on the mass and energy conservation laws using the single particle approach. Fig. 1 shows schematically a cocurrent moving bed reactor and the control volume for which the analysis is performed. The MBR is modelled to lumped parameters to solid particles and lumped parameters to fluid phase; it is considered tubular, vertical and diluted, with each particle surrounded only by the dragging fluid; inside the particles a first-order irreversible chemical reaction takes place uniformly. Other assumptions are (Bertoli, 1989, 2000, 2020; Meier et al., 2009; Medeiros et al., 2021): steady state operation; physical and transport properties uniform and constant; spherical particles with uniform and constant

radius and uniformly distributed over the cross-section of the reactor; developed flow; fluid temperature and velocity profiles considered uniform in the cross-section of the reactor (particles and fluid may have different velocities); conveyor fluid transparent to thermal radiation; reactor wall considered as an isothermal blackbody; axial heat dispersion considered negligible in comparison with the advective energy flux; wall-particle radiative heat flux described by a linearized form of the Stefan-Boltzmann equation; interaction effects between particles and particle-wall, neglected; thermal effects due to viscous dissipation or particle friction, neglected.

Insert Figure 1

Figure 1. Schematic representation of the cocurrent moving-bed reactor and the differential control volume considered for the analysis.

2.1 Governing equations

Considering the previous hypotheses and introducing the dimensionless particle residence time

$$\tau \equiv \frac{3h_p}{\rho_p c_p R_p} t = \mathrm{Bi_p Fo'} \qquad (1a, b)$$

the dimensionless temperatures,

$$\theta_f(\tau) \equiv \frac{T_f(t_1\tau) - T_{fi}}{T_{pi}} \qquad (2)$$

$$\theta_p(\tau) \equiv \frac{T_p(t_1\tau) - T_{pi}}{T_{pi}} \qquad (3)$$

the reactant conversion, and the dimensionless heat source term due to a first order irreversible chemical reaction,

$$X(\tau) \equiv \frac{C_{Ai} - C_A(t_1\tau)}{C_{Ai}} \qquad (4)$$

$$g(\tau) \equiv \mathrm{Da}_{\mathrm{dev}}\big(1 - X(\tau)\big) \tag{5}$$

and finally, the dimensionless groups:

$$\mathrm{P}_{\mathrm{y}}' \equiv \frac{3h_p}{\rho_p c_p R_p K} \tag{6}$$

$$\beta \equiv \frac{\dot{m}_p c_p}{\dot{m}_f c_f} \tag{7}$$

$$\varphi \equiv 1 + \frac{h_r}{h_p} \tag{8}$$

$$\omega \equiv 1 + r_{ws}\frac{h_f}{h_p} \tag{9}$$

Then, considering the differential control volume in Fig. 1, the LPM is

$$\frac{dX(\tau)}{d\tau} = \frac{1-X(\tau)}{\mathrm{Py}'} \tag{10}$$

$$\frac{1}{\beta}\frac{d\theta_f(\tau)}{d\tau} = \theta_p(\tau) - \theta_p(\infty) + \omega\left(\theta_f(\infty) - \theta_f(\tau)\right) \tag{11}$$

$$\frac{d\theta_p(\tau)}{d\tau} = \theta_f(\tau) - \theta_f(\infty) + \varphi\left(\theta_p(\infty) - \theta_p(\tau)\right) + g(\tau) \tag{12}$$

subject to the initial conditions (at the reactor's inlet) presented in Eqs. (13) – (15),

$$X(0) = 0 \tag{13}$$

$$\theta_f(0) = 0 \tag{14}$$

$$\theta_p(0) = 0 \tag{15}$$

In the previous equations,

$$\theta_f(\infty) \equiv \frac{T_w - T_{fi}}{T_{pi}} \tag{16}$$

$$\theta_p(\infty) \equiv \frac{T_w - T_{pi}}{T_{pi}} \tag{17}$$

3. Model solution

3.1 Solution procedure

The development of SAS for the Eqs. (14) - (19), proceeds according to the following steps:

i. The reactor is sectioned into a k_{max} number of intervals.

ii. In the interval k, i.e., $[\tau_{k-1}, \tau_k]$, K and φ are evaluated at temperature $T_p(\tau_{k-1})$, and kept constant (K_{k-1} and φ_{k-1}, respectively), making the model equations linear.

iii. The associated linear problem is solved analytically and locally (i.e., in the interval k).

iv. The local solution is iteratively regressed to the reactor inlet $(k = 0)$, thus obtaining the SAS.

v. A representation of the SAS in continuous variables, is obtained through limit operations and the definition of integral.

In the next sections, this methodology will be developed. It should be noted, however, that for the computational implementation of SAS, only the results of step *iii* are required.

Note that this procedure differs from that of Vanti et al. (2008) and Bertoli et al. (2015a), because in these works, given the simplicity of the models studied, the SAS in continuous variables was obtained directly from the model equations - i.e., without the previous steps *i-iv* - through integrating factors.

3.2 Model linearization

Initially the reactor is sectioned into k_{max} intervals. In the k interval, i. e., $[\tau_{k-1}, \tau_k]$, K and φ are evaluated at the temperature $T_p(\tau_{k-1})$ and made constant. Then, we can write from Eqs. (10)-(12), the following linear system of ordinary differential equations (ODEs):

$$\frac{dX(\tau)}{d\tau} = \frac{1-X(\tau)}{\mathrm{Py}'_{k-1}} \tag{18}$$

$$\frac{1}{\beta}\frac{d\theta_f(\tau)}{d\tau} = \theta_p(\tau) - \theta_p(\infty) + \omega\big(\theta_f(\infty) - \theta_f(\tau)\big) \tag{19}$$

$$\frac{d\theta_p(\tau)}{d\tau} = \theta_f(\tau) - \theta_f(\infty) + \varphi_{k-1}\left(\theta_p(\infty) - \theta_p(\tau)\right) + g_{k-1}(\tau) \tag{20}$$

Where

$$g_{k-1}(\tau) \equiv \mathrm{Da}_{\mathrm{dev,k-1}}\big(1 - X(\tau)\big) \tag{21}$$

Subject to the following conditions at the beginning of the interval:

$$X(\tau_{k-1}) = X_{k-1} \tag{22}$$

$$\theta_f(\tau_{k-1}) = \theta_{f,k-1} \tag{23}$$

$$\theta_p(\tau_{k-1}) = \theta_{p,k-1} \tag{24}$$

3.3 Local (interval) solution of the linearized model

Integrating Eq. (28), and using the boundary condition of Eq. (22), we have

$$X_k(\tau) = 1 - (1 - X_{k-1})e^{-\left(\frac{\tau-\tau_{k-1}}{\mathrm{Py}'_{k-1}}\right)} \tag{25}$$

Thus, substituting Eq. (25) into Eq. (21), the thermal generation rate becomes

$$g_{k-1}(\tau) = \mathrm{Da}_{\mathrm{dev},k-1}(1 - X_{k-1})e^{-\left(\frac{\tau-\tau_{k-1}}{\mathrm{Py}'_{k-1}}\right)} \tag{26}$$

As seen, the approach used causes decoupling of reaction kinetics from energy balances, but not vice versa. Therefore, isolating $\theta_p(\tau)$ in Eq. (19), we have

$$\theta_p(\tau) = \theta_p(\infty) + \frac{1}{\beta}\frac{d\theta_f(\tau)}{d\tau} + \omega\left(\theta_f(\tau) - \theta_f(\infty)\right) \tag{27}$$

Substituting Eq. (27) into Eq. (20), one obtains:

$$\frac{d\theta_p(\tau)}{d\tau} = (\omega\varphi_{k-1} - 1)\big(\theta_f(\infty) - \theta_f(\tau)\big) + g_{k-1}(\tau) - \frac{\varphi_{k-1}}{\beta}\frac{d\theta_f(\tau)}{d\tau} \tag{28}$$

