PDAE Formulations of Gas Pipes with Gas Mixtures

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Abstract

A PDAE model of a multicomponent gas pipeline has been formulated and solved using the `ode15s` solver of Matlab. The model with boundary conditions allows for reactions and diffusion. Also, general cubic equations of state for pressure and enthalpy are described. To simplify the implementation at this stage, a non-reactive, non-diffusional model with fixed feed composition is considered, and multicomponent versions of the Redlich-Kwong-Soave and Peng-Robinson equations of state, as well as a multicomponent second order virial equation of state have been implemented.

Depending on the use of the model, the results showed the importance of considering the feed composition in the model, as well as using a high quality pressure equation of state (EOS). Furthermore, in order to achieve accurate temperature predictions, it is necessary to use a high quality enthalpy EOS, and to include a transient energy balance.

1 Introduction

When using mechanistic/physical laws to model systems, the result is often a combination of partial differential equations (PDEs), ordinary differential equations (ODEs), and algebraic equations (AEs). For dynamic models, the traditional approach has been to eliminate algebraic equations, leading to differential equations in the relevant variables. The advantage of this approach is that the resulting model equations are relatively well understood when it comes to analyzing the existence and uniqueness of solutions, as well as the well-posedness. Furthermore, there is a plethora of well understood numerical techniques to solve the problems. In fact, eliminating the algebraic equations may well be the best strategy, numerically speaking, when attempting to solve the model.

Eliminating the algebraic equations has, however, some important disadvantages. If it is of interest to know the values of the variables that have been eliminated, a post processing of the already established solution is necessary. But more importantly, eliminating the algebraic equations often requires a considerable amount of manipulation such as differentiation, etc. In addition to the necessary model manipulation, the resulting model becomes more complex.

There are thus many reasons to preserve models of systems as e.g. a combination of ODEs and AEs; such model forms are known as Differential Algebraic Equations (DAEs). The existence and uniqueness of such models, as well as solution strategies, are discussed in e.g. (Brenan, Campbell & Petzold 1989), (Ascher & Petzold 1998), and (Hairer & Wanner 2002). An important concept of DAEs is that of the index of the problem, which essentially tells how many times the equations must be differentiated in order to eliminate the algebraic variables. Numerical solvers such as `DASSL` and `RADAU` solve models formulated as DAEs, but with increasing difficulties as the index of the problem increases. Other solvers such as `ode15s`, which is available for Matlab, (Shampine, Reichelt & Kierzenka 1999), solve problems of index 0 and 1 only.

Models that include PDEs pose the additional difficulty of boundary conditions and their location, as well as how to discretize them. The most general models formed by combinations of PDEs, ODEs, and AEs, are known as Partial Differential Algebraic Equations (PDAEs). The analysis of index and the location of boundary conditions for linear PDAEs are discussed e.g. in (Martinson & Barton 2001) and (Martinson & Barton 2002); see (Carlson & Lie 2002) for an elementary discussion of boundary condition location. In general, hyperbolic modes of such models represent conservation equations and are characterized by restrictions on the location of boundary conditions as well as discretization techniques. Parabolic modes, on the other hand, represent modes with entropy production (friction, diffusion, etc.) and are less restrictive both with regards to the

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location of the boundary condition and the discretization scheme. Additional difficulties show up for nonlinear systems, where shock waves and alternating locations of boundary conditions may occur, e.g. (Smoller 1994) and (Martinson & Barton 2001).

Gas pipelines are of interest for distributing natural gas to consumers. Typical models of such pipelines involve the mass, momentum, and energy balances which typically are posed as PDEs in one spatial variable: position along the pipeline. In addition, algebraic equations such as a friction model, a pressure state equation, an enthalpy state equation, the defining equation for total energy, etc. are needed, see e.g. (Fincham & Goldwater 1979), (Osiadacz 1987), (Osiadacz & Chaczykowski 2001), (Hofsten 2001), (Carlson & Lie 2002), as well as (Sandler 1989), (Prausnitz, Lichtenthaler & de Azevedo 1986), (Reid, Prausnitz & Sherwood 1977). The resulting model is a PDAE, and a simplified model of such a system is linearized and analyzed in (Martinson & Barton 2001). (Chua & Dew 1984) gives an early account of numerical methods for solving models of gas pipelines. (Osiadacz & Chaczykowski 2001) propose to use the Method of Lines (MOL)[1] for solving this model, see e.g. (Schiesser 1991), (Silebi & Schiesser 1992), and (Wouwer, Saucez, Schiesser & Saucez 2001) for a discussion of MOL. A potential problem with using MOL is that a gas pipeline model often is quite close to being hyperbolic, and for hyperbolic systems MOL must be used with care, see (Brenan et al. 1989) and (Wouwer et al. 2001). Quite often, simplified models are used such as models in quasi steady state, e.g. it may be assumed that the energy balance is at steady state, or that both the energy balance and the momentum balance are at steady state, see (Osiadacz 1987) and (Hofsten 2001). In (Osiadacz & Chaczykowski 2001), the importance of a dynamic energy balance is studied. In that study, a relatively advanced pressure state equation is used, while a very simple enthalpy state equation is used. Their view on the importance of a dynamic energy balance is supported by (Carlson & Lie 2002), who in addition considered more accurate enthalpy state equations.

The main aim of this paper is to extend the study in (Carlson & Lie 2002) by including the possibility that the gas consists of a gas mixture. The developed model is relatively general in the sense that the possibilities of chemical reactions and diffusion are included. Furthermore, a more general presentation of cubic equations of state is included. In order to limit the presentation, the simplified case of no reaction and no diffusion is considered, where also the feed composition is constant. Then a discretized model with PDAEs turned into index 1 DAEs using MOL, is simulated using the `ode15s` solver of Matlab©. The paper is organized as follows. In section 2, we pose the model in the form of PDAEs, and discuss the choice of boundary conditions. In section 3, model parameters and operating conditions are given, and the models are simulated. Conclusions are drawn in section 4.

2 Model of gas pipeline

2.1 PDAE for gas mixture

Consider a gas mixture of n_c components which are transported in a gas pipe line. The following general notation is used: column vector $\mathbf{y} \in \mathbb{R}^{n_c}$ is used to denote some quantity of the components in the mixture. Operator $*$ denotes array multiplication[2], hence $\mathbf{y} * \mathbf{z}$ has elements $y_i \cdot z_i$. Likewise, / denotes array division[3], hence $\mathbf{y}/\mathbf{z}$ has elements y_i/z_i. Furthermore, $y = \mathbf{y}^T \mathbf{1}_{n_c}$, where column vector $\mathbf{1}_{n_c} \in \mathbb{R}^{n_c}$ with every element being 1; thus y is the sum of the elements in $\mathbf{y}$. Figure 1 gives a sketch of the gas pipe line where gas mixture is transported.

Here, A is the cross sectional area of the pipe, and Ω is the circumference. We consider a one-dimensional spatial problem, where quantities vary with time t and axial position x. At co-ordinates (t, x), the velocities of the various components are collected in vector $\mathbf{v}$, element v_i of $\mathbf{v}$ is assumed to have axial direction and have the same value across the pipeline.

