16th Australasian Fluid Mechanics Conference Crown Plaza, Gold Coast, Australia 2-7 December 2007

CFD Modeling of Globe Valves for Oxygen Application

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Abstract

Components used in high-pressure, high-temperature, flowing oxygen are susceptible to ignition and combustion in presence of restriction or when particles impact these restriction. The valves in any systems are the common flow restrictors, hence, the design and analyses of valves are most critical tasks. The flow of oxygen through valves distinguishes itself by accentuating auto-ignition and consequent flame propagation in metals and non-metals, apart from other usual characteristics present with gases/liquids. The combination of ignition resistance, proper and reliable performance and fabrication economy marks the specification of material and design of valves in oxygen-enriched environment. The analyses have been performed by applying the commercial computational fluid dynamics (CFD) code, FLUENT, to obtain the solution of the two-dimensional turbulent flow field through a globe valve for its different openings in the GOX environment. The flow control valves in high velocity oxygen systems for different openings are simulated for turbulence and eddy dissipation. The influence of pressure, flow rate and opening of the valve on the rise in temperature and eddy dissipation rate is also obtained for compressible flow range. The simulation for turbulence is done by k- ε and k- ω turbulence models and the results have been compared.

Introduction

Valves control the fluid flow and pressure in a system or a process. The selection of their types, design and material plays a vital role in the performance and reliability of any system. A number of researchers have experimented and analyzed valves for all its parts, fluid types, operating parameters, discharge coefficient, stiction and eroding characteristics and have improved the valve technology. Now, with the emergence of robust computational fluid dynamics (CFD) tools and powerful computers, the analysis of valve performance, and thus the job of designing valves to suit a particular application can be done much faster. Apart from this, CFD analysis can reveal the complex flow structure and the sonic characteristics around the valve, which the experiments hardly provide. Even otherwise, experimentation needs to be supplemented with CFD analysis because of the complex geometry as well as complexities like turbulence during the sonic flow through a valve. The experimental results were validated by CFD analysis or vice versa. In the present study, CFD analysis of a specific globe valve design has been carried out to understand its performance and reliability during the high pressure flow of gaseous oxygen.

The analyses of the flow behavior inside a valve using CFD method have provided the relation between flow, geometry and pressure loses (Amirante et al. [2, 4]; Beeson et al. [5]; Chern et al. [7]; Vu et al. [33]). Valve-related problems like

the stiction, erosion, vibration, cavitation etc. were also modeled for effective performance of the valve using CFD methods (Choudhury et al. [8, 9]; FLUENT User's Guide [12]; Forder et al. [13]; Kalsi et al. [17]; Newton et al. [23]). Many analyses have specifically provided the flow patterns for different ports and opening gaps in the valves, which eventually determined the design and operation of the hardware (Oza et al. [25]; Parslow et al. [26]; Stevenson et al. [31]; Slockers et al. [32]). Experimentation and CFD analyses were also performed to investigate the cause of vibrations that cause valve instability (Morita et al. [22]). The turbulence modeling around the valve opening for both steady and unsteady flow were carried out in both compressible and incompressible ranges, as a part of determination of flow and viscous forces on valves (Ahuja et al. [1]; Davis et al. [10]; Forsyth et al. [15]; Mazur et al. [20]).

Selection of Valve for High Pressure and High Flow Rate Gaseous Stream

There are different kinds of valves available and each one is used for a specific purpose (Vu et al. [33]). Gate valves are generally used in systems where low flow resistance for a fully open valve and no throttling are desired. Globe valves are used in systems where good throttling characteristics and low seat leakage are desired with relatively high head loss allowable in an open valve. Ball valves allow quick, quarter turn on-off operation and have poor throttling characteristics. Plug valves are used for changing flow direction between different ports via a single valve. Diaphragm valves and pinch valves are used in systems wherein the system is required to be completely isolated from the fluid. Butterfly valves provide significant advantages over other valves in weight, space, and cost for large valve applications. Check valves are used in applications where open flow in one direction and prevention of flow in the reverse direction are desirable. A combination of characteristics of lift check valve and a globe valve gives a stop check valve. Safety relief valves are used to provide automatic protection for over-pressurization in a system. Researchers have extensively experimented with all the above categories of the valves in order to identify the valves for specific applications (Zappe et al. [36]). The computational analyses have not been performed that extensively as the experimental study. The application of valves in high pressure and high flow rate gaseous streams calls for thorough research and analysis. The methodology adopted in these systems focus on the analyses, design and then experimental validation of the analyzed results.