Deriving Eq. (19) with respect to τ and substituting Eq. (28) into the result, then $\theta_p(\tau)$ is decoupled from $\theta_f(\tau)$, according to the following equation

$$\frac{1}{\beta}\frac{d^2\theta_f(\tau)}{d\tau^2}+\left(\omega+\frac{\varphi_{k-1}}{\beta}\right)\frac{d\theta_f(\tau)}{d\tau}+(\omega\varphi_{k-1}-1)\left(\theta_f(\tau)-\theta_f(\infty)\right)=g_{k-1}(\tau) \tag{29}$$

Now, defining

$$\Theta_f(\tau)\equiv\theta_f(\tau)-\theta_f(\infty) \tag{30}$$

then Eq. (29) is rewritten in the form,

$$\frac{1}{\beta}\frac{d^2\Theta_f(\tau)}{d\tau^2}+\left(\omega+\frac{\varphi_{k-1}}{\beta}\right)\frac{d\Theta_f(\tau)}{d\tau}+(\omega\varphi_{k-1}-1)\Theta_f=g_{k-1}(\tau) \tag{31}$$

The solution of Eq. (31) (inhomogeneous) can be obtained by the Complementary Function Method, in the form (see for instance Butkov, 1973)

$$\Theta_f(\tau)=\Theta_{f(hom)}(\tau)+\Theta_{f(part)}(\tau) \tag{32}$$

Where $\Theta_{f(hom)}$ is the general solution of the associated homogeneous (complementary function) and $\Theta_{f(part)}$ is a particular solution.

The solution of the associated homogenous $\Theta_{f(hom)}$ - a 2nd order ODE with constant coefficients -, is standard (Wylie and Barrett, 1990):

$$\Theta_{f(hom)}(\tau)=b_{1,k-1}e^{-r_{1,k-1}\tau}+b_{2,k-1}e^{-r_{2,k-1}\tau} \tag{33}$$

with characteristic equation with the following roots

$$r_{(1,2),k-1}=\frac{-(\beta\omega+\varphi_{k-1})\pm\sqrt{(\beta\omega-\varphi_{k-1})^2+4\beta}}{2}= \frac{-(\beta\omega+\varphi_{k-1})\pm\sqrt{(\beta\omega+\varphi_{k-1})^2+4\beta(1-\varphi_{k-1})}}{2} \tag{34a-d}$$

The solution $\Theta_{f(part)}$ is obtained by the method of undetermined coefficients (Jenson and Jeffreys, 1963):

$$\Theta_{f(part)}(\tau)=b_{3,k-1}\,e^{r_{3,k-1}\tau} \tag{35}$$

Where

$$r_{3,k-1}=-\frac{1}{\mathrm{Py}'_{k-1}} \tag{36}$$

$$b_{3,k-1}e^{r_{3,k-1}\tau_{k-1}}\equiv b'_{3,k-1}=\frac{\beta\,\mathrm{Da}_{\mathrm{dev},k-1}(1-X_{k-1})}{r_{3,k-1}^2+(\beta\omega+\varphi_{k-1})r_{3,k-1}+\beta\omega\varphi_{k-1}-\beta} \tag{37a, b}$$

Thus, substituting the results of Eqs. (33) and (35) into Eq. (32), the general solution of Eq. (35) is

$$\Theta_f(\tau) = \sum_{l=1}^{3} b_{l,k-1} e^{r_{l,k-1}\tau} \tag{38}$$

That is,

$$\theta_f(\tau) = \theta_f(\infty) + \sum_{l=1}^{3} b_{l,k-1} e^{r_{l,k-1}\tau} \tag{39}$$

Substituting Eq. (39) into Eq. (27), we obtain the local solution for the particle temperature

$$\theta_p(\tau) = \theta_p(\infty) + \sum_{l=1}^{3} \left(\frac{r_{l,k-1}}{\beta} + \omega\right) b_{l,k-1} e^{r_{l,k-1}\tau} \tag{40}$$

The coefficients $b_{1,k-1}$ and $b_{2,k-1}$ are determined from Eqs. (39) and (40), and the conditions Eqs. (23) and (24), as follows:

$$b_{1,k-1} e^{r_{1,k-1}\tau_{k-1}} \equiv b'_{1,k-1} = \frac{b'_{3,k-1}(r_{3,k-1} - r_{2,k-1}) + (\beta\omega + r_{2,k-1})\left(\theta_{f,k-1} - \theta_f(\infty)\right) - \beta\left(\theta_{p,k-1} - \theta_p(\infty)\right)}{r_{2,k-1} - r_{1,k}} \tag{41a, b}$$

$$b_{2,k-1} e^{r_{2,k-1}\tau_{k-1}} \equiv b'_{2,k-1} = \frac{b'_{3,k-1}(r_{3,k-1} - r_{1,k-1}) + (\beta\omega + r_{1,k-1})\left(\theta_{f,k-1} - \theta_f(\infty)\right) - \beta\left(\theta_{p,k-1} - \theta_p(\infty)\right)}{r_{1,k-1} - r_{2,k-1}} \tag{42a, b}$$

3.4 Difference equations

Difference equations to integrate the system of Eqs. (10)-(15) are obtained from Eqs. (25), (36), (39) and (40), as follows:

$$X_k = 1 - (1 - X_{k-1}) e^{r_{3,k-1}(\tau_k - \tau_{k-1})} \tag{43}$$

$$\theta_{f,k} = \theta_{fk-1} + \sum_{l=1}^{3} b_{l,k-1}(e^{r_{l,k-1}\tau_k} - e^{r_{l,k-1}\tau_{k-1}}) \tag{44}$$

$$\theta_{p,k} = \theta_{p,k-1} + \sum_{l=1}^{3} \left(\frac{r_{l,k-1}}{\beta} + \omega\right) b_{l,k-1}(e^{r_{l,k-1}\tau} - e^{r_{l,k-1}\tau_{k-1}}) \tag{45}$$

In the above equations, $(\tau_{k-1} \le \tau \le \tau_k)$ and $(1 \le k \le k_{max})$.

Eqs. (43)-(45), together with Eqs. (34), (36), (37), (41) and (42), are used to calculate, recursively, the conversion and temperatures along the MBR. Alternatively, and for numerical stability purposes, one can rewrite the above equations as follows:

$$X_k = 1 - (1 - X_{k-1})e^{r_{3,k-1}\Delta\tau} \tag{46}$$

$$\theta_{f,k} = \theta_{f,k-1} + \sum_{l=1}^{3} b'_{l,k-1}\,(e^{r_{l,k-1}\Delta\tau} - 1) \tag{47}$$

$$\theta_{p,k} = \theta_{p,k-1} + \sum_{l=1}^{3} \left(\frac{r_{l,k-1}}{\beta} + \omega\right) b'_{l,k-1}\,(e^{r_{l,k-1}\Delta\tau} - 1) \tag{48}$$

Where $b'_{1,k-1}$, $b'_{2,k-1}$ and $b'_{3,k-1}$, are respectively given by Eqs. (41), (42) and (37), and

$$\Delta\tau = \tau_k - \tau_{k-1} \tag{49}$$

3.5 SAS (recursive solution)

From Eqs. (46)-(48) and using the inlet conditions Eqs. (13)-(15), the SAS is obtained by recursion:

$$X_k = 1 - e^{\Delta\tau \sum_{j=1}^{k} r_{3,j-1}} \tag{50}$$

$$\theta_{f,k} = \sum_{j=1}^{k} \sum_{l=1}^{3} b_{l,j-1}(e^{r_{l,j-1}\tau_j} - e^{r_{l,j-1}\tau_{j-1}}) \tag{51}$$

$$\theta_{p,k} = \sum_{j=1}^{k} \sum_{l=1}^{3} \left(\frac{r_{l,k-1}}{\beta} + \omega\right) b_{l,j-1}(e^{r_{l,j-1}\tau_j} - e^{r_{l,j-1}\tau_{j-1}}) \tag{52}$$

3.6 Modification to the τ-marching procedure

The implementation of SAS is performed through a τ-marching procedure using the difference equations of Section 3.4. However, once the analytical solution of the linear problem is known, one can take advantage of this in favor of accuracy, through the following modification: for the k interval, instead of K and h_r being evaluated at the temperature $T_{p,k-1}$, as described in Section 3.2, this calculation is now carried out at the average temperature of the k interval, obtained from Eq. (40), in the following form

$$\theta_{pm,k} = \theta_{p,k-1} + \frac{1}{\Delta\tau}\sum_{l=1}^{3}\left(\frac{r_{l,k-1}}{\beta} + \omega\right) b'_{l,k-1}\left(\frac{e^{r_{l,k-1}\Delta\tau}-1}{r_{l,k-1}} - \Delta\tau\right) \tag{53}$$

The results obtained with and without this modification are presented in Section 7.