The momentum balance is based on the barycentric (mass averaged) velocity v_b:

$$v_b = \frac{1}{\rho} \mathbf{v}^T \boldsymbol{\rho}$$

where $\boldsymbol{\rho}$ contains the mass concentrations (mass/volume) of the components. It is common to introduce the

[1] The name MOL originates from solving the ODEs of a material description of a system: the solution is valid in a co-ordinate system that moves along the *characteristic line* in the space of independent variables of the equivalent spatial description. MOL is also used to denote the idea of discretizing PDEs in all but one independent variable, leading to ODEs which can be solved using a standard ODE solver.

[2] In Matlab: `.*`

[3] In Matlab: `./`

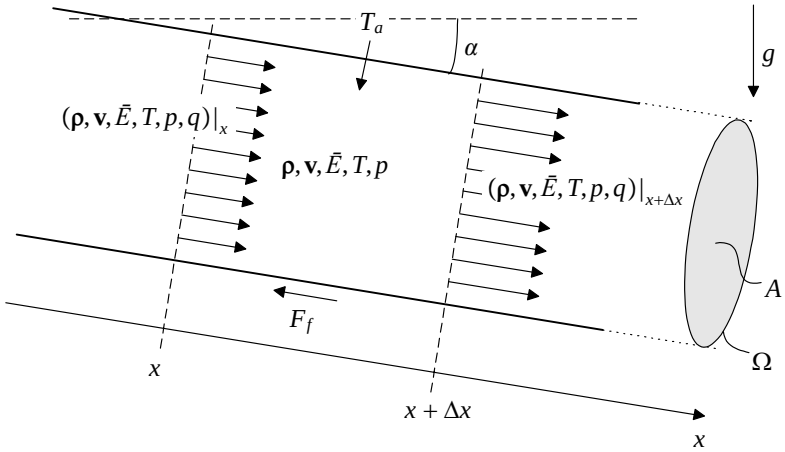

Figure 1: Sketch of gas pipeline with cross sectional area A and circumference Ω.

diffusional mass flux $\mathbf{j}$ defined by the difference between $\mathbf{v}$ and v_b as:

$$\mathbf{j} = \boldsymbol{\rho} * (\mathbf{v} - v_b \mathbf{1}_{n_c}).$$

In a material description where the co-ordinate system moves with the gas at velocity v_b, the mass, momentum, and energy balances lead to:

$$\begin{aligned}
\frac{D}{Dt}\boldsymbol{\rho} &= -\frac{\partial}{\partial x}\mathbf{j} + \mathbf{r} \\
\frac{D}{Dt}(\rho v_b) &= -\frac{\partial}{\partial x}p - \frac{1}{2}\rho v_b |v_b| \frac{\Omega f}{A} + \rho g \sin\alpha \\
\frac{D}{Dt}(\bar{E}) &= -\frac{\partial}{\partial x}(v_b p + q) + \frac{h\Omega}{A}(T_a - T) - \frac{\partial}{\partial x}\left(\left(\frac{\partial U}{\partial \mathbf{m}}\right)^T \mathbf{j}\right) + \frac{1}{2}\rho v_b^2 |v_b| \frac{\Omega f}{A}.
\end{aligned}$$

Here, D/Dt is the substantial derivative, $\mathbf{r}$ is the rate of reaction, p is the hydrostatic pressure, f is Fanning's friction factor, $\bar{E}$ is volumetric total energy, q is axial heat conduction, U is internal energy, the elements of $\mathbf{m}$ are the masses of the compoents, $\partial U/\partial \mathbf{m}$ is a column vector containing the partial derivatives of U wrt. m_i, and h is the heat transfer coefficient between the gas pipe and the surroundings of temperature T_a. See e.g. (de Groot & Mazur 1984), (Lavenda 1978), and (Bird, Stewart & Lightfoot 2002) for details.

In the momentum balance, it may be convenient to introduce the volumetric momentum $\bar{\pi} = \rho v_b$ as a variable instead of v_b, and substitute $\bar{\pi}/\rho$ for v_b. An alternative is to introduce the mass flow $w = A\boldsymbol{\rho}^T\mathbf{v} = A\rho v_b$ and replace v_b by $w/(A\rho)$. By simultaneously switching to a spatial description where $Dy/Dt = \partial y/\partial t + \partial(v_b y)/\partial x$, in the interior $x \in (0, L)$ of the gas pipe the mass, momentum, and energy balances become:

$$\frac{\partial}{\partial t}\boldsymbol{\rho} = -\frac{1}{A}\frac{\partial}{\partial x}\left(\frac{w}{\rho}\boldsymbol{\rho}\right) - \frac{\partial}{\partial x}\mathbf{j} + \mathbf{r} \tag{1}$$

$$\frac{\partial w}{\partial t} = -\frac{1}{A}\frac{\partial}{\partial x}\left(\frac{w^2}{\rho} + A^2 p\right) - \frac{\Omega f}{2A^2}\frac{w}{\rho}|w| + Ag\sin\alpha \cdot \rho \tag{2}$$

$$\frac{\partial \bar{E}}{\partial t} = -\frac{1}{A}\frac{\partial}{\partial x}\left(\frac{w\bar{E}}{\rho} + \frac{pw}{\rho} + Aq\right) + \frac{h\Omega}{A}(T_a - T) - \frac{\partial}{\partial x}\left(\left(\frac{\partial U}{\partial \mathbf{m}}\right)^T \mathbf{j}\right) + \frac{\Omega f}{2A^4}\frac{w^2}{\rho^2}|w|, \tag{3}$$

which can be considered a generalization of the model in (Carlson & Lie 2002).[4]

In addition, the following algebraic equations are needed:

1. An expression for diffusional mass flux $\mathbf{j}$, e.g. a generalized Fick's law:

$$\mathbf{j} = -D\frac{\partial \boldsymbol{\rho}}{\partial x}$$

[4] Note that an erroneous sign in the heat of friction of (Carlson & Lie 2002) has be corrected.

where D is a (possibly non-symmetric) matrix, or the Stefan-Maxwell equation, see e.g. (Cussler 1997) and (Bird et al. 2002).

2. An expression for the rate of reaction $\mathbf{r}$, see e.g. (Rawlings & Ekerdt 2002).

3. A state equation for pressure, e.g. the ideal gas law:

$$p = cRT, \tag{4}$$

where the molar concentration $c = \mathbf{c}^T \mathbf{1}_{n_c}$ is related to the mass concentration $\boldsymbol{\rho}$ as

$$\boldsymbol{\rho} = \mathbf{c} * \mathbf{M}. \tag{5}$$

A more realistic group of equations of state (EOS) is the cubic EOS, see e.g. Table 1 for a description of the Peng-Robinson cubic EOS. For mixtures of components, the various components will have different critical data (T_c, p_c, ω). In that case, pseudo components are considered, where a and b are found by mixing rules, e.g.:

$$\begin{aligned} a(T) &= \boldsymbol{\xi}^T \mathbf{A} \boldsymbol{\xi} \\ b &= \boldsymbol{\xi}^T \mathbf{b} \end{aligned}$$

where $\boldsymbol{\xi}$ contains the mole fractions

$$\boldsymbol{\xi} = \frac{1}{c}\mathbf{c}, \tag{6}$$

the elements of column vector $\mathbf{b}$ is the b's of the various components, and the elements of matrix $\mathbf{A}$ are $a_{jk}(T)$ given as

$$a_{jk}(T) = (1 - \delta_{jk}) \sqrt{a_j(T)\, a_k(T)},$$

with δ_{jk} a binary interaction parameter; $\delta_{jj} = 0$. For simple models, δ_{jk} is assumed to be independent of the composition, temperature, and pressure. Binary interaction parameter δ_{jk} usually have small values, and it is common to assume they are zero when they are not known. Other choices of EOS than a cubic EOS are also mentioned in Table 1.

