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Vapor Recompression Distillation: Multi-Scale Dynamics and Control

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Abstract— **This paper focuses on the dynamics and control of a vapor recompression distillation column. A dynamic modeling framework is presented and the presence of multi-time-scale behavior is documented. Using singular perturbations, a model reduction procedure is outlined to arrive at reduced order models capturing the dynamics in each time-scale. A hierarchical control scheme is proposed based on the multi-scale nature of the system. The theoretical results are illustrated via a simulation case study on a propane-propylene system.**

I. INTRODUCTION

Distillation is one of the most energy consuming units in a chemical plant, motivating the need for energy integration. Vapor recompression distillation (VRD) is one such energy integrated distillation configuration, wherein the vapor coming from the top of the distillation column is used to provide energy for the vaporization of the bottoms stream [1]. Vapor recompression distillation is favored for separations involving close-boiling liquids. Such separations result into large reflux ratios and a small compressor duty is needed to facilitate the heat transfer in a combined reboiler-condenser.

Most research on vapor recompression distillation has emphasized steady state economics (*e.g.* [2], [3]), focusing on capital costs, operating costs and optimal steady state operating conditions. In a vapor recompression distillation column, there is a significant amount of energy recycle through the combined reboiler-condenser, which introduces strong interactions between different units in this system. Furthermore, there is also a large amount of material recycle owing to the large reflux flows. The tight material and energy integration in vapor recompression distillation shows a potential for intricate dynamics. However, very few papers have focused on the dynamics and control of these columns (*e.g.* [3], [4]).

In this paper, we propose a comprehensive modeling, analysis and control framework for such columns. We document that the discrepancies in material and energy flows in this system lead to a multi-time-scale behavior. Through a nested application of singular perturbations, reduced order non-stiff models valid in each time-scale are obtained. We then propose a hierarchical control scheme exploiting this time-scale multiplicity. The theoretical results are illustrated via a simulation case study on a propane-propylene system.

II. DYNAMIC ANALYSIS

Figure 1 shows a typical configuration for a direct (column fluid itself being used as a refrigerant) vapor recompression distillation system. The vapor coming out from the top of the distillation column is compressed in the compressor so as to facilitate the heat transfer to the bottoms stream. A major part of the compressed vapor condenses in the reboiler-condenser and this in turn boils the bottoms stream, generating the vapor entering the stripping section of the column. A trim condenser is used to condense the residual vapor. An auxiliary cooler is used to bring the temperature of the reflux back to the required value. For simplicity, we assume constant specific heats ($c_{p,l}, c_{p,v}$), constant relative volatility (α) and constant molar holdup on each tray (M_i). The pressure drop in the column is assumed to be negligible. We further assume that the liquid flow rate in the rectifying section is constant from plate to plate, which is usually a good assumption for a mixture of close-boiling components. Further, we assume that the kinetic and potential energy contributions to energy are negligible. To simplify the analysis, let us also assume:

- The liquid in the reboiler in thermal equilibrium with the vapor.
- Fast (instantaneous) heat transfer in the reboiler-condenser.
- No subcooling in the condensers.

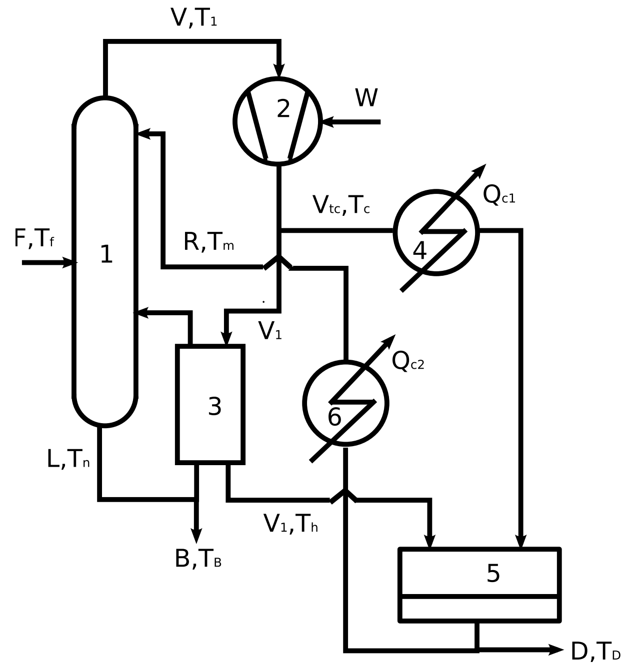

Fig. 1. Vapor recompression distillation (1 - Column, 2 - Compressor, 3 - Reboiler-condenser, 4 - Trim condenser, 5 - Reflux drum and 6 - Auxiliary cooler

Based on these assumptions, the material and energy balance equations of the system can be written as:

Distillation column (n trays)
$1 \leq i < nf$

$$\begin{aligned}\frac{dx_i}{dt} &= \frac{1}{M_i}\left[V(y_{i+1}-y_i)+R(x_{i-1}-x_i)\right]\\ \frac{dT_i}{dt} &= \frac{1}{M_i c_{p,l}}\left[V(\tilde{h}_v(T_{i+1})-\tilde{h}_v(T_i))+R(\tilde{h}_l(T_{i-1})-\tilde{h}_l(T_i))\right]\end{aligned}$$

$$\begin{aligned}\frac{dx_{nf}}{dt} &= \frac{1}{M_{nf}}\left[V(y_{nf+1}-y_{nf})+R(x_{nf-1}-x_{nf})\right.\\ &\quad \left.+F(x_f-x_{nf})\right]\\ \frac{dT_{nf}}{dt} &= \frac{1}{M_{nf}c_{p,l}}\left[V(\tilde{h}_v(T_{nf+1})-\tilde{h}_v(T_{nf}))+\right.\\ &\quad \left.R(\tilde{h}_l(T_{nf-1})-\tilde{h}_l(T_{nf}))+F(\tilde{h}_l(T_f)-\tilde{h}_l(T_{nf}))\right]\end{aligned}$$

$nf < i \leq n$

$$\begin{aligned}\frac{dx_i}{dt} &= \frac{1}{M_i}\left[V(y_{i+1}-y_i)+(R+F)(x_{i-1}-x_i)\right]\\ \frac{dT_i}{dt} &= \frac{1}{M_i c_{p,l}}\left[V(\tilde{h}_v(T_{i+1})-\tilde{h}_v(T_i))+\right.\\ &\quad \left.(R+F)(\tilde{h}_l(T_{i-1})-\tilde{h}_l(T_i))\right]\end{aligned}$$

Compressor

$$\begin{aligned}\frac{dT_c}{dt} &= \frac{1}{M_c c_v}\left[V(\tilde{h}_v(T_1)-\tilde{h}_v(T_c))+\eta W\right]\\ \frac{dP_c}{dt} &= (V-V_1-V_{tc})\frac{RT_c}{V_c}\end{aligned}$$

Reboiler-condenser

$$\begin{aligned}\frac{dM_B}{dt} &= R+F-V-B\\ \frac{dx_B}{dt} &= \frac{1}{M_B}\left[(R+F)(x_n-x_B)-V(y_B-x_B)\right]\\ 0 &= V_1(\tilde{h}_v(T_c)-\tilde{h}_l(T_h))-Q\\ 0 &= (R+F)(\tilde{h}_l(T_n)-\tilde{h}_l(T_B))-\\ &\quad V(\tilde{h}_v(T_B)-\tilde{h}_l(T_B))+Q\end{aligned}$$

Trim condenser

$$\frac{dT_o}{dt} = \frac{1}{M_t c_{p,l}}\left[V_{tc}(\tilde{h}_v(T_c)-\tilde{h}_l(T_o))-Q_{c1}\right]$$

Reflux drum

$$\begin{aligned}\frac{dM_D}{dt} &= V-R-D\\ \frac{dx_D}{dt} &= \frac{1}{M_D}\left[V(y_1-x_D)\right]\\ \frac{dT_D}{dt} &= \frac{1}{M_D c_{p,l}}\left[V_1(\tilde{h}_l(T_h)-\tilde{h}_l(T_D))+\right.\\ &\quad \left.V_{tc}(\tilde{h}_l(T_o)-\tilde{h}_l(T_D))\right]\end{aligned}$$

Auxiliary cooler

$$\frac{dT_m}{dt} = \frac{1}{M_a c_{p,l}}\left[R(\tilde{h}_l(T_D)-\tilde{h}_l(T_m))-Q_{c2}\right]$$

where D, B and F are the distillate, bottoms and the feed molar flow rates and x_F is the feed composition. V and R are the vapor and reflux flows, V_{tc} is the flow through the trim condenser and V_1 is the condenser section inlet flow for the reboiler-condenser. $\tilde{h}$ represents partial molar enthalpy with subscripts v and l denoting the vapor and liquid stream respectively. Q is the heat duty of the reboiler-condenser. Q_{c1} and Q_{c2} are the duties for the trim condenser and the auxiliary cooler respectively. W is the compressor power and η is the compressor efficiency.

For this vapor recompression distillation, we make the following assumptions regarding the magnitude of various material and energy flows.

1) VRD favors separation of species with close-boiling points. Such a difficult separation requires a large operating reflux ratio (R/D). At steady state, we thus define a small parameter $D_s/R_s = \varepsilon_1 << 1$.
2) The contribution of latent heat to the enthalpy is much larger than that of the sensible heat. So at steady state, we define another small parameter $\tilde{h}_l(T_f)/\tilde{h}_v(T_f) = \varepsilon_2 << 1$.
3) The material flows V and V_1 are comparable in magnitude to R and the material flows F, V_{tc} and B are comparable in magnitude to D.
4) The energy flows W and Q_{c2} are $\mathcal{O}(1/\varepsilon_1)$ and Q_{c1} is $\mathcal{O}(1/\varepsilon_2)$. At steady state, we define $W_s/F_s\tilde{h}_l(T_f) = k_w/\varepsilon_1$, $Q_{c2,s}/F_s\tilde{h}_l(T_f) = k_{qc2}/\varepsilon_1$ and $Q_{c1,s}/F_s\tilde{h}_l(T_f) = k_{qc1}/\varepsilon_2$.
5) The energy transfer rate across the reboiler-condenser is $\mathcal{O}(1/\varepsilon_1\varepsilon_2)$ and thus we define $Q_s/F_s\tilde{h}_l(T_f) = k_q/\varepsilon_1\varepsilon_2$.

