

RIGOROUS DYNAMIC SIMULATION OF DISTILLATION COLUMNS BASED ON UV-FLASH

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Abstract. The paper demonstrates that a rigorous dynamic simulation for distillation columns, including varying pressure and vapor holdup is feasible using a UV-flash approach. A strategy is presented for calculating this flash efficiently when used in dynamic simulation. The paper also considers use of local thermodynamic models combined with look-up tables, where all variables are continuous in time. The results are illustrated on a propane-butane fractionator where the vapor holdup is considerable and should not be neglected.

Key Words. Distillation; Process dynamics; Stiff systems; Numerical efficiency

1 INTRODUCTION

Most static and dynamic models for distillation columns are based on a staged model with equilibrium between the vapor and the liquid. Energy and material balances on each stage result in a model with the internal energy U and the component holdups n_j as the mathematical states. Since the volume \mathcal{V} of each stage is constant, this leads directly to a problem formulation where the solution of a UV-flash is a key element. The definition of a UV-flash is: Given the internal energy U , volume \mathcal{V} and the component holdups (n_j), do a flash calculation to find the vapor fraction f , the composition in the vapor and liquid phase (y_j and x_j), the pressure (P) and the temperature (T).

$$(U, \mathcal{V}, n_j) \rightarrow (T, P, f, x_j, y_j) \quad (1)$$

This approach allows both for varying pressure and including the vapor holdup. Surprisingly, as noted in a review paper by Skogestad (1992), there are almost no references in the literature where this seemingly most natural solution approach is taken; one exception seems to be a recent paper by Gani *et al.* (1990). Why is the U -approach not used more?

1. One likely reason is numerical difficulties, that is, that the resulting set of differential equations (ODEs) is very stiff when the pressure is allowed to vary, and that a UV-flash calculation can be very time consuming, in particular when implemented as an outer iteration around a more conventional flash calculation.

2. A trivial possibility is that the approach has been used, but not published.

3. Another trivial reason is that most dynamic distillation programs are derived from steady-state packages where the stage volume (and the liquid and vapor holdup) does not affect the solution, and where the pressure at some point in the column is almost always specified, which means that bubble-point flashes may be used. Therefore, most dynamic simulators have incorporated assumptions like neglected vapor holdup or constant pressure which lead to a bubble-

point flash.

One of the objectives of our work was therefore to find out whether there could be any fundamental problems that made the rigorous UV-flash approach undesirable.

In the paper we also discuss several other issues such as: a) Modeling assumptions in distillation leading to a UV-flash approach. b) Efficient flash algorithms for dynamic simulation. c) Use of local thermodynamics models, particularly with the aim to avoid discontinuities in the parameters.

2 DYNAMIC DISTILLATION MODELS

In this paper we only consider equilibrium-based distillation models using a fixed number of equilibrium stages. Even for an equilibrium model one may divide each tray in a distillation column into several control volumes, for example, one for the downcomer and one for each of the phases on the tray. One may also introduce a plate efficiency calculations to correct for nonequilibrium. However, in this paper we make the simplifying assumption that each tray is a single equilibrium stage with complete equilibrium between the two phases, leading to an UV-flash approach as noted in the introduction. The assumptions we have made:

A1 *Perfect mixing in both liquid and vapor phase on each stage.*

A2 *The two phases are in thermodynamic equilibrium (assume 100 % tray efficiency).*

In this work we also make the following assumptions:

A3 *Neglect heat loss and neglect thermal capacity of the column walls and internals.*

A4 *"Normal operation", with no flooding, weeping, flow reversal, etc.*

Assumptions A3 are discussed by McGreavy *et al.* (1986). It is easy to extend the model to overcome assumptions A3 and A4.