3.7 SAS in continuous variables

A representation of SAS in continuous variables can be obtained from Eqs. (50)-(52) by making $\Delta\tau \to 0$ (i.e., $k_{max} \to \infty$), summing the series, and using the definition of definite integral. Proceeding in this way, one obtains:

$$X(\tau) = 1 - e^{\int_0^\tau r_3 d\tau} \tag{54}$$

$$\theta_f(\tau) = \sum_{l=1}^{3}\int_0^\tau b_l r_l e^{r_l\tau} d\tau \tag{55}$$

$$\theta_p(\tau) = \sum_{l=1}^{3}\int_0^\tau \left(\frac{r_l}{\beta} + \omega\right) b_l r_l e^{r_l\tau} d\tau \tag{56}$$

Where

$$r_{(1,2)} = \frac{-(\beta\omega+\varphi)\pm\sqrt{(\beta\omega-\varphi)^2+4\beta}}{2} \tag{57a, b}$$

$$r_3 = -\frac{1}{\mathrm{Py}'} \tag{58}$$

$$b_1 = \frac{b_3(r_3-r_2)e^{r_3\tau}+(\beta\omega+r_2)\left(\theta_f(\tau)-\theta_f(\infty)\right)-\beta\left(\theta_p(\tau)-\theta_p(\infty)\right)}{r_2-r_1} e^{-r_1\tau} \tag{59}$$

$$b_2 = \frac{b_3(r_3-r_1)e^{r_3\tau}+(\beta\omega+r_1)\left(\theta_f(\tau)-\theta_f(\infty)\right)-\beta\left(\theta_p(\tau)-\theta_p(\infty)\right)}{r_1-r_2} e^{-r_2\tau} \tag{60}$$

$$b_3 = \frac{\beta\mathrm{Da}_{\mathrm{dev}}\left(1-X(\tau)\right)}{r_3^2+(\beta\omega+\varphi)r_3+\beta\varphi\omega-\beta} e^{-r_3\tau} \tag{61}$$

In Eqs. (54-61), the parameters r_l, b_l $(l = 1, 2, 3)$, $\mathrm{Da}_{\mathrm{dev}}$, Py' and φ, are now continuous functions of $T_p(\tau)$. Thus, the SAS in continuous variables is expressed by a system of coupled implicit integral equations. In Appendix A, it is shown that SAS in continuos varables satisfies the model equations and, therefore, is an exact representation of the model.

4. Residence time scales

To deepen the physical understanding of the results, the following particle residence time scales (see also, Bertoli et al., 2012, 2016, 2017, 2019, 2022; Tribess et al., 2022) are introduced in Table 1.

Table 1 - t' scales of phenomena for co-current vertical MBR

Insert Table 1

Once these scales are defined, is interesting to note that:

$$\mathrm{Bi_p} = \frac{t_1}{t_2}, \quad \mathrm{Bi_r} = \frac{t_1}{t_3}, \quad \mathrm{Da_{IV}} = \frac{t_1}{t_6}, \quad \mathrm{Da_{dev}} = \frac{t_2}{t_6}, \quad \mathrm{Fo'} = \frac{t'}{t_1}, \quad \mathrm{Py} = \frac{t_7}{t_1} \qquad (62a\text{-}f)$$

$$\mathrm{Py'} = \frac{t_7}{t_2}, \quad \mathrm{Th^2} = \frac{t_1}{t_7}, \quad \beta = \frac{t_2}{t_4}, \qquad \varphi \equiv 1 + \frac{t_2}{t_3}, \quad \tau = \frac{t'}{t_2}, \qquad \omega = 1 + \frac{t_4}{t_5} \qquad (63g\text{-}h)$$

In addition to enabling a clear physical understanding of the system parameters, scale analysis is also useful in the preliminary model selection. This analysis is postponed to Section 7.4.

5. Case studies

The same case studies seen by Medeiros et al. (2021) were chosen for analysis, for comparison purposes:

a) Heat transfer in a moving bed of oil shale fines (Lisbôa, 1987)

Oil shale fines are a residue from moving bed pyrolysis of oil shale. One solution for using these residues is pyrolysis in co-current MBR (Lisbôa, 1987). Thus, the heating of

a mixture of oil shale fines and air, in a co-current moving bed, is chosen as case study *a*, and represented by thermal test (TT) nº 4 of Lisbôa (1987) - also described in Bertoli (2000) and Bertoli et al. (2019) -.

b) Flash calcination of kaolinite in a moving bed (Teklay et al., 2016)

The flash calcination of kaolin-rich clays is an important aspect in the metakaolin production. The process is carried out in moving bed reactors (Teklay et al., 2015) or fluidized bed reactors (Salvador, 1995), at temperatures between 450 and 750 ºC, producing only water vapor (Salvador, 1995; Sperinck et al., 2011; Teklay et al., 2016) and metakaolin, according to the reaction (Bridson et al., 1985; Slade et al., 1992)

$$Al_2Si_2O_5(OH)_4 \xrightarrow{\Delta} Al_2O_3 \,.\, 2\ SiO_2 + 2\ H_2O \tag{64}$$

In this work, kaolinite calcination kinetics is selected as case study *b*, and will be represented in a simplified way by the kaolinite dehydroxylation step. The conditions, properties and correlations are those used by Teklay et al. (2014) - also described in Medeiros et al (2021) -. The specific heat of the granular solids (c_p) was calculated iteratively at an average temperature between the inlet and outlet, based on the method described by Waples and Waples (2004). Air is chosen as the dragging fluid.

6. Methodology

6.1 SAS verification and relative performance

The SAS is initially verified by comparison with the linear model solution. Nonlinearities are removed from the model, making constants K and h_r, evaluated at an average temperature along the reactor. Two discretization levels, $k_{max} = 1$ and $k_{max} = N$, are considered. The discretization of the SAS with $k_{max} = 1$ is particularly important

since it represents the exact linear problem solution. Moreover, the linearized solution allows a comprehensive investigation of the error sources in the SAS, as described in Section 6.2.1. Then, we proceed by considering T_p varying in the calculation of K and h_r and comparing the SAS results with other numerical methods: explicit Euler, Heun, Ralston, and Runge-Kutta of 3rd, 4th and 5th order. All calculations are performed on a computer with Intel® Core™ i5-9400F (10400F?) CPU @ 2.90 GHz, 64 GB RAM, and MS Windows 10 x 64 operating system.

6.2 Model validation

The model validation (at least partial) is made by comparing the thermogravimetric analysis (TGA) data (Teklay et al., 2014) - see case study *b* - with model predictions. Validation is said to be partial because the TGA only partially represents the conditions of a MBR. For the SAS to mimic the operating conditions of the TGA, the following settings are made (see Medeiros et al., 2021): $\tau =$ TGA clock time; $v_p = v_f$; h_f and h_r low enough to nullify thermal exchanges with the wall; c_f sufficiently high so that T_f does not change; T_g a linear function of the heating rate and particle residence time; and T_w is changed to the equilibrium temperature $T_{eq,k}$, calculated for each k section.

