Fast Dynamic Simulation of Distillation Columns
with Local Thermodynamic Models and Adomian Decomposition

Pedro R. B. Fernandes

GIMSCOP/Chemical Engineering Department, Federal University of
Rio Grande do Sul, Brazil (e-mail: pedro@ enq.ufrgs.br)

Abstract: Dynamic simulation of first-principles distillation models is a very time-consuming task, yet it is necessary for monitoring, control and optimization of such processes. In this sense, this work proposes a discretized Adomian decomposition method coupled with the Local Thermodynamic Model technique in order to speed up the integration of dynamic responses for distillation columns with acceptable accuracy loss. Results show that the combination of both approximation methods can lead to at least 150x faster simulations with respect to a reference solution with equivalent model characteristics.

Keywords: Dynamic simulation; Distillation Column; Adomian Decomposition; Thermodynamic model.

1. INTRODUCTION

Distillation columns are very important equipment in the process industries because they are responsible for the separation and specification of final products and for the intermediate recovery of raw materials, among other functions. Therefore, distillation columns are essential for the operation, profit, efficiency and environmental compliance of chemical processes. Nevertheless, distillation columns are complex systems, due to the high number of internal states (hundreds, in most cases), low number of measurements, slow dynamics, and their multivariable and nonlinear characteristics. One important issue regarding distillation columns is the estimation of product composition, since in most cases these are not analyzed on-line, and even in favourable situations measurements are only available with sampling times and/or delays that can reach several hours. In this sense, any techniques destined to the monitoring, control and optimization of units involving distillation columns are valuable, especially those model-based, as, for example, predictive control, sensor fusion/Kalman filtering, data reconciliation, etc. However, the computational cost and reliability of obtaining numerical solutions from dynamic first principles distillation models, which can be constituted by systems of hundreds (even thousands) of differential or differential-algebraic equations, can be prohibitive for on-line applications (Ito et al., 2018).

In the literature, there have been several proposals to reduce the complexity and, as a result, the computational burden in integrating the dynamic equations of distillation models as well as applications thereof. Examples in this regard are alternative model formulations like the nonlinear wave propagation theory (Fu and Liu, 2017; Hankins, 2007; Hwang, 1995), stage aggregation, also called compartmentalization (Kamath et al., 2010; Linhart and Skogestad, 2009, 2010; Schäfer et al., 2019), or specialized simulation algorithms, as orthogonal polynomial collocation (Cao et al., 2016; Valleriote et al., 2012), among others

(Abrol et al., 2010; Dones and Preisig, 2010). Particularly, Schäfer et al. (2019) report approximately 95% time savings relative to conventional models in optimal control applications. Another approach is related to the great extent of the computational time associated to solving the thermodynamic equilibrium equations that determine phase compositions in this type of model. In this sense, an interesting alternative is to use simplified property models, which can reduce significantly the time cost (Fernandes and Trierweiler, 2009; Ledent and Heyen, 1994), or by approximating phase equilibrium properties with, for example, artificial neural networks (Nentwich and Engell, 2016). This is particularly beneficial for conventional property models that are themselves implicit functions of the state variables (like volumetric equations of state or Helmholtz energy models, for example).

1.1 Adomian decomposition method

The Adomian series expansion, or decomposition (Adomian, 1984, 1988, 1991), is an analytical method that can solve a wide class of mathematical problems, either linear or non-linear. The key idea of the method is to obtain recursively the terms of an expansion of the solution by reverting its Taylor series in the independent variable. Considering an equation in operator form

$$\mathcal{L}v = g + \mathcal{R}v + \mathcal{N}v \qquad (1)$$

where $\mathcal{L}$ is a general linear operator, $\mathcal{R}$ a linear function or operator and $\mathcal{N}$ a nonlinear one, g an inhomogeneous term and v the dependent variable. The formal solution of this problem is, obviously,

$$v = \mathcal{L}^{-1}g + \mathcal{L}^{-1}\mathcal{R}v + \mathcal{L}^{-1}\mathcal{N}v \qquad (2)$$