2.1 Model based on UV -flash

The equations for a stage in a distillation column are the mass and energy balances, together with the hydraulic equations (to describe the overall liquid and vapor flows) and the vapor-liquid equilibrium (VLE). This leads to the following set of equations for a stage with no feed, product or heat exchange:

Molar balances for n_c components ($j = 1, n_c$):

$$\frac{d(n_{i,j})}{dt} = V_{i-1}y_{i-1,j} + L_i x_{i,j} - V_i y_{i,j} - L_{i+1} x_{i+1,j} \quad (2)$$

Energy balance :

$$\frac{d(U_i)}{dt} = V_{i-1}h_{V,i-1} + L_i h_{L,i} - V_i h_{V,i} - L_{i+1} h_{L,i+1} \quad (3)$$

Flash relationship (VLE):

$$(U_i, V_i, n_{j,i}) \rightarrow (T_i, P_i, x_{i,j}, y_{i,j}, h_{V,i}, h_{L,i}, f_i, M_{V,i}, M_{L,i}) \quad (4)$$

Vapor flow :

$$V_i = f_V(P_i - P_{i+1}, M_{L,i+1}, \text{geometry}...) \quad (5)$$

Liquid flow :

$$L_i = f_L(M_{L,i}, P_i - P_{i-1}, V_{i-1}, \text{geometry}...) \quad (6)$$

The mathematical states are the component holdups $n_{i,j}$ (in both phases combined) and the internal energy U_i . Here subindex i denotes stage number (which is sometimes deleted in the following), subindex j denotes component number, $y_{i,j}$ and $x_{i,j}$ denote mole fractions, V_i denotes stage volume, f_i denotes vapor fraction, V_i, L_i , denotes molar streams leaving stage i , $h_{V,i}, h_{L,i}$ denotes molar enthalpies, and $M_{V,i} = f_i \sum_j n_{i,j}$ and $M_{L,i} = (1 - f_i) \sum_j n_{i,j}$ denote total vapor and liquid holdup. The vapor and liquid flows are calculated from hydraulic equations as indicated by (5) and (6). Lockett (1986) gives an excellent overview over different approaches.

Solution. This set of differential and algebraic equations (DAEs) may be solved simultaneously using a DAE-solver like DASSL. In the alternative ODE-approach, which is the one taken in this paper, one reduces by elimination the DAE system to a set of ordinary differential equations (ODEs). That is, at each integration step one knows the states ($n_{i,j}$ and U_i) and the volume (V_i) at each stage, and solves separately the algebraic equations, including the resulting UV -flash in Eq. (4). The main advantage of the ODE-approach compared to the simultaneous DAE-approach is that it is easier to make use of any special structure in the flash equations. The main disadvantage is that one has to converge the algebraic equations for each case the ODE solution algorithm

requires an evaluation of the derivatives. Pantelides and Barton (1992) point out that this can be very inefficient if there is a large number of implicit algebraic equations. However, Perregaard *et al.* (1992) compared the two approaches numerically on three distillation column examples, and found that with their algorithms the ODE approach is between one and three times more efficient.

2.2 Model based on bubble-enthalpy flash

Another very common simplification in distillation models is to:

A5 Neglect the vapor holdup.

We then have $x_{j,i} = n_{i,j}/M_{L,i}$. Choe and Luyben (1987) conclude that the vapor holdup should be included if the pressure is greater than 5-10 bar. For liquids the following assumption is also valid:

A6 The liquid specific enthalpy is equal to the specific internal energy, $h_L = u_L$.

With these two additional assumptions the UV -flash is replaced by a bubble-point flash with given (h_L, x_j) . Note that the stage pressure is not assumed fixed in this approach. Gani *et al.* (1986) and Choe and Luyben (1987) use this approach.

It is often claimed that the equations are easier to solve when we neglect the vapor holdup, but this is not correct as the vapor flows are still calculated from equation (5) resulting in a stiff set of equations due to the small pressure driving forces. We therefore conclude that neglecting the vapor holdup :

1. Does not affect the number of mathematical states.
2. Does not imply immediate vapor response.
3. Does not reduce the stiffness (the effect is rather opposite).

2.3 Model based on bubble-pressure flash

To reduce the stiffness and make the flash even simpler the following additional assumption is often introduced:

A7 Fixed pressure on the trays.

