DYNAMIC OPTIMIZATION OF COUNTERCURRENT HEAT EXCHANGERS WITH PHASE CHANGE

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This paper addresses dynamic optimization of shell and tube countercurrent heat exchangers with phase change, through first principles mathematical models, within a simultaneous approach. Partial condensation of natural gas takes place on the shell side. Dynamic mass, energy and momentum balances are formulated for the condensing fluid. The resulting distributed parameter problem is transformed into a lumped parameter one by applying the method of Lines for the spatial coordinate. Additional constraints to prevent temperatures crosses and to ensure spatial temperature monotonicity are directly handled as path constraints within the simultaneous dynamic optimization approach. The differential algebraic equation system is transformed into a large nonlinear programming problem through orthogonal collocation over finite elements in time and solved with an interior point algorithm. The model provides temporal and spatial profiles of control and state variables that are in good agreement with plant data.

1. INTRODUCTION

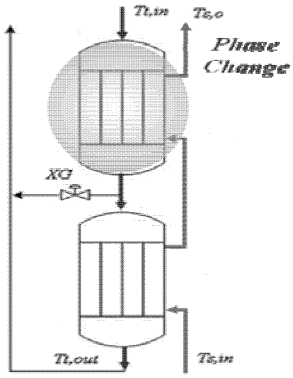
Process industries usually have unit operations involving heat transfer between fluids. Apart from the steady state operation, heat exchangers also present transients, produced by different reasons such as startup, shutdown, disturbances or deliberate variations in flowrates and thermal condition of the fluids entering the unit. Optimal operation, accident handling, dynamic design and real time dynamic optimization require a detailed description of the dynamic behavior of heat exchangers. Dynamic analysis of heat exchangers also provides information on the dynamic responses subject to different disturbances. Therefore, knowledge on transient behavior of heat exchangers is indispensable for process control, optimal operation and accident prevention. Dynamic information is useful for the evaluation of the effects on the fluid streams, and also to foresee the effects downstreams, on the process control system, new steady state and the time required to reach it, changes in the operating conditions to have a more stable operation or to minimize the transient time if the system is stable, amongst others. In all cases, dynamic simulation is a useful tool for operation (control or regulation) and design. During the last years, safety and environmental aspects together with process intensification, have increased the interest on studying the dynamic behavior of heat exchangers. Mathisen et al. (1994) propose a dynamic model for determining controllability of heat exchangers and heat exchanger networks. Romie (1984) proposes a dynamic model with distributed parameters for countercurrent heat exchangers studying the dynamic responses to step disturbances in the fluid entrance temperature, and he solves the problem applying the explicit finite differences method. Correa and Marchetti (1987) develop a dynamic simulation with a multicell model, describing the dynamic behavior of multipath heat exchangers with bafles in transient states. They propose to divide the heat exchanger in distributed elements where a small part of the heat exchange takes place. The resulting model is adequate to simulate some startup alternatives which allow to obtain the dynamic response to disturbances in the feed flowrate or temperature. Roetzel and Xuan (1992) apply Laplace transform to solve the equations describing the dynamic energy balances arising from arbitrary perturbations on feed temperatures. Lakshmanan and Potter (1994) develop a mathematical model which provides analytical solutions for the