Based in these, we define the $\mathcal{O}(1)$ steady state ratios $B_s/D_s = k_B$, $F_s/D_s = k_F$, $V_{tc,s}/D_s = k_{tc}$, $V_{1,s}/R_s = k_{V1}$, $V_s/R_s = k_V$, the scaled material flows $B/B_s = u_B$, $F/F_s = u_F$, $V_{tc}/V_{tc,s} = u_{tc}$, $V_1/V_{1,s} = u_{V1}$, $V/V_s = u_V$, $R/R_s = u_R$ and $D/D_s = u_D$, and the scaled energy flows $W/W_s = u_w$, $Q_{c1}/Q_{c1,s} = u_{qc1}$, $Q_{c2}/Q_{c2,s} = u_{qc2}$ and $Q/Q_s = u_q$. We also define the following $\mathcal{O}(1)$ ratios of specific enthalpies $\tilde{h}_l(T_i)/\tilde{h}_l(T_f) = k_{i,l}$, $\tilde{h}_v(T_i)/\tilde{h}_v(T_f) = k_{i,v}$, $\tilde{h}_l(T_h)/\tilde{h}_l(T_f) = k_h$, $\tilde{h}_l(T_B)/\tilde{h}_l(T_f) = k_b$, $\tilde{h}_l(T_o)/\tilde{h}_l(T_f) = k_o$, $\tilde{h}_l(T_D)/\tilde{h}_l(T_f) = k_d$, $\tilde{h}_l(T_m)/\tilde{h}_l(T_f) = k_m$, $\tilde{h}_v(T_c)/\tilde{h}_v(T_f) = k_c$ and $\tilde{h}_v(T_B)/\tilde{h}_v(T_f) = k_{bv}$. The material and energy balance dynamics now take the form:

Distillation column
$1 \leq i < nf$

$$\begin{aligned}\frac{dx_i}{dt} &= \frac{D_s}{M_i\varepsilon_1}\left[k_V u_V(y_{i+1}-y_i)+u_R(x_{i-1}-x_i)\right]\\ \frac{dT_i}{dt} &= \frac{D_s\tilde{h}_l(T_f)}{M_i c_{p,l}\varepsilon_1}\left[k_V u_V\left(\frac{k_{i+1,v}-k_{i,v}}{\varepsilon_2}\right)+u_R(k_{i-1,l}-k_{i,l})\right]\end{aligned}$$

$$\begin{aligned}\frac{dx_{nf}}{dt} &= \frac{D_s}{M_{nf}}\left[\frac{k_V u_V}{\varepsilon_1}(y_{nf+1}-y_{nf})+\frac{u_R}{\varepsilon_1}(x_{nf-1}-x_{nf})\right.\\ &\quad \left.+k_F u_F(x_f-x_{nf})\right]\\ \frac{dT_{nf}}{dt} &= \frac{D_d\tilde{h}_l(T_f)}{M_{nf}c_{p,l}}\left[\frac{k_V u_V}{\varepsilon_1}\left(\frac{k_{nf+1,v}-k_{nf,v}}{\varepsilon_2}\right)+\right.\\ &\quad \left.\frac{u_R}{\varepsilon_1}(k_{nf-1,l}-k_{nf,l})+k_F u_F(1-k_{nf,l})\right]\end{aligned}$$

$nf < i \leq n$

$$\frac{dx_i}{dt} = \frac{D_s}{M_i}\left[\frac{k_V u_V}{\varepsilon_1}(y_{i+1}-y_i)+\left(\frac{u_R}{\varepsilon_1}+k_F u_F\right)(x_{i-1}-x_i)\right]$$
$$\frac{dT_i}{dt} = \frac{D_s\tilde{h}_l(T_f)}{M_i c_{p,l}}\left[\frac{k_V u_V}{\varepsilon_1}\left(\frac{k_{i+1,v}-k_{i,v}}{\varepsilon_2}\right)+\left(\frac{u_R}{\varepsilon_1}+k_F u_F\right)(k_{i-1,l}-k_{i,l})\right]$$

Compressor

$$\frac{dT_c}{dt} = \frac{D_s\tilde{h}_l(T_f)}{M_c c_v \varepsilon_1}\left[k_V u_V\left(\frac{k_{1,v}-k_c}{\varepsilon_2}\right)+\eta k_F k_w u_W\right]$$
$$\frac{dP_c}{dt} = \frac{D_s R T_c}{V_c}\left[\frac{k_V u_V}{\varepsilon_1}-\frac{k_{V1}u_{V1}}{\varepsilon_1}-k_{tc}u_{tc}\right]$$