The proposed solution involves the infinite series of the form

$$v = \sum_{n=0}^{\infty} v_n \qquad (3)$$

where the v_n are partial solutions, with v_0 the solution of

$$\mathcal{L}v = g \qquad (4)$$

and the following terms obtained by the recurrence relation

$$v_i = \mathcal{L}^{-1}\mathcal{R}v_{i-1} + \mathcal{L}^{-1}\mathcal{A}_{i-1}, \text{ for } i = 1,..,\infty \qquad (5)$$

where $\mathcal{A}_i$ are particular functions of v_j, $j = 0,..,i$, called the *Adomian polynomials*, which can be found on the basis of derivatives of $\mathcal{N}$ with respect to a dummy argument (Adomian, 1984; Elsaid, 2012). The Adomian decomposition has been employed to solve a number of different problems, as partial differential equations (Adomian, 1986; Arabia, 2015), boundary value problems (Kumar and Singh, 2010) and ordinary differential equations (Younker, 2011). Although the method has been applied for nonlinear root finding with separation processes, for example in flash solving and steady-state distillation (Fatoorehchi et al., 2015; Fatoorehchi and Abolghasemi, 2014), no work has been found concerning dynamic simulation of such processes.

This paper proposes the combination of the Adomian decomposition method, using a discretization scheme (Younker, 2011), and the local thermodynamic model approach (Fernandes and Trierweiler, 2009) to accelerate the dynamic simulation of distillation columns. The next section describes the phenomenological dynamic model considered in the paper. The thermodynamic approximation method is shown in Section 3, and the application of the Adomian technique to the distillation equations is explained in Section 4. Simulation results comparing the original problem with the approximations are in Section 5.

2. DYNAMIC MODEL

The considered dynamic model for the distillation column consists of a set of coupled ordinary differential equations (ODE's) representing the liquid mole fractions in each stage of the column. The main hypotheses of this model are the homogeneity of properties in the control volume, constant internal flows in each section, 100% efficient stages in thermodynamic equilibrium, and constant stage holdup. The column is depicted in Figure 1, where F and z are respectively feed rate and molar composition, L is the reflux rate, W is the reboiler boilup, D is the distillate flow and x_D its molar composition, B is the bottoms rate and x_B its composition.
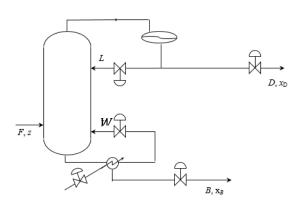

Fig. 1. Scheme of the distillation column (one feed and two products, total condenser).

For the condenser, the equations are ($i = 1,..,N_c$):

$$M_1 \frac{dx_{i,1}}{dt} = V_2(y_{i,2} - x_{i,1}) \qquad (6)$$

For the internal stages, except the feed stage, the equations are ($i = 1,..,N_c \; j = 2,..,N_s - 1, j \neq N_f$):

$$M_j \frac{dx_{i,j}}{dt} = L_{j-1}x_{i,j-1} - L_j x_{i,j} + V_{j+1}y_{i,j+1} - V_j y_{i,j} \qquad (7)$$

On-stage feed ($i = 1,..,N_c$):

$$M_{Nf} \frac{dx_{i,Nf}}{dt} = Fz_i + L_{Nf-1}x_{i,Nf-1} - L_{Nf}x_{i,Nf} + V_{Nf+1}y_{i,Nf+1} - V_{Nf}y_{i,Nf} \qquad (8)$$

For the reboiler, the equations are of the form ($i = 1,..,N_c$):

$$M_{Ns} \frac{dx_{i,Ns}}{dt} = L_{Ns-1}x_{i,N-1} - (L_{Ns} - W)x_{i,Ns} - Wy_{i,Ns} \qquad (9)$$

In each stage, the molar holdup is M_j. The internal flows are given by:

$$L_j = \begin{cases} R, \text{ if } j < N_f \\ R + qF, \text{ if } j \geq N_f \end{cases} \qquad (10)$$

$$V_j = \begin{cases} W + (1-q)F, \text{ if } j \leq N_f \\ W, \text{ if } j > N_f \end{cases} \qquad (11)$$

where q is the feed quality. Therefore, the model contains $NsNc$ differential states (the liquid compositions in each stage, $x_{i,j}$).