Valves, when used in high pressure systems, often get damaged by the frequent and severe movement of the metal pieces, back and forth, against each other over an extended period of time and by shock waves during the closing of the valves. Leakage is another problem in the valves used in high pressure systems. The repair or replacement requires demounting of the valve from an existing piping structure. The inconvenience and attendant damage to the surrounding piping structure poses major impediment to the valve replacement. Another shortcoming in the valves employed in high pressure applications is the requirement of considerable pressure for actuating the valve. This is because the high seal pressure and related high friction forces are necessary to insure sealing. Further, the contaminants affect the seal life so severely that the life of the valves reduces to nearly half of its prescribed life time. In addition to all these, the geometry of the valve and the drop in velocity around the downstream region involves the risk of particle accumulation.

Globe valve is commonly used as the control valve for high pressure system due to lesser leakage and higher erosion resistance compared to other valves. Gate valves are good for low pressure systems and can perform efficiently without leakage only for low pressure systems. For high pressure systems, the vibration and shock waves due to the turbulence causes rapid erosion of the gate of the gate valve. This makes gate valve vulnerable to failure in high pressure gaseous systems.

The high pressure oxygen system is more prone to incidents and accidents as compared to other fluid owing to its oxidizing property. For any system to be in flames the presence of fuel, the igniter and oxidizer is required. In oxygen systems, valve materials act as fuel and once the ignition occurs, the oxygen itself acts as oxidizer. Ignition sources are the only ones which need to be avoided. Thus, the material compatibility along with the configuration plays a vital role for the safe performance of the Globe valves used in high pressure and high flow rate gaseous oxygen systems (GOX).



The computational modeling along with the turbulent and unstable flow condition (flow eddies) for GOX in higher pressure and temperature ranges has not yet been done by any researcher. In this paper, the turbulent modeling of a globe valve, shown in Fig. 1, for pressures near and above 250 bara and mass flow rate of 7 kg/s has been performed in order to understand its performance and estimate its reliability with respect to oxygen hazard.

Oxygen System Hazard and its Analysis using CFD

Oxygen is reactive at ambient conditions, and its reactivity increases with increasing pressure, temperature, and concentration. Most materials, both metals and non-metals, are flammable in high-pressure oxygen, therefore, systems must be designed to reduce or eliminate ignition hazards. With oxygen systems, unlike other systems, the design and material selection is very critical to avoid ignition hazards. This risk is caused since oxygen is a strong oxidizer that causes ignition and vigorously supports combustion. The use of oxygen, therefore, always involves risk. Normal engineering materials, like the carbon steel, stainless steel, polymers etc. utilized in oxygen systems without precautions, often cause incidents and accidents when ignition mechanisms are not appropriately mitigated. Examples of such events are numerous in all areas of engineering that utilize oxygen. It includes combustion of steel pipelines along a considerable length because of high gas velocity and low levels of cleanliness, burning of aluminum alloy pumps because of metal impacts and fires in oxygen cylinder (and other gas) regulators in industrial, commercial and medical applications. Fires in pumps, compressors, valves, regulators, life support systems and aerospace/space system units containing oxygen-enriched atmospheres often result in losses of lives and properties. In the oxygen systems, the igniting fuel is often non-metals, while it causes propagation in the metal or alloy structure itself.

Sr.	Components	Possible Ignition Source
No.		
1	Ball Valve	Particle impact, adiabatic
		compression, promoted
		ignition
2	Relief Valve	Mechanical impact or
		frictional heating, promoted
		ignition
3	Globe Valve	Particle impact, promoted
		ignition
4	Butterfly Valve	Particle impact, promoted
		ignition
5	Check valve	Mechanical impact or
		frictional heating, promoted
		ignition
6	Fittings	Particle impact, promoted
		ignition
7	Flex Hose	Adiabatic compression
8	Soft goods	Pneumatic impact,
		mechanical impact, and
		particle impact
9	Compressor &	Friction, fresh metal
	Pump	exposure
10	Cylinders	Adiabatic compression,
		over pressurization
11	Filters	Particle impact, static
		electricity
12	Measuring	Particle impact, pneumatic
	Equipment	impact, resonance

Table 1: Oxygen System Components with Possible Ignition Source (Stevenson, et. al. [31])