Reboiler-condenser

$$\frac{dM_B}{dt} = D_s\left[\frac{u_R}{\varepsilon_1}+k_F u_F-\frac{k_V u_V}{\varepsilon_1}-k_B u_B\right]$$
$$\frac{dx_B}{dt} = \frac{D_s}{M_B}\left[\left(\frac{u_R}{\varepsilon_1}+k_F u_F\right)(x_n-x_B)-\frac{k_V u_V}{\varepsilon_1}(y_B-x_B)\right]$$
$$0 = \frac{D_s\tilde{h}_l(T_f)}{M_h c_{p,l}}\left[\frac{k_{V1}u_{V1}}{\varepsilon_1}\left(\frac{k_c}{\varepsilon_2}-k_h\right)-\frac{k_F k_q u_q}{\varepsilon_1\varepsilon_2}\right]$$
$$0 = \frac{D_s\tilde{h}_l(T_f)}{M_B c_{p,l}}\left[\left(\frac{u_R}{\varepsilon_1}+k_F u_F\right)(k_{n,l}-k_b)-\frac{k_V u_V}{\varepsilon_1}\left(\frac{k_{bv}}{\varepsilon_2}-k_b\right)+\frac{k_F k_q u_q}{\varepsilon_1\varepsilon_2}\right]$$

Trim condenser

$$\frac{dT_o}{dt} = \frac{D_s\tilde{h}_l(T_f)}{M_t c_{p,l}}\left[k_{tc}u_{tc}\left(\frac{k_c}{\varepsilon_2}-k_o\right)-\frac{k_F k_{qc1}u_{qc1}}{\varepsilon_2}\right]$$

Reflux drum

$$\frac{dM_D}{dt} = D_s\left[\frac{k_V u_V-u_R}{\varepsilon_1}-u_D\right]$$
$$\frac{dx_D}{dt} = \frac{D_s}{M_D\varepsilon_1}\left[k_V u_V(y_1-x_D)\right]$$
$$\frac{dT_D}{dt} = \frac{D_s\tilde{h}_l(T_f)}{M_D c_{p,l}}\left[\frac{k_{V1}u_{V1}}{\varepsilon_1}(k_h-k_d)+k_{tc}u_{tc}(k_o-k_d)\right]$$

Auxiliary cooler

$$\frac{dT_m}{dt} = \frac{D_s\tilde{h}_l(T_f)}{M_a c_{p,l}\varepsilon_1}\left[u_R(k_d-k_m)-k_F k_{qc2}u_{qc2}\right] \tag{1}$$

The presence of the small parameters ε_1 and ε_2 make this model stiff. For simplicity, let us assume that ε_1 and ε_2 are comparable ($\varepsilon_2 = k\varepsilon_1$, where k is $\mathcal{O}(1)$). Let us also define another small parameter $\varepsilon_3 = \varepsilon_1\varepsilon_2$ so that $\varepsilon_3 << \varepsilon_1, \varepsilon_2 << 1$. We note that the dynamic system (1) involves terms which are $\mathcal{O}(1)$, $\mathcal{O}(1/\varepsilon_1)$ and $\mathcal{O}(1/\varepsilon_3)$, showing a potential for the evolution of the state variables over three time-scales. The control problem for such a multi-time-scale system can be addressed by obtaining reduced order models valid in each time-scale and using them to derive controllers in the respective time-scales. Such a model reduction can be done through a successive application of singular perturbation techniques to model (1) [5].

III. Model reduction and Control

In order to derive the description of the dynamics in the fast time-scale, let us define a stretched fast time-scale $\tau = t/\varepsilon_3$. Substituting τ in the dynamic equations (1) and taking the limit $\varepsilon_3 \to 0$, we obtain the reduced order dynamic model valid in the fast time-scale as:

Distillation column
$1 \leq i \leq n$

$$\frac{dT_i}{d\tau} = \frac{D_s\tilde{h}_l(T_f)}{M_i c_{p,l}}\left[k_V u_V(k_{i+1,v}-k_{i,v})\right]$$

Compressor

$$\frac{dT_c}{d\tau} = \frac{D_s\tilde{h}_l(T_f)}{M_c c_v}\left[k_V u_V(k_{1,v}-k_c)\right]$$

Reboiler-condenser

$$\begin{aligned} 0 &= k_{V1}u_{V1}k_c - k_F k_q u_q \\ 0 &= -k_V u_V k_{bv} + k_F k_q u_q \end{aligned} \tag{2}$$

We note that all the temperatures in a loop comprising of the column, the compressor and the reboiler-condenser (the energy recycle loop) have a component in this fast time-scale, while the material balance dynamics does not evolve in this time-scale. This fast dynamics converge to a quasi-steady state captured by the constraints:

$$\begin{bmatrix} 0 \\ \vdots \\ 0 \\ \vdots \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \mathbf{g}_f = \begin{bmatrix} k_V u_V(k_{2,v}-k_{1,v}) \\ \vdots \\ k_V u_V(k_{i+1,v}-k_{i,v}) \\ \vdots \\ k_V u_V(k_{n+1,v}-k_{n,v}) \\ k_V u_V(k_{1,v}-k_c) \\ k_{V1}u_{V1}k_c - k_F k_q u_q \\ -k_V u_V k_{bv} + k_F k_q u_q \\ k_V u_V - k_{V1}u_{V1} \end{bmatrix} \tag{3}$$

We can note that these quasi-steady state constraints are not linearly independent (note that $k_{n+1,v} = k_{bv}$). Thus the quasi-steady state for the fast dynamics does not specify an isolated equilibrium point; rather it specifies a lower dimensional equilibrium manifold. The large internal (to the system) energy flows do not affect the total enthalpy of the system. Only $n+3$ (out of $n+4$) constraints are linearly independent and thus, there is a slower dynamics for these temperatures in the energy recycle loop.