2.1 Thermodynamic equilibrium

In an equilibrium stage j, vapour composition can be related to the liquid composition by a generally implicit relation of the form:

$$y_{i,j} = K_i(T_j, P_j, x, y) \cdot x_{i,j}, \; i = 1,..,N_c \qquad (12)$$

with K_i, called the *K-values*, obtained by means of thermodynamic relationships for the properties (*fugacities*) of each phase. Vapor compositions y_i and stage temperatures T_j must be obtained by solving the so-called *bubble-point problem* involving (12) and the constraint on mole fractions

$$\sum_{i=N_c} y_{i,j} = 1, \forall j \qquad (13)$$

for given $x_{i,j}$ and stage pressure P_j.

3. THERMODYNAMIC APPROXIMATIONS

As shown in (Fernandes and Trierweiler, 2009), thermodynamic approximation methods can improve the computational time for the solution of separation problems, especially the dynamic simulation of distillation columns. In this paper, an alternative method called *Simplified Thermodynamic Model* (STM) is employed, which has the form:

$$\ln(K_i P) = \theta_{1,i} + \frac{\theta_{2,i}}{\theta_{3,i}+T} + \sum_{k=1,k\neq i}^{Nc} \theta_{r[k],i} \cdot x_j^2 \qquad (14)$$

where $\theta_{p,i}$ are model parameters ($r = 4,5,...,N_c + 2$), fitted previously on the basis of data generated with an adequate conventional thermodynamic model covering the operating space both in terms of composition and pressure. The simplified model (14) employed in this work consists in a single equation for each component and not in a network of such models, as in Fernandes and Trierweiler (2009), in order

to improve simulation speed. Moreover, there is no model update during the simulation, as in (Ledent and Heyen, 1994)

3.1 Bubble Point Problem Acceleration (BPPA)

By exploiting the structure of (14), it has been shown (Fernandes and Trierweiler, 2009) that the bubble point problem can be solved explicitly, at least in an approximate fashion, avoiding iterative solutions of the equilibrium problem for each stage at every time step. With this method, the bubble point temperature can be directly determined for stage j by means of the following relations:

$$T_j = \frac{-C_{2,j} + \sqrt{C_{2,j}^2 - 4C_{1,j}C_{3,j}}}{2C_{1,j}} \qquad (15)$$

$$C_{p,j} = \phi_{p,j} + \sum_{i=1}^{N_c} \beta_{p,i} R_{i,j}, \; p = 0, \dots, 3 \qquad (16)$$

$$R_{i,j} = x_{i,j} \exp\left(\theta_{1,i} + \sum_{k=1, k \neq i}^{N_c} \theta_{r[k],i} \cdot x_{k,j}^2\right) \qquad (17)$$

where $\phi_{0,j} = -P_j$ and $\phi_{1,j} = \phi_{2,j} = 0$. The coefficients $\beta_{p,i}$, $p = 1, \dots, 3$ are specific of the method and determined solely on the basis of $\theta_{p,i}$, and thus are not additional approximation parameters. The vapor compositions can be finally calculated by

$$y_{i,j} = \frac{x_{i,j}}{P_j} exp\left(\frac{\theta_{2,i}}{\theta_{3,i} + T_j}\right) R_{i,j} \qquad (18)$$