This assumption, often justified because pressure is tightly controlled, replaces the vapor flow hydraulic equation (5). Since the pressure, which is a dependent variable in the original formulation, is now specified we get an index problem. The minimum number of independent states are reduced by one for each stage, but the number of differential equations remains the same. We may solve this problem by rearranging the energy balance to compute the vapor flow.

$$V_i = \frac{1}{h_{V,i} - h_{L,i}} (V_{i-1}(h_{V,i-1} - h_{L,i}) + L_{i+1}(h_{L,i+1} - h_{L,i}) - M_{L,i} \frac{d(h_{L,i})}{dt}) \quad (7)$$

Conceptually, this an algebraic equation since we may express $d(h_{L,i})/dt$ as a function of the states, for example, by obtaining the differential of h_L with respect to the states numerically or analytically. However, this may be difficult and time consuming. Fuentes and Luyben (1982) proposed to estimate $d(h_{L,i})/dt$ numerically using previous time step and we use same approach in this paper. One problem with such an *ad hoc* scheme (which corresponds to an outer Euler integration) is that it destroys the convergence of high-order integration methods like Runge-Kutta or Gear. One way to avoid this problem is to use the following common assumption:

A8 Assume $d(h_{L,i})/dt = 0$

Fuentes and Luyben (1982) concluded that this assumptions should *not* be used, and the simulations we present later seem confirm this. However, the validity of assumption **A8** depends entirely on the reference state. Both in Fuentes and Luyben (1982) and in our work the reference state is the pure components as liquid at a fixed temperature, and in this case assumption **A8** will hold only if the temperature differences along the column are small. However, if we want to make use of assumption **A8** a better choice is to use as a reference state the pure components as boiling liquids at a *fixed pressure*. This makes h_L a function of both composition and temperature (even for the case when c_{pL} is the same for all components), and due to cancelling effects h_L will remain approximately constant along the column, and we find that $dh_{L,i}/dt$ is small.

It should be noted that Eq.7, which is now used to compute V_i , depends on the liquid flow, whereas Eq.6, which is used to compute L_i , depends on the vapor flow (because the froth density depends on the vapor flow). Thus, these two equations should be solved simultaneously. If one fails to do this, and for example uses the vapor flow from the previous integration step when evaluating L_i , then one will again destroy the accuracy of a high-order integration method, and the integration may stall.

Partly because of problems as just noted we did not obtain a considerable reduction in simulation time when assuming constant pressure, in spite of the fact that the stiffness of the equations was reduced several orders of magnitude.

3 FLASH CALCULATIONS

We here consider algorithms to solve the UV -flash at each stage (the index i denoting the stage number is deleted in the following). The first step is to introduce intensive variables, i.e., the specific molar energy, u , the specific molar volume, v , and the overall phase composition, z_j .

$$u = \frac{U}{M}; \quad v = \frac{V}{M}; \quad z_j = \frac{n_j}{M} \quad (8)$$

where $M = \sum_{j=1}^{n_c} n_j$ denotes the total holdup on a stage. The UV -flash then becomes

$$(u, v, z_j) \rightarrow (T, P, f, x_j, y_j) \quad (9)$$

The set of equations indicated by (9) consists of $2n_c + 3$ equations in $2n_c + 3$ unknowns (T, P, f, x_j, y_j). The following equations are used:

n_c component material balances:

$$(1 - f)x_j + fy_j - z_j = 0 \quad (10)$$

n_c equilibrium relations:

$$f_j^V - f_j^L = 0 \quad (11)$$

where the fugacities f_j^L and f_j^V are known functions of T, P, x_j, y_j .

1 summation of molefraction :

$$\sum_{j=1}^{n_c} (y_j - x_j) = 0 \quad (12)$$

(The above $2n_c + 1$ equations apply to any two-phase system.) Finally, for the UV -flash the internal energy and volume is specified, yielding two additional constraints:

$$g_u(T, P, f, x_j, y_j) = u - (1 - f)u_L - fu_V = 0 \quad (13)$$

$$g_v(T, P, f, x_j, y_j) = v - (1 - f)v_L - fv_V = 0 \quad (14)$$

Here the specific molar energies (u_L, u_V) and the specific molar volumes (v_L, v_V) in the two phases are known functions of the composition, temperature and pressure. One obvious way to solve this set of coupled equations is to use a Newton-Raphson scheme with $2n_c + 3$ variables. However, for many components this may be very time consuming and we would like to reduce the number of iteration variables. First introduce the equilibrium constant ("K-value"):

$$\frac{y_j}{x_j} = K_j(T, P, x_j, y_j) \quad (15)$$

Introducing this into (10) and (12) yields the Rachford-Rice equation:

$$g_r(T, P, f, x_j, y_j) = \sum_{j=1}^{n_c} \frac{z_j(K_j - 1)}{1 + f(K_j - 1)} = 0 \quad (16)$$

If we in addition assume that K_j, u_L, u_V, v_L and v_V are mainly functions of pressure and temperature then there are only three independent variables (T, P and f) in equations (13), (14) and (16). This may be used to derive a simplified Newton-Raphson procedure with only 3 iteration variables. The algorithm for the UV -flash used in this paper is then:

Step 0 Initial guess of T, P, f, x_j and y_j .