6.3 Stability

Given the semi-analytical character, the roots (eigenvalues) and form of the SAS are known. Thus, SAS stability analysis can be carried out in a simple way, by analyzing the signal of the roots and inspecting its implementation.

6.4 Consistency and convergence

To test consistency, a methodology similar to that for verifying an analytical solution is introduced: SAS in continuous variables is substituted into the model equations; then, if the system is satisfied, consistency is demonstrated. This methodology is more general than that of Vanti et al. (2008) and Bertoli et al. (2015a), since in these works, given the simplicity of the models studied, the SAS in continuous variables can be obtained directly from the model equations (see comments in Section 3.1) - and consequently, consistency is ensured.

If stability and consistency are demonstrated, SAS consistency is automatically guaranteed. (Ref.?)

6.5 SAS error analysis

Initially, we define ζ as a generic variable that represents T_f, T_p or X. Then, for ζ calculated with k_{max} intervals, the following SAS error expressions are written:

$$E^T_{\zeta;k_{max}}(\tau) \equiv \zeta_{k_{max}}(\tau) - \zeta(\tau) = E^R_{\zeta;k_{max}}(\tau) + E^L_{\zeta;k_{max}}(\tau) \quad (65)$$

$$\mathrm{RMSE}_{\zeta;kmax} \equiv \sqrt{\sum_{j=1}^{M} \frac{1}{M}\left(E_{\zeta;k_{max}}(\tau_j)\right)^2} \quad (66)$$

Where, $E^T_{\zeta;k_{max}}$ is the total error, given by the sum of the machine rounding error, $E^R_{\zeta;k_{max}}$ (roundoff error) with the error due to model linearization, $E^L_{\zeta;k_{max}}$ (linearization error), and $\mathrm{RMSE}_{\zeta;k_{max}}$ is the Root Mean Squared Error (RSME). The following presents the analysis methodology for these types of error.

6.5.1 Roundoff error $\left(E^R_{\zeta;k_{max}}\right)$

In this work, roundoff errors are estimated using two independent methods: the first - known from the literature - is based on accounting for floating point operations; and the

second - developed here - makes use of characteristics of SAS. These methods are described respectively below.

- Method *A* - Estimation based on expressions from the literature

The randon and non-randon round-off errors in the calculation of ζ can be estimated as a function of number of intervals from assessment of the number of arithmetic operations of each calculation. The MATLAB code developed by Qian (2023) was used to calculate the number of arithmetic operations (FLOPS) for the SAS, considering an average (and constant) T_p in the calculation of h_r and K, for each k_{max} tested. Then, estimates of random and non-random round-off errors were performed by multiplying the machine precision ($\epsilon_M = 2.220446049250313 \times 10^{-16}$) by FLOPS at the power ½ and 1, respectively (Ref?).

- Method *B* - Estimation based on SAS characteristics

SAS can provide an excellent estimate of this error if we consider that: the linearized model solution is exact; (if K and h_r are made constant - e.g., at an average temperature along the reactor -, SAS can be used to solve the linear problem; estimating K and h_r at an average temperature, one has approximately the same order of magnitude for the arguments of the exponential functions and for the coefficients of the solution, in comparison with the non-linear problem; for the same number of intervals, the SAS can be programmed to perform approximately the same number of operations both on the linear problem and on the corresponding non-linear problem; for a given τ, the difference between the results of the linear problem, using $k_{max} = 1$ and $k_{max} = N$, is due only to the roundoff error. As a result of the previous considerations, it is concluded that an excellent estimate of $E^R_{\zeta;k_{max}}$ can be obtained from the difference between the results of the SAS for the linear problem with $k_{max} = 1$ and with $k_{max} = N$.

6.5.2 Linearization error $\left(E^{L}_{\zeta;k_{max}}\right)$

To evaluate the linearization error, the following iterative procedure is adopted:

(a) A set $S = \left\{k_{max_1},\ k_{max_2}, \cdots, P\right\}$ of increasing k_{max} intervals is composed, assuming that for each element $E^{R}_{\zeta;k_{max}} \ll E^{L}_{\zeta;k_{max}}$, and that $E^{L}_{\zeta;P} \ll E^{L}_{\zeta;k_{max}\neq P}$;

(b) the $E^{L}_{\zeta;k_{max}}$ for calculations with $kmax$ intervals is given approximately by the following expression

$$E^{L}_{\zeta;k_{max}}(\tau_j) \cong \zeta_{k_{max}\neq P}(\tau_j) - \zeta_P(\tau_j) \tag{67}$$

(c) the RMSE for calculations with $kmax$ intervals is given approximately by the following expression

$$\mathrm{RMSE}_{\zeta;k_{max}} \cong \sqrt{\sum_{j=1}^{M} \frac{1}{M}\left(\zeta_{k_{max}\neq P}(\tau_j) - \zeta_P(\tau_j)\right)^2} \tag{68}$$

(d) the linearization error trend line is plotted as a function of k_{max};

(e) if the results agree with the assumptions in (a), the procedure ends, otherwise a new choice of S is made and the procedure is restarted.

6.6 Stifness

Stifness is a characteristic of interest in the integration of an ODE system, and is normally quantified by the stiffness ratio (SR) (Davis, 1984). In the present study, the SR for the linearized model can be defined in the following form

$$\mathrm{SR} \equiv \frac{\max_i |r_i|}{\min_i |r_i|},\ i = 1,2,3 \tag{69}$$

Although the model under study is a nonlinear system of ODEs, whose stiffness may vary over time (Davis, 1984), SAS is based on "interval solutions of the linearized model" whose form is independent of them. Therefore, if for a given SR (say SR_1) it is possible

to integrate the model equations keeping K and h_r constant - i.e., the linear problem -, then, the integration of the nonlinear problem can be guaranteed as long as $\mathrm{SR}(\tau) < \mathrm{SR}_1$ for $(0 \leq \tau \leq \tau_L)$. Therefore, to evaluate SAS in relation to system stiffness, the SR is varied over several orders of magnitude and the performance of SAS is compared to that of conventional ODE integrators. The variation in the order of magnitude of the SR is achieved through the variation of the pre-exponential factor (A)..

This artificial variation can generate non-physical results - for example, negative absolute temperatures -, however, this does not interfere with this numerical analysis.

7. Results and discussion

7.1 Model verification

SAS is verified by comparison with the analytical solution of the linear (and simpler) model, and with results from other numerical methods. Case study *a* (Section 5) is used in the comparison, with the following modifications: h_r and K evaluated at a constant temperature of 597.2035 K ??? and inclusion of the hypothetical kinetic data... .

Thus, following the methodology of Section 6.1, two discretization levels are considered, $k_{max} = 10^4$ and $k_{max} = 1$. As illustrated in Fig. 2, excellent agreement was obtained for ζ at the reactor outlet, for the different discretization levels studied.

Insert Figure 2

Figure 2. ζ at L, calculated with $k_{max} = 10^4$ and $k_{max} = 1$, for case study *a*, with the following modifications: h_r and K evaluated at a constant temperature of 597.2035 K ??? and inclusion of the hypothetical kinetic data...

Then, we proceed to investigate the SAS performance considering variable T_p in calculating h_r and K. Fig. 3 shows the predictions for ζ profiles - numerical solutions of Eqs. (10)-(15) - from SAS and the ..... methods.

Insert Figure 3

Figure 3. ζ profiles calculated with SAS ($k_{max} = 10^4$) and 4th order Runge-Kutta method, for case study *a*, with the following modifications: ..... .

As can be seen, excellent agreement was found between the different solution methods.

