



# Numerical simulation of real gas flows in natural gas supersonic separation processing



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## ABSTRACT

The real gas effects on natural gas supersonic separation were investigated using a computational fluid dynamics approach with ideal gas and real gas models. The computed results showed that the fluid properties calculated by the ideal gas law diverged significantly from the real gas cases in the supersonic zones, while the real gas models predicted a similar result from one to the other. The deviation of the gas Mach number between the ideal and real gas models was about 13.50% at the nozzle exit, while the error in the gas density was more than 20% in the whole supersonic separators. The shock wave position calculated by the real gas model was ahead of the one calculated by the ideal gas law. The shock position moved forward with the increasing inlet pressure, while the real gas predicted value was always in front of the ideal gas value. The relative error of the gas Mach number exceeded 15% with an inlet temperature of 283 K.

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## 1. Introduction

As the global economy rises, the demand for energy supply is increasing continuously over the last two decades. Natural gas plays a significant strategic role in the global energy supply. Natural gas is a gaseous mixture, primarily composed of methane, ethane, propane and butane, with some heavier alkanes, carbon dioxide, hydrogen sulfide, nitrogen and a small amount of water vapor. The presence of water vapor in natural gas increases the risk of the formation of gas hydrates and line plugging due to hydrate deposition on the pipe walls. The free water or water vapour results in corrosion when combined with acid gases including carbon dioxide and hydrogen sulfide. It also reduces the delivery capacity of the pipelines as a result of a collection of free water. Therefore, water vapor must be removed from natural gas early on to prevent these effects.

Natural gas dehydration plays an important role in industrial processes around the world. Many different techniques are employed to dehydrate water vapor from natural gas, such as absorption, adsorption, refrigeration, membrane permeation and so on. The supersonic swirling separation is a revolutionary technique

which can be used to condense and separate water vapor and higher hydrocarbons from natural gas (Okimoto and Brouwer, 2002; Betting and Epsom, 2007). It works mainly on two principles of gas expansion and supersonic cyclonic separation. The supersonic separator is a static device composed of a swirl generation device, a Laval nozzle, a cyclonic separation part and a diffuser. The supersonic separator enables high reliability and availability because it has no rotating parts. Moreover, this new separation process prevents hydrate formation and eliminates the need for inhibitor and regeneration systems due to the short residence time of gas in the device.

Alferov et al. (2005) investigated the separation characteristics of a supersonic separator compared to the Joule-Thomson valve and turbo-expander for natural gas. Jassim et al. (2008a,b) studied the high-pressure natural gas flows through a Laval nozzle using the computational fluid dynamics technique. Karimi and Abdi (2009) combined the MATLAB and HYSYS packages to predict the effect of the operating parameters on natural gas flows in a high pressure Laval nozzle. Malyshkina (2008) obtained the distribution of gas dynamic parameters of natural gas through a supersonic separator with a computational method. In another study, a procedure was developed to predict the separation capability of water vapor and higher hydrocarbons from natural gas in a supersonic separator (Malyshkina, 2010). A supersonic separator was compared to a Joule-Thomson valve with

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TEG and demonstrated the high economic performance and natural gas liquids recovery of a supersonic separator (Machado et al., 2012). The generalized radial basis function artificial neural networks were used to optimize the geometry of a supersonic separator (Mahmoodzadeh and Shahsavand, 2013). Rajae and Shahsavand (2013) developed a new theoretical approach based on mass transfer rates to calculate the liquid droplet growth in supersonic conditions for binary mixtures. Castier (2014) modelled the supersonic flows through the properly sized converging–diverging nozzles. In our preliminary studies, a series of numerical studies were conducted to predict the natural gas flows in a supersonic separator, including the swirling flow (Wen et al., 2012a; Yang et al., 2014b) and the particle flows (Wen et al., 2012b). Also, without considering a swirling flow, the gas mass flow rates and the pressure recovery coefficient were evaluated using the computational fluid dynamics methods (Wen et al., 2013; Yang et al., 2014a).

The main objective of our study was to develop various real gas models to predict the flow parameters of natural gas through a supersonic separator at supersonic velocities. The parametric studies were performed to clarify the effects of real gas models with different operational parameters.