4. ADOMIAN COLUMN APPROXIMATION

Casting the equations describing the composition dynamics of a distillation column in the matrix form

$$\mathcal{L}\{X\} = \mathbf{g}(t) + \mathcal{R}\{X\} + \mathcal{N}\{X\} \qquad (19)$$

where $\mathcal{L}$ is the differential operator d/dt, X is a vector representation of $x_{i,j}$ ($i = 1, \dots, N_c, j = 1, \dots, N_s$), $\mathcal{R}$ is a linear operator and $\mathcal{N}$ a nonlinear operator. Then, by following Adomian method, and considering the discretization of the integration interval suggested by Younker (2011), in order to avoid polynomial divergence, the solution at each time sub-interval k up to approximation order N_a is given by

$$X_{N_a}^{(k)} = \sum_{r=N_a} X_r^{(k)} \qquad (20)$$

where the partial solutions are

$$X_0^{(k)} = S_0^{(k)} + \mathcal{L}^{-1}\{\mathbf{g}\} \qquad (21)$$

$$X_r^{(k)} = \mathcal{L}^{-1}\left\{\mathcal{R}\{X_{r-1}\}\right\} + \mathcal{L}^{-1}\left\{\mathcal{A}_{r-1}\{X_{r-1}\}\right\} \qquad (22)$$

for $r = 1, \dots N_a$, where $S_0^{(k)}$ is the vector of initial conditions in each sub-interval, equal to $X_{N_a}^{(k-1)}$ for the discretized implementation to ensure solution continuity, $\mathcal{L}^{-1}$ is the definite integration from t_{k-1} to t_k, and $\mathcal{A}_{r-1}$ is the Adomian polynomial of order $r - 1$. For the column equations, the linear part $\mathcal{R}$ corresponds to the component liquid flows of the form $L_j x_{i,j}$, and the non-linear term $\mathcal{N}$ corresponds to vapor component flows $V_j y_{i,j} = V_j K_{i,j} x_{i,j}$. The non-homogeneous term $\mathbf{g}$ has elements $g_{i,j}$ given by $F z_i / M_{N_f}$ if $j = N_f$ (feed stage) and 0 otherwise, and is considered constant for simplicity in this work.

Although the original method is exact (analytic), for practical purposes the solution is truncated after a number of terms N_a. Such discretization renders the integration method explicit and of finite order. Moreover, since the main objective of this work is to achieve a low computational time with satisfactory precision, and in order to avoid the integration of the nonlinear Adomian terms, the *K-values* are considered constant at each time step. Although the Adomian solution is general, the direct application of the method for more rigorous column model formulations can be prohibitive in terms of computational time, due the arising integrals of Adomian polynomials, which can be cumbersome (Younker, 2011). Tailored schemes must be devised in this case.

With these considerations, (19) can be rewritten as

$$\mathcal{L}\{X\} = \mathbf{g} + \Phi^{(k)} X \qquad (23)$$

where $\Phi^{(k)}$ is the permutation of a block tridiagonal matrix with the following elements

- lower diagonal: L_j / M_j, $j = 1, \dots, N_s - 1$

- main diagonal: $\Phi_{i,1}^{(k)} = -(R + D)/M_i$; $\Phi_{i,j}^{(k)} = -(L_j + V_j K_{i,j}^{(k)})/M_j$, $j = 2, \dots, N_s - 1$; and $\Phi_{i,Ns}^{(k)} = -(B + W K_{i,Ns}^{(k)})/M_{N_s}$

- upper diagonal: $V_{j+1} K_{i,j+1}^{(k)} / M_{j+1}, j = 1, \dots, Ns - 1$

Therefore, by applying the Adomian method in the column equations (19), it is possible to obtain the following series solution with N_a terms:

$$X_{N_a}^{(k)} = \sum_{n=0}^{N_a} \frac{1}{n!} \left(\Phi^{(k)}\right)^n S_0^{(k)} \delta_k{}^n + $$
$$\sum_{n=0}^{N_a} \frac{1}{n+1!} \left(\Phi^{(k)}\right)^n \mathbf{g} \, \delta_k{}^{n+1} \qquad (24)$$

where $\delta_k = t_{k-1} - t_k$ is the time step. Note that, for computational efficiency, the matrix power $\left(\Phi^{(k)}\right)^n$ can be calculated by accumulating the matrix product between $\Phi^{(k)}$ and the previous term. This solution can be also implemented in Horner-type form:

$$X_{N_a}^{(k)} = \left(\mathbf{I} + \frac{\Phi^{(k)} \delta_k}{1}\left(\mathbf{I} + \frac{\Phi^{(k)} \delta_k}{2}(\cdots)\right)\right) S_0^{(k)} + \left(\mathbf{I} + \frac{\Phi^{(k)} \delta_k}{2}\left(\mathbf{I} + \frac{\Phi^{(k)} \delta_k}{3}(\cdots)\right)\right) \mathbf{g} \, \delta_k \qquad (25)$$