4. Friction is given by expressions of type $f = F(\mathrm{Re}, \varepsilon/D)$ which relates Fanning's friction factor f to the Reynold number Re

$$\mathrm{Re} = \frac{wD/A}{\mu} \tag{7}$$

where D is pipe diameter and μ is viscosity, and ε describes the roughness of the pipe. Viscosity of gas may be given e.g. as in (Lydersen 1979):

$$\mu = \frac{bT^{3/2}}{S + T} \tag{8}$$

where b and S are parameters depending on gas type, while the temperature is absolute temperature. One common example of a friction model is the Colebrook model, which gives an implicit expression for f. An explicit algebraic approximation for the Colebrook model is e.g. the Colebrook-Haaland model, (Elseth 2001):

$$f = \left(\frac{1}{1.8 \log_{10}\left(\frac{6.9}{\mathrm{Re}} + \left(\frac{\varepsilon}{3.7D} \right)^{1.1} \right)} \right)^2 \frac{1}{4}. \tag{9}$$

The factor $\frac{1}{4}$ is introduced to compensate for a difference in the definition of the friction factor in this paper, which follows (Bird, Stewart & Lightfoot 1960), and in the referenced thesis. Other possibilities are listen in Table 1.

5. The definition of the volumetric total energy:

$$\bar{E} = \bar{U} + \frac{1}{2A^2}\frac{w^2}{\rho} + \bar{P}_0 + \rho g x \sin\alpha, \tag{10}$$

where $\bar{U}$ is volumetric internal energy, and $\bar{P}_0$ is volumetric potential energy at position $x = 0$. It is convenient to express $\bar{U}$ as

$$\bar{U} = \bar{H} - p, \tag{11}$$

Table 1: Various alternative algebraic equations for the gas pipe model.

Model	Equation	Name
Pressure state equation	$\frac{pM}{\rho RT} = 1 + \frac{B(T)\rho}{M}$	Second order virial equation; see e.g. (Reid et al. 1977) for $B(T)$
—"—	$p = \frac{RT}{\tilde{V}-b} - \frac{a(T)}{(\tilde{V}+\varepsilon b)(\tilde{V}+\sigma b)}; a(T) = \frac{\Omega_a R^2 T_c^2}{p_c}\alpha(T_r;\omega); b = \frac{\Omega_b R T_c}{p_c}$	General cubic EOS; see e.g. (Reid et al. 1977) for (T_c, p_c, ω)
	$\varepsilon = 0$, $\sigma = 1$, $\Omega_a = 0.42748$, $\Omega_b = 0.08664$, $\alpha(T_r;\omega) = \left[1 + \left(0.480 + 1.574\omega - 0.176\omega^2\right)\left(1 - \sqrt{T_r}\right)\right]^2$	Redlich-Kwong-Soave EOS
	$\varepsilon = 1 + \sqrt{2}$, $\sigma = 1 - \sqrt{2}$, $\Omega_a = 0.457235$, $\Omega_b = 0.077796$, $\alpha(T_r;\omega) = \left[1 + \left(0.37464 + 1.54226\omega - 0.26992\omega^2\right)\left(1 - \sqrt{T_r}\right)\right]^2$	Peng-Robinson EOS
—"—	—	S-GERG 88, (Int 1997)
Friction law	$\sqrt{\frac{1}{f}} = 4\log_{10}\left(\frac{3.7D}{\varepsilon}\right)$	Rough pipe law
—"—	$\sqrt{\frac{1}{f}} = 0.92 \cdot 6.78\,\mathrm{Re}^{0.073}$	Panhandle law
Molar enthalpy state equation	$\tilde{H}^{\mathrm{ig}}(T) = \int_0^T \tilde{c}_p^{\mathrm{ig}}(T)\,dT$, where $\tilde{c}_p^{\mathrm{ig}}(T) = \mathbf{a}_{c_p}^T\boldsymbol{\xi} + \mathbf{b}_{c_p}^T\boldsymbol{\xi}T + \mathbf{c}_{c_p}^T\boldsymbol{\xi}T^2 + \mathbf{d}_{c_p}^T\boldsymbol{\xi}T^3$	Ideal gas law; $\tilde{c}_p^{\mathrm{ig}}$ is molar heat capacity. See e.g. (Reid et al. 1977) for coefficients.
—"—	$\tilde{H}(T) = \tilde{H}^{\mathrm{ig}}(T) + RT(z-1) + \frac{a(T) - T\frac{\partial a(T)}{\partial T}}{b(\sigma-\varepsilon)}\ln\left(\frac{\tilde{V}+\varepsilon b}{\tilde{V}+\sigma b}\right)$, where: $z = \frac{M}{RT}\frac{p}{\rho}$, while $a(T)$ and b are found from mixing rules	Cubic EOS, see pressure EOS and e.g. (Sandler 1989). z is the compressibility coefficient

where volumetric enthalpy $\bar{H}$ can be expressed as

$$\bar{H} = c\tilde{H} \tag{12}$$

where $\tilde{H}$ is molar enthalpy.

6. A simple state equation for molar enthalpy is based on a constant molar heat capacity vector $\tilde{\mathbf{c}}_v$ at constant volume:

$$\tilde{H} = \tilde{U}_0 + \tilde{\mathbf{c}}_v^T\boldsymbol{\xi}T + pc, \tag{13}$$

where $\tilde{U}_0$ is molar internal energy at some reference state; we could set $\tilde{U}_0 = 0$. Other possible molar enthalpy EOS are listed in Table 1,[5] where in the case of a cubic EOS:

$$\frac{\partial a}{\partial T} = \left(\boldsymbol{\xi} * \frac{\partial \mathbf{a}}{\partial T}/\mathbf{a}\right)^T \mathbf{A}\boldsymbol{\xi}.$$

7. Assuming Fourier's law for heat conduction:

$$q = -k\frac{\partial T}{\partial x} \tag{14}$$

where k is thermal conductivity.

8. In the heating term caused by diffusion, $U = \bar{U} \cdot V$. Since $\bar{H} = c\tilde{H}$ where $\tilde{H}$ is based on mole fractions $\boldsymbol{\xi}$, it is convenient to rephrase $\partial U/\partial \mathbf{m} = \partial \bar{U}(\boldsymbol{\xi})/\partial \boldsymbol{\rho}$. Since

$$\begin{aligned} \boldsymbol{\xi} &= \frac{1}{c}\mathbf{c} \\ \boldsymbol{\rho} &= \mathbf{c} * \mathbf{M}, \end{aligned}$$

[5] A typo in the Matlab implementation of $\tilde{H}^{\mathrm{ig}}(T)$ of (Carlson & Lie 2002) has been corrected.

it follows that $\partial\bar{U}/\partial\boldsymbol{\rho}$ can be expressed by:

$$c \cdot \mathbf{M} * \frac{\partial \bar{U}}{\partial \boldsymbol{\rho}} = \frac{\partial \bar{U}}{\partial \boldsymbol{\xi}} - \mathbf{1}_{n_c} \cdot \left(\frac{\partial \bar{U}}{\partial \boldsymbol{\xi}}\right)^T \boldsymbol{\xi}.$$

With

$$\bar{U} = c\tilde{H} - p,$$

the following quantities are needed:

$$\frac{\partial}{\partial \boldsymbol{\xi}}\left(c\tilde{H}\right) = c\frac{\partial \tilde{H}}{\partial \boldsymbol{\xi}} + \tilde{H}\mathbf{c} \text{ and } \frac{\partial p}{\partial \boldsymbol{\xi}}$$

where $\partial\tilde{H}/\partial\boldsymbol{\xi}$ and $\partial p/\partial\boldsymbol{\xi}$ are found from differentiating the EOS for enthalpy and pressure.

