

On estimating the error of local thermodynamic models. A general approach†

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A general method is developed for predicting the deviation between local and rigorous thermodynamic property models. The method is based on a quadratic error structure. The curvature matrix is updated after each parameter revision. The updating scheme utilizes the observed deviation as a measure for correcting the matrix and thus does not require any additional rigorous model evaluations. A recursive least squares procedure with variable forgetting is adopted for the parameter updating. A local model structure for K-value evaluations is applied in a dynamic simulation model of a batch distillation column. The efficiency and accuracy of the proposed method are tested for two different mixtures; a nearly ideal and a strongly non-ideal mixture.

1. Introduction

As more sophisticated thermodynamic models are introduced, which more accurately take into account highly non-ideal systems, they become computationally more expensive. Costly thermodynamic model evaluations are primarily caused by complicated correlations, solution of non-linear equations by iteration (often slowly converging) and numerical differentiation to generate partial derivatives. Therefore, methods are needed which are more efficient in their use of these models. The computational burdens involved in large scale, process flow sheeting simulations are extensive; as much as 70-90% of the time is spent on thermodynamic and physical (TP) property estimations. It is easy to see that there is much to gain from more efficient use of these models. For dynamic process simulation, it may even become a necessity, if the computations are to proceed in real time or faster.

There are several possible strategies for more efficient use of TP models. According to Grens (1983), four approaches are usually taken to improve phase-equilibrium calculations:

1. Reformulation of the calculation – the convergence properties of the iteration procedure can be influenced by the choice of convergence function and iteration variables.

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2. Convergence acceleration of fix-point schemes – the convergence rate of fix-point schemes can be improved by various methods such as by the dominant eigenvalue method.
3. Free-energy minimization techniques – this is an alternative statement of the equilibrium condition.
4. Use of local approximations to the thermodynamic functions – this is accomplished by replacement of the rigorous TP models by local approximations. The local approximation is a simple analytic function fitted to the rigorous model over a limited range and periodically revised to provide the best fit in the region of interest.

Among the remedial actions listed above, the last approach is the one treated here. Besides having a modular structure, this approach seems to have the widest applicability. It is independent of the actual rigorous model used and it is especially well-suited for dynamic process simulation. The idea is to have a general procedure that can be applied to a wide variety of local TP property models. It is also desirable to have a procedure that is transparent so that the application program does not see any difference between the rigorous TP package and the local TP procedure as depicted in Fig. 1. As it appears in Fig. 1, the independent variables of the local and the rigorous models are not identical. This is because the local model is explicitly dependent on only a subset (x) of the variables (z) that the rigorous model is a function of.

It is essential that the local model has an explicit structure. Furthermore, the local approximation, \hat{y} , should be based on a simplification of the rigorous model if possible, but polynomials and other arbitrary functions may also be used. Local models based on physical considerations will, however, be more efficient as they are valid over a much larger region before the parameters need to be revised. Major effects should therefore be represented by an approximately correct mathematical structure, whereas minor effects are represented by the adjustable parameters. It is, however, desirable to have as few parameters as possible for each local model. Another desirable quality of local thermodynamic models is that they can provide the partial derivatives directly by analytical differentiation, although the reliability of such a measure is questioned by Chimowitz *et al.* (1983).

Several papers have been published on local models during the last ten years or so, and a review of some works is given by Grens (1983), while more recent works include Chimowitz *et al.* (1984), Macchietto *et al.* (1986), Clark and Reklaitis (1986) and Johns (1985). Models are mainly developed for K-values and fugacity coefficients, but others, such as vapour pressure, liquid activity coefficients and enthalpy

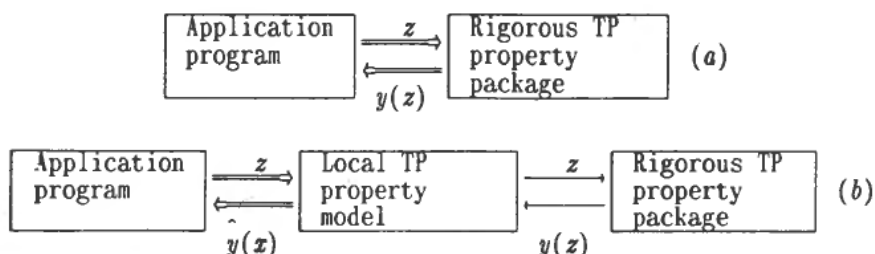


Figure 1. The conventional approach (a) and the application of local model (b). Frequent and less frequent calls are indicated by (=) and (—), respectively.

evaluations, are also treated. The simplified K-value model applied here is one that neglects the interaction between the component itself and the remaining mixture constituents. Only pressure, temperature and liquid mole fraction dependencies are explicitly represented in the following mathematical structure:

$$\ln(K_i P) = \theta_{1i} + \theta_{2i}/T + \theta_{3i}(1 - x_i)^2 \quad (1)$$

More advanced local models that take into account non-ideal effects are proposed by Chimowitz *et al.* (1983), though these are found not to be necessary here.

The class of local models that is investigated here includes the one above and most other known local models suggested. All are linear in the parameters and can be expressed as:

$$\hat{y}(x) = \theta^T x \quad (2)$$

Here, x may be labeled the observation vector or the vector of independent variables and contains some of the process state variables or transformations of these. θ is the vector of adjustable parameters. For model (1) above, the property for the i th component is $\ln(K_i P)$ and the observation vector is given by:

$$x^T = [1, 1/T, (1 - x_i)^2] \quad (3)$$

Note that the observation vector x in (2) will normally contain a constant element. Then, x cannot attain all possible values and therefore the local model will normally not go through the origin. Alternatively, the local model can be written as $\hat{y}(x) = c + \theta^T x$. Here the dimension of the θ vector and the x vector is one less than in equation (2). When x is augmented with a constant, it does not affect the analysis as presented here. Expression (2) is chosen because the parameters are gathered in one single vector.

