INFLUENCE OF THERMODYNAMIC GAS MODELS IN NATURAL GAS TURBO-EXPANDER FLOW SIMULATIONS

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ABSTRACT
During transport and storage of natural gas, natural gas turbo-expanders are used to throttle the high pressure gas and to increase the system efficiency extracting additional work. This paper reports on how three thermodynamic gas models affect prediction of the flow field in the turbo-expander. The tested thermodynamic gas models include the polytropic ideal gas law (PIG), Peng-Robinson equation of state (PR), and Redlich-Kwong equation of state (RK). Simulations have been performed with Ansys CFX 17.0. Methane has been selected as the working fluid and Hanwha Techwin expander geometry has selected. Simulation with the RK model (often considered to be the most accurate of the three models) has been selected as the reference. Density values calculated with the PIG model shows deviations ranging from 9 to 22%. PR and RK models show similar results, showing less than 2% difference in predicted static temperature and flow rate, respectively. However, PIG model shows 15% and 13.4% differences in the static temperature and flow rate, respectively.

INTRODUCTION
Turbo expanders are widely used in industry to chill the gas or vapor stream, reduce pressure, and obtain mechanical work [1]. This paper deals with an expander for throttling high temperature and high pressure gas.

Computational fluid dynamic (CFD) simulation is usually used to design or analyze turbomachinery flows. In general, ideal-gas laws are used. Flow with ideal gas assumption can be different from the actual flow field. In particular, various thermodynamic properties, such as dynamic viscosity and specific heat capacity, are assumed to be constant. This assumption results in inaccurate flow predictions at high pressures.


Thus researchers have focused on characterizing the natural gas properties. However, simulations of natural gas flow in turbo-expanders have not yet been reported in the open literature. Therefore, this paper reports on how the real gas effects influence prediction of the flow field in the turbo-expander.

EQUATIONS OF STATE FOR GASES
Equation of state describes the relations among thermodynamic properties. In this study, ideal gas assumption and two equations considering real gas effects have been used.

Polytropic Ideal Gas Law (PIG)
The PIG law assumes that there is no attraction between gas molecules. It is known that the PIG is well satisfied at low pressures. The PIG equation is:

\[ P = \frac{RT}{v} \] (1)

where P is pressure, T is temperature, and v is molar volume, which is volume occupied by one mole of a substance. R is universal gas constant. In the PIG, specific heat ratio, dynamic viscosity, and thermal conductivity are assumed to be constant.

Real Gas Law
Real gas law considers compressibility effect. Generally, compressibility factor is expressed as Z, the equation is:

\[ Z = \frac{RT}{Pv} \] (2)

Z has a value of 1 in the PIG law and is used to describe the deviation of a real gas from the ideal gas.

The Redlich-Kwong (RK) and the Peng Robinson (PR) Equations of State are most commonly used and are known to be accurate. [3]

The RK equation of state is:

\[ P = \frac{RT}{v} \left(1 - \frac{a(T)}{v(v+b)}\right) \] (3)

where a and b are constants for correcting attractive potential of molecules and volume, respectively.

The PR equation of state is:
where \( a \) and \( b \) again characterize the molecular properties.

The above three equations have been internally coupled to the CFD solver to calculate the thermodynamic properties of natural gas. For real gas EOS, zero pressure coefficient of specific heat capacity is used as reference. This variable is calculated as a fourth order polynomial \[8\].

\[
P = \frac{RT}{v - \frac{a(T)}{v(b + 1)}}
\] (4)

where \( a \) and \( b \) again characterize the molecular properties.

The above three equations have been internally coupled to the CFD solver to calculate the thermodynamic properties of natural gas. For real gas EOS, zero pressure coefficient of specific heat capacity is used as reference. This variable is calculated as a fourth order polynomial \[8\].

NUMERICAL METHOD
Simulations have been performed with Ansys CFX 17.0. The natural gas of interest has methane greater than 96%. Therefore, methane has been selected as the working fluid. Hanwha Techwin expander geometry has used for expander simulations. The simulation was performed at the design point.

Mesh Quality Assessment
Mesh quality assessment was carried out in 3 element numbers. 3 cases are named coarse, mid, and fine. Each value was predicted at the impeller exit and divided by value of fine case.

<table>
<thead>
<tr>
<th>Element (million)</th>
<th>0.48</th>
<th>2.14</th>
<th>6.65</th>
</tr>
</thead>
</table>

Figure 2. Mesh quality assessment.

Solver Setup
A steady state simulation is performed. CFD domain is restricted to one passage per row and periodic boundary conditions are used. The CFD domain is also described in Figure (3). The Flow is modeled as a fully turbulent flow using the shear-stress transport (SST) turbulence model. The total energy, including viscous work term, is used to calculate heat transfer. All solid walls including nozzle and impeller blades, are rough walls with 19 \( \mu \) m roughness. No-slip boundary condition is used for all solid walls. Mixing plane is selected for the rotating interface. Total pressure and total temperature are applied to the inlet boundary condition. Inlet flow direction is normal to inlet plane. Turbulence rate is set at 5%. Average static pressure is applied at the outlet.