In this way, the solution in each subinterval is the exponential matrix function updated with state values reached at the end of the previous interval. Therefore, the proposed simulation algorithm using the Adomian technique can be stated as follows:

1. Calculate the *K-values* at the step k with the STM/BPPA technique using liquid composition given in the initial condition vector $S_0^{(k)}$ and stage pressure P_j;

2. Determine the system matrix for the k-th interval, $\Phi^{(k)}$;

3. Determine recursively the solution $X_{N_a}^{(k)}$ for a specified approximation order, N_a;

4. Make $S_0^{(k+1)} = X_{N_a}^{(k)}$ and advance one time step δ_k;

5. Return to 1 until the endpoint is reached.

In this paper, three different possible algorithms with the Adomian technique were also tested:

    I.   Fixed order N_a and fixed time step δ (ADM-I);

    II.   Fixed order N_a and adaptation of variable time step δ_k to achieve a specified tolerance ε (ADM-II);

    III. Fixed time step δ and adaptation of variable order $N_{a,k}$ to achieve a specified tolerance ε (ADM-III).

In cases II and III, error control is done based on the improvement of the solution after a new term is added in the solution, that is,

$$\Delta_X = \left\| X_r^{(k)} - X_{r-1}^{(k)} \right\|_2 \tag{26}$$

For case II, if the method fails to achieve the specified tolerance in a given sub-interval, the step is then reduced by a factor ε/Δ_X, and it is increased by a maximum of 25% if the step is successful.

5. RESULTS AND DISCUSSION

In order to compare the methods, the original model (6)-(11) and the Adomian algorithms were implemented in Python (*v.* 3.8.5, *numpy* v. 1.19.2). Conventional integration was done with *scipy* (v.1.5.0) *odeint* function (algorithm *lsoda*).

5.1 Case Study

The case study was a 34-stage (including condenser and reboiler) distillation column separating the mixture benzene, toluene and m-xylene, which shows a moderate departure from ideality. Feed stage was the 16th from top, and the feed is a saturated liquid mixture ($q = 1$) with composition 0.625 (benzene), 0.250 (toluene) and 0.125 (m-xylene) and molar flow of 7.330 kmol/min. Molar holdups were 100 kmol for each internal stage and 1000 kmol for condenser and reboiler. Specified flows were $D = 4.794$ and $B = 2.899$ kmol/min. For the base case (initial steady state), reflux flow was $L = 12.41$ kmol/min. Pressure (1.4 atm) was considered constant in all stages for simplicity. The conventional thermodynamic model was constituted by the Peng-Robinson equation of state for the vapor phase and by the UNIQUAC activity coefficient model for the liquid phase. The STM was obtained by means of 364 equilibrium points around a nominal steady-state composition profile by solving a least-squares regression to determine the parameters $\theta_{p,i}$. Figure 2 displays a diagonal plot of the resulting approximated *K-values*.

5.2 Test setup

Several simulation types were compared in this paper with regard to computational time and simulation error:

- Type A (reference): conventional thermodynamic model, iterative bubble problem solution and integration with *odeint*, default tolerance ($1.49 \cdot 10^{-8}$);
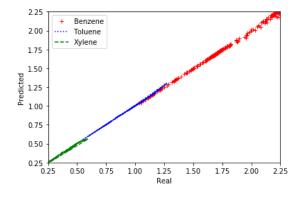

Fig. 2. Diagonal plot of the *K-values* from the STM (*predicted*) and the conventional model (*real*).