dynamic behavior of countercurrent heat exchangers. Later, Sarit and Roetzel (1995) propose a dispersion model for countercurrent plate exchangers, to predict dynamic responses to temperature changes. The model includes lengthwise conduction along the tube walls and determines the outlet temperature of both fluids for arbitrary perturbations in both entrance temperatures. Roetzel and Balzereit (2000) studied the effect of axial dispersion in tridimensional flow for the shell side, considering overlapping of axial dispersion in the fluid. Ranong and Roetzel (2002) study the dynamic behavior of a system with two one-stream coupled heat exchangers. For the dynamic case, responses to disturbances in temperatures and feed flowrates are calculated using Laplace transform and explicit finite differences. They also include the global heat transfer coefficient dependency on stream mass flowrate. Yin and Jensen (2003) investigate the transient response of temperature in heat exchangers, using an integral method, assuming that one of the fluids remains at constant temperature and the other does not undergo phase change. Luo et al. (2003) study the dynamic behavior of heat exchangers with one-dimensional flow (co- and countercurrent). Both models are solved in the transformed field. Moita et al. (2005) present a distributed model for plate countercurrent heat exchangers without phase change.
When phase change takes place in one or both heat exchanging fluids, mass and heat transfer are simultaneous and coupled. Schoenberg (1966) analyzes the responses of the condensing pressure and interfacial movement to sinusoidal variations on the steam feed flowrate. Mayinger and Schult (1981) propose a simplified transient model for condensers. Zinemanas et al. (1984) propose an algorithm for the simulation of horizontal or vertical shell and tube heat exchangers with phase change and one or more components. The algorithm determines the local values along the heat exchanger, taking into account the different flow schemes. The calculation is based on numerical integration with constant enthalpy steps. Liao et al. (1988) analyze the flow transient behavior in a single tube condenser, and report the dynamic of the vaporized fraction and outlet velocity to changes on the heat flux through the wall and vapor inlet flowrate. Liao and Wang (1990) propose a two fluid model wth two phases, introducing momentum balances, to study the essential mechanisms in the dynamic behavior of the condensing fluid. Wang and Touber (1991) propose a distributed dynamic model of an aero-cooler, presenting many examples. Mandler and Brochu (1991) present a distributed dynamic simulator based on first principles of cryogenic heat exchangers of LNG for process control. Dynamic optimization of heat exchangers with phase change has received little attention in the literature. In this regard, Rodriguez and Diaz (2006, 2007) address dynamic optimization of cryogenic heat exchangers through rigorous models, applying the Bell-Delaware method for pressure drop calculation and the Soave Redlich Kwong equation of state (Soave, 1972).
In this work, we propose first principles models for a system of countercurrent heat exchangers where partial phase change occurs in natural gas on the shell side, within an ethane extraction plant. The model is formulated within a simultaneous optimization approach and includes mass, energy and momentum balances for the condensing fluid, as well as energy balances for the noncondensing one. The Soave Redlich Kwong equation provides thermodynamic equilibrium predictions. Constraints to prevent temperature crosses at each cell in the heat exchangers have been added to the optimization problem, together with additional constraints to ensure monotonicity in temperature spatial profiles. The control variable is the bypass flowrate in one heat exchanger to keep outlet temperature at a specified value. A ramp change in inlet gas flowrate has been analyzed and compared to plant data, with good agreement.

2. DYNAMIC MODELING OF HEAT EXCHANGERS WITH PHASE CHANGE

In this work, dynamic models for countercurrent shell and tube heat exchangers with and without phase change are formulated, in an equation oriented environment. As a particular case, the heat exchangers have baffles and single path in the shell and the tubes. More complex heat exchangers can be modeled from basic models, with series and parallel equipment. Figure 1 shows a typical system of heat exchangers and a bypass valve. In the single phase model, the energy balance for each fluid, after spatial discretization in *Ncell1* cells is as follows:

$$\frac{dT_{j,i}}{dt} = -\frac{v_{j,i}}{\Delta z}\left(T_{j,i} - T_{j,i-1}\right) \pm \frac{h_j * A_{sup}}{\rho_{j,i} * Cp_j * A_j * L}\Delta T_{s-t} \qquad i = 1,\ldots, Ncell1,\ j = Tube, Shell$$



In heat exchangers with phase change, two submodels are considered: A submodel with the two phase flow, and a submodel of single phase flow. Basic simplifying assumptions for the two phase flow are that vapor and liquid be in thermodynamic equilibrium, but they can have different rates and that there is only one-dimensional flow, meaning that both liquid and vapor phases have an average cross sectional velocity. Mass and momentum balances are formulated for liquid and vapor phases. As both phases are in thermodynamic equilibrium at each time t, one energy balance is required for the vapor-liquid system, where E is the internal energy.

Fig. 1: System of countercurrent heat exchangers.