Table 1. Element number
<table>
<thead>
<tr>
<th></th>
<th>Coarse</th>
<th>Mid</th>
<th>Fine</th>
</tr>
</thead>
</table>

Figure 3. CFD domain.
RESULTS AND DISCUSSION

Table 2. Mass flow rate

<table>
<thead>
<tr>
<th></th>
<th>PIG law</th>
<th>RK EOS</th>
<th>PR EOS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass Flow Rate [kg/s]</td>
<td>0.661</td>
<td>0.764</td>
<td>0.779</td>
</tr>
</tbody>
</table>

The mass flow rate of the PIG is 13% less and the mass flow rate of the PR EOS is 3% higher than the RK EOS flow rate. The relative big difference of the PIG law is due to the predicted density difference and the blockage effect of the separation bubble on the impeller blade.

Density

The temperature predicted by the PIG law is higher than the reference. Therefore, the PIG density shows 13% error when compared to REFPROP data at the same state. Thus the mass flow rate of PIG law is lower.

Table 3. Temperature and density

<table>
<thead>
<tr>
<th></th>
<th>Ts [K]</th>
<th>Density [kg/ m³]</th>
<th>Refprop Density [kg/ m³]</th>
<th>Density Error [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>PIG law</td>
<td>179.9</td>
<td>14.59</td>
<td>16.74</td>
<td>12.9</td>
</tr>
<tr>
<td>RK EOS</td>
<td>161.8</td>
<td>20</td>
<td>19.9</td>
<td>0.5</td>
</tr>
<tr>
<td>PR EOS</td>
<td>160</td>
<td>20.7</td>
<td>20.36</td>
<td>1.67</td>
</tr>
</tbody>
</table>

Table (4) lists the blockage area ratio for the three thermodynamic models. The PIG law case has the largest blockage effect.

\[
\frac{A_B}{A} = 1 - \frac{U}{U_c}
\]  

(5)

Table 4. Blockage area ratio

<table>
<thead>
<tr>
<th></th>
<th>PIG law</th>
<th>RK EOS</th>
<th>PR EOS</th>
</tr>
</thead>
<tbody>
<tr>
<td>An/A</td>
<td>0.07</td>
<td>0.038</td>
<td>0.031</td>
</tr>
</tbody>
</table>

Figures show chordwise pressure distribution on the impeller blade at the mid span predicted by PIG law, RK EOS and PR EOS, respectively. The upper line is the pressure side and the lower line is the suction side. The pressure coefficient decreases on both sides with real gas EOS, but there is a slight increase followed by a plateau on the suction side in the case of PIG law. This plateau indicates flow separation.

\[
c_p = \frac{P - P_{\infty}}{\frac{1}{2} \rho U^2}
\]  

(6)

Figures show the velocity vectors of the flow through impeller at the mid span of predicted by the PIG law, RK EOS and PR EOS, respectively. Color of vector is the velocity in the theta-z plane non-dimensionalized by the impeller tip speed. The scale is uniformed for the three thermodynamic cases. In the PIG law case, there is a separation bubble of with a length of about 37% of the impeller chord length. Separation bubbles are also visible in the RK EOS and PR EOS cases. However, they are significantly smaller with lengths of 9% and 7% of impeller chord length, respectively.
The impeller from the hub to the shroud are analyzed to confirm that the separation bubble occurs at all spanwise locations. Blade loading and velocity vectors from near hub, 25% span, 75% span, and near shroud are shown in Figures. In the near hub and near shroud, the flow is reflected on the wall surface.
CONCLUSIONS
Influence of thermodynamic gas models in natural gas turbo expander flow has been numerically investigated with PIG law, RK EOS, and PR EOS. The following are the conclusions from the investigation:
1. All three models predict separation bubbles on the impeller blade. The largest separation bubble is predicted by the PIG law.
2. The PIG law predicts the lowest mass flow rate.
3. Differences in the predicted mass flow rates among the three thermodynamic models arise from the blockage effects due to the separation bubble on blade suction side and density calculated from each equation.
4. Real gas effects need to be considered for turboexpander design and analysis.

ACKNOWLEDGEMENTS
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NOMENCLATURE
P pressure, Pa
T temperature, K
v molar volume, m³/mol
R universal gas constant, 8.314J/K mol
Z compressibility
U velocity
A area, m²
cp pressure coefficient
ρ density, kg/m³
Subscripts
B blockage
c core
∞ impeller outlet

REFERENCES
(8) Ansys CFX-Solver Theory Guide.