- Type B: the same as Type A, but with precision reduced to a specified tolerance ε;

- Type C: STM, iterative bubble problem solution and integration with *odeint*, default tolerance;

- Type D: STM/BPPA and integration with *odeint*, default tolerance;

- Type E: STM/BPPA and integration with Adomian-I of order N_a (referred to as ADM$_{Na}$-I);

- Type F: STM/BPPA and integration with Adomian-I of order N_a with the Horner scheme (referred to as ADM$_{Na}$-IH).

In each case, step perturbations from a fixed steady state were simulated. Ten runs were performed with simultaneous multiplicative step disturbances in L and V in the range [0.5, 1.5], plus ten runs with additive disturbances in z_1 in the range [-0.125, 0.125] (with opposite perturbations in z_2 and z_3). The dynamic responses were simulated up to 100 min, with time steps of 0.1 min (note that for *odeint* this value is only used to interpolate intermediate solutions at variable intervals). Three different values of ε ($5 \cdot 10^{-2}$, $1 \cdot 10^{-2}$, $5 \cdot 10^{-3}$) were also tested, although this has effect solely on type B. Therefore, 60 simulations were done with each method.

Errors at the endpoint were calculated as the 2-norm of the distance of a given solution and that of the reference solution, that is, for $l = B, ..., F$:

$$e_l = \left\| X_A \, (t = 100 \text{ min}) - X_l \, (t = 100 \text{ min}) \right\|_2 \tag{27}$$

Observe that (27) is related to the global error of each integration scheme, and that the individual component/stage composition error is of the order of $10^{-2} \cdot e_l$. The computational time T for each simulation was measured with the function *timer* of the *timeit* package and then averaged. An "acceleration factor" with respect to the reference solution was calculated in each case by

$$\Gamma_l = T_A/T_l, \ l = B, ..., F \tag{28}$$

A qualitative comparison of the average computational times for all simulations is shown in Fig. 3. For reference, the vertical grid represents 100s in an Intel i5 3.2GHz PC with 4Gb RAM. As it can be seen, there are at least 2 orders of

magnitude between the conventional solution (*A*) and the Adomian schemes (*E* and *F*).
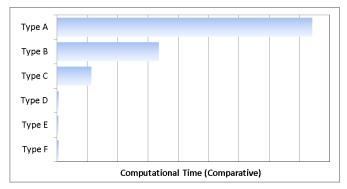

Fig. 3. Overall comparison of the simulation types with regard to computational time.

Figure 4 illustrates the transient responses of benzene liquid mole fractions in all stages for a step increase of 50% in the benzene feed composition. In this plots, tolerance ε was $1 \cdot 10^{-2}$ for simulation type *B* and Adomian order was 3 for types *E* and *F*. Clearly, all responses are very close.
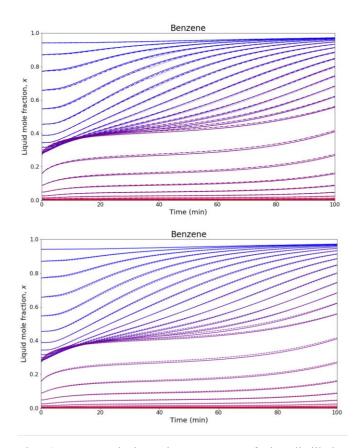

Fig. 4. Integrated dynamic responses of the distillation column for a 50% step in z_1. Top: simulation types *A* (full lines), *B* (dotted), *C* (dashed), *D* (dashed-dotted); Bottom: simulation types *A* (full lines), *E* (dotted), *F* (dashed).

Table 1 exhibits the average simulation errors e_l (27) and acceleration factors Γ_l (28) for each simulation type. As one could expect, type *B* has the smallest error with respect to the reference simulation, since it has the same model structure of

the original problem, although it is only approximately 3x faster. Types *C* and *D* have very similar errors, showing that the BPPA causes a very small precision loss, but with a time burden 20x smaller than the iterative solution with STM (and 150x faster than the original solution). The additional gain with the Adomian approximation is further 25%, and the approximations of order 3 (ADM$_3$-I and ADM$_3$-IH) show already a similar precision to the conventional integration with the STM. Simulation types *E* and *F* have the same errors, since the only difference is the implementation form. ADM-I is slightly more efficient then ADM-IH, probably due to the fact that, although it is Horner form, (25) has two terms which have to be calculated separately. Moreover, the approximated methods show fairly less variations in computational time, what is very desirable for on-line applications.