One of the problems with applying local thermodynamic models in process simulation, which is the main issue of concern in this work, is that there are no adequate procedures for deciding when to update the local model parameters. Since the local parameters are to be updated in an adaptive manner, the deviation of the local model from the exact rigorous model has to be estimated somehow. As soon as the error exceeds the specified tolerance, the parameters must be updated to give a good fit to the rigorous model in the region of interest. The local model should be sufficiently accurate, but at the same time it should *not* be updated more than needed to attain the required accuracy.

While the method, as proposed by Macchietto *et al.* (1986), based on selecting a time interval where the next update is to be done, may be effective, it is found to be theoretically inadequate because the error is not an explicit function of time. Also the error function proposed by Clark and Reklaitis (1986) is found to be insufficient as it is an *ad hoc* method. In the present paper, however, we propose a method for predicting the error, that is general in character and that is based on the true independent variables. With this method, changes in the independent variables which fall outside the region of validity are detected immediately and the local model is updated.

2. Parameter estimation

The deterministic local model (2) is estimated by means of ordinary least squares fitting to the rigorous model. As the local parameters are to be updated in an adaptive manner, a recursive least squares procedure is applied. In such procedures it is

common to introduce forgetting in the updating of the covariance matrix in order to weight adjacent information more than remote. The algorithm may also be implemented with variable forgetting as the one proposed by Fortescue *et al.* (1981).

$$\theta_{k+1} = \theta_k + K_{k+1}\mu_{k+1} \quad (4)$$

$$\mu_{k+1} = y_{k+1} - y_k(x_{k+1}) \quad (5)$$

$$K_{k+1} = P_k x_{k+1} [1 + x_{k+1}^T P_k x_{k+1}]^{-1} \quad (6)$$

$$P_{k+1} = [I - K_{k+1} x_{k+1}^T] P_k / \lambda_{k+1} \quad (7)$$

$$\lambda_{k+1} = 1 - \mu_{k+1}^2 [1 - x_{k+1}^T K_{k+1}] / \Sigma_0 \quad (8)$$

A problem that may occur with this algorithm is that the covariance matrix P_{k+1} will increase exponentially if there is no or little excitation of x and if λ is less than one. This may create a situation known as blow-up, implying that the parameter vector will become extremely sensitive to even small deviations between the rigorous and the local model. Sælid *et al.* (1985) have solved this problem by proposing an algorithm where the amount of information introduced for each parameter is equal to the amount forgotten. The diagonal elements of the covariance matrix P_{k+1} are thus held constant. Although there could be possibilities that some elements of the observation vector may be insufficiently excited during the simulation and thereby the danger of encountering blow-up situations, this was not observed, and therefore algorithm (4)–(8) was used without problems for the examples studied here.

The local model parameters and the covariance matrix have to be initialized since the procedure is recursive. The approach applied here is to postpone the simulation until the parameters and the covariance matrix are estimated. During this initialization phase, the independent variables of the local model are excited independently to obtain good estimates of both the parameters and the covariance matrix. These initial updates require evaluations of the rigorous model which are not used in the simulation. In most cases, however, these redundant rigorous evaluations are few compared to the total number of updates during the simulation.

3. Error estimation

The most essential concern with the application of local TP property models is knowing when to update the model parameters. A procedure that is economic in its use of the rigorous model should call for the rigorous routines only when the deviation between the rigorous and the local model exceeds a specified tolerance. Therefore, in order to employ an adaptive strategy, it is necessary to have an approximate estimate of the error. Whenever the process state variables fall outside the region of validity, the model parameters will be updated.

3.1. Error structure

Since this approach is intended to be of general character, the rigorous model is approximated by a Taylor series expansion around the last updated point x_k and the series is truncated after three terms.

$$y(x) \approx y_k + [\partial y / \partial x]_k^T (x - x_k) + \frac{1}{2} (x - x_k)^T [\partial^2 y / \partial x^2]_k (x - x_k) \quad (9)$$

Here, y_k is the exact rigorous value at x_k . Let us assume that the local parameter vector is fitted to the rigorous model such that:

$$\theta_k = [\partial y / \partial x]_k \quad (10)$$

This is not exactly true, but θ_k is after all the best approximation to the first derivative of y available at x_k . Since the local model is given $\hat{y}_k(x) = c_k + \theta_k^T x$, the deviation between the rigorous and the local model can be expressed as:

$$\begin{aligned} \varepsilon_k(x) &= y(x) - \hat{y}_k(x) \\ &\approx y_k - \hat{y}_k(x_k) + \frac{1}{2}(x - x_k)^T [\partial^2 y / \partial x^2]_k (x - x_k) \end{aligned} \quad (11)$$

Hence, the estimated error is assumed to attain a quadratic structure and may be written briefly as:

$$\varepsilon_k(x) = \varepsilon_k(x_k) + \frac{1}{2}(x - x_k)^T Q_k (x - x_k) \quad (12)$$

$\varepsilon_k(x_k) = y_k - \hat{y}_k(x_k)$ is known exactly from the last updating, but it is a small quantity and might as well be neglected from the expression. Q_k is an estimate of the Hessian matrix, but it includes higher derivatives as well. It is a measure of the curvature of the rigorous model and thus the deviation from a linear model.

3.2. Updating scheme

The problem which confronts us is how to get an estimate of the curvature, or more precisely, how to estimate the matrix Q_k . A possible way is by numerical approximation of the Hessian by perturbation of x around x_k . This approach will, however, require too many calls to the rigorous package and thus the whole idea of applying local models becomes fruitless. Needless to say, a necessary condition for applying local thermodynamic models is that the computational procedure is efficient.