The discretized balances applying the Method of Lines with backward finite differences are:
Vapor phase mass balance

$$\frac{dM_{V,i}}{dt} = V_{i-1} - V_i + m_{LV,i} \qquad i = 1,\ldots,Ncell2$$

where $m_{LV,i}$ corresponds to the interfacial mass transport rate from liquid to vapor in cell i.
Liquid phase mass balance

$$\frac{dM_{L,i}}{dt} = L_{i-1} - L_i - m_{LV,i}$$

Energy Balance

$$\frac{dE_i}{dt} = L_{i-1}{*}h_{i-1} + V_{i-1}{*}H_{i-1} - L_i{*}h_i - V_i{*}H_i + Q_i^t$$

Momentum balance – vapor phase

$$\frac{d(M_{V,i}v_{V,i})}{dt} = V_{i-1}v_{V,i-1} - V_i v_{V,i} + F_{P,i} - F_{in,i} + m_{LV,i}v_{L,i}$$

Momentum balance – liquid phase

$$\frac{d(M_{L,i}v_{L,i})}{dt} = L_{i-1}v_{L,i-1} - L_i v_{L,i} + F_{P,i} + F_{in,i} - m_{LV,i}v_{L,i} - F_{w,i} \qquad i = 1,\ldots,Ncell2$$

where $M_{V,i}$ and $M_{L,i}$ represent vapor and liquid accumulation in each cell i, defined as:

$$M_{V,i} = A_T Le_i \theta_i \rho_{V,i} \qquad i = 1,\ldots,Ncell2$$

$$M_{L,i} = A_T Le_i (1-\theta_i)\rho_{L,i} \qquad i = 1,\ldots,Ncell2$$

θ_i is the vaporized fraction in cell i, calculated as the ratio between transversal areas for vapor ($A_{V,i}$) and total (A_T):

$$\theta_i = \frac{A_{V,i}}{A_T} \qquad i = 1,\ldots,Ncell2$$

$v_{V,i}$ and $v_{L,i}$ represent fluid velocity of each phase

$$v_{V,i} = \frac{V_i}{A_{V,i}\rho_{V,i}} \qquad i = 1,\ldots,Ncell2$$

$$v_{L,i} = \frac{L_i}{(1-A_{V,i})\rho_{L,i}} \qquad i = 1,\ldots,Ncell2$$

$F_{P,i}$, is the driving force, depending on the pressure drop in cell i:

$$F_{P,i} = \left(P_{s,i-1}\ \theta_{i-1} - P_{s,i}\ \theta_i\right)A_T \qquad i = 1,\dots,Ncell2$$

$F_{in,i}$ is the interfacial shear stress, calculated for condensation inside a tube with internal diameter D_S (Liao and Wang, 1990), as a function of the vaporized fraction, the squared difference of velocities between phases and the interfacial friction factor $f_{f,i}$:

$$F_{in,i} = \frac{4\sqrt{\theta_i}}{D_S} f_{f,i} \frac{\rho_{L,i}}{2}\left(v_{V,i} - v_{L,i}\right)^2 \qquad i = 1,\dots,Ncell2$$

$f_{f,i}$ is calculated with a correlation proposed by Whalley and Hewitt (1977):

$$f_{f,i} = f_v\left[1 + 24\left(\frac{\rho_{L,i}}{\rho_{V,i}}\right)^{1/3}\frac{\delta}{D_S}\right] \qquad i = 1,\dots,Ncell2$$

where f_v depends on the Reynolds number :

$$f_v = \begin{cases} 0.079\,Re^{-0.25}, 4000 \le Re \le 30000 \\ 0.046\,Re^{-0.20}, Re > 30000 \end{cases}$$

and δ is the liquid film thickness, calculated as a fraction of the vaporized fraction for an anular model as:

$$\frac{\delta_i}{D_S/2} = 1 - \sqrt{\theta_i} \qquad i = 1,\dots,Ncell2$$

$m_{LV,i}v_{L.i}$ represents the momentum of mass transfer between the two phases. The velocity is assumed to be the liquid velocity. Finally, the last term represents friction on the wall. For the condensation process it has been calculated as:

$$F_{w,i} = \frac{4}{D_S}\tau_{w,i} \qquad i = 1,\dots,Ncell2$$

where $\tau_{w,i}$ is the shear stress of the fluid on the wall, calculated as a function of vapor and liquid flows, densities and the respective friction factors.

$$\tau_{w.i} = -f_{v,i}\frac{V_i^2}{2\rho_{vi}}\left[1 + 2.85\frac{f_{Li}\rho_{vi}V_i}{f_{vi}\rho_{Li}L_i}\right]^2 \qquad i = 1,\dots,Ncell2$$