2.2 Simplified model

As stated, in this paper it is assumed that $\mathbf{j} = 0$, and that no reactions take place: $\mathbf{r} = 0$. In *addition*, assume that the composition of the feed gas is constant over time wrt. the molar composition, i.e. $\boldsymbol{\xi}$ of the feed gas is constant. Based on these assumptions, it follows that the molar composition $\boldsymbol{\xi}$ must the *constant* for all (t, x), and equal to the constant feed composition. In that case, the gas mixture can be considered as a single gas component with properties given by mixing rules. Thus no mass balances for for the individual components are needed, instead the total mass balance is needed, $\rho = \boldsymbol{\rho}^T \mathbf{1}_{n_c}$. In sum, in the interior $x \in (0, L)$ of the gas pipe the mass, momentum, and energy balances become identical to the model presented in (Carlson & Lie 2002)[6] — with the modification that the mixing rules are applied to the EOS with $\boldsymbol{\xi}$ fixed and equal to the feed composition.

In general, it would seem natural to choose the state equation for enthalpy to conform with the state equation for pressure, but simplifications are common in order to make the elimination of the enthalpy state equation tractable. In this paper, the algebraic state equations are preserved in the PDAE formulation, and the tractability of the elimination step is not an issue.

In addition to this model which is valid in the internal of the system, boundary conditions are needed. These will be discussed in the next section. Initial conditions are also needed; typically it is assumed that $\rho(t = 0, x)$, $w(t = 0, x)$, and $\bar{E}(t = 0, x)$ are known functions of the spatial variable x.

2.3 Boundary conditions

A simplified analysis of the requirements for boundary conditions were given in (Carlson & Lie 2002). Based on physical reasoning, it is natural to extend the multi-component case as follows: The feed pressure is given at position $x = 0$, together with the composition $\boldsymbol{\xi}$, and the temperature. Likewise, the mass flow to the consumer is specified at $x = L$. Thus:

$$\begin{aligned} p(t, x = 0) &= p_0(t) \\ \boldsymbol{\xi}(t, x = 0) &= \boldsymbol{\xi}_0(t) \\ T(t, x = 0) &= T_0(t) \\ w(t, x = L) &= w_L(t). \end{aligned}$$

When it comes to the heat conduction $q(t, x)$, it is less clear where to put the boundary conduction; in (Carlson & Lie 2002) the choice

$$q(t, x = L) = 0$$

was made, and the same condition is used here.

With mass diffusion, it is natural to require no mass diffusion at $x = 0$:

$$\mathbf{j}(t, x = 0) = \mathbf{j}_0(t).$$

In this paper, the case of $\mathbf{j}(t, x) \equiv 0$ is considered, together with $\boldsymbol{\xi}_0(t) =$ constant.

To conclude, the functions $p_0(t)$, $w_L(t)$, $T_0(t)$, and $\xi_0(t)$ are specified by the surroundings of the gas pipe, and the boundary conditions specify how these functions interact with the gas pipe.

[6] Except for a corrected sign in the heat of friction.

Table 2: Some approximations of the gradient with fixed spatial step length. Upwind formulaes are listen below; the corresponding down-wind formulaes are found by substituting $-\Delta x$ for Δx in the approximations.

True value	**Approximation**	**Residual**
$\left.\frac{du(x)}{dx}\right\|_{x=x_0}$	$\frac{u(x_0+\Delta x)-u(x_0)}{\Delta x}$	$\mathcal{O}\left(\Delta x\right)$
$\left.\frac{du(x)}{dx}\right\|_{x=x_0}$	$\frac{u(x_0+\Delta x)-u(x_0-\Delta x)}{2\cdot\Delta x}$	$\mathcal{O}\left(\Delta x^2\right)$
$\left.\frac{du(x)}{dx}\right\|_{x=x_0}$	$\frac{-3u(x_0)+4u(x_0+\Delta x)-u(x_0+2\cdot\Delta x)}{2\cdot\Delta x}$	$\mathcal{O}\left(\Delta x^2\right)$
$\left.\frac{du(x)}{dx}\right\|_{x=x_0}$	$\frac{u(x_0-2\cdot\Delta x)-8u(x_0-\Delta x)+8u(x_0+\Delta x)-u(x_0+2\cdot\Delta x)}{12\cdot\Delta x}$	$\mathcal{O}\left(\Delta x^4\right)$
$\left.\frac{du(x)}{dx}\right\|_{x=x_0}$	$\frac{-3u(x_0-\Delta x)-10u(x_0)+18u(x_0+\Delta x)-6u(x_0+2\cdot\Delta x)+u(x_0+3\cdot\Delta x)}{12\cdot\Delta x}$	$\mathcal{O}\left(\Delta x^4\right)$
$\left.\frac{du(x)}{dx}\right\|_{x=x_0}$	$\frac{-25u(x_0)+48u(x_0+\Delta x)-36u(x_0+2\cdot\Delta x)+16u(x_0+3\cdot\Delta x)-3u(x_0+4\cdot\Delta x)}{12\cdot\Delta x}$	$\mathcal{O}\left(\Delta x^4\right)$

2.4 PDAE formulation vs. PDE formulation

The model of the gas pipeline clearly demonstrates the advantage in posing the model as a PDAE, instead of as a PDE where the algebraic equations have been eliminated. With the PDAE formulation, switching to alternative algebraic equations such as alternative friction laws, alternative pressure state equations, alternative enthalpy state equations, alternative viscosity models, etc. is achieved by just changing the call to a different function where a different algebraic equation is evaluated.

In the traditional formulation, on the other hand, extensive manipulations are required in order to eliminate the algebraic equations so that one is left with three PDEs with e.g. density ρ, mass flow w, and temperature T are the unknowns. The advantage with the elimination is that the resulting PDEs may be simpler to solve than PDAEs.

In sum, posing the model of the gas pipeline as a PDAE is much simpler then posing it as a PDE, since a considerable amount of formula manipulation is avoided. In particular, this is true if we have not settled on some of the algebraic equations such as the friction law, the pressure state equation, and the molar enthalpy state equation. With a PDAE model, we simply switch the algebraic equations, while with a PDE model, we need to go through considerable formulae manipulation for each new algebraic equation that we want to test. Another advantage of the PDAE formulation is that there is no need for post processing of the computed solution in order to find how other quantities then ρ, w, and T develop over time. The main disadvantage of the PDAE formulation is that there are simply more unknowns in the problem, and that we leave a possibly difficult problem of solving the algebraic equations to the DAE solver.