In Fig. 4, further comparisons for the conditions described for Fig. 3, with other numerical methods (explicit Euler, Heun, Ralston, and Runge-Kutta of 3rd and 5th order), also show excellent agreement. For the relative difference defined by Eq. (70), a maximum of $\mathcal{O}(10^{-1})\%$ was found for T_f and T_p,

$$\Delta\zeta\% = \frac{\zeta^{\mathrm{OM}} - \zeta^{\mathrm{SAS}}}{\zeta^{\mathrm{SAS}}} \times 100 \tag{70}$$

Insert Figure 4

Figure 4.: ζ profiles $(\mathrm{A}) - (\mathrm{J})$; $\Delta\zeta\%$ profiles (L,K). Profiles for case study *a*, with the following modifications:... . For SAS, $k_{max} = 10^4$, and for the other methods the sectioning was....

Fig. 5 presents a comparison of the computation time of different numerical methods, for integrating the model equations over the length of the reactor, under the conditions described in Fig. 4.

Insert Figure 5

Figure 5. Computation time for integrating the model equations over L, under conditions described in Fig. 4.

As indicated in Fig. 5, the SAS calculation time is approximately half that observed in the solution by the explicit Euler method. The advantage of the SAS is therefore evident: not only is it unconditionally stable - unlike the explicit Euler method that can diverge depending on the step size -, but it also requires significantly less computation time when compared with the other numerical methods.

7.2 Model validation

Following the methodology described in Section 6.2, the (partial) validation of this model is performed by comparison with TGA data from Teklay et al. (2014) - case study *b*. For a heating rate of 40 K/min, Fig. 6 shows the SAS results using the dehydrolyxation kinetic parameters (KP) from Table 2 and the TGA data from Teklay et al. (2014).

`

Table 2. Kinetic parameters for kaolinite dehydrolyxation from different sources.

Insert Table 2

Insert Figure 6

Figure 6. Comparison of model predictions with TGA data (Teklay et al., 2014) at the heating rate of 40 K/min.

As seen in Fig. 6, despite the simplification in the kaolinite calcination kinetics - reduced in the analysis, to the kaolinite dehydroxylation step -, for sets K1 – K3 there is a reasonable agreement between the model predictions and the TGA data, (partially) validating the model. Full validation however requires comparison with MBR data.

Figs. 7A and 7B show a comparison between results of the present model and more complex models, for particle temperature as a function of residence time, at a heating rate of 40 K/min.....

Insert Figure 7

Figure 7. (A) Particle temperatures predicted by the present model and the model of Teklay et al. (2014), at a heating rate of 40 K/min.; (B) Particle temperatures predicted by the present model and the model of Medeiros et al. (2021), at a heating rate of 40 K/min.

As can be seen, the results agree satisfactorily, enabling cross-validation between the present model and the others mentioned. Note, however, that the model by Teklay et al. (2014) - more complex in the description of the phenomena in the solid phase and the chemical kinetics of the flash calcination of kaolinite - is intended for the simulation of the calcination of kaolinite in a fluidized bed reactor (for which τ should be interpreted as the "clock" team). Medeiros et al. (2021).

This good prediction capacity in relation to the more complex models analyzed is discussed in Section 7.4.

7.3 Numerical analysis

In this section, a numerical analysis of the SAS is developed, aiming at the following aspects: stability, consistency and convergence, round-off and linearization errors, as well as the ability to solve stiff problems.

7.3.1 SAS stability

By definition, $\varphi_{k-1} > 1$ and $\mathrm{Py}'_{k-1} > 0$. Thus, from Eqs. (34c,d) and (36), we have $r_{l,k-1} < 0 \;\; (l = 1 - 3)$. Therefore, following the methodology in Section 6.3, it can be concluded that the implementation of SAS in the form of Eqs. (46)-(48) is unconditionally stable, since a perturbation on a single value of ζ_{k-1} produces a variation in subsequent values that does not increase step by step, regardless of the value of $\Delta\tau$ (Gear, 1971?).

7.3.2 Consistency and convergence

Following the methodology of Section 6.4, the SAS in continuos variables - Eqs. (54)-(61) - is substituted into the model equations, Eqs. (10)-(15). It is shown in Appendix A that by carrying out this substitution, each equation in the model is satisfied. Thus, for $\Delta\tau \to 0$, SAS converges to the exact solution and therefore consistency is demonstrated.

Since the stability of SAS has already been demonstrated, these results allow us to conclude - according to Section 6.4 - that SAS is a consistent and convergent numerical scheme.

7.3.3 Round-off error

Fig. 8(A) presents the estimates of absolute round-off error for ζ, as a function of k_{max}, for case study *a*, with the following modifications: ....., .

The results are presented according to the methods described in Section 6.5.1: *A* (markers), and *B* (solid and dashed lines for random and non-random round-off errors, respectively). Using method *B*, the round-off error was estimated by comparing the SAS at each k_{max} considered (10^1 to 10^8) with the exact solution when $k_{max} = 1$. These calculations were carried out considering an average (and constant) T_p in h_r and K.

Insert Figure 8(A)

Figure 8 (A). Estimates of absolute round-off error for ζ (markers), at $z = \frac{L}{2}$, as a function of k_{max}, for case study *a*, with the following modifications: .....,, solid and dashed lines for random and non-random round-off errors, respectively.

As can be seen, for $k_{max} > 10^4$ the values obtained with method B are located at intermediate points to those obtained with method A, thus demonstrating consistency.

Figs. 8(C)-(E) presents the ζ profiles for the conditions described for Fig. 8(A) as a function of k_{max}.

Insert Figures 8(C)-(E)

Interestingly, in Figs. 8(C)-(E) the estimated round-off error presents regular behavior, only when $k_{max} > 10^4$. This is due to the fact that for $k_{max} > 10^4$, SAS maintains a pattern in the ξ profile, that is refined as k_{max} increases.

7.3.4 Linearization error

Fig. 8(B) presents the estimates of the linearization error for ζ, as a function of k_{max},

for case study a, with the following modifications: ....., . The results were obtained according to the methodology in Section 6.5.2, considering $P = 10^8$.

Insert Figure 8(B)

Figure 8 (B). Estimates of linearization error for ζ (markers), at $z = \frac{L}{2}$, as a function of k_{max}, for case study a, with the following modifications: .....,

Fig. 9(A) presents the root mean squared linearization error for T_f as a function of k_{max}^{-1} for the conditions described for Fig. 8(B). The calculations were performed following the methodology described in Section 6.5.2, considering $P = 10^8$ and variable T_p in h_r and K.

Insert Figure 9(A)

Figs. 9(B)-(D) details in a semilogarithmic scale, the behavior of the linearization error for large values of k_{max}.

Insert Figures 9(B)-(D)

As discussed in Appendix B, for very large values of k_{max}, exact knowledge of this behavior is only accessible through theoretical analysis. However, observing the behavior of $\mathrm{RMSE}_{\zeta;k_{max}}$ in these figures, we can consistently infer the theoretical results Eqs. (B1) and (B2).

Among the various functions proposed (see Supplementary Material) to adjust $\mathrm{RMSE}_{\xi;kmax}$ as a function of $kmax^{-1}$, the hyperbolic sine function

$$f(k_{max}^{-1}) = a\sinh(k_{max}^{-1}) \quad (71)$$

showed an $R^2 = 0.9999$ for all ζ, with $\text{RMSE}_{\zeta;k_{max}}$ of 5.606×10^{-6}, 8.074×10^{-6} and 3.441×10^{-7} for $\zeta = T_f, T_p$ and X, respectively. When compared with other proposed functions, this function does not present the smallest RMSE, however, it is of interest because it has the theoretical properties P_1 and P_2 (Appendix B), as well as it presents the expected increase in $\text{RMSE}_{\zeta;k_{max}}$ for k_{max}^{-1} approaching 1 - with the exception of $k_{max} < 10^2$, as will be seen below -.

In Figs. 9(B)-(D) the solution when $k_{max} < 10^2$ does not represent the physical behavior of the problem under study. For $k_{max} > 10^2$ the phenomena are properly described and refinement is obtained as k_{max} increases. Moreover, a limiting discretization level with $k_{max} = 10^7$ should be adopted considering an error control strategy with the machine error three orders of magnitude lower than the linearization error.