Ignition of the metal or alloy can occur directly through impact of particles entrained in the gas flow, due to friction between surfaces within the unit, or due to the kindling chain, or burning of a more flammable material. While some of the ignition potential can be eliminated through a sound system design, the use of appropriate procedural controls to limit the contamination and ensuring appropriate operating limits, the practical solution is to select the proper metallic materials, such as the burn resistant alloys like copper alloys, Inconel, Monel etc. and/or the mitigation of the important ignition mechanisms (Jackson et al. [16]; Ramanath et al. [28]). The commonly recognized ignition sources (or their combination) that can raise the thermal energy within the system above its ignition threshold include the following:

1) Friction 7) Resonance 2) Particle impact 8) External heat sources 3) Mass impact 9) Internal Flexing 4) Promoted ignition 10) Flow friction 5) Static electric discharge 11) Fresh metal exposure 6) Electric arc and spark

Table 1 shows the probable cause of ignition source in some components used in the oxygen environment. Reduction of ignition and fire risk requires consideration of following factors:

- Equipment design
- Selection of materials .
- Design, configuration and construction of devices/systems
- Operating parameters (including flow characteristics)

Computational analyses for systems ranging from cryogenic control valves and pressure regulator systems to cavitating venturis used to support rocket engine and component testing have been made (Choudhury et al. [8]). A CFD model was developed to investigate the combustion and gas dynamics in a high velocity oxygen-fuel (HVOF) thermal spray gun using the liquid fuel propane (Newton et al. [23]). Studies on the complex three-dimensional flow field of oxygen safety pressure relieve valve, check valves and ball valves have been performed. The pressure, temperature and velocity profiles have been obtained for various opening gaps for the valves. The particle impact testing in the valves along with the erosion characteristics were studied experimentally in many organizations (Parslow et. al. [26]) Although, computational analysis have been performed in valve performance in liquids and other gases, such analysis in oxygen or oxygen enriched systems have not yet been done exhaustively.

The k - ϵ and k - ω turbulence model for compressible flow range has been compared. The performance and comparison of both the models have been done for orifice flow in a pipeline, irregular geometries and nozzles. However, the comparison for valves has not been yet performed by any investigator. Hence, the present analyses involve the comparison of the above models for globe valve.

System Considered

Fig. 2 shows a segment of 2-D piping and instrumentation (P&I) diagram of a process using high pressure gaseous oxygen. The manually controlled globe valve (GV 1) is the subject of consideration for the analyses here. The filter (FL 1) is placed just after the T-section, joining GV 1, GV 2 and FL 1. The body of the valve is made of cast carbon steel, while the valve seat and the stem are made of Monel and the sealing elements like the gland packing, disc seal, back seal, body seal etc are of PTFE (polytetrafluroethylene) material. The P & I diagram indicates that the globe valves are used in numerous places along other components such as sensors, like pressure transducer (PT), safety valves (SV), pressure regulators (PR) etc. Such a system may be a part of a larger system used for testing as well as actual firing of rocket engines. Therefore, any failures of such systems or sub-systems need to be prevented through reliable design of these components with appropriate operation and selection of materials.



Fig. 3 shows the cross section of a single seat globe valve. The plug and the seat region, unlike the inlet and the exit region could be considered as axisymmetric. Thus the inlet and exit geometry have been simplified as shown in Fog. 4. This assumumption is justified as within the plug and seat region the flow complexities due to the inlet/outlet 3-D flow will not be significant.



Fig. 4 Axisymmetric view of grid for the plug and seat region (rotated 90°)

The ground level testing of components to be used in rockets calls for testing with the parameters with appropriate range within which it shall actually be subjected to in reality. Hence, the present study involves the analyses of the globe valve subjected to high pressure and high temperature gaseous oxygen (GOX).

CFD and Selection of Turbulent Model

Ball valve and butterfly valves have been analyzed using CFD. The CFD analyses with ball and butterfly valves in oxygen systems provided key insights into the ignition mechanism through visualization of the flow through the valves and identification of the most probable impact targets of the carried over particulate matters (Newton et al. [23]). It also provides the probable gas pressure and velocity inside the valve which aides in evaluating the ignition and possible propagation phenomenon. However, the experimental or computational evaluation of the reliability of globe valve vis-à-vis the ball or butterfly valves has not yet been done. Thus the CFD based analysis of flow of GOX at high pressure through a globe valve was taken up, with the focus on safety from fire hazard under oxygen-enriched atmosphere.