Rather, let us assume that expression (12) is provided with an approximate matrix Q_k which can be applied for estimating the error in the neighbourhood of a fixed point x_k . If the predicted error exceeds the tolerance at x_{k+1} , a rigorous model evaluation is made and the local parameters are updated. At the same time, the exact error is made available by measuring the difference between the rigorous and the local value at x_{k+1} . By fitting the same error structure (12) to the measured error (μ_{k+1}), but now with the corrected curvature matrix H_k , we have a possible scheme for correcting Q_k . The predicted and the measured error at x_{k+1} may thus be written:

$$\varepsilon_{k+1} = \frac{1}{2} p_{k+1}^T Q_k p_{k+1} \quad (13)$$

$$\mu_{k+1} = \frac{1}{2} p_{k+1}^T H_k p_{k+1} \quad (14)$$

The vector p_{k+1} is the difference between two succeeding updatings; $p_{k+1} = x_{k+1} - x_k$. The difference between the measured and predicted errors is defined as:

$$\delta_{k+1} = \mu_{k+1} - \varepsilon_{k+1} = \frac{1}{2} p_{k+1}^T [H_k - Q_k] p_{k+1} \quad (15)$$

The way equation (15) is written, δ_{k+1} may attain all real values. However, in order to avoid failing to update the model when it should be updated, the absolute value of the predicted error should be greater or preferably equal to the absolute measured error. This is the desired situation, but may not always be the case.

Since one measurement (μ_{k+1}) is available at each parameter revision, the corrected matrix may be written as a rank-one update of the one used for prediction.

$$H_k = Q_k + uv^T \quad (16)$$

Substituting equation (16) into (15), it reduces to

$$\delta_{k+1} = \frac{1}{2} p_{k+1}^T uv^T p_{k+1} \quad (17)$$

So long as v is not orthogonal to p_{k+1} , we have a well-defined u vector and thus any rank-one update will satisfy (17). A possible choice of v is a vector parallel to p_{k+1} . By choosing $v = p_{k+1}$ and by defining the scalar $s_{k+1} = p_{k+1}^T p_{k+1}$, equation (17) becomes

$$p_{k+1}^T u = 2\delta_{k+1}/s_{k+1} \quad (18)$$

The vector u is not uniquely determined by a single equation, but u can at least be chosen such that equation (18) is satisfied, and a possible choice is

$$u = p_{k+1} 2\delta_{k+1}/s_{k+1}^2 \quad (19)$$

With this choice of u , the correction of Q_k to obtain H_k can be made according to the following equation

$$H_k = Q_k + p_{k+1} p_{k+1}^T 2\delta_{k+1}/s_{k+1}^2 \quad (20)$$

We may easily convince ourselves that equation (20) satisfies (13) and (14) by pre- and post-multiplication of p_{k+1} .

Finally, in order to have a complete updating scheme, the curvature of the rigorous model is assumed to be constant over the interval p_{k+1} such that the matrix used for predicting the error around next working point, x_{k+1} , is set equal to H_k . Thus, the complete recursive updating scheme reads

$$Q_{k+1} = Q_k + p_{k+1} p_{k+1}^T 2\delta_{k+1}/s_{k+1}^2 \quad (21)$$

In process simulations, the Q matrix will possibly be updated several times along the state trajectory. At each updating, the new estimate of the Q matrix will only be improved in the direction of the last movement, p_{k+1} . In directions perpendicular to the last movement, however, the error function with Q_{k+1} will predict the same error as with Q_k .

As with the parameter covariance matrix, the initialization of the Q matrix is made by perturbation of the independent variables. During this initialization phase, the local parameters, the covariance matrix and the Q matrix are estimated.

4. Application of dynamic simulation

The methods described here for recursive parameter estimation and for predicting the error of the local thermodynamic models are applied in studies of dynamic simulation of a batch distillation column (cf. the Appendix). The batch distillation model requires repetitive bubble point calculations, and it is a typical case where the application of local K-value models may be advantageous. Only equilibrium ratios are approximated by the use of local models, while enthalpies are supplied by rigorous thermodynamic routines. The local K-value models are interfaced with the process model through a completely transparent thermodynamic property routine.

The differential-algebraic equations describing the column are solved by means of a diagonal implicit Runge-Kutta integration method with step length control. Although the model is sparse, a full matrix solver is used with the integrator. Many functional evaluations may surely be saved by using a sparse solver, but this is of little importance to the main issue addressed here, namely the number of rigorous property evaluations compared to the total number of property evaluations.

Two different mixtures are distilled. The first is a nearly ideal hydrocarbon mixture while the second is a strongly non-ideal system. For each of the two mixtures, two solutions are obtained; first, the conventional solution by using only rigorously calculated K-values, and the second solution is obtained by the use of local model K-value models. A local K-value model corresponding to the one in equation (1) is selected for both mixtures.

The column trays, including the reboiler and the condenser, are viewed as separate process units with distinct sets of local model data. Each process unit is updated independently of each other, but all the K-value models within each unit are chosen to be updated simultaneously.

Before starting the simulation with the local approximations, the parameters, the covariance matrix and the Q matrix for all local models in each unit are initialized by perturbation around the initial point. After the initialization phase, forgetting is introduced in the update of the local model covariance matrices as described by Fortescue *et al.* (1981).

Obviously, the number of evaluations of the distillation model and thus also the number of TP property evaluations are dependent on the integration accuracy. The number of local model updates, however, is found to be nearly independent of the integration accuracy in the two examples studied here. Therefore, the proportion of rigorous TP calls decreases with increasing integration accuracy.

Example 1: ideal mixture

In Example 1, the mixture consists of *n*-butane, *n*-pentane and *n*-hexane which is distilled with constant distillate flow rate and constant external reflux ratio. The local K-value model (1) is updated with reference to a rigorous model based on the SRK equation of state. The simulation is performed according to the specifications given in Table 1 in the Appendix.