Step 1 Calculate u_L, u_V, v_V, v_L and K_j

Step 2 Calculate x_j and y_j from

$$x_j = \frac{z_j}{1 + f(K_j - 1)}; \quad y_j = K_j x_j \quad (17)$$

Step 3 Write equations (13), (14) and (16) on the form $g(x) = 0$ with $g = (g_u, g_v, g_r)^T$ and $x = (T, P, f)^T$. Perform one Newton-Raphson iteration to update T, P and f :

$$\Delta x = - \left(\frac{\partial g}{\partial x} \right)^{-1} g(x) \quad (18)$$

Step 4 Go to step 1 and repeat until convergence for all variables (T, P, f, x_j and y_j) is reached.

Remarks: 1) A direct substitution method is applied for the iteration on x_j and y_j which will slow down the quadratic convergence usually associated with a Newton-Raphson scheme. However, this is not a major problem for the propane-butane mixture studied in this paper, since here the K -value depends only weakly on composition. 2) One may consider using more than one Newton-Raphson iteration in step 3. 3) Values from previous times are used for initialization in step 0. 4) The Jacobian inverse, $(\partial g / \partial x)^{-1}$, is computed only once for each flash at each time step. 5) The implemented algorithm is more complicated because it also handles problems like switching between one and two phases. 6) Hendriks *et al.* (1992) propose a reduction method to phase equilibria calculations which may be viewed as a generalization of our approach where we iterate only on 3 variables. They report a reduction in computational effort by a factor of 6-7. Michelsen (1986) has presented a similar approach which applies for cubic equations of state. He also discusses the importance of having good initial estimates and presents a modification of the Newton-Raphson method to solve the flash problem. 7) In this paper the explicit virial equation is used to calculate the specific molar density. However, often one uses cubic equations of state (EOS) which are iterative. In this case the EOS should also be solved simultaneously with the three other equations ($g(x) = 0$).

The above flash algorithm has significantly reduced the simulation time compared to a simple nested loop solution in terms of the variables p, T, f, x_j and y_j .

4 THERMODYNAMICS

Hillestad *et al.* (1989) report that as much as 70 % to 90 % of the time is spent on thermodynamic and physical property estimators in dynamic simulations. The use of a simplified thermodynamic models provide a simple means for reducing this time. The methods can be divided into two groups :

1. Look-up tables.
2. Local thermodynamics models on each stage.

A combination of the two methods is also possible and is used in this work. For local models the parameters should be updated such that discontinuities are avoided. Otherwise, this may cause difficulties for the

equation solver and increase the simulation time. For real-time simulation (e.g., training simulators) look-up tables are often used. For the UV -flash one can generate a table off-line and interpolate in the table during simulation. One major problem with look-up tables is that they become huge if the system have many components and the interpolation become difficult and time consuming. One way to solve this problem is to reduce number of independent variables, for example by using principal component regression similar to the approach of Hendriks *et al.* (1992).

Hillestad *et al.* (1989) discuss the use of local thermodynamics in general and use the following local model for calculating the $K_j = y_j / x_j$:

$$\ln(K_j P) = \theta_{1j} + \theta_{2j}/T + \theta_{3j}(1 - x_j)^2 \quad (19)$$

where the parameters θ are estimated by a recursive least squares procedure with variable forgetting. They also discuss error estimation and updating schemes.

In this paper K_j is computed using an activity coefficient model for the liquid phase and a fugacity coefficient model for the vapor phase:

$$K_j = \frac{\gamma_j P_j^s \phi_j^s \theta_j}{\phi_j P} \quad (20)$$

where γ_j denotes the activity coefficient, ϕ_j denotes the fugacity coefficient, P_j^s denotes the vapor pressure and θ_j denotes the Poynting factor. This equation is well suited for polar components, and another advantage is that the all the local parameters have physical significance. In the local model for each stage the parameters $\gamma_j, \phi_j^s, \theta_j$ and ϕ_j are treated as simple time-varying functions

$$k(t) = k_0 + k_1(t - t_1) \quad (21)$$

where the parameters are updated such that discontinuities in $k(t)$ are avoided, which would otherwise slow down the numerical integration.