Additional equations stand for thermodynamic properties and vapor liquid equilibrium:
Internal energy:

$$E_i = M_{V,i}H_i + M_{L,i}h_i \qquad i = 1,\dots,Ncell2$$

Equilibrium relationship for component j ($K_{i,j}$):

$$K_{i,j} = \frac{\phi_{i,j}^L}{\phi_{i,j}^V} \qquad i = 1,\dots,Ncell2,\ j = 1,\dots,nc$$

$$y_{i,j} = K_{i,j}x_{i,j} \qquad i = 1,\dots,Ncell2,\ j = 1,\dots,nc$$

Summation equations:

$$\sum_j y_{i,j} - \sum_j x_{i,j} = 0 \qquad i = 1,\dots,Ncell2$$

Vapor enthalpy (Hi) and liquid enthalpy (hi):

$$H_i = H_i^{ideal} - \Delta H_i \qquad i = 1,\dots,Ncell2$$

$$H_i^{ideal} = \sum_{j=1}^{nc} H_{i,j}^{ideal}(T_i)y_{i,j} \qquad i = 1,\dots,Ncell2$$

$$h_i = h_i^{ideal} - \Delta h_i \qquad i = 1,\dots,Ncell2$$

$$h_i^{ideal} = \sum_{j=1}^{nc} h_{i,j}^{ideal}(T_i)x_{i,j} \qquad i = 1,...,Ncell2$$

where ΔHi y Δhi are residual enthalpies. These functions, the fugacity coefficients and compressibility factors are calculated with the Soave-Redlich-Kwong equation of state (Soave, 1972). This equation of state is recommended for the prediction of vapor liquid equilibrium in mixtures of light hydrocarbons, even for near critical conditions (Christiansen et al., 1979), as it is the case of the partially condensed stream.

3. OPTIMIZATION ALGORITHM

The dynamic model for the system of countercurrent shell and tube heat exchangers, described in Section 2, is formulated within a simultaneous dynamic optimization framework. In this approach, both state and control variables are represented by piecewise polynomials over finite elements in time and the ordinary differential algebraic equation (DAE) system is discretized by orthogonal collocation over these finite elements. Therefore, the optimization problem subject to a DAE is transformed into a large scale nonlinear programming (NLP) problem that is solved with a barrier method with Successive Quadratic Programming (SQP) techniques within program IPOPT (Biegler et al., 2002).

4. OPTIMIZATION PROBLEM FOR HEAT EXCHANGERS

A dynamic optimization problem is formulated for the system of cryogenic heat exchangers HX1-HX2 that are part of a natural gas processing plant. The dynamic optimization problem is formulated as

$$\begin{aligned}
& min \int_0^{tf} \left(Ts - T_{SP}\right)^2 dt \\
& st. \\
& \{DAE\ HE\ Model\} \\
& 0 \le x_{bypass} \le 1. \\
& Ts_k - Tt_{k+1} \ge \Delta T_{min}; k = 1,...Ncells1-1 \\
& Ts_k - Tt_{IN1} \ge \Delta T_{min}; k = Ncells1 \\
& Ts_j - Tt_{j+1} \ge \Delta T_{min}; j = 1,...Ncells2-1 \\
& Ts_j - Tt_{IN} \ge \Delta T_{min}; j = Ncells2 \\
& Ts_{m,IN} \ge Ts_{m,1}; m = 1,2 \\
& Ts_{m,i} \ge Tsm,_{i+1}; i = 1,..., Ncellsm-1; m = 1,2 \\
& Tt_{m,i} \ge Tt_{m,i+1}; i = 1,...Ncellsm-1; m = 1,2 \\
& Tt_{m,Ncellsm} \ge Tt_{m,IN}; m = 1,2 \\
& z(t=0) = z_0; y_L \le y \le y_U; z_L \le z \le z_U
\end{aligned}$$

where inequalities correspond to constraints to prevent from temperature crosses in each cell of the system of heat exchangers, HX1 and HX2. There are additional constraints to ensure temperature monotonicity along the heat exchangers. Inlet natural gas temperature at the heat exchangers outlet is controlled by manipulating the cold stream flowrate fraction, x_G, through a bypass valve which is considered as the degree of freedom for the optimization problem. The objective is to minimize the transient to get the set point temperature at the outlet of HX2, from the initial temperature of partially condensed (T_S) to a desired value (T_{SP}). T_{SP} = 212K for this special case. The integral objective function is handled as an additional differential equation.