The maximum allowed relative deviation between rigorous properties and local model approximations is set to 1%. In Fig. 2, the liquid mole fractions in the condenser obtained by the two solutions are shown. Likewise, Fig. 3 shows the corresponding K-value solutions. In Fig. 4, the observed relative errors in the local model approximations are shown.

As little as 0.8 and 0.4% of the total number of property evaluations were calls to the rigorous package when the integration accuracy were 10^{-3} and 10^{-4} , respectively. Although the number of rigorous evaluations becomes significantly less by applying a local K-value model, the CPU reduction is not very substantial for this example because the SRK model is in itself not very heavy.

Example 2: non-ideal mixture

In Example 2, the batch column is run with the strongly non-ideal mixture of acetone, acetonitrile and water. A TP property package based on the NRTL equation of state is used for obtaining the rigorous K-values, while model (1) is still

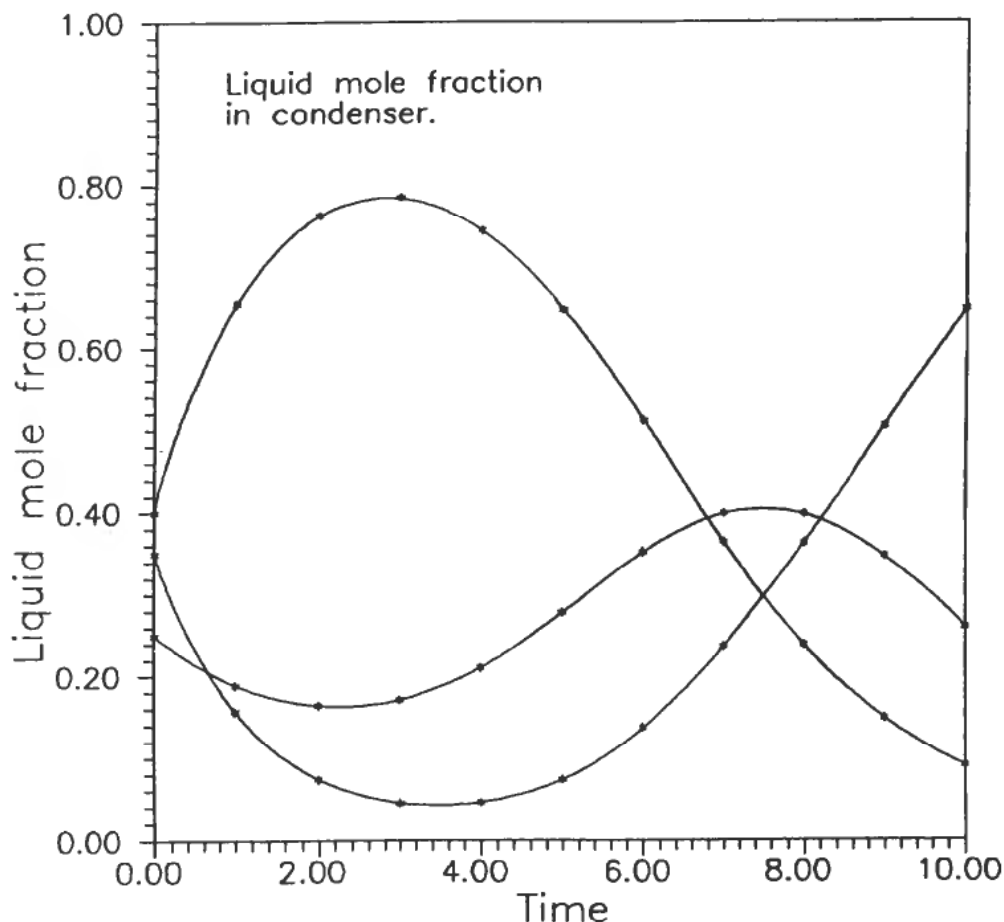


Figure 2. Liquid mole fraction transients in the condenser of Example 1; solutions obtained with local models (lines) and with rigorous models (dots).

employed as local model. During the first part of the simulation, the column is run with total external reflux until it reached stationary conditions. The column is operated at steady state condition for some time before the distillate flow rate is set to a constant value which induces a transition state in the system.

Also here, the maximum allowed relative deviation between the rigorous and the local models is 1%. Diagrams indicating the accuracy of the local solutions are given in Fig. 5 and 6 where both the rigorous and the local solutions are plotted. Due to non-ideality and longer periods of transients, the proportion of updates of the local model parameters increased as expected compared to Example 1. The proportion of rigorous updates amounted to 10 and 4.2% of the total number of rigorous TP evaluation when the integration tolerance were 10^{-3} and 10^{-4} , respectively. Figure 7 shows the measured relative error at the updated points.

Compared to the local model, the rigorous K-values based on the NRTL equation are computationally much more expensive. The CPU time spent on one call to the thermodynamic package based on local models, with and without an update, and the time spent on a call to the rigorous NRTL K-value routine are measured. A