Let us consider the same limiting case $\varepsilon_3 \to 0$ in the original time-scale t, to obtain the description of the dynamics after the fast boundary layer. This takes the form:

Distillation column
$1 \leq i < nf$

$$\frac{dx_i}{dt} = \frac{D_s}{M_i\varepsilon_1}\left[k_V u_V(y_{i+1}-y_i)+u_R(x_{i-1}-x_i)\right]$$
$$\frac{dT_i}{dt} = \frac{D_s\tilde{h}_l(T_f)}{M_i c_{p,l}}\left[z_i+\frac{u_R(k_{i-1,l}-k_{i,l})}{\varepsilon_1}\right]$$

$$\frac{dx_{nf}}{dt} = \frac{D_s}{M_{nf}}\left[\frac{k_V u_V(y_{nf+1}-y_{nf})+u_R(x_{nf-1}-x_{nf})}{\varepsilon_1}+k_F u_F(x_f-x_{nf})\right]$$

$$\frac{dT_{nf}}{dt} = \frac{D_d\tilde{h}_l(T_f)}{M_{nf}c_{p,l}}\Big[z_{nf} + \frac{u_R}{\varepsilon_1}(k_{nf-1,l} - k_{nf,l}) + k_F u_F(1 - k_{nf,l})\Big]$$

$nf < i \leq n$

$$\frac{dx_i}{dt} = \frac{D_s}{M_i}\left[\frac{k_V u_V}{\varepsilon_1}(y_{i+1} - y_i) + \left(\frac{u_R}{\varepsilon_1} + k_F u_F\right)(x_{i-1} - x_i)\right]$$

$$\frac{dT_i}{dt} = \frac{D_s\tilde{h}_l(T_f)}{M_i c_{p,l}}\left[z_i + \left(\frac{u_R}{\varepsilon_1} + k_F u_F\right)(k_{i-1,l} - k_{i,l})\right]$$

Compressor

$$\frac{dT_c}{dt} = \frac{D_s\tilde{h}_l(T_f)}{M_c c_v}\left[z_c + \frac{\eta k_F k_w u_W}{\varepsilon_1}\right]$$

$$\frac{dP_c}{dt} = \frac{D_s R T_c}{V_c}\left[\frac{k_V u_V - k_{V1}u_{V1}}{\varepsilon_1} - k_{tc}u_{tc}\right]$$

Reboiler-condenser

$$\frac{dM_B}{dt} = D_s\left[\frac{u_R - k_V u_V}{\varepsilon_1} + k_F u_F - k_B u_B\right]$$

$$\frac{dx_B}{dt} = \frac{D_s}{M_B}\left[\left(\frac{u_R}{\varepsilon_1} + k_F u_F\right)(x_n - x_B) - \frac{k_V u_V}{\varepsilon_1}(y_B - x_B)\right]$$

$$0 = \frac{D_s\tilde{h}_l(T_f)}{M_h c_{p,l}}\left[z_h - \frac{k_{V1}u_{V1}k_h}{\varepsilon_1}\right]$$

$$0 = \frac{D_s\tilde{h}_l(T_f)}{M_B c_{p,l}}\left[\left(\frac{u_R}{\varepsilon_1} + k_F u_F\right)(k_{n,l} - k_b) + \frac{k_V u_V k_b}{\varepsilon_1} - \left(\sum_{i=1}^{n} z_i + z_c + z_h\right)\right]$$

Trim condenser

$$\frac{dT_o}{dt} = \frac{D_s\tilde{h}_l(T_f)}{M_t c_{p,l}}\left[k_{tc}u_{tc}\left(\frac{k_c}{k\varepsilon_1} - k_o\right) - \frac{k_F k_{qc1}u_{qc1}}{k\varepsilon_1}\right]$$

Reflux drum

$$\frac{dM_D}{dt} = D_s\left[\frac{k_V u_V - u_R}{\varepsilon_1} - u_D\right]$$

$$\frac{dx_D}{dt} = \frac{D_s}{M_D\varepsilon_1}\left[k_V u_V(y_1 - x_D)\right]$$

$$\frac{dT_D}{dt} = \frac{D_s\tilde{h}_l(T_f)}{M_D c_{p,l}}\left[\frac{k_{V1}u_{V1}}{\varepsilon_1}(k_h - k_d) + k_{tc}u_{tc}(k_o - k_d)\right]$$

Auxiliary cooler

$$\frac{dT_m}{dt} = \frac{D_s\tilde{h}_l(T_f)}{M_a c_{p,l}\varepsilon_1}\left[u_R(k_d - k_m) - k_F k_{qc2}u_{qc2}\right] \qquad (4)$$

along with the constraints $\mathbf{g}_f = 0$. The algebraic variables $\mathbf{z}$ denote the limiting terms corresponding to the difference between large energy flows (in the energy recycle loop) which are indeterminate, but finite. We can note that the model (4) after the fast boundary layer is also stiff, owing to the presence of the small parameter ε_1 (equivalently the large term $1/\varepsilon_1$). This indicates the presence of intermediate and slow dynamics.