3 Simulation of gas pipeline

3.1 Discretization of PDAEs into DAEs

In practice, the PDAEs must be discretized, e.g. by the Method of Lines. Here, the model in eqs. 1 – 14 is discretized in spatial variable x. First we divide the spatial region $x \in [0, L]$ into N compartments of equal width Δx, $\Delta x = L/N$. Denoting location $x_i = (i-1)\cdot\Delta x$, we see that $x = 0 \Leftrightarrow x_1$, while $x = L \Leftrightarrow x_{N+1}$. We thus need $N+1$ elements to store results for $x_i, i \in \{1, 2, \cdots, N+1\}$. We consider. We approximate the spatial gradient using a linear combination of neighboring points, i.e. we consider the problem of approximating $\left.\frac{du(x)}{dx}\right|_{x=x_0}$ with a weighted sum $\sum_{i=I_1}^{I_2} c_i \cdot u\left(x_0 + i\cdot\Delta x\right)$. The result will be:

$$\left.\frac{du\left(x\right)}{dx}\right|_{x=x_0} = \sum_{i=I_1}^{I_2} c_i \cdot u\left(x_0 + i\cdot\Delta x\right) + \mathcal{O}\left(\Delta x^d\right)$$

where d is the order or degree of the approximation. Some examples of approximations are given in Table 2. In (Osiadacz & Chaczykowski 2001), a fourth order approximation of the gradient is used.

The result is then a set of DAEs of form

$$M\left(t, y\right)\frac{dy}{dt} = f\left(t, y\right),$$

which is a DAE form supported by Matlab solver `ode15s`.

Table 3: Data for the simulations.

Variable	Value + unit in (Osiadacz & Chaczykowski 2001)	Value + unit in SI	Comment
D	1422 mm	1.422 m	diameter
$A = \pi \frac{D^2}{4}$	—	$1.588\,\mathrm{m}^2$	cross sectional area
$\Omega = \pi D$	—	4.467 m	circumference
L	122 km	122×10^3 m	length of pipe
$\frac{R}{M}$	493 J/ (kg K)	493 J/ (kg K)	gas constant
T_a	12 °C	285 K	ground temperature
ε	0.1 mm	—	Roughness of pipe
k	3.4×10^{-2} W/ (m K)	3.4×10^{-2} W/ (m K)	Thermal conductivity coefficient
h	25 W/ (m K) /Ω	$5.597\,\mathrm{W}/\left(\mathrm{m}^2\,\mathrm{K}\right)$	heat transfer coefficient
f	—	≈ 0.00028	friction factor; Colebrook-White law
g	$9.81\,\mathrm{m/s^2}$	$9.81\,\mathrm{m/s^2}$	gravity
α	0°	0°	angular slope of pipe
c_v	1.34×10^3 J/ (kg K)	22.6 J/ (mol K)	specific heat at constant volume
ρ_s	$0.8226\,\mathrm{kg/m^3}$	$0.8226\,\mathrm{kg/m^3}$	normal density
p_0	8.4 MPa	—	B.C.
$Q_{s,x=L}$	$Q_{s,x=L}(t) = f(t)$, see fig.2	—	B.C.
w_L	—	457 kg/ s	$w_L = Q_{s,x=L} \cdot \rho_s$
T_0	42.5 °C	315 K	B.C.
q_L	0 W	0 W	B.C.
$\rho(t=0,x)$	—		I.C.
$w(t=0,x)$	—		I.C.

3.2 Implementation issues

The solution of DAEs requires consistent initial values that satisfy all the constraints at $t = 0$, i.e. $y(t=0)$ and $dy/dt|_{t=0}$ must be consistent with the DAE above. This is only possible if $f(y,t)|_{t=0}$ lies in the column space of $M|_{t=0}$. If $M|_{t=0}$ has a non-trivial nullspace, then the value of $dy/dt|_{t=0}$ is non-unique. In that case, a possible strategy is to choose $dy/dt|_{t=0}$ as a minimum norm solution. In sum, if we have chosen $y(t=0)$, we can find $dy/dt|_{t=0}$ as $dy/dt|_{t=0} = M^{\dagger} y(t=0)$, where $M^{\dagger}$ denotes the pseudo-inverse of M. The danger with using the pseudo inverse, is that a solution is found even when $f(y,t)|_{t=0}$ does not lie in the column space of $M|_{t=0}$.

In (Carlson & Lie 2002), it was found that a straightforward implementation of the DAEs worked if the energy balance was assumed to be in steady state. However, with a transient energy balance, the straightforward implementation of the DAEs became numerically unstable, and a Gauss-Seidel like strategy was used to overcome this problem: the boundary condition $T(t, x=0) = T_f$ was removed, and instead an equivalent boundary condition for molar enthalpy was used, with $\tilde{H}(t, x=0) = \tilde{H}(\rho(t, x=0), T(t, x=0))$. Similarly, eq. 10 was inserted into the right hand side of eq. 3. The resulting code appears to work for the algebraic models used in this paper.

3.3 Simulation data

The model parameters, boundary conditions, etc. are taken from (Osiadacz & Chaczykowski 2001). Since a Matlab version of the pressure state equation used by (Osiadacz & Chaczykowski 2001), S-GERG 88, has not been available, we used simpler state equations based on a single component gas (methane). Translated into the variables used here, these data are given in table 3.

The boundary condition for mass flow, $w_L = w(t, x=L)$ varies with time; this implies that the gas consumption varies — see fig. 2.

In (Osiadacz & Chaczykowski 2001), a gas constant of $R/M = 493\,\mathrm{J/(kg\,K)}$ was used. With $R = 8.31\,\mathrm{J/(mol\,K)}$, this implies that $M = 16.86\,\mathrm{g/mol}$. Postulating that their gas mixture was composed of methane and CO_2, with molar weights of $M_{C_1} = 16.043\,\mathrm{g/mol}$ and $M_{CO_2} = 44.010\,\mathrm{g/mol}$, respectively, this gives a methane content ξ of:

$$16.86 = 16.043\xi + 44.010\,(1-\xi) \Leftrightarrow \xi = 0.971\,\mathrm{mol/mol}.$$

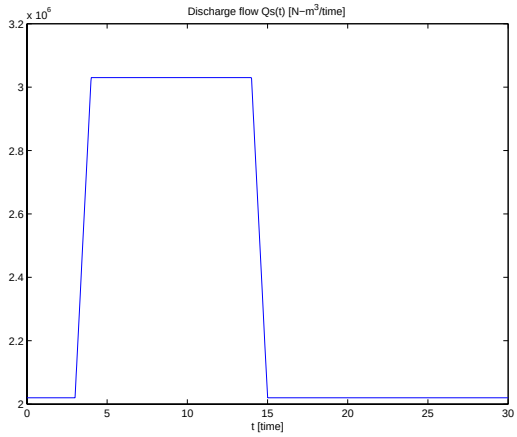

Figure 2: Change of mass flow at $x = L$ is $w_L = Q_{x=L} \cdot \rho_s$.