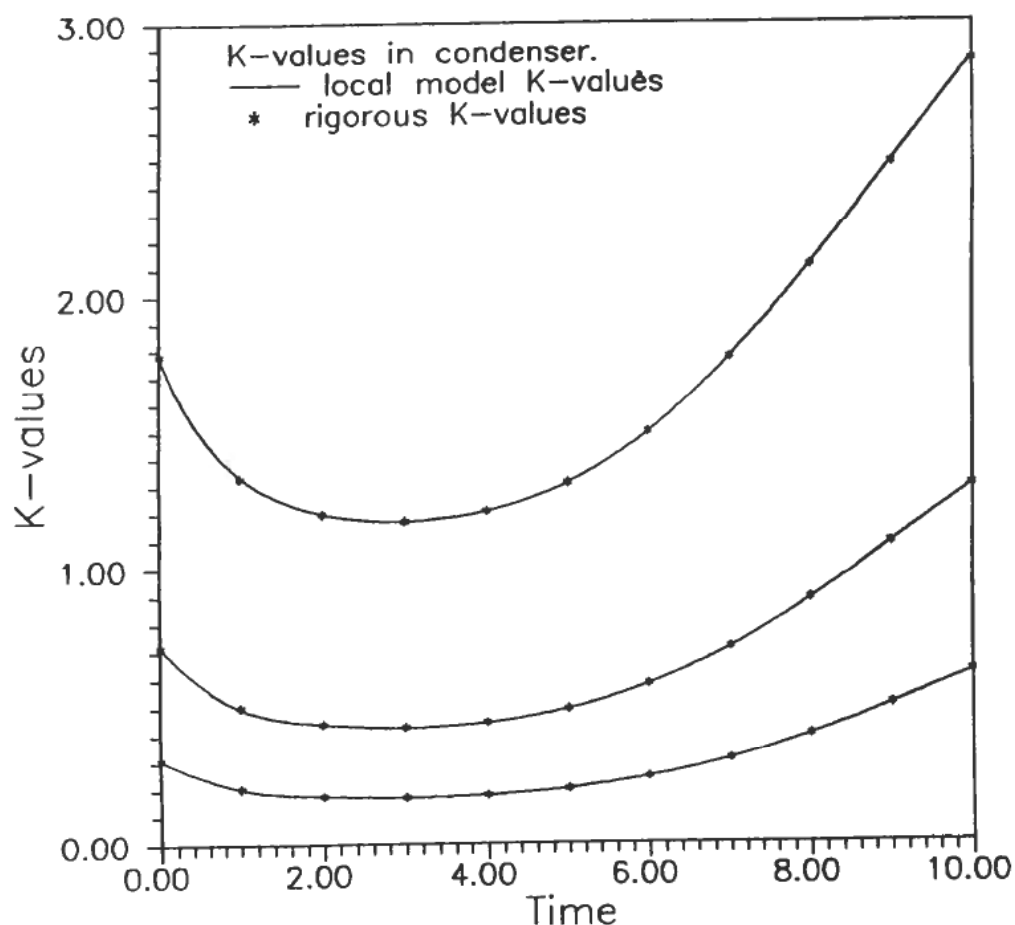


Figure 3. The local (lines) and the rigorous (dots) K-values as function of time.

ratio of about 7 : 1 between local K-value approximations with and without an update is observed. While the ratio between a call to the rigorous NRTL K-value routine, and a local model call without any update is measured to about 4 : 1. This should indicate that simulations using less than 50% updates of the local models will have a reduction in the time spent on the calculation of thermodynamic properties. Less than 10% updates of the local model gives more than 43% savings in the CPU time.

5. Discussion

It is obvious from the assumptions and the specifications of the column model that it is not intended to simulate a completely realistic operation of a batch distillation. The physical property routines, however, are realistic enough. Rather, the intention of this work has been to develop a transparent program that can be inserted between any rigorous TP property package and an application program, as for example a model for dynamic simulation of a batch distillation column. This is

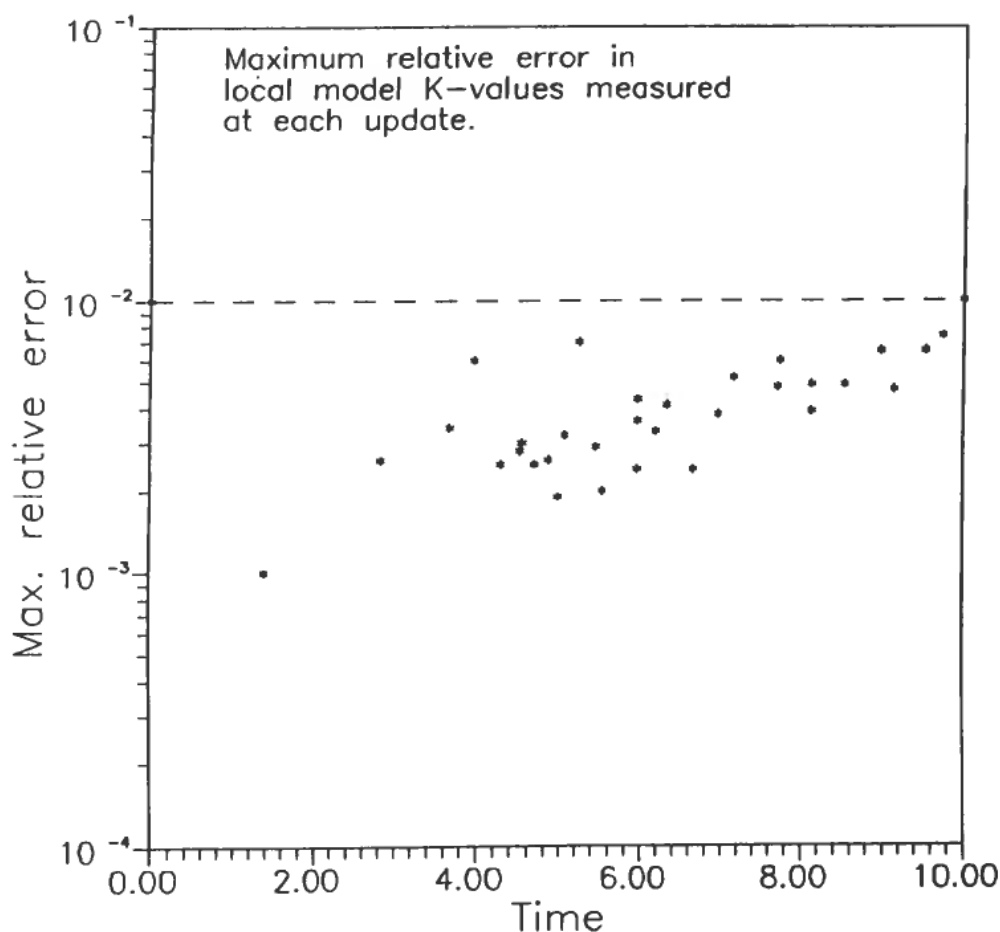


Figure 4. The maximum relative error measured at each update of Example 1; the property tolerance limit is indicated by the dashed line.

accomplished, and the developed procedure for predicting the deviation between the local and the rigorous models has proven to be both effective and accurate. The accuracy of the error prediction is illustrated in Fig. 4 and 7, which show that the measured error is mostly within the tolerance limit and at the same time not far below.