Remark III.1 *There are two approaches to proceed with the model reduction at this point. We can obtain an ODE (ordinary differential equation) representation of model (4), through substitution of the algebraic variables* $\mathbf{z}$*, which can be obtained from the differentiation of the constraints. The resulting ODE model will be stiff and using singular perturbations, we can further decompose this model to an intermediate and a slow dynamic component. On the other hand, we can also directly apply singular perturbations to the differential algebraic equation (DAE) system (4) to resolve the dynamics in the intermediate time-scale in DAE form, which can subsequently be converted into an equivalent ODE form. It can be shown that the two approaches lead to the same ODE representations. We will use the latter approach which allows for a more concise derivation.*

To this end, let us define the intermediate time-scale $\theta = t/\varepsilon_1$. Substituting θ in (4) and taking the limit $\varepsilon_1 \to 0$, we have:

Distillation column

$1 \leq i < nf$

$$\frac{dx_i}{d\theta} = \frac{D_s}{M_i}\left[k_V u_V(y_{i+1} - y_i) + u_R(x_{i-1} - x_i)\right]$$

$$\frac{dT_i}{d\theta} = \frac{D_s\tilde{h}_l(T_f)}{M_i c_{p,l}}\left[\tilde{z}_i + u_R(k_{i-1,l} - k_{i,l})\right]$$

$$\frac{dx_{nf}}{d\theta} = \frac{D_s}{M_{nf}}\left[k_V u_V(y_{nf+1} - y_{nf}) + u_R(x_{nf-1} - x_{nf})\right]$$

$$\frac{dT_{nf}}{d\theta} = \frac{D_d\tilde{h}_l(T_f)}{M_{nf}c_{p,l}}\left[\tilde{z}_{nf} + u_R(k_{nf-1,l} - k_{nf,l})\right]$$

$nf < i \leq n$

$$\frac{dx_i}{d\theta} = \frac{D_s}{M_i}\left[k_V u_V(y_{i+1} - y_i) + u_R(x_{i-1} - x_i)\right]$$

$$\frac{dT_i}{d\theta} = \frac{D_s\tilde{h}_l(T_f)}{M_i c_{p,l}}\left[\tilde{z}_i + u_R(k_{i-1,l} - k_{i,l})\right]$$

Compressor

$$\frac{dT_c}{d\theta} = \frac{D_s\tilde{h}_l(T_f)}{M_c c_v}\left[\tilde{z}_c + \eta k_F k_w u_W\right]$$

$$\frac{dP_c}{d\theta} = \frac{D_s R T_c}{V_c}\left[k_V u_V - k_{V1}u_{V1}\right]$$

Reboiler-condenser

$$\frac{dM_B}{d\theta} = D_s\left[u_R - k_V u_V\right]$$

$$\frac{dx_B}{d\theta} = \frac{D_s}{M_B}\left[u_R(x_n - x_B) - k_V u_V(y_B - x_B)\right]$$

$$0 = \frac{D_s\tilde{h}_l(T_f)}{M_h c_{p,l}}\left[\tilde{z}_h - k_{V1}u_{V1}k_h\right]$$

$$0 = \frac{D_s\tilde{h}_l(T_f)}{M_B c_{p,l}}\left[u_R(k_{n,l} - k_b) + k_V u_V k_b - \left(\sum_{i=1}^{n}\tilde{z}_i + \tilde{z}_c + \tilde{z}_h\right)\right]$$

Trim condenser

$$\frac{dT_o}{d\theta} = \frac{D_s\tilde{h}_l(T_f)}{M_t c_{p,l}k}\left[k_{tc}u_{tc}k_c - k_F k_{qc1}u_{qc1}\right]$$

Reflux drum

$$\frac{dM_D}{d\theta} = D_s\left[k_V u_V - u_R\right]$$

$$\frac{dx_D}{d\theta} = \frac{D_s}{M_D}\left[k_V u_V(y_1 - x_D)\right]$$

$$\frac{dT_D}{d\theta} = \frac{D_s\tilde{h}_l(T_f)}{M_D c_{p,l}}\left[k_{V1}u_{V1}(k_h - k_d)\right]$$

Auxiliary cooler

$$\frac{dT_m}{d\theta} = \frac{D_s \tilde{h}_l(T_f)}{M_a c_{p,l}} \left[u_R(k_d - k_m) - k_F k_{qc2} u_{qc2} \right] \tag{5}$$

along with the constraints $\mathbf{g}_f = 0$. The terms $\tilde{\mathbf{z}}$ capture the evolution of the variables $\mathbf{z}$ in the intermediate time-scale. This intermediate dynamics converge to a quasi-steady state captured by the constraints:

$$\begin{bmatrix} \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix} = \begin{bmatrix} \mathbf{g}_f \\ \mathbf{g}_x \\ \mathbf{g}_\theta \end{bmatrix}$$

where $\mathbf{g}_x$ represents the constraints arising from the material balance dynamics and $\mathbf{g}_\theta$ represents the constraints arising from the energy balance dynamics. Here, $\mathbf{g}_x$ is:

$$\mathbf{g}_x = \begin{bmatrix} k_V u_V(y_2 - y_1) + u_R(x_0 - x_1) \\ \vdots \\ k_V u_V(y_{i+1} - y_i) + u_R(x_{i-1} - x_i) \\ \vdots \\ k_V u_V(y_{n+1} - y_n) + u_R(x_{n-1} - x_n) \\ u_R - k_V u_V \\ u_R(x_n - x_B) - k_V u_V(y_B - x_B) \\ k_V u_V - u_R \\ k_V u_V(y_1 - x_D) \end{bmatrix}$$