From the previous results and Figs. ???, it can be concluded that the analysis meets item (e) of the methodology in Section 6.5.2 and therefore can be completed.

As an application, the exact solution for the position in the middle of the reactor will be estimated for case study??, with the following modifications:..... Thus, considering $k_{max} = 10^2$ - the lower limit of the linear region in Fig.??- the absolute linearization errors for T_p, T_f and X are 1.67447, 1.59637 and 0.00143172, respectively. On the other hand, the corresponding round-off errors at the same discretization level are 2.27374×10^{-13}, zero and zero, respectively. Therefore, at $\frac{L}{2}$, the exact solution can be estimated as (696.774 ± 1.67447) K, (723.847 ± 1.59637) K and $(0.486343 \pm 0.00143172)$ for T_p, T_f and X, respectively,

7.3.5 Stiffness ratio (SR)

Following the methodology of Section 6.6, Table 3 lists the order of magnitude of SR that the different numerical methods were able to integrate for the case study??, with the following modifications:.....

Insert Table 3

Table 3. Performance of different ODE solvers at different SR, for integration of model equations along the length of the reactor, for case study ??, with the following modifications...

Table 3 clearly shows the superior performance of SAS, followed by the variable-step methods - ODE23s and ODE15s - and the other methods

Insert Figure 10

Notably, SAS was able to integrate for all tested SRs (i.e., up to SR $= 10^{35}$). Also, the implicit variable step methods - ODE23s and ODE15s - stand out for solving very stiff systems, with SR $= 10^{16}$.

Figure 10 illustrates, the computation time as a function of the stiffness ratio, for ODE23s and ODE15s for the conditions described for Table 3.

Figure 10. Computation time as a function of SR, for ODE23s and ODE15s, for the conditions described for Table 3.

Depending on the SR, the calculation time for ODE solvers can become very high. This can be easily seen in Fig. 10 where the ODE15s calculation time presents an exponential behavior.

In Tests 10, 11 and 12, with SR 1×10^{30}, 1×10^{31} and 1×10^{32}, respectively, the ODE15s computation time was 0.179294, 0.624987 and 9.581942 s, respectively. In order to make the behavior of computation time clear, Test 13 (SR $= 1 \times 10^{33}$) was not shown in Fig. 10, however, its calculation time was 676.732586 s with 5,735,317 steps. It should then be considered notable that for SR $= 1 \times 10^{33}$, SAS integrated the system in 5.514555 s with 100,000 intervals.

The exceptional performance of SAS can be explained based on its unconditional stability (Section 6.1) together with a relatively small number of operations in each interval. Hence, SAS has the capability to address stiff problems both numerically and computationally.

7.4 Scale analysis for MBR model selection

Model selection must consider accuracy and required resources; thus, the simplest model with sufficiently accurate results is indicated (Çengel and Ghajar, 2011). In the literature, there are several detailed studies on lumped model selection criteria for different types of moving bed heat exchangers (Depew and Farbar, 1963; Kern and Hemmings, 1978; Fan and Zhu, 1998; Saastamoinen, 2004; Haim and Kalman 2008; Bertoli et al., 2017, 2020). In the present work, a rough analysis, based only on scale analysis, will be sufficient to understand the model selection.

Thus, based on the scales in Table 1 and the assumptions made, it can be said that the present model - to lumped parameters in both phases - is more suitable for systems with negligible mass transfer effects, and small Bi and small $\mathrm{Da_{IV}}$.

7.5 SAS selection criteria - quantitative analysis

To verify the previous statements based on scale analysis, as well as to obtain some quantitative information about the SAS selection criteria, a comparative analysis of SAS was developed with a distributed parameter model (DM) in the solid phase - Medeiros et al. (2021) -, described in Appendix C for completeness.

Insert Table 4

Insert Figure 11

8. Conclusion

The continuous search for improving and optimizing reaction processes in moving beds motivates research in modeling and simulation. Thus, this work could contribute in the following ways:

- Develops a local analytical solution for a kinetic and heat transfer lumped model of a tubular MBR, with a first-order chemical reaction occurring uniformly in the particles.
- Implements the local solution in the FAM framework.
- Develops an unconditionally stable, consistent and convergent numerical scheme for a kinetic and heat transfer lumped model of a tubular MBR, with a first-order chemical reaction occurring uniformly in the particles.
- Develops a numerical scheme capable of fast integration of model equations, for systems with stiffness ratio SR $= 10^{33}$ (highest SR tested).
- Demonstrates the accuracy of the SAS in comparison with other methods, with the advantage of simple programming.
- Develops a specific methodology for SAS error analysis.

- Demonstrates analytically the unconditional stability of SAS in the implemented form.
- Demonstrates analytically the consistency and convergence and of the solution.
- Generalizes a previous method for proving consistency of SAS.
- Improves the physical understanding of model parameters through scale analysis.
- Performs model validation through comparison with experimental data.
- Presents a solution that can be used as a benchmark for MBR simulations.

Finally, it is noteworthy that the solution obtained performs stable, fast, and accurate with a minimum of computation time and memory.

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Nomenclature

A	pre-exponential factor, $\left(\frac{1}{\mathrm{s}}\right)$
A_p	particle area $= 4\pi R_p^2$, (m^2)
a_1	wall area per unit volume of the reactor $= \frac{2}{R}$, $\left(\frac{1}{m}\right)$
Bi	compound Biot number $= \mathrm{Bi}_p + \mathrm{Bi}_r$, $(-)$
Bi_p	particle Biot number for convection heat transfer $= \frac{3h_p R_p}{k_p}$, $(-)$
Bi_r	particle Biot number for radiation heat transfer $= \frac{3h_r R_p}{k_p}$, $(-)$

B $= \frac{\mathrm{Bi}}{3} = B_p + B_r$, $(-)$

B_p $= \frac{\mathrm{Bi}_p}{3}$, $(-)$

B_r $= \frac{\mathrm{Bi}_r}{3}$, $(-)$

$b_{l,k-1}$ SAS coefficient defined by Eqs. (37a), (41a) and (42a), $(-)$

$b'_{l,k-1}$ modified SAS coefficient defined by Eqs. (37b), (41b) and (42b), $(-)$

C $=$ cooling

C_A concentration of species A, $\left(\frac{\mathrm{mol}}{\mathrm{m}^3}\right)$

c specific heat at constant pressure, $\left(\frac{\mathrm{J}}{\mathrm{kg{\cdot}K}}\right)$

DPM MBR distributed parameter model of Medeiros et al.,

$\mathrm{Da}_{\mathrm{IV}}$ Damköhler fourth number for a first order irreversible chemical reaction $= \frac{(-\Delta H_R)KC_{Ai}R_p^2}{k_p T_{pi}}$, $(-)$

$\mathrm{Da}_{\mathrm{dev}}$ external thermal Damköhler number for pyrolysis/devolatilization, for convection heat transfer $= \frac{(-\Delta H_R)KC_{Ai}R_p}{3h_p T_{pi}}$, $(-)$

$\mathrm{Da}_{\mathrm{dev},k-1}$ $= \frac{(-\Delta H_R)K_{k-1}C_{Ai}R_p}{3h_p T_{pi}}$, $(-)$

D_p solids thermal diffusivity $= \frac{k_p}{\rho_p c_p}$, $\left(\frac{m^2}{\mathrm{s}}\right)$

d_p particle diameter, (m)