The application of local TP property models in distributed parameter systems is, naturally, not restricted to our example with a distillation column. In the general case, where partial differential equations are to be solved, local models are assigned to each component for each discrete point in space. As each model may have its own error control, the data sets are updated independently. If it is desirable to move the discretization points in space to track a moving front of the solution, for example, this will not cause any difficulties for the application of local property models as described here. This is because the applied error structure is based on the true independent variables.

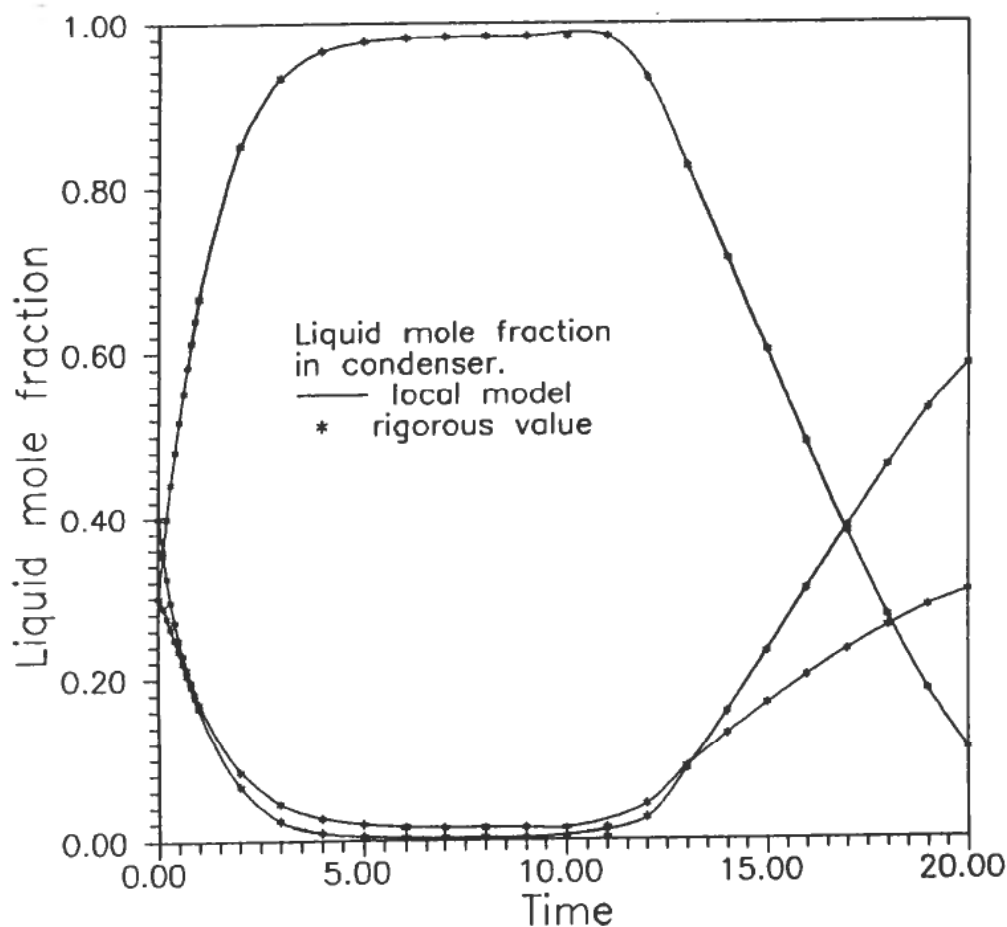


Figure 5. Liquid mole fraction transients in the condenser of Example 2: solutions obtained with local models (lines) and with rigorous models (dots).

5.1. Efficiency

The efficiency of the proposed method for predicting the deviation between the local and the rigorous TP property models is close to optimal. This is because the method does not pose any additional property evaluations except for a few in the initialization phase. Compared to the total number of updates needed during the simulation, the initialization requires minor work.

The overall reduction in CPU time, when the method is implemented in a dynamic process simulation model, must be seen in context with the efficiency and the accuracy of the error prediction. Obviously, the number of rigorous property evaluations required will also depend on the problem characteristics, such as the duration of transients, the non-ideality of the system and the local model structure. For the two systems studied here, which are not considered untypical, less than 10% rigorous property evaluations are needed in order to attain the required accuracy of 1% relative. This will give substantial reductions of the overall computational costs in dynamic process simulations and can undoubtedly have a great impact in study-