The model has been implemented in a Fortran 90 environment and integrated to program IPOPT (Biegler et al., 2002, Zabala and Biegler, 2008). Analytical first partial derivatives are calculated with the symbolic mathematical program Maple and incorporated into the Fortran code. Information on the Jacobian structure is required. In this environment, the dynamic optimization problem is discretized in time using orthogonal collocation over finite elements, thus transforming it into an NLP problem, which is solved with IPOPT using an interior point method (Barrier method) using successive quadratic programming techniques in a reduced space (rSQP).

5. NUMERICAL RESULTS

The system of heat exchangers object of this study is part of the cryogenic sector of an ethane extraction plant. Heat exchanger HX1 is discretized into ten cells (3 m total length, considering three modules in series, four in parallel) and HX2, in six cells (1m, one module in series, two in parallel). The model includes 57 differential equations and 236 algebraic ones, plus 63 ineaquality constraints thata are treated as equalities through the incllusion of slack variables. The temporal discretization is done with 20 finite elements with two collocation points, rendering an NLP with 15518 variables and 15498 equality constraints. An initial value of 0.01 was used for the barrier parameter. We perform a comparison of numerical results with plant data when a ramp perturbation is introduced into inlet gas flowrate, as shown in Fig. 2. As the system of heat exchangers allows heat integration between the demethanizer top stream (Ttop, cold stream) and inlet natural gas (hot stream), the cold stream is also perturbed after the initial perturbation in inlet gas flowrate, as it is shown in Fig. 2. For confidentiality reasons, actual data scale in not shown.

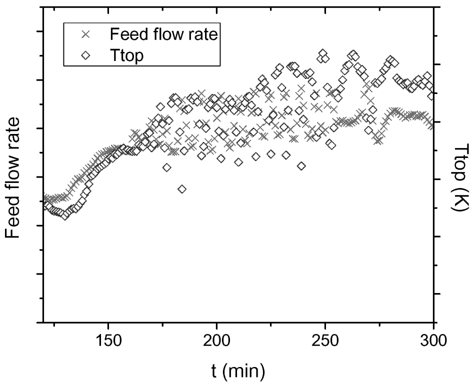


Fig. 2. Plant data: Feed flowrate (inlet hot stream to HX1) and residual gas temperature (Ttop, inlet cold stream to HX2)

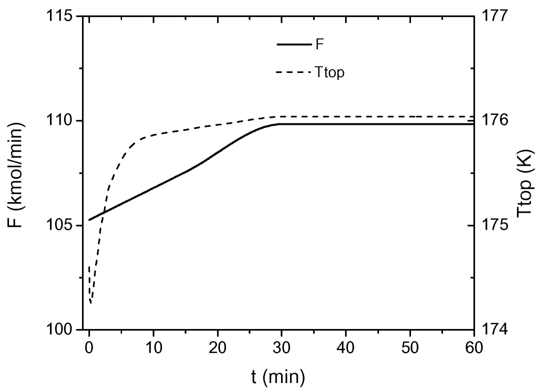


Fig. 3. Feed flowrate (F, inlet hot stream to HX1) and residual gas temperature (Ttop, inlet cold stream to HX2) predictions

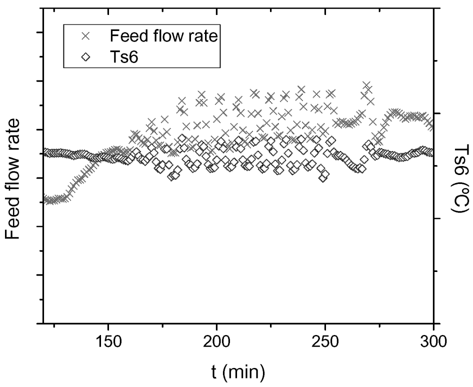


Fig. 4. Plant data: Feed flowrate and natural gas temperature (Ts6, outlet hot stream from HX2)