We can note that the constraints $\mathbf{g}_x$ are also not linearly independent (note that $x_0 = x_D$). In fact, the last two constraints can be represented in terms of the first $n+2$ constraints. The deficiency in the linearly independent constraints, in this time-scale, can be attributed to the fact that large internal material flows do not affect the total material holdup of the system. This gives rise to a two-dimensional slow dynamics corresponding to the material balance equations.

The constraints corresponding to the energy balance ($\mathbf{g}_\theta$) are:

$$\mathbf{g}_\theta = \begin{bmatrix} \tilde{z}_1 + u_R(k_{0,l} - k_{1,l}) \\ \vdots \\ \tilde{z}_i + u_R(k_{i-1,l} - k_{i,l}) \\ \vdots \\ \tilde{z}_n + u_R(k_{n-1,l} - k_{n,l}) \\ \tilde{z}_c + \eta k_F k_w u_W \\ \tilde{z}_h - k_{V1} u_{V1} k_h \\ u_R(k_{n,l} - k_b) + \left(-\sum_{i=1}^n \tilde{z}_i - \tilde{z}_c - \tilde{z}_h\right) + k_V u_V k_b \\ k_{tc} u_{tc} k_c - k_F k_{qc1} u_{qc1} \\ k_{V1} u_{V1}(k_h - k_d) + k_{tc} u_{tc}(k_o - k_d) \\ u_R(k_d - k_m) - k_F k_{qc2} u_{qc2} \end{bmatrix}$$

which are linearly independent. Thus the energy balance dynamics does not have any component in the slow time scale and the slow model is two dimensional.

Let us now derive the description of the material balance dynamics in the slow time-scale. We take the limit $\varepsilon_1 \to 0$ in the original time-scale for the system (1) to obtain:

Distillation column

$1 \leq i < nf$

$$\begin{aligned} \frac{dx_i}{dt} &= \frac{D_s}{M_i} w_i \\ \frac{dx_{nf}}{dt} &= \frac{D_s}{M_{nf}} \left[w_{nf} + k_F u_F (x_f - x_{nf}) \right] \end{aligned}$$

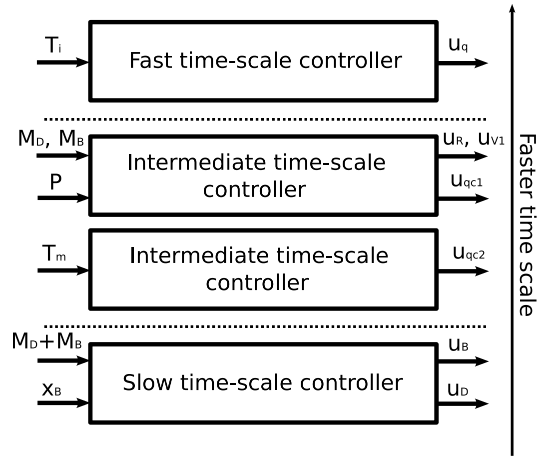

Fig. 2. Hierarchical control structure

$nf < i \leq n$

$$\frac{dx_i}{dt} = \frac{D_s}{M_i} \left[w_i + k_F u_F (x_{i-1} - x_i) \right]$$

Reboiler-condenser

$$\begin{aligned} \frac{dM_B}{dt} &= D_s \left[w_B + k_F u_F - k_B u_B \right] \\ \frac{dx_B}{dt} &= \frac{D_s}{M_B} \left[w_{xb} + k_F u_F (x_n - x_B) \right] \end{aligned}$$

Reflux drum

$$\begin{aligned} \frac{dM_D}{dt} &= D_s \left[-w_B - u_D \right] \\ \frac{dx_D}{dt} &= \frac{D_s}{M_D} \left(-\sum_{i=1}^n w_i - w_{xb} - (x_B - x_D) w_B \right) \end{aligned} \tag{6}$$

along with the constraints $\mathbf{g}_x = 0$. The algebraic variables $\mathbf{w}$, in this time-scale, denote the indeterminate (but finite) limiting terms corresponding to the difference between large material flows.

Thus what we have is a model decomposition of the original multi-scale, stiff model (1) into three non-stiff reduced order models (2), (5) and (6), valid in the fast, intermediate and slow time-scale.

In this paper, we focus on the control of exit concentration of the bottoms stream ($1 - x_B = \mathbf{y_1}$), material holdups (M_D and M_B) and the pressure (P_c) in the system. The time scale separation helps us to propose a hierarchical control structure, as shown in Figure 2.