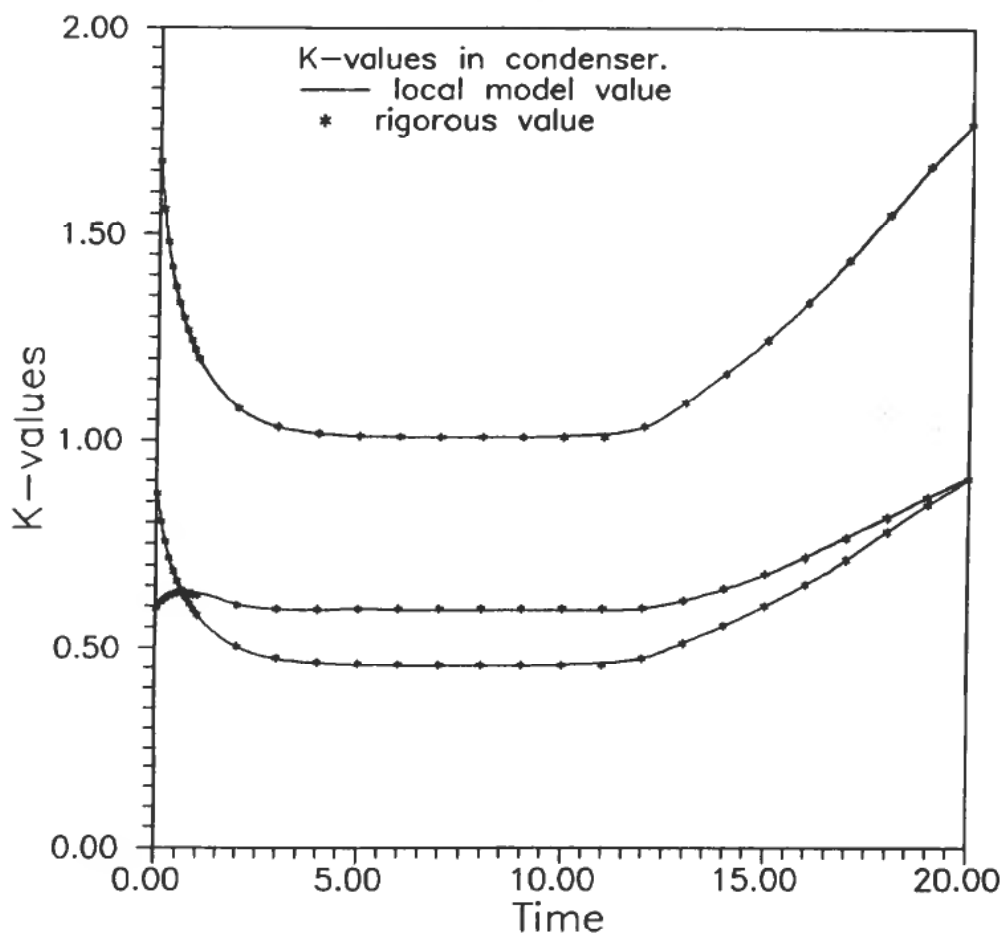


Figure 6. Local (lines) and rigorous (dots) K-values as function of time.

ing transient behaviour of large scale process systems and in attempting real time simulations.

Another observation, made from the simulations, is that integrating the model with local property models required fewer right-hand side evaluations than if the rigorous property models were called directly. This has also contributed to increasing the overall efficiency. However, the number of integration steps taken by the two approaches are the same. In fact, the model equations with the use of local property models will become more sparse than if only rigorous models were applied since the weak couplings are neglected in the former. In reality, two different models are solved which have approximately the same solution. Since an implicit integration method is used, a possible explanation of the difference in the number of right-hand side evaluations could be that the sparser model converges the non-linear algebraic equations faster than the other.

5.2. Stored information

The principal disadvantage of applying local thermodynamic property models, instead of using merely the rigorous models, is that the former requires much additional information to be stored. Therefore, the reductions in CPU time are to some

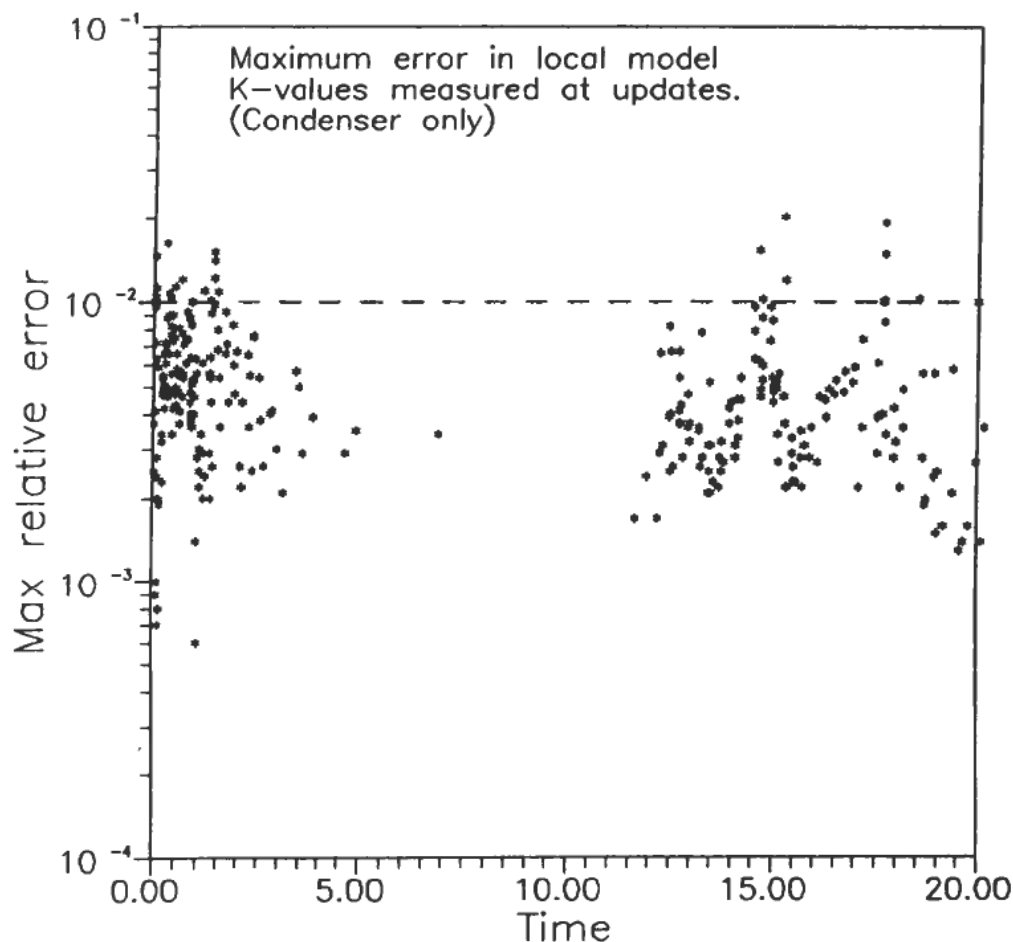


Figure 7. Maximum relative error measured in local K-values of Example 2.