One may easily include higher-order terms, for example, using a Newton interpolation polynomial. At present the updating of the parameters k_0 and k_1 is implemented like a first order filter rather than a predictor. This gives a "lag effect" and reduces the accuracy, but on average the parameters are correct, and instability is avoided. The time between updates, Δt , is presently adjusted based on the error, ϵ , between the local model and the rigorous model for the parameters $\gamma_j, \phi_j^s, \theta_j$ and ϕ_j . We have $\Delta t = \Delta t_{old} \frac{\epsilon}{\epsilon_{max}}$ where ϵ_{max} is the maximum allowed error. This approach worked well in the absence of feedback control, but it does not work well under feedback which yields sudden changes in the derivatives, and other approaches will be tested.

Finally, we list some features that should be included in a thermodynamic package which is intended used for dynamic simulation.

1. Minimize redundancy in thermodynamic calculations.

2. Minimize use of nested loop in iterative calculations, like flashes.
3. Avoidance of discontinuities, e.g., when going from two phases to only one liquid phase, which can lead to discontinuity in liquid density.
4. Adjustable accuracy for all iterative calculations, like flashes.
5. Option to give initial values for all iterative calculations.
6. Option to evaluate directly quantities that can be computed explicitly, for example, possible explicit expressions for the specific energy, activity coefficients or fugacity.
7. Option to evaluate directly any implicit equations included in iterative calculations, such as the flash equations $g(x)$ in Section 3.
8. Options for local models and look-up tables.

5 EXAMPLE COLUMN

We consider an industrial propane-butane column with 40 single-pass sieve trays. The feed is located at tray 17. The column operates at 13.2 bar and the product specifications are 95 % propane in the distillate and 95 % butane in the bottom. We use an LV-configuration where the top pressure is controlled by heat removed in the condenser, the flux drum level is controlled by the distillate flow, the bottom level is controlled by the bottom flow, the propane fraction in the distillate is controlled by the reflux flow, and the butane fraction in the bottom is controlled by the amount of heat added to the reboiler. All controllers are simple PI controllers.

Four different models based on the following sets of assumptions have been tested:

Model	Assumptions	Flash
M1	A1-A4	uv-flash
M2	A1-A6	hx-bubble
M3	A1-A7	px-bubble
M4	A1-A8	px-bubble

For each of these models one may also consider various simplifications to the thermodynamic model:

T1	Rigorous activity-fugacity coefficient model
T2	Local models and tables with updating
T3	Local models and tables with no updating

To study the stiffness of the differential equations we computed the eigenvalues of the model without control. The inverse of the largest eigenvalue which is equal to the smallest time constant is for models M1-M3:

$$M1 : 0.125 \cdot 10^{-3} \text{ s}$$

$$M2 : 0.054 \cdot 10^{-3} \text{ s}$$

$$M3 : 1.52 \text{ s}$$

Thus, models M1 and M2 which include pressure dynamics have very fast modes with time constants

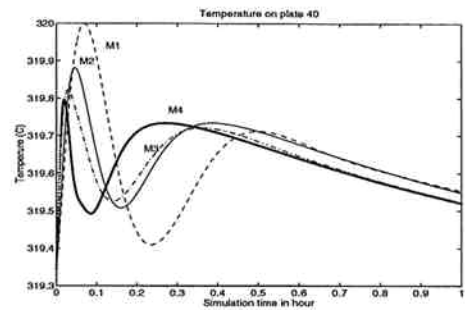


Fig. 1: Response of top plate temperature to step in feed rate. Thermodynamic model T3

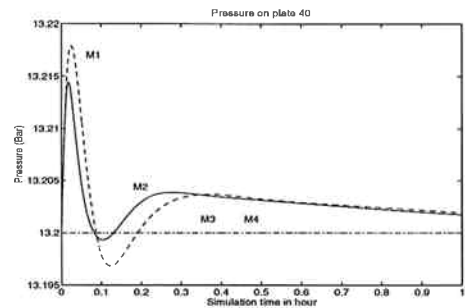


Fig. 2: Response of top plate pressure to step in feed rate.(T3).

of about 0.1 milliseconds. The reason for the small time constant is that small changes in pressure causes large changes in vapor flow. Also note that model M2 with neglected vapor holdup has an even smaller time constant than the rigorous model M1. As expected, the fastest mode is much slower (about 1.5 s) when the pressure is assumed constant as in model M3. In this case the fastest mode is due to the liquid tray hydraulics.