In the intermediate time-scale, only the scaled flows corresponding to the internal material flows are available for manipulation. So we can address the control of M_D and M_B in the intermediate time-scale, using u_R and u_{V1} respectively. Pressure, which is a critical variable in the operation of vapor recompression distillation, should be regulated in the intermediate time-scale. The natural choice for the manipulated variable for pressure control is Q_{c1}. We can use simple P controllers to address these control actions:

$$\begin{aligned} u_R &= 1 - k_{ro}(M_{D,set} - M_D) \\ u_{V1} &= 1 - k_{v1o}(M_{B,set} - M_B) \\ u_{qc1} &= 1 - k_{po}(P_{set} - P) \end{aligned} \tag{7}$$

Parameter	Value	Parameter	Value
n	95	F	100 mol/min
n_f	48	x_f	0.5
R	608 mol/min	D	50 mol/min
V	658 mol/min	x_D	0.95
W	$7.91{\times}10^5$ J/min	B	50 mol/min
Q_c	$2.77{\times}10^5$ J/min	x_B	0.05
V_1	640 mol/min	$c_{p,v}$	72.1 $J/mol/K$
T_f	296.4 K	$c_{p,l}$	118.3 $J/mol/K$
T_1	293.3 K	M	1000 mol
T_n	300.1 K	M_c	200 mol
T_c	310.0 K	M_t	1000 mol
T_h	302.8 K	M_B	1000 mol
T_m	296.2 K	α	1.162
P_{col}	10.13 bar	P_c	14.11 bar
ε_1	0.082	ε_2	0.025

TABLE I
NOMINAL PROCESS PARAMETERS

The total material holdup ($M_D + M_B$: $\mathbf{y_2}$) also needs to be controlled in the slow time-scale, alongwith $\mathbf{y_1}$, the purity of the bottoms stream. The available manipulated inputs are u_D and u_B. A model based controller can be derived to address these control objectives using the slow model (6). To illustrate these results, let us consider a simulation case study of propane-propylene separation in a vapor recompression distillation system.

IV. SIMULATION RESULTS

We consider a simulation case of propane-propylene separation in a vapor recompression distillation column shown in Figure 1. The nominal values for various variables are listed in table I. We used control laws (7) with $k_{ro} = 0.33$, $k_{v1o} = 0.31$ and $k_{po} = 0.28$, based on Ziegler-Nichols technique. We used an input/output linearizing controller to address the control objectives in the slow time-scale. The slow model (6) is a differential algebraic equation (DAE) system. In order to obtain a state-space representation of the slow dynamics, the algebraic constraints $\mathbf{g}_x = 0$ are differentiated, after substituting the control laws (7). This allows to obtain expressions for the algebraic variables w. These are substituted in (6) to obtain the state space representation of the slow model, which is used for the controller derivation. The relative degree for the two outputs, in this case, is 1 and therefore we requested first order responses:

$$\beta_1 \frac{d\mathbf{y_1}}{dt} + \mathbf{y_1} = v_1, \quad \beta_2 \frac{d\mathbf{y_2}}{dt} + \mathbf{y_2} = v_2 \tag{8}$$

with $\beta_1 = \beta_2 = 20\ min$ using a state feedback controller. In order to get offset free response, we added external error feedback PI controllers, tuned following the arguments in [6].

To test the proposed controller scheme, we applied a set point change of +3% to $\mathbf{y_1}$ and the corresponding response of the system is shown in Figure 3. We can note a smooth set point transition demonstrating the efficacy of the proposed control structure.

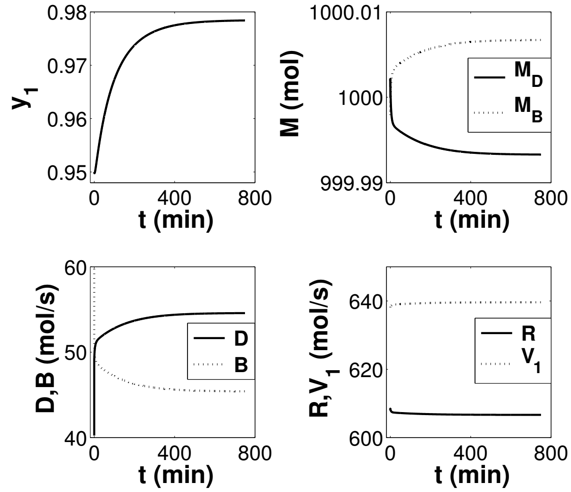

Fig. 3. Closed loop performance for a set point chance in $\mathbf{y_1}$

V. CONCLUSIONS

In this paper, we considered an energy integrated distillation scheme - vapor recompression distillation. We showed that the dynamic equations governing the material and energy balance are stiff, giving rise to a three time-scale dynamic behavior. We used singular perturbations to derive reduced order non-stiff models valid in each time-scale and proposed a hierarchical control strategy exploiting this time-scale separation. A simulation case study was performed on propane-propylene separation to illustrate the performance of the proposed controllers. We demonstrated that the proposed controllers exhibit excellent performance in enabling steady state transitions.

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