## 2. Governing equations

In a supersonic separator, natural gas is accelerated to supersonic velocities resulting in lower gas pressure and temperature. The gas flows can be described by the partial differential equations including mass equation (continuity equation), momentum equation, and energy equation, which are the basis for the calculation and simulation. To close the partial differential equations, the standard  $k$ – $\varepsilon$  model was employed in solving the supersonic gas flows in a nozzle (Pougatch et al., 2008). For the gas modelling at supersonic velocities, the assumptions were as follows:

- It was assumed here that the gas flow in a supersonic separator was steady state.
- The gas was a single flow without considering a condensation process.
- The swirl generation part was removed from the device and the swirling flow was not considered accordingly.
- The flow in a supersonic separator was hypothesized to be an isentropic flow.

### 2.1. Mass conservation equation

The mass equation of gas phase (continuity equation) is described as:

$$\frac{\partial}{\partial x_i}(\rho u_i) = 0 \quad (1)$$

where  $\rho$  and  $u$  are the gas density and velocity, respectively.

### 2.2. Momentum conservation equation

The conservation of momentum for gas phase can be written as follows:

$$\frac{\partial}{\partial x_j}(\rho u_i u_j + p \delta_{ij} - \tau_{ji}) = 0 \quad (2)$$

where  $p$  is the gas pressure;  $\tau_{ij}$  is the viscous stress;  $\delta_{ij}$  is the Kronecker delta.

### 2.3. Energy conservation equation

The energy equation for gas phase is expressed as Eq. (3).

$$\frac{\partial}{\partial x_j}(\rho u_j E + u_j p + q_j - u_i \tau_{ij}) = 0 \quad (3)$$

where  $E$  is the total energy;  $q_j$  is the heat flux;  $t$  is the time.

### 2.4. Turbulent kinetic energy equation

$$\frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k + G_b - \rho \varepsilon - Y_M + S_k \quad (4)$$

where  $k$  is the turbulent kinetic energy;  $G_k$  is the generation of turbulence kinetic energy due to the mean velocity gradients;  $G_b$  represents the generation of turbulence kinetic energy due to buoyancy;  $Y_M$  represents the contribution of the fluctuating dilatation in compressible turbulence to the overall dissipation rate.  $S_k$  is the source term.

### 2.5. Turbulent kinetic energy dissipation rate equation

$$\frac{\partial}{\partial x_i}(\rho \varepsilon u_i) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + C_{\varepsilon 1} \frac{\varepsilon}{k} (G_k + C_{\varepsilon 3} G_b) - C_{\varepsilon 2} \rho \frac{\varepsilon^2}{k} + S_\varepsilon \quad (5)$$

where  $\varepsilon$  is the turbulent dissipation rate;  $C_{\varepsilon 1}$ ,  $C_{\varepsilon 2}$  and  $C_{\varepsilon 3}$  are constants;  $S_\varepsilon$  is the source term.

### 2.6. Equation of state

As the supersonic separation process is performed at high pressure and low temperature, natural gas properties may be far from a perfect gas. The equation of state (EOS) plays a significant role in evaluating the gas properties. Errors in pressure and temperature evaluation lead to poor prediction of the flow structures. Hence, in this simulation, the ideal gas and various real gas models were employed to predict gas dynamic parameters including Redlich–Kwong (RK), Redlich–Kwong–Soave (RKS), Redlich–Kwong–Aungier (RKA) and Peng–Robinson (PR) EOSs (Redlich and Kwong, 1949; Soave, 1972; Peng and Robinson, 1976; Aungier, 1995).

The classical ideal gas law may be written:

$$p = \rho RT \quad (6)$$

where  $p$ ,  $\rho$  and  $T$  are the gas absolute pressure, density and absolute temperature, respectively.  $R$  is the gas constant.

Since van der Waals presented an EOS to describe the pressure–volume–temperature ( $PVT$ ) behaviour of fluids in 1873, many EOSs have been proposed to predict the thermodynamic properties of pure compounds and mixtures, such as its temperature, density, viscosity, enthalpy, entropy and so on. These simple cubic equations of state are so attractive for their reduced computational time and the required parameters are available for almost all compounds of interests. The cubic equations of state can be expressed in the following general form:

$$p = \frac{RT}{V - b + c} - \frac{\alpha(T)r a_c}{V^2 + \lambda_1 V - \lambda_2^2} \quad (7)$$

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