Though the CFD results in the present study have not been experimentally validated, they provide useful information on the flow dynamics across the globe valve seat during the initial opening sequences, the temperature rise in the valve, the velocity profile, the turbulent kinetic energy rise and eddy dissipation around the plug region. The CFD analyses are used as an intermediate step towards the determination of the safety of the system.

Turbulent flows are characterized by fluctuating velocity fields. Turbulence brings fluids of differing momentum content into contact. Turbulence is characterized by eddies or instabilities. During turbulence, large eddies extract energy from the flow and the smaller eddies extract energy from the larger eddies. The energy continues to flow to still smaller eddies until the eddies are too small to be sustained and in that case the energy is dissipated by turbulent viscous forces. The reduction of the velocity gradients, in the presence of restrictions, due to the action of viscosity reduces the kinetic energy of the flow and this mixing is dissipative. Hence the energy "cascades" down through smaller length scales.

The choice of turbulence model depends on consideration such as the physics encompassed in the flow, the established practice for a specific class of problem, the level of accuracy required, the available computational resources, and the amount of time available for the simulation. The selection of particular model for specific application from the general guidelines (Kamnis et al. [18]; Leutwyler et al. [19]; Min et al. [21]) is not easy. In general terms, a good turbulence model requires minimum complexity (i.e. contain a minimum number of differential equations, empirical constants and functions, but still provide sufficiently accurate and physically realistic results), robustness (i.e. promote stable convergence and not have difficulty resolving the steep gradients in nearwall regions), possess extensive universality (i.e. can be applied to a wide variety of flows without adjusting the empirical constants). For engineering calculations, twoequation turbulence models have become the most popular, since they are relatively simple to program and place much lower requirements on computer resources than other more complex models (e.g. algebraic and Reynolds stress models). Consequently, when cost effective, timely solutions of flows

spanning large domains with complicated geometries are required, only two-equation models are currently practical. The k - ϵ model relates the turbulence viscosity, μ_t (Pa-s), the turbulence kinetic energy, k (m²s⁻²), and the turbulence dissipation rate, ϵ (m²s⁻³). The k - ω turbulence model is similar to the low Reynolds number $k - \varepsilon$ model, with ω replacing ε , which represents the specific dissipation rate (s⁻¹). The development and improvisation of the models (Amirante et al. [3]; Chern et al. [6]) and their comparison led to the general inference that the near-wall simulation results for turbulent flow with $k - \omega$ model were more accurate than the $k - \varepsilon$ model. The $k - \omega$ model is known to behave well for wall-bounded problems and is simpler and faster in convergence than the $k - \varepsilon$ model. On the contrary, k -- ε model gives better results in the free stream region. The k - ε model captures the features of the flow more accurately when compared with the one-equation and mixing length model.

The grid used in the study is a structured grid. The grid independence investigation leads to the optimum grid with 744 cells and 1565 faces. Fig.5 shows the grid independence test results. The increase in cells beyond 744 had no significant variation in the parameter values. Symmetry boundary conditions have been used in the centerline. All solid boundaries have been represented using the no slip velocity conditions. The governing equations are discretized in FLUENT using finite volume formulations with the second order spatial accuracy. The continuity is satisfied by SIMPLE (semi-implicit pressure linked equations) algorithm. The residuals used for the convergence criteria have been normalized with three orders of magnitude.



Results and Discussion

The results for both the turbulence models for 20% and 50% openings are shown in Fig. 6 through 26

In each case, the flow initially accelerates through the plug and seat region, and then flows downstream in the form of a wall jet while remaining attached to the plug. In addition, a recirculation region develops on the downstream side of the seat. As the valve percent opening increases, the plug begins to retract beyond the plane of the seat as shown in Fig. 6.







Fig.9 Contour for Mach number for 20% opening (k - ε model)















Fig. 13 Velocity Profile 20 % opening (k - ω model)



Fig. 14 Contour for Turbulent Kinetic Energy for 20% opening (k - ω model)



Fig. 15 Contour for Turbulent Eddy Dissipation Rate for 20% opening $(k - \omega \mod 1)$



Fig. 16 Turbulent Kinetic Energy value Comparison for 20% opening $\bigwedge k - \varepsilon$ model $\coprod k - \omega$ model





Fig. 19 Turbulent Kinetic Energy profile for 50% opening

Aug 24, 2007 ILUENT 6.2 (wi, sogregated, sko)



natours of Turbulence Kinetic Zuergy (k) (m8/s8)