E activation energy, $\left(\frac{\mathrm{J}}{\mathrm{mol}}\right)$

$E_{\xi;kmax}$ error for ξ calculated with $kmax$ intervals, $(-)$

$EP\%$ relative error between SAS and DM, defined by Eq. (72), $(-)$

FAM $=$ finite-analytic method

Fo' modified Fourier number $= \frac{D_p \acute{t}}{R_p^2}$, $(-)$

g dimensionless heat source, defined by Eq. (5), $(-)$

g_{k-1} linearized dimensionless heat source defined by Eq. (21), $(-)$

H $=$ heating

ΔH_R enthalpy of reaction, $\left(\frac{\text{J}}{\text{mol}}\right)$

h_f fluid-wall convective heat transfer coefficient, $\left(\frac{\text{W}}{\text{m}^2\cdot\text{K}}\right)$

h_p fluid-particle convective heat transfer coefficient, $\left(\frac{\text{W}}{\text{m}^2\cdot\text{K}}\right)$

h_r wall-particle radiative heat transfer coefficient $= \sigma\epsilon_p\left(T_w^2 + T_p^2\right)\left(T_w + T_p\right)$, $\left(\frac{\text{W}}{\text{m}^2\cdot\text{K}}\right)$

$h_{r,k-1}$ $= \sigma\epsilon_p\left(T_w^2 + T_{p,k-1}^2\right)\left(T_w + T_{p,k-1}\right)$, $\left(\frac{\text{W}}{\text{m}^2\cdot\text{K}}\right)$

K reaction rate constant $= Ae^{-\frac{E}{\Re T_p}}$, $\left(\frac{1}{\text{s}}\right)$

K_{k-1} $= Ae^{-\frac{E}{\Re T_{p,k-1}}}$, $\left(\frac{1}{\text{s}}\right)$

k interval index

k_{max} number of intervals in which the reactor is axially sectioned

k_p solids thermal conductivity, $\left(\frac{\text{W}}{\text{m}^2\cdot\text{K}}\right)$

LHS $=$ left-hand side

L reactor length, (m)

MBR $=$ moving bed reactor

$\dot{m}_f$ fluid mass flow rate $= \rho_f v_f \pi R^2$, $\left(\frac{\text{kg}}{\text{s}}\right)$

$\dot{m}_p$ solids mass flow rate $= \rho_p v_p (1-\varepsilon)\pi R^2$, $\left(\frac{\text{kg}}{\text{s}}\right)$

n_v particle number density $= \frac{6\dot{m}_p}{\rho_p v_p \pi^2 R^2 d_p^3} = \frac{1-\varepsilon}{V_p}$, $\left(\frac{1}{\text{m}^3}\right)$

ODE $=$ ordinary differential equation

$\mathcal{O}(a)$	order a
P	largest element of S, $(-)$
Py	pyrolysis first number $= \frac{k_p}{\rho_p c_p R_p^2 K} = \mathrm{Th}^{-2}$, $(-)$
Py′	pyrolysis second number for convection heat transfer $= \frac{3h_p}{\rho_p c_p R_p K}$, $(-)$
Py'_{k-1}	$= \frac{3h_p}{\rho_p c_p R_p K_{k-1}}$, $(-)$
RHS	= right-hand side
RMSE	= root mean squared error
R	reactor inner radius, (m)
$\mathfrak{R}$	gas constant $= 8.314\ \left(\frac{\mathrm{J}}{\mathrm{mol \cdot K}}\right)$
R_p	particle radius, (m)
r	radial position within the particle, (m)
$r_{l,k-1}$	root defined by Eqs. (34) and (36), $(-)$
r_{ws}	wall area / particulate phase area $= \frac{2R_p}{3R(1-\varepsilon)}$, $(-)$
SAS	= semi-analytical solution
SR	= stiffness ratio
S	set defined in Section 6.2.2
TGA	= thermogravimetric analysis
T	temperature, (K)
Th	thermal Thiele modulus $= R_p\sqrt{\frac{K}{D_p}}$, $(-)$
$\acute{t}$	particle residence time $= \frac{z}{v_p}$, (s)
t_2	$\acute{t}$ scale defined in Table 1, (s)
V	reactor volume, (m^3)

V_p particle volume $= \frac{4}{3}\pi R_p^3$, (m^3)

v_f superficial velocity of the conveyor fluid, $\left(\frac{\mathrm{m}}{\mathrm{s}}\right)$

v_p particle axial velocity, $\left(\frac{\mathrm{m}}{\mathrm{s}}\right)$

X reactant conversion, $(-)$

z axial spatial coordinate, (m)

Greek Symbols

α $= \alpha_f + \alpha_p = \alpha_p \omega$, $(-)$

α_f $= \alpha_p(\omega - 1)$, $(-)$

α_p $= \mathrm{Bi}_p \beta$, $(-)$

β capacity rate ratio $= \frac{\dot{m}_p c_p}{\dot{m}_f c_f} = \frac{\rho_p v_p c_p (1-\varepsilon)}{\rho_f v_f c_f}$, $(-)$

$\Delta\zeta\%$ relative difference of ζ between OM and SAS, defined by Eq. (70), $(-)$

$\Delta\tau$ dimensionless time step $= \frac{3 h_p L}{\rho_p v_p c_p R_p k_{max}}$, $(-)$

ε void fraction $= 1 - \frac{\dot{m}_p}{\rho_p v_p \pi R^2}$, $(-)$

ϵ surface emissivity, $(-)$

ϵ_M machine precision = $2.220446049250313 \times 10^{-16}$, $(-)$

ζ generic variable $= T_f$, T_p or X, $(-)$

θ dimensionless temperature $= \frac{T - T_i}{T_{pi}}$, $(-)$

$\theta_f(\infty)$ defined by Eq. (16), $(-)$

$\theta_p(\infty)$ defined by Eq. (17), $(-)$

ξ dimensionless particle radial coordinate $= \frac{r}{R_p}$, $(-)$

ρ	density, $\left(\frac{\mathrm{kg}}{\mathrm{m}^3}\right)$
σ	Stefan-Boltzmann constant $= 5.6697 \times 10^{-8} \left(\frac{\mathrm{W}}{\mathrm{m}^2 \cdot \mathrm{K}^4}\right)$
τ	dimensionless residence time $= \frac{3h_p}{\rho_p c_p R_p} \acute{t}$, $(-)$
τ_L	dimensionless residence time at L, $(-)$
φ	$= 1 + \frac{h_r}{h_p}$, $(-)$
φ_{k-1}	$= 1 + \frac{h_{r,k-1}}{h_p}$, $(-)$
ω	$= 1 + r_{ws} \frac{h_f}{h_p}$, $(-)$

Subscripts

f	fluid
hom	homogeneous
i	inlet
j	discrete point j in τ
k	discrete point k in τ
l	root index
p	particle
$part$	particular
pm	average taken over an interval, for the particle
pc	particle center
ps	particle surface
w	wall

Superscripts

L	linearization
OM	other method
R	machine rounding
T	total

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Appendix A – Verification of SAS in continuous variables

Initially, it is easy to see that the boundary conditions Eqs. (13)-(15) are satisfied by Eqs. (54)-(56) and, to verify the governing equations, we substitute into Eqs. (10)-(12) the solution in continuous variables, Eqs. (54)-(61):

- Substituting Eq. (54) in the LHS of Eq. (10) and developing, we have

$$\frac{dX(\tau)}{d\tau} = -r_3 e^{\int_0^\tau r_3 d\tau} = r_3(X(\tau) - 1) = \frac{1-X(\tau)}{\mathrm{Py}'} \equiv \text{RHS of Eq. (10)} \qquad \text{(A1a – d)}$$

- Substituting Eq. (55) in the LHS of Eq. (11) and developing, we have

$$\frac{1}{\beta}\frac{d\theta_f(\tau)}{d\tau} = \frac{1}{\beta}\sum_{l=1}^{3} r_l b_l e^{r_l \tau} =$$

$$\frac{1}{\beta}\left(r_1 \frac{b_3(r_3-r_2)e^{r_3\tau}+(\beta\omega+r_2)\left(\theta_f(\tau)-\theta_f(\infty)\right)-\beta\left(\theta_p(\tau)-\theta_p(\infty)\right)}{r_2-r_1} + \right.$$

$$\left. r_2 \frac{b_3(r_3-r_1)e^{r_3\tau}+(\beta\omega+r_1)\left(\theta_f(\tau)-\theta_f(\infty)\right)-\beta\left(\theta_p(\tau)-\theta_p(\infty)\right)}{r_1-r_2} + r_3 b_3 e^{r_3\tau} \right) =$$

$$\theta_p(\tau) - \theta_p(\infty) + \omega\left(\theta_f(\infty) - \theta_f(\tau)\right) \equiv \text{RHS of Eq. (11)} \qquad \text{(A2a – d)}$$