5.1 Closed-loop simulations.

The simulations show the closed-loop response to a 25% step increase in the feed flowrate. The effect of neglecting the vapor holdup and assuming constant pressure is shown in Figure 1 and 2. The molar vapor holdup is about 40 % of that in the liquid, and therefore the response is significantly faster when the vapor holdup is neglected (models M2-M4), and the responses become even faster when the pressure is assumed constant (models M3-M4). The difference between models M3 and M4 shows that the terms dh_i/dt can not be neglected with our choice of reference state (which is liquid at a fixed temperature) due to large temperature differences across the column.

The effect of using local thermodynamic models is illustrated in Figure 3. The error is large when using approach T3 where we do not update the activity and fugacity coefficients, but also for approach T2 the error is quite large, and the "lag effect" caused by the present updating scheme is clearly seen in Fig. 3. It is

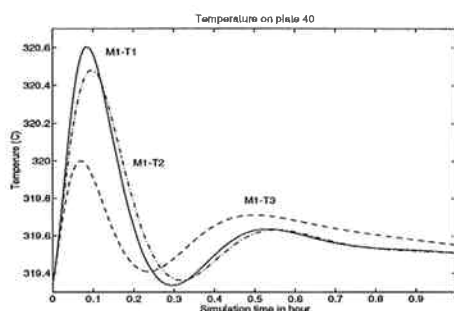


Fig. 3: Response of top temperature to step in feed rate

concluded that further work must be done to improve the updating scheme. The simulations shown are for a step change in the feed rate of about 12.5 %. For smaller steps the difference will be smaller.

In terms of computer time, approach T3 is almost 10 times faster than T1, whereas T2 is about 2-3 times faster. Obviously, the saving in computer time for approach T2 depends on the error limit and scheme used for updating the local model.

5.2 Numerical analysis.

The following integrations methods available in SIMULINK™ have been used: Euler, Runge-Kutta, Adams and Gear. For the case with pressure variations (models M1 and M2) resulting in extremely stiff equations Gear's method was by far the most efficient, whereas the differences were small for models M3 and M4 with constant pressure. This is consistent with the results of hoe and Luyben (1987) who used a model similar to M2. In terms of computer times with Gear's method there was no significant difference between model M1 (*UV*-flash) and M2 (bubble-enthalpy flash), whereas models M3 and M4 were about 2 times faster.

As noted above, the extreme stiffness for the case with varying pressure is caused by the small pressure differences between the stages. In our case this difference is only 300 Pa which is 0.02% of the total pressure of 13 bar. Another related problem is that the vapor flow rates are then very sensitive to small changes in the pressure. Specifically, if the pressure on a stage is calculated with 7 significant digits (i.e. ± 1 Pa), then this may cause changes in the third significant digit in the tray pressure difference and thus in the vapor flow. The consequence is that one must require very high accuracy both in the flash algorithm as well as in the integration algorithm. Our experience so far using Gear's method is to use a relative tolerances of about 10^{-7} in the integration algorithm and about 10^{-9} in the flash algorithm. Reducing the tolerance in the integration algorithm may yield instability, and reducing the tolerance in the flash algorithm leads to very long simulation times. Gani *et al.* (1986) noticed similar problems.

In the introduction we asked whether there were fundamental reasons for why the rigorous *UV*-approach is not more widely used, or whether it was due to more trivial reasons like that the fact that it simply was not published or that most steady-state distillation packages are based on bubble-point flashes. Our results indicate that the latter reasons are most likely. We find that although the resulting set of equations is indeed stiff, this does not seem to increase the simulation time drastically compared the case where the pressure is fixed provided an efficient solution method is used.

An efficient *UV*-flash is required for use in dynamic simulation, and we have proposed some methods to speed it up. We also propose using local thermodynamics model where the local parameters are functions of time such that discontinuities are avoided. Further work is needed on how this updating should be performed.

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