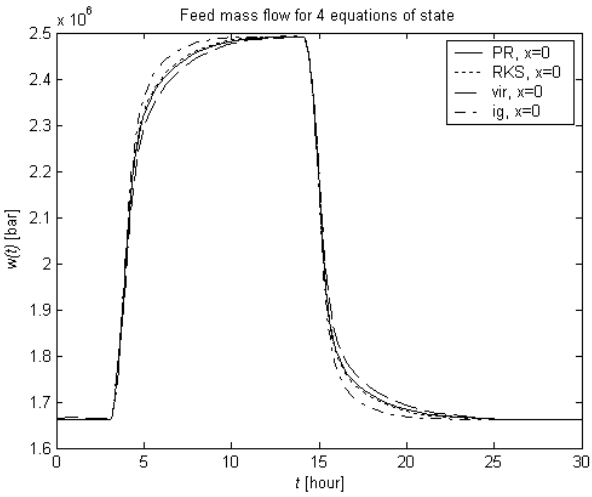

Figure 3: Feed mass flow $w_{x=0}(t)$ with constant c_v internal energy, using pressure equations of state: Peng-Robinson (solid), Redlich-Kwong-Soave (dotted), virial equation (dashed), and ideal gas (dash-dot). Exit mass flow is as given in fig. 2.

3.4 Simulation results

In this section, selected simulation results are presented. In all simulations, the simulation time is 30 h, 10 compartments are used in the discretization, the Colebrook-Haaland friction model is used, both kinetic and potential energies are included, and a fourth order spatial gradient approximation is used, both within the pipeline and on the boundaries. The results are displayed in figures, showing the time development of the feed mass flow, the exit pressure, and the exit temperature.

3.4.1 Enthalpy based on the constant c_v assumption

It is of interest to compare the various equations of state (EOS). In this section, four pressure EOSs are compared, while a simplified EOS for the enthalpy expression is use: the molar enthalpy is based on the assumption of constant c_v. This case is similar to the study of (Osiadacz & Chaczykowski 2001), where the constant c_v assumption was used — they used a different EOS, though. Figure 3 displays the response in feed mass flow $w_{x=0}(t)$, fig. 4 displays the response in exit pressure $p_{x=L}(t)$, while fig. 5 displays the response in the exit temperature $T_{x=L}(t)$ for the four different pressure equations.

From fig. 3, we see that the feed mass flow is virtually independent of the choice of pressure EOS. Figure 4 shows the expected result that the pressure response is highly dependent on the choice of pressure EOS: in

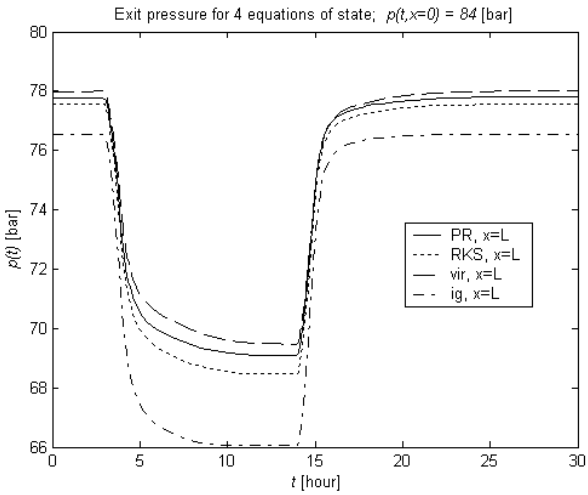

Figure 4: Exit pressure $p_{x=L}(t)$ with constant c_v internal energy, using pressure equations of state: Peng-Robinson (solid), Redlich-Kwong-Soave (dotted), virial equation (dashed), and ideal gas (dash-dot). Feed pressure is 84 bar.

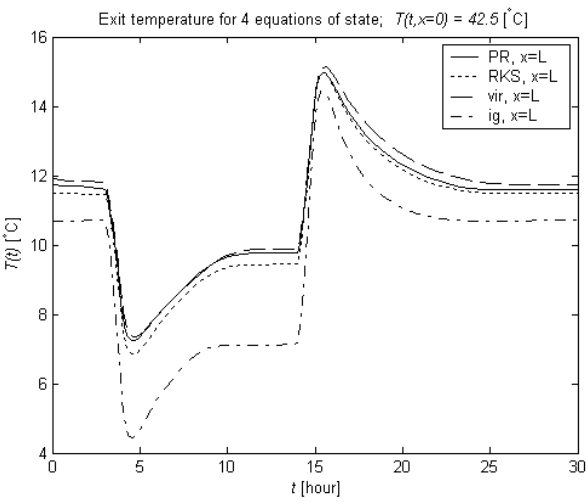

Figure 5: Exit temperature $T_{x=L}(t)$ with constant c_v internal energy, using pressure equations of state: Peng-Robinson (solid), Redlich-Kwong-Soave (dotted), virial equation (dashed), and ideal gas (dash-dot). Feed temperature is 42.5 °C.

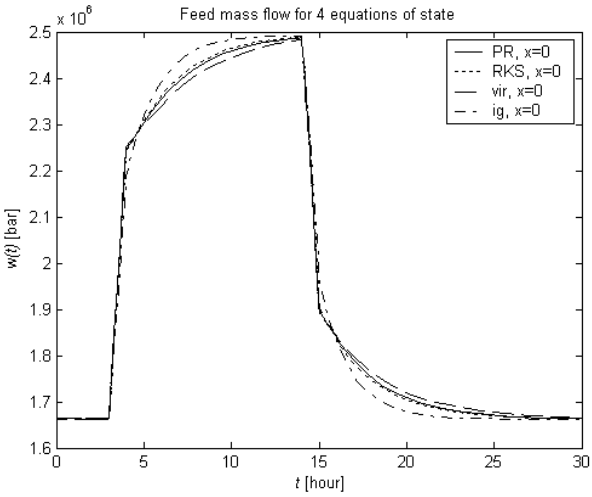

Figure 6: Feed mass flow $w_{x=0}(t)$ with constant c_v internal energy and assuming steady-state energy balance, using pressure equations of state: Peng-Robinson (solid), Redlich-Kwong-Soave (dotted), virial equation (dashed), and ideal gas (dash-dot). Exit mass flow is as given in fig. 2.

particular the ideal gas law deviates considerable from the other ones (about 5%), while the two cubic equations of state (Redlich-Kwong-Soave, Peng-Robinson) and the second order virial equations give predictions that deviate by around 1 bar at most. Figure 5 indicates that the temperature response depends on the chosen EOS to a similar degree as the pressure response. Furthermore, the ideal gas law appears to indicate a shorter time constant than the other EOSs.

3.4.2 Steady-state energy balance with enthalpy based on the constant c_v assumption

A relatively common assumption in the simulation of gas pipelines, is that the energy balance is at steady-state. The comparison of this assumption with that of a transient energy balance as in the previous section, was also studied by (Osiadacz & Chaczykowski 2001). As in the previous section, the constant c_v assumption is used. Figure 6 displays the response in feed mass flow $w_{x=0}(t)$, fig. 7 displays the response in exit pressure $p_{x=L}(t)$, while fig. 8 displays the response in the exit temperature $T_{x=L}(t)$ for the four different pressure equations.

Figures 6 and 7 compared to figures 3 and 4 show that the mass flow and the pressure predictions are relatively independent of the steady-state energy balance assumption, although the results under the transient energy assumption are smoother. The temperature response has the same general characteristics — compare fig. 8 with fig. 5. In addition, the temperature amplitude is considerably larger under the steady-state assumption — some 2-3 times larger.