- Substituting Eq. (56) in the LHS of Eq. (12) and developing, we have

$$\frac{d\theta_p(\tau)}{d\tau} = \frac{1}{\beta}\sum_{l=1}^{3} r_l^2 b_l e^{r_l\tau} + \omega\sum_{l=1}^{3} r_l b_l e^{r_l\tau} =$$

$$\frac{1}{\beta}\sum_{l=1}^{3} r_l^2 b_l e^{r_l\tau} + \omega\frac{d\theta_f(\tau)}{d\tau} = \frac{r_3^2-(r_1+r_2)r_3+r_1 r_2}{\beta} b_3 e^{r_3\tau} - \left(\omega(r_1+r_2) + \right.$$

$$\left.\frac{r_1 r_2}{\beta}\right)\left(\theta_f(\tau) - \theta_f(\infty)\right) - (r_1+r_2)\left(\theta_p(\tau) - \theta_p(\infty)\right) + \omega\frac{d\theta_f(\tau)}{d\tau} =$$

$$g(\tau) + (\beta\omega^2+1)\left(\theta_f(\tau) - \theta_f(\infty)\right) + (\beta\omega+\varphi)\left(\theta_p(\tau) - \theta_p(\infty)\right) +$$

$$\omega\left(\beta\omega\left(\theta_f(\infty) - \theta_f(\tau)\right) + \beta\left(\theta_p(\tau) - \theta_p(\infty)\right)\right) = g(\tau) + \theta_f(\tau) -$$

$$\theta_f(\infty) - \varphi\left(\theta_p(\tau) - \theta_p(\infty)\right) \equiv \text{RHS of Eq. (12)} \qquad \text{(A3a – e)}$$

Therefore, the SAS in continuous variables satisfies the governing equations and the boundary conditions, thus constituting an exact representation - in integral form - of the system of model equations. This result is therefore a proof of consistency of the solution.

Appendix B – Properties of interest of the SAS inearization error for $k_{max} \to \infty$

As seen in Section 6.5.2, it is of interest to know the behavior of the SAS linearization error as a function of the number of intervals. However, for very large values of k_{max}, it is difficult at present - due to the large associated machine error or even technological limitations - to know exactly this behavior using only computational resources. Thus, the theoretical analysis of the SAS for this limit, reveals the following properties of interest:

$$P_1 : \lim_{kmax \to \infty} E^L_{\xi;kmax} = 0 \tag{B1}$$

which follows immediately from the results in Appendix A; and

$$P_2 : \lim_{kmax \to \infty} \mathcal{O}\left(\frac{dE^L_{\xi,kmax}}{dk^{-1}_{max}}\right) < \mathcal{O}(k^2_{max}) \tag{B2}$$

as a necessary result so that $\lim_{kmax \to \infty} \frac{dE^L_{\xi,kmax}}{dk_{max}}$ can be null in the following derivative

$$\lim_{kmax \to \infty} \frac{dE^L_{\xi,kmax}}{dk_{max}} = -\lim_{kmax \to \infty} \left(\frac{1}{k^2_{max}} \frac{dE^L_{\xi,kmax}}{dk^{-1}_{max}}\right) \tag{B3}$$

Note that the previous properties P_1 and P_2 follow, by extension, to $\mathrm{RMSE}_{\xi;k_{max}}$.

Appendix C – MBR distributed parameter model (Medeiros et al., 2021)

The MBR model studied by Medeiros et al. (2021) (DM) is to distributed parameters in the particles and to lumped parameters in the fluid phase, and the assumptions on which

it is based are the same as those in Section 2 of this study, except that the thermal conductivity of the particle is considered finite. The equations of DM are written below:

Governing equations

$$\frac{\partial X}{\partial \mathrm{Fo}'} = \mathrm{Th}^2(1-X) \tag{C1}$$

$$\frac{d\theta_f}{\mathrm{dFo}'} = \alpha_p\left(\theta_{ps} - \theta_p(\infty)\right) + \alpha\left(\theta_f(\infty) - \theta_f\right) \tag{C2}$$

$$\frac{\partial \theta_p}{\partial \mathrm{Fo}'} = \frac{1}{\xi^2}\frac{\partial}{\partial \xi}\left(\xi^2 \frac{\partial \theta_p}{\partial \xi}\right) + G \tag{C3}$$

Where $X = X(\xi, \mathrm{Fo}')$, $\theta_f = \theta_f(\mathrm{Fo}')$, $\theta_p = \theta_p(\xi, \mathrm{Fo}')$.

Particle boundary conditions

$$\text{At } \xi = 0,\ \mathrm{Fo}' > 0:\ \left.\frac{\partial \theta_p}{\partial \xi}\right|_{(0,\mathrm{Fo}')} = 0 \tag{C4}$$

$$\text{At } \xi = 1,\ \mathrm{Fo}' > 0:\ -\left.\frac{\partial \theta_p}{\partial \xi}\right|_{(1,\mathrm{Fo}')} = B\left(\theta_{ps} - \theta_p(\infty)\right) - B_p\left(\theta_f - \theta_f(\infty)\right) \tag{C5}$$

And conditions at the reactor entrance

$$\text{At } \mathrm{Fo}' = 0, \forall\, \xi:\ X(\xi, 0) = 0 \tag{C6}$$

$$\text{At } \mathrm{Fo}' = 0:\ \theta_f(0) = 0 \tag{C7}$$

$$\text{At } \mathrm{Fo}' = 0, \forall\, \xi:\ \theta_p(\xi, 0) = 0 \tag{C8}$$

In the above equations, $\theta_f(\infty)$ and $\theta_p(\infty)$ are given by Eqs. (16) and (17), respectively, and G is the dimensionless heat source term due to a first order irreversible chemical reaction

$$G = \mathrm{Da_{IV}}\,(1-X) \tag{C9}$$

Where $G = G(\xi, \mathrm{Fo}')$, and the reaction rate constant is dependent on the temperature within the particle, according to the Arrhenius equation:

$$K\left(\theta_p(\xi, \mathrm{Fo}')\right) = A\exp\left(\frac{-E}{\Re\, T_p}\right) = A\exp\left(\frac{-E}{\Re T_{pi}(\theta_p+1)}\right) \tag{C10a, b}$$

Medeiros et al. (2021) semi-analytically solved this model introducing the additional simplification of constant rate inside the particle in each interval - calculated

at the corresponding volumetric average particle temperature -. In the present study, this simplification is not made and the model equations are solved using CFD resources, as described in Section 7.4.

Table 1 - t' scales of phenomena for co-current vertical MBR

Scale	Associated phenomenon
$t_1 \equiv \frac{R_p^2}{D_p}$	heat conduction at a distance R_p within the particle
$t_2 \equiv \frac{\rho_p c_p R_p}{3h_p}$	H of the particle by fluid-particle convection
$t_3 \equiv \frac{\rho_p c_p R_p}{3h_r}$	H of the particle by wall-particle radiation heat transfer
$t_4 \equiv \frac{\rho_f c_f v_f}{n_v A_p h_p v_p}$	C of the fluid by fluid-particle convection
$t_5 \equiv \frac{\rho_f v_f c_f}{a_1 h_f v_p}$	H of the fluid by fluid-wall convection
$t_6 \equiv \frac{\rho_p c_p T_{pi}}{(-\Delta H_R) K C_{Ai}}$	H of the particle by the first-order chemical reaction
$\tau_7 \equiv \frac{1}{K}$	first order chemical reaction in the solid phase