Table 1. Average simulation results

Simulation	Acceleration factor, Γ_l	Final error, e_l
Type *B*		
$\varepsilon = 5 \cdot 10^{-2}$	2.97	0.0321
$\varepsilon = 1 \cdot 10^{-2}$	2.66	0.0096
$\varepsilon = 5 \cdot 10^{-3}$	2.24	0.0028
Type *C**	7.86	0.0274
Type *D**	155.8	0.0275
Type *E*		
ADM$_2$-I	184.7	0.0355
ADM$_3$-I	185.3	0.0283
ADM$_4$-I	181.7	0.0281
Type *F*		
ADM$_2$-IH	180.6	0.0355
ADM$_3$-IH	176.8	0.0283
ADM$_4$-IH	167.7	0.0281

* these simulations do not depend on ε.

5.2 Variable Step Implementations

Tests were also conducted with the variable step implementations described in section 4 (ADM-II and ADM-III) as shown in Table 2 for $\varepsilon = 5 \cdot 10^{-2}$ and order 3.

Table 2. Average simulation results for the variable step implementations

Simulation	Acceleration factor, Γ_l	Final error, e_l
ADM$_3$-I	185.4	0.0283
ADM$_3$-II	396.0	0.1888
ADM$_3$-III	171.9	0.0610

The results are highly dependent on fine-tuning the algorithm (step increase factor). Nevertheless, simulations with ADM-II can be 2x faster in comparison to ADM-I at crude tolerances (with 40% less steps at the cost of 50% larger final error), specially for steps in *L* and *V*. This is 400x faster than the original simulation.

6. CONCLUSIONS

The combined use of thermodynamic model simplification (STM), an algorithm to avoid implicit solutions of the bubble point problem (BPPA), plus the Adomian decomposition technique led in this paper to a speeding factor of 2 orders of magnitude in the dynamic simulation of distillation columns (that is, time savings above 99,5%). This improvement can make possible the on-line implementation of several model-based techniques when accuracy is not of paramount importance. This is particularly true for composition estimation, due to the fact that the saved time can allow for model correction with plant data. Moreover, since the proposed method does not depend on internal iterations, which may fail to converge, it is also more reliable for real time applications. Although the integration with the Adomian decomposition in original form (type F, ADM-I) contributes to a lesser extent in this time reduction, optimized variable-step implementations can further boost the time savings. Moreover, the ADM analytic structure has the potential to allow for the efficient implementation of optimal control problems, for example.

REFERENCES

Abrol, S., Lu, M., Hill, D., Herrick, A., and Edgar, T. F. (2010). Faster dynamic process simulation using in situ adaptive tabulation. *Industrial and Engineering Chemistry Research*, *49*(17), 7814–7823.

Adomian, G. (1984). Convergent series solution of nonlinear equations. *Journal of Computational and Applied Mathematics*, *11*(2), 225–230.

Adomian, G. (1986). A New Approach to the Heat Equation - An Application of the Decomposition Method. *Journal of Mathematical Analysis and Applications*, *113*, 202–209.

Adomian, G. (1988). A review of the decomposition method in applied mathematics. *Journal of Mathematical Analysis and Applications*, *135*(2), 501–544.

Adomian, G. (1991). A review of the decomposition method and some recent results for nonlinear equations. *Computers and Mathematics with Applications*, *21*(5), 101–127.

Arabia, S. (2015). Some Modifications of Adomian Decomposition Methods for Nonlinear Partial Differential Equations. *Ijrras*, *23*(May), 164–173.

Cao, Y., Swartz, C. L. E., Flores-Cerrillo, J., and Ma, J. (2016). Dynamic modeling and collocation-based model reduction of cryogenic air separation units. *AIChE Journal*, *62*(5), 1602–1615.