3.4.3 Enthalpy based on fixed c_v vs. enthalpy based on a cubic EOS

It is of interest to compare the model predictions and how they depend on the enthalpy expression. A common model for gas pipelines is that the enthalpy is expressed by a constant heat capacity c_v, see e.g. (Osiadacz & Chaczykowski 2001). Here, we compare the responses under this assumption as well as a cubic pressure EOSs, to a cubic EOSs in both pressure and enthalpy. Figure 9 displays the response in feed mass flow $w_{x=0}(t)$, fig. 10 displays the response in exit pressure $p_{x=L}(t)$, while fig. 11 displays the response in the exit temperature $T_{x=L}(t)$ for the cubic EOSs.

Figures 9 and 10 show that the mass flow and pressure predictions are almost independent of the chosen enthalpy models. The temperature response does, however, give 1-2 °C higher value with a more accurate enthalpy expression, fig. 11.

3.4.4 Composition change

Finally, with a gas mixture, it is of interest to study the effect of changes in the composition. Here, the nominal case of $\xi_{C_1} = 0.971\,\mathrm{mol/mol}$ is compared to a 10% decrease in the methane content, which also means a 10% increase in the CO_2 content. In this section, the Peng-Robinson EOS is used. Figure 12 displays the response

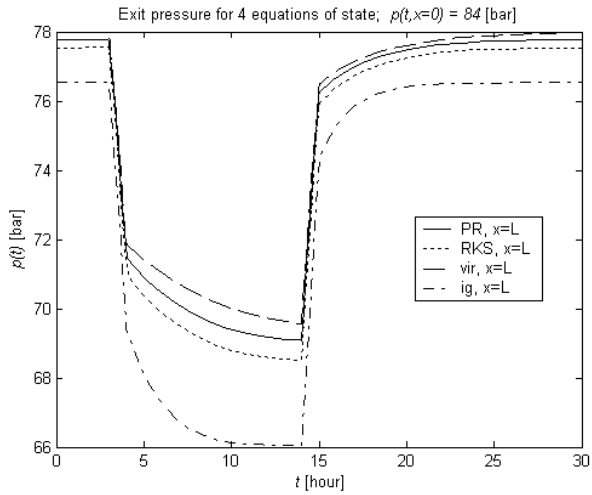

Figure 7: Exit pressure $p_{x=L}(t)$ with constant c_v internal energy and assuming steady-state energy balance, using pressure equations of state: Peng-Robinson (solid), Redlich-Kwong-Soave (dotted), virial equation (dashed), and ideal gas (dash-dot). Feed pressure is 84 bar.

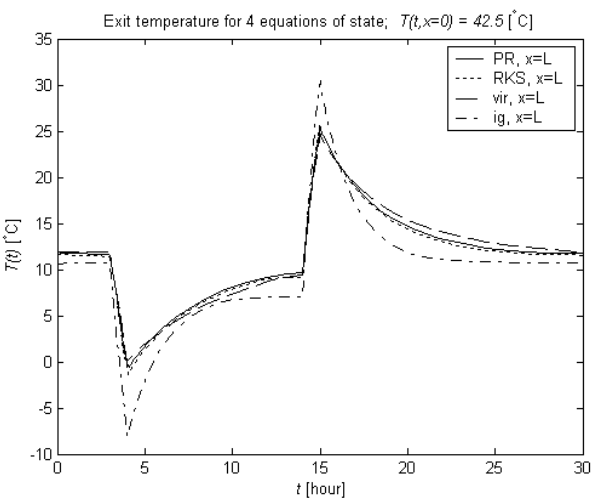

Figure 8: Exit temperature $T_{x=L}(t)$ with constant c_v internal energy and assuming steady-state energy balance, using pressure equations of state: Peng-Robinson (solid), Redlich-Kwong-Soave (dotted), virial equation (dashed), and ideal gas (dash-dot). Feed temperature is 42.5 °C.

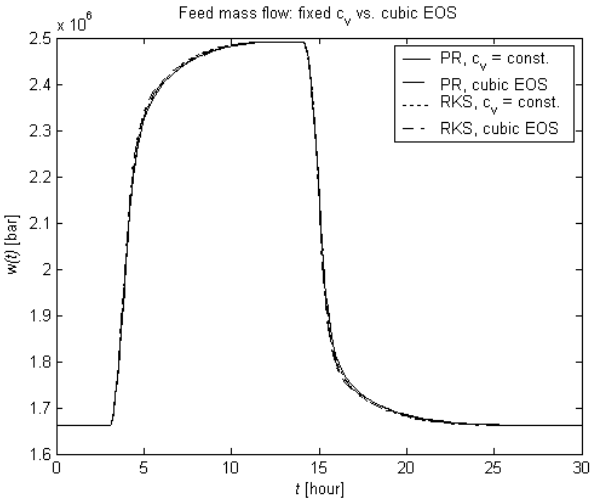

Figure 9: Feed mass flow $w_{x=0}(t)$: comparison of basing $\tilde{H}$ on fixed c_v or cubic EOS: PR & constant c_v (solid), PR & cubic EOS (dashed), RKS & constant c_v (dotted), and RKS & cubic EOS (dash-dot). Exit mass flow is as given in fig. 2.

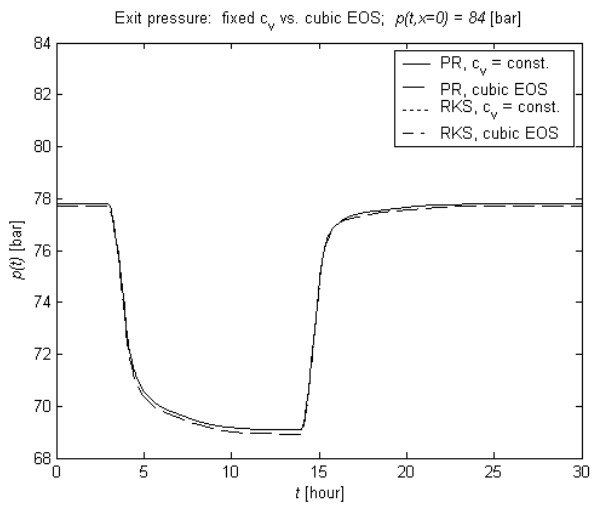

Figure 10: Exit pressure $p_{x=L}(t)$: comparison of basing $\tilde{H}$ on fixed c_v or cubic EOS: PR & constant c_v (solid), PR & cubic EOS (dashed), RKS & constant c_v (dotted), and RKS & cubic EOS (dash-dot). Feed pressure is 84 bar.