extent compensated by an increase in the storage requirements. On the other hand, the cost of memory is no longer critical. For example, each component on each tray in our distillation column requires a distinct set of data which includes the parameter vector, the covariance matrix and the curvature matrix. In addition, each component may also have different kinds of local property models as for example K-values, activity coefficients, etc. Fortunately, the dimensions of the vectors and matrices are small, typically four, and only half the information of the matrices needs to be stored as they are symmetric.

6. Conclusions

The proposed method for predicting the deviation between the local and the rigorous thermodynamic models has proven to be both accurate and efficient. The proportion of rigorous property evaluations, which depends on the duration of transients, the non-ideality of the mixture and the local model structure, is reduced

almost to a minimum by the proposed method. Substantial savings in CPU time are obtained by simulating the dynamic behaviour of a batch distillation column with the use of local K-value approximations.

Nomenclature:

H_k	The corrected curvature matrix at x_k .
K_{k+1}	Kalman gain vector defined in equation (6).
p_{k+1}	Calculated difference between two succeeding updatings; $p_{k+1} = x_{k+1} - x_k$.
P_k, P_{k+1}	Parameter covariance matrices at x_k and x_{k+1} , respectively.
Q_k, Q_{k+1}	Matrix used for predicting the error around x_k and x_{k+1} .
s_{k+1}	$s_{k+1} = p_{k+1}^T P_{k+1}$
u	vector defined in equation (16).
v	Vector defined in equation (16).
x, x_k	Independent variables of the local model, continuous and discrete.
$y(x)$	Rigorous property model.
y_k	Rigorous property evaluated at x_k ; i.e. $y_k = y(x_k)$.
$\hat{y}_k(x)$	Local property model; $\hat{y}_k(x) = \theta_k^T x$.
z	Independent variables of the rigorous model.

Greek letters:

δ_{k+1}	Difference between the measured and predicted error, defined in equation (15).
ε_{k+1}	Predicted error at the border of the region; $\varepsilon_{k+1} = \varepsilon_k(x_{k+1})$.
$\varepsilon_k(x)$	Function for predicting the error around x_k , defined in equation (12).
λ_{k+1}	Forgetting factor for updating the covariance matrix.
μ_{k+1}	Measured error between the rigorous and the local model.
θ_k	Parameter vector updated at x_k .
Σ_0	Amount of information in the forgetting procedure.

Appendix

Batch distillation model

Assumptions

- Constant molar holdup on trays
- Constant molar holdup in condenser
- Negligible rate of change of internal energies in the column
- Negligible vapour holdup
- Negligible fluid dynamic loop
- Theoretical trays
- Chemical equilibrium on each tray
- Adiabatic operation
- Stationary and linear pressure profile along the column

Model equations

Condenser: (tray 1)

$$n_c \dot{x}_{i,1} = V_2 K_{i,2} x_{i,2} - D(R+1)x_{i,1}$$

$$V_2 H_2 = D(R+1)h_c + Q_c$$

$$V_2 = D(R+1)$$

*j*th tray: ($1 < j < r$)

$$n_j \dot{x}_{i,j} = L_{j-1}x_{i,j-1} + V_{j+1}K_{i,j+1}x_{i,j+1} - (L_j + V_j K_{i,j})x_{i,j}$$

$$V_{j+1}H_{j+1} + L_{j-1}h_{j-1} = V_j H_j + L_j h_j$$

$$L_j = V_{j+1} - D$$

Reboiler: (tray *r*)

$$n_r \dot{x}_{i,r} = L_{r-1}x_{i,r-1} - V_r x_{i,r} K_{i,r} + x_{i,r} D$$

$$Q_r = V_r H_r - L_{r-1}h_{r-1}$$

$$\dot{n}_r = -D$$

Nomenclature

n_j	number of moles on tray <i>j</i>	n_c	number of moles in the condenser
L_j	liquid molar flowrate	V_j	vapour molar flowrate
h_j	liquid molar enthalpy	H_j	vapour molar enthalpy
$K_{i,j}$	equilibrium ratio	$x_{i,j}$	liquid mole fraction
Q_c	condenser duty	Q_r	reboiler duty
D	distillate flowrate	R	external reflux ratio
i	<i>i</i> th component	j	<i>j</i> th tray
r	total number of trays		

		Example 1	Example 2
Mixture	(1)	n-butane	acetone
	(2)	n-pentane	acetonitrile
	(3)	n-hexane	water
Initial vapor and liquid molefrac. ($x_i = y_i$)	(1)	0.40	0.3
	(2)	0.35	0.3
	(3)	0.25	0.4
Condenser and reboiler pressure		4.5 bar	1.0 bar
		5.0 bar	1.9 bar
Molar liquid holdup			
condenser:		20.0 mol	10.0 mol
trays:		1.0 mol	1.0 mol
reboiler: (initial)		110.0 mol	110.0 mol
Distillate			
time interval:		0-10 hour	0-11/11-20 hour
reflux ratio:		1.4	$\infty/3$
distillate flow rate:		10.0 mol/h	0/7.5 mol/h
Number of trays		5	10

Table 1. Problem specifications.

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