Fig. 20 Velocity profile for 50% opening



Fig. 21 Turbulent Eddy Dissipation Rate profile for 50%

Flow separation from the plug with the formation of a second recirculation zone occurs around the region between the jet and the plug. This may result in either flow reattachment to the plug at a point downstream or it is flowing as a free jet until the impingement on the surface of the valve body. In each case the pressure decreases in the downstream direction with more pressure gradients occurring around the plug and seat region. No significant pressure changes are observed upstream of the seat and only minor changes are observed downstream of the seat. Minor pressure recovery. This is desirable in a control valve. But in globe valves the flow path being complex, the pressure gradient is observed to be more than that of ball or butterfly valve.

The turbulent kinetic energy values are higher in the plug region for the fifty percent opening than the twenty percent opening. The restriction is more towards the downstream, hence, explaining more energy dissipation and turbulence. The drop in the velocity (Fig. 6) at the back seal position in all the opening contours enhances the particulate accumulation. The seal, being made of flammable material, along with the particulate accumulation might cause the initiation of ignition in presence of source of heating or a electrostatic charge (Amirante et al. [3]).



Fig. 22 Total Temperature profile for 50% opening



Fig. 23 Velocity profile for 50% opening (k- ω model)



Fig. 25 Turbulent Kinetic Energy for 50% opening (k-ω model)

Ang 24, 2007 FLUENT 6.3 (axi, segregated, skm)

e Kinetic Energy (k) (m8/s8)



Fig. 26 Specific Dissipation Rate Profile for 50% opening (K- ω model)

The simulations of the valve have been done with both $k - \epsilon$ method and $k - \omega$ model of turbulence. The $k - \epsilon$ model converges slower as compared to $k-\omega$ model. But $k-\omega$ model gives higher values of velocities, temperature and turbulent parameters then that of the $k - \epsilon$ method. This is because the latter produces lesser recirculation effect that the former (Dhinsa et al. [11]; Rodi et al. [29]). The $k - \omega$ model does not utilize wall functions and therefore needs a relatively fine meshing around the plug zone, increasing the computational time, on the other hand, $k - \epsilon$ method shows thicker boundary layer. The $k - \epsilon$ model converges well for all openings with the same boundary conditions poses convergence problem for 80% opening of the valve.

The temperature rise, apart from the flow, depends on the thermal conductivity and thickness of the valve material. In the present study, the valve body material has been taken to be cast steel and the plug and the seat material to be Monel. The thickness of the material is taken to be 5 cm. Based on the simulations, the temperature value has been found to be less than 10K, which is not significant to cause ignition.

Committees and organizations like the European Industrial Gas Association (EIGA), the British Compressed Gas Association, The International Fire Protection Association, National Fire Protection Association (NFPA) of America, Bundesanstalt für Materialforschung und Prüfung (BAM) of Germany, Deutsches Institut für Normung (DIN), the National Aeronautics and Space Administration (NASA) American Society for Testing and Materials (ASTM) G-4 committee and the Compressed Gas Association (CGA) have performed a thorough survey on the material used in any type of LOX/GOX application and have generated data of the material properties, such as the auto-ignition temperature, threshold pressure etc., which are relevant for selection of materials for components in oxygen system. Nickel and Nickel alloys are used in the stem, seat and some downstream parts of the valve since they pose good resistance to the propagation of ignition in the component. These materials being costly are not used to fabricate the whole body of the component. The present work suggests that cast steel can be used along with Monel in critical portions in the globe valve shown in Fig.1.

Conclusion

The CFD simulation for globe valve here resulted from the curiosity to better understand its performance in high pressure oxygen environment. The simplified axisymmetric numerical model predicted the inherent valve characteristic for globe style control valves. The turbulent kinetic energy increases as the plug retracted beyond the plane of seat. The k- ω model gave higher values of velocity and turbulent kinetic energy than the k $-\varepsilon$ model since the latter captures lesser recirculation and is more suitable for boundary level flow. The k $-\varepsilon$ model is more suitable for free stream simulation. There

are probabilities of particulate accumulation around the back seal region of the plug due to the velocity drop by nearly 90% towards the wall region and the recirculation of the flow. The material considered in the simulation was taken to be the same as existing in reality. The temperature rise in the simulation was less than 10K, hence, the selection of Monel in the sensitive areas would resist the ignition initiation, since it is used only in those regions prone to get ignited.

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