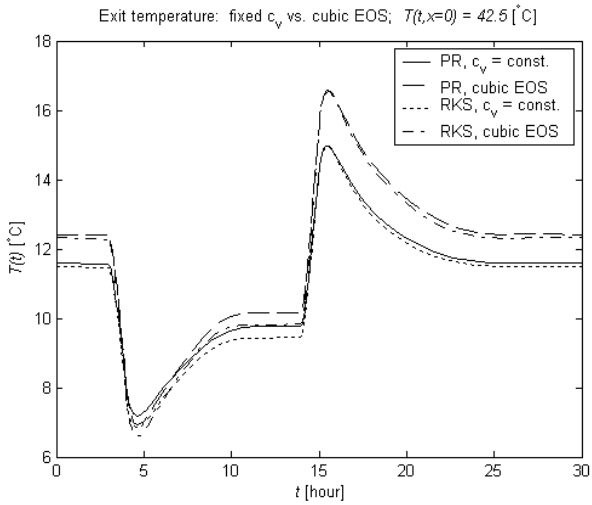

Figure 11: Exit temperature $T_{x=L}(t)$: comparison of basing $\tilde{H}$ on fixed c_v or cubic EOS: PR & constant c_v (solid), PR & cubic EOS (dashed), RKS & constant c_v (dotted), and RKS & cubic EOS (dash-dot). Feed temperature is 42.5 °C.

in feed mass flow $w_{x=0}(t)$, fig. 13 shows the response in exit pressure $p_{x=L}(t)$, while fig. 14 shows the response in the exit temperature $T_{x=L}(t)$ for the nominal case of $\boldsymbol{\xi}_0$ and for the 10% increase in CO_2 content.

Figure 12 shows that the feed mass flow is virtually independent of the feed composition. However, figures 13 and 14 show that the exit pressure and the exit temperature responses are sensitive to the feed composition.

4 Conclusions

In this paper, the study of (Carlson & Lie 2002) is extended to consider gas mixtures, and to more general cubic equations of state (EOS). The model of the gas pipeline is posed as PDAEs — partial differential algebraic equations. A model allowing for a multicomponent system with reactions and mass diffusion is developed. Several alternative algebraic expressions for pressure, total energy, enthalpy, friction, and spatial discretization order are given, and the PDAE formulation makes it simple to mix-and-match between the various alternatives. Simplified models without reactions and mass diffusion, and with fixed feed composition are implemented in the `ode15s` DAE solver of Matlab.

The gas pipeline with parameters and operating points as in (Osiadacz & Chaczykowski 2001) is used, with the modification that a gas mixture is specified containing methane and carbon dioxide to achieve the average molar weight given by (Osiadacz & Chaczykowski 2001).

Overall, it appears that the feed mass flow to the gas pipe is virtually independent of the chosen pressure and enthalpy EOS, whether the energy balance is assumed to be in the steady-state or transient, and whether the composition is changed or not. This is the result of a forced exit mass flow, and the mechanisms of nature where mass tends to be conserved.

Pressure is a key quantity in the operation of a gas pipeline. The exit pressure appears to be sensitive to the choice of pressure EOS and to the composition of the feed, but to be relatively insensitive to the chosen enthalpy model, and whether or not a steady-state energy balance is used.

Finally, the temperature response is relatively sensitive to all variations studied here: choice of pressure and enthalpy EOS, whether a transient or steady-state energy balance is used, and the feed composition.

The main quantities for a gas pipeline from the customer point of view, are the mass flow and the pressure. From this preliminary study, the following guidelines for model accuracy can be drawn. If the mass flow is the quantity of main interest, it appears that a single component model with a simple pressure EOS under the steady-state assumption for the energy balance, is adequate. If the pressure is also of interest, whether to satisfy the customer or for operational reasons, an accurate multi component pressure EOS under the steady-state energy balance, appears to be adequate. Finally, if the temperature is also of interest, perhaps because of heat loss to the surroundings and transient operation, then a further refinement with an accurate enthalpy EOS together with a transient energy balance, should be used.

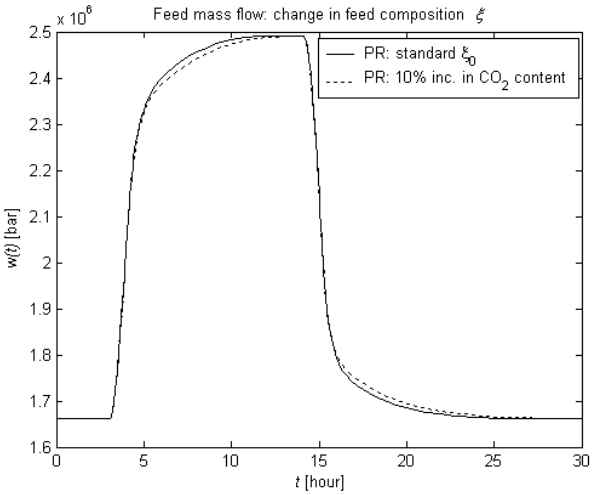

Figure 12: Feed mass flow $w_{x=0}(t)$, with Peng-Robinson EOS and $\tilde{H}$ based on cubic EOS: effect of feed composition. Nominal (standard) feed composition ξ_0 (solid) and 10% increase in CO_2 composition (dotted). Exit mass flow is as given in fig. 2.

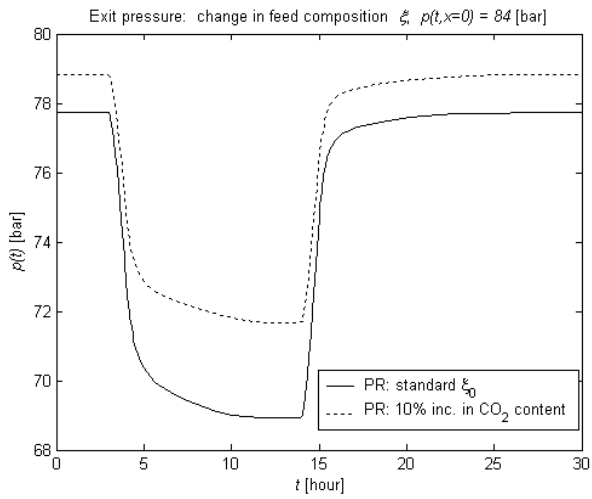

Figure 13: Exit pressure $p_{x=L}(t)$, with Peng-Robinson EOS and $\tilde{H}$ based on cubic EOS: effect of feed composition. Nominal (standard) feed composition ξ_0 (solid) and 10% increase in CO_2 composition (dotted). Feed pressure is 84 bar.

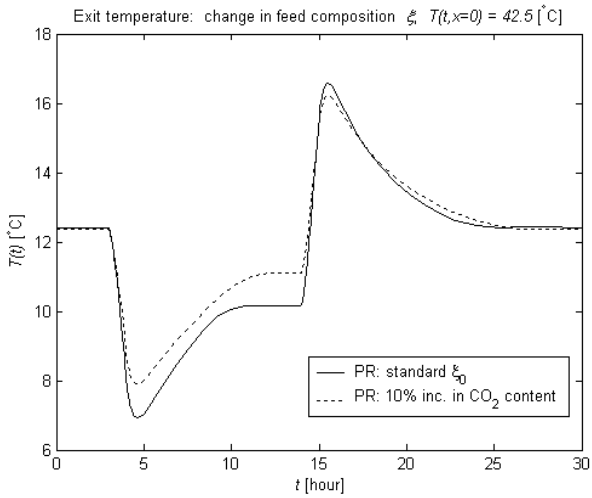

Figure 14: Exit temperature $T_{x=L}(t)$, with Peng-Robinson EOS and $\tilde{H}$ based on cubic EOS: effect of feed composition. Nominal (standard) feed composition ξ_0 (solid) and 10% increase in CO_2 composition (dotted). Feed temperature is 42.5 °C.

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