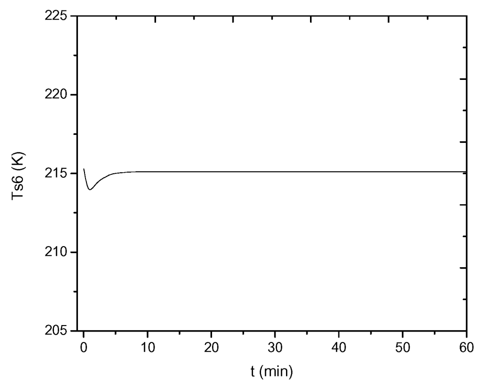


Fig. 5. Natural gas temperature profile (Ts6, outlet hot stream from HX2)

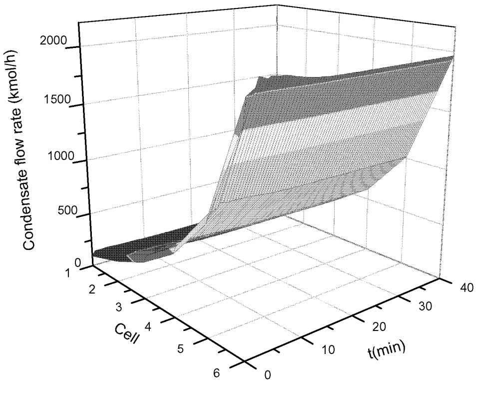


Fig. 6. Optimal profile for condensate flowrate

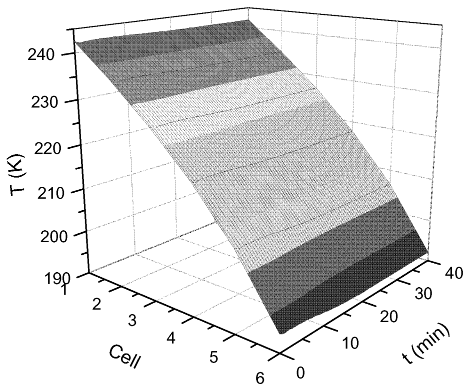


Fig. 7. Optimal spatial and temporal profile for cold stream in HX2

At time t=128 minutes, a ramp-type perturbation is introduced such that the final value of the flowrate is 3.5% higher than initial one, as follows:

$$Fin =,\begin{cases} 105.26 + 0.152627\,t, 0 \le t \le 15 \\ 109.844760 - 0.611460\,t + 0.0407481333\,t^2 - 0.000679047407\,t^3, 15 < t \le 30 \\ 109.84, t \ge 30 \end{cases}$$

Figure 3 shows the simulated ramp perturbation in feed flowrate, as well as inlet cold stream temperature profile (demethanized top stream) to HX2, where natural gas partial condensation takes place.
Figures 4 and 5 show plant data and numerical results for natural gas outlet temperature from HX2, respectively. This temperature is controlled through a bypass valve between both heat exchangers, as shown in Fig. 1. The outlet temperature of this partially condensed vapor shows an initial decrease due to the instantaneous shutdown of the bypass valve (in the initial steady state, 10% of the residual gas is bypassing the first cryogenic heat exchanger). The model determines the immediate shutdown of the bypass valve (which is the optimization variable), emulating the action of a control system regulating outlet natural gas temperature. The increase in temperature of the top demethanizer stream (inlet cold stream) leads the system to a new steady state where this temperature is 0.2K higher than the initial one (215.10K). The initial outlet temperature could be reached if external refrigeration were considered (not this case). Fig. 6 shows condensate flowrate in HX2, showing an initial increase due to the complete shutdown of the bypass valve and a lower final value. Fig. 7 shows residual gas temperature (tube side) in HX2, where natural gas is partially condensed on the shell side.

6. CONCLUSIONS

In this work, we have formulated dynamic models of shell and tube heat exchangers based on first principles within an equation oriented approach, for systems with and without phase change. The partial differential algebraic system was spatially discretized applying the method of lines with backwards finite differences. Thermodynamic predictions were made using the cubic equation of state of Soave-Redlich-Kwong (Soave, 1972) for the fugacity coefficients of each component in each phase, and the corresponding compressibility factors. The formulation within a simulatenous dynamic optimization framework allows the direct inclusion of minimum temperature differences between the interchanging streams as path constraints, guaranteeing the operative feasibility of process units in the transients. The models have allowed the study of the dynamic behavior of a system of cryogenic heat exchangers in an ethane extraction plant, where partial condensation of the hot stream takes place. The comparison with actual plant data confirms response trends and velocity.

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