Dones, I., and Preisig, H. A. (2010). Model simplification and time-scale assumptions applied to distillation modelling. *Computers and Chemical Engineering*, *34*(5), 732–743.

Elsaid, A. (2012). *Adomian Polynomials : a Powerful Tool for Iterative Methods of Series Solution of Nonlinear Equations*. *2*(4), 381–394.

Fatoorehchi, H., and Abolghasemi, H. (2014). Approximating the minimum reflux ratio of multicomponent distillation columns based on the Adomian decomposition method. *Journal of the Taiwan Institute of Chemical Engineers*, *45*(3), 880–886.

Fatoorehchi, H., Abolghasemi, H., and Rach, R. (2015). A new parametric algorithm for isothermal flash calculations by the Adomian decomposition of Michaelis-Menten type nonlinearities. *Fluid Phase Equilibria*, *395*, 44–50.

Fernandes, P. R. B., and Trierweiler, J. O. (2009). Local thermodynamic models networks for dynamic process simulation. *Industrial and Engineering Chemistry Research*, *48*(18), 8529–8541.

Fu, Y., and Liu, X. (2017). An advanced control of heat integrated air separation column based on simplified wave model. *Journal of Process Control*, *49*, 45–55.

Hankins, N. P. (2007). A Non-Linear Wave Model with Variable Molar Flows for Dynamic Behaviour and Disturbance Propagation in Distillation Columns. *Chemical Engineering Research and Design*, *85*(1 A), 65–73.

Hwang, Y. L. (1995). Wave Propagation in Mass-Transfer Processes: From Chromatography to Distillation. *Industrial and Engineering Chemistry Research*, *34*(8), 2849–2864.

Ito, E. H. C., Secchi, A. R., Gomes, M. V. C., and Paiva, C. R. (2018). Development of a gas composition soft sensor for distillation columns: A simplified model based and robust approach. In M. R. Eden, M. G. Ierapetritou, & G. P. B. T.-C. A. C. E. Towler (Eds.), *13 International Symposium on Process Systems Engineering (PSE 2018)* (Vol. 44, pp. 661–666). Elsevier.

Kamath, R. S., Grossmann, I. E., and Biegler, L. T. (2010). Aggregate models based on improved group methods for simulation and optimization of distillation systems. *Computers and Chemical Engineering*, *34*(8), 1312–1319.

Kumar, M., and Singh, N. (2010). Modified Adomian Decomposition Method and computer implementation for solving singular boundary value problems arising in various physical problems. *Computers and Chemical Engineering*, *34*(11), 1750–1760.

Ledent, T., and Heyen, G. (1994). Dynamic approximation of thermodynamic properties by means of local models. *Computers & Chemical Engineering*, *18*(Suppl.), S87–S91.

Linhart, A., and Skogestad, S. (2009). Computational performance of aggregated distillation models. *Computers & Chemical Engineering*, *33*(1), 296–308.

Linhart, A., and Skogestad, S. (2010). Reduced distillation models via stage aggregation. *Chemical Engineering Science*, *65*(11), 3439–3456.

Nentwich, C., and Engell, S. (2016). Application of surrogate models for the optimization and design of chemical processes. *2016 International Joint Conference on Neural Networks (IJCNN)*, 1291–1296.

Schäfer, P., Caspari, A., Kleinhans, K., Mhamdi, A., and Mitsos, A. (2019). Reduced dynamic modeling approach for rectification columns based on compartmentalization and artificial neural networks. *AIChE Journal*, *65*(5), e16568.

Valleriote, A., Dorigo, L., Secchi, A. R., and Biscaia, E. C. (2012). Reduced Rigorous Models for Efficient Dynamic Simulation and Optimization of Distillation Columns. In I. D. L. Bogle & M. B. T.-C. A. C. E. Fairweather (Eds.), *22 European Symposium on Computer Aided Process Engineering* (Vol. 30, pp. 1262–1266). Elsevier.

Younker, J. M. (2011). Numerical integration of the chemical rate equations via a discretized adomian decomposition. *Industrial and Engineering Chemistry Research*, *50*(6), 3100–3109.