PSV Sizing Using DWSIM:

A Free and Open-Source Chemical Process Simulator

By

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PREFACE

The manual "Process Simulation Using DWSIM" presents a set of PSV Sizing exercises using a free and open-source chemical process simulator "DWSIM" and can be utilized to establish process simulation laboratory as part of undergraduate chemical engineering degree or in allied degree curriculum. The problem statements are of intermediate level of some advanced theories using API 520 and API 521.

Prerequisite

- Must know about DWSIM UI/UX.
- Flow sheeting in DWSIM
- Selection of Thermodynamic Packages.
- Manipulating variables

Thanks

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P.E. O&G

Disclaimer

All the exercises are strictly restricted to learning only and not meant to be used in real world application.

PROCESS SIMULATION USING DWSIM: A FREE AND OPEN-SOURCE CHEMICAL PROCESS SIMULATOR

PREAMBLE

DWSIM is an open-source CAPE-OPEN compliant chemical process simulator. It features a Graphical User Interface (GUI), advanced thermodynamics calculations, reactions support and petroleum characterization / hypothetical component generation tools. DWSIM can simulate steady-state, vapor–liquid, vapor–liquid-liquid, solid–liquid and aqueous electrolyte equilibrium processes and has built-in thermodynamic models and unit operations (https://en.wikipedia.org/wiki/DWSIM). It is available for Windows, Linux and Mac OS.

The objective of the course is to create awareness of the open-source process simulator "DWSIM" among prospective graduates and practicing process engineers. The course will cover Intermediate aspects of create flow sheet in DWSIM and simulation of simple units such as Mixer, Splitters, CSTR, Distillation column, Pumps, Turbines, Compressors, etc.

Target Audience

- Junior Interns in Process Firms
- III / Final year B. Tech. Chemical Engineering students
- M. Tech. Chemical Engineering students
- Practicing Process Engineers

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1 BACKGROUND

Pressure relief valves or other relieving devices are used to protect piping and equipment against excessive over-pressure. Proper selection, use, location, and maintenance of relief devices are essential to protect personnel and equipment as well as to comply with codes and laws.

Determination of the maximum relief required may be difficult. Loads for complex systems are determined by conservative assumptions and detailed analysis. By general assumption, two unrelated emergency conditions caused by unrelated equipment failures or operator error will not occur simultaneously (no double jeopardy). The sequence of events must be considered. The development of relief loads requires the engineer to be familiar with overall process design, including the type of pump drives used, cooling water source, spares provided, plant layout, instrumentation, and emergency shut-down philosophy.

This section suggests methods to calculate relief capacity for most emergency conditions, including fire. A common reference for determining individual relieving rates is contained in Section 3 of API RP 521.1 The design of the proper relieving device must take into consideration all of the following upset conditions for the individual equipment item if such upset can occur. Each upset condition must be carefully evaluated to determine the "worst case" condition which will dictate the relieving device capacity.

Blocked Discharge

The outlet of almost any vessel, pump, compressor, fired heater, or other equipment item can be blocked by mechanical failure or human error. In this case, the relief load is usually the maximum flow which the pump, compressor, or other flow source produces at relief conditions.

Fire Exposure

Fire is one of the least predictable events which may occur in a gas processing facility but is a condition that may create the greatest relieving requirements. If fire can occur on a plant-wide basis, this condition may dictate the sizing of the entire relief system; however, since equipment may be dispersed geographically, the effect of fire exposure on the relief system may be limited to a specific plot area. Vapor generation will be higher in any area which contains a large number of uninsulated vessels. Various empirical equations have been developed to determine relief loads from vessels exposed to fire. Formula selection varies with the system and fluid considered. Fire conditions may overpressure vapor-filled, liquid-filled, or mixed-phase systems.

Tube Rupture

When a large difference exists between the design pressure of the shell and tube sides of an exchanger (usually a ratio of 1.5 to 1 or greater), provisions are required for relieving the low-pressure side. Normally, for design, only one tube is considered to rupture. Relief volume for one tube rupture can be calculated using appropriate sizing equations in this section. When a cool media contacts a hot stream, the effects of flashing should be considered. Also, the possibility of a transient over-pressure caused by the sudden release of vapor into an all-liquid system should be considered.

Control Valve Failure

The failure positions of instruments and control valves must be carefully evaluated. In practice, the control valve may not fail in the desired position. A valve may stick in the wrong position, or a control loop may fail. Relief protection for these factors must be provided. Relief valve sizing requirements for these conditions should be based on flow coefficients (manufacturer data) and pressure differentials for the specific control valves and the facility involved.

Thermal Expansion

If isolation of a process line on the cold side of an exchanger can result in excess pressure due to heat input from the warm side, then the line or cold side of the exchanger should be protected by a relief valve. If any equipment item or line can be isolated while full of liquid, a relief valve should be provided for thermal expansion of the contained liquid. Low process temperatures, solar radiation, or changes in atmospheric temperature can necessitate thermal protection. Flashing across the relief valve needs to be considered.

Utility Failure

Loss of cooling water may occur on an area-wide or plant-wide basis. Affected are fractionating columns and other equipment utilizing water cooling. Cooling water failure is often the governing case in sizing flare systems. Electric power failure, similar to cooling water failure, may occur on an area-wide or plant-wide basis and may have a variety of effects. Since electric pump and air cooler fan drives are often employed in process units, a power failure may cause the immediate loss of reflux to fractionators. Motor driven compressors will also shut down. Power failures may result in major relief loads. Instrument air system failure, whether related to electric power failure or not, must be considered in sizing of the flare system since pneumatic control loops will be interrupted. Also control valves will assume the position as specified on "loss of air" and the resulting effect on the flare system must be considered.

2 PSV SIZING

Objective

Find the appropriate orifice areas of the PSV for the given problem statement

Data

- Protected equipment: Reboiler
- Relief service: Steam
- Reason for relief: Blocked steam discharge
- Relieving rate:10000 kg/hr.
- Gas Density: 2.5 kg/m3
- Ratio of specific heats for gas (Cp/Cv): 1.3
- Compressibility factor: 1.1
- Molecular weight of gas = 250 °C
- Set pressure: 5 barg
- Accumulation: 10%
- Back pressure at relief valve discharge: 0.5 barg
- Type of relief valve: Conventional pressure relief valve
- Inlet stream 2: 80 mol % Methanol solutions flowing at 10 kmol/h
- Both the streams are at 30 °C and at 1 bar pressure
- The liquid streams can be considered as ideal

DWSIM Blocks Used

- Valve
- Material Stream
- Indicators (Digital or Analog)

Procedure

1. Start a new DWSIM Simulation (DWSIM VER 8.0 - CLASSIC UI). Click on "New steady state Simulation" as a template for new simulation
2. The simulation configuration window will be opened. It shows a specification page. Add components required to solve the problem statement. In the present case, add water. Ensure all components are added from the same property database. For instance, in this case, both components are added from "ChemSep" database.
3. Specify the thermodynamic package as Stea m table (IAPWA-IF97).
4. Customize the system of units for the simulation and click "Next".
5. The flow sheeting section of simulation window will be opened. First, let provide input and output streams for the unit operation to be performed. Drag and drop two Material streams available at the right, in the object palette. Rename them stream as "Inlet-Stream-1"and "Inlet-Stream-2". These serve as input streams.
6. On clicking the "Inlet Stream" stream, general information about the stream will be displayed on the left side of screen. Specify the feed compositions, temperature, and

pressure for the inlet streams. Once credentials are specified for the inlet streams, the color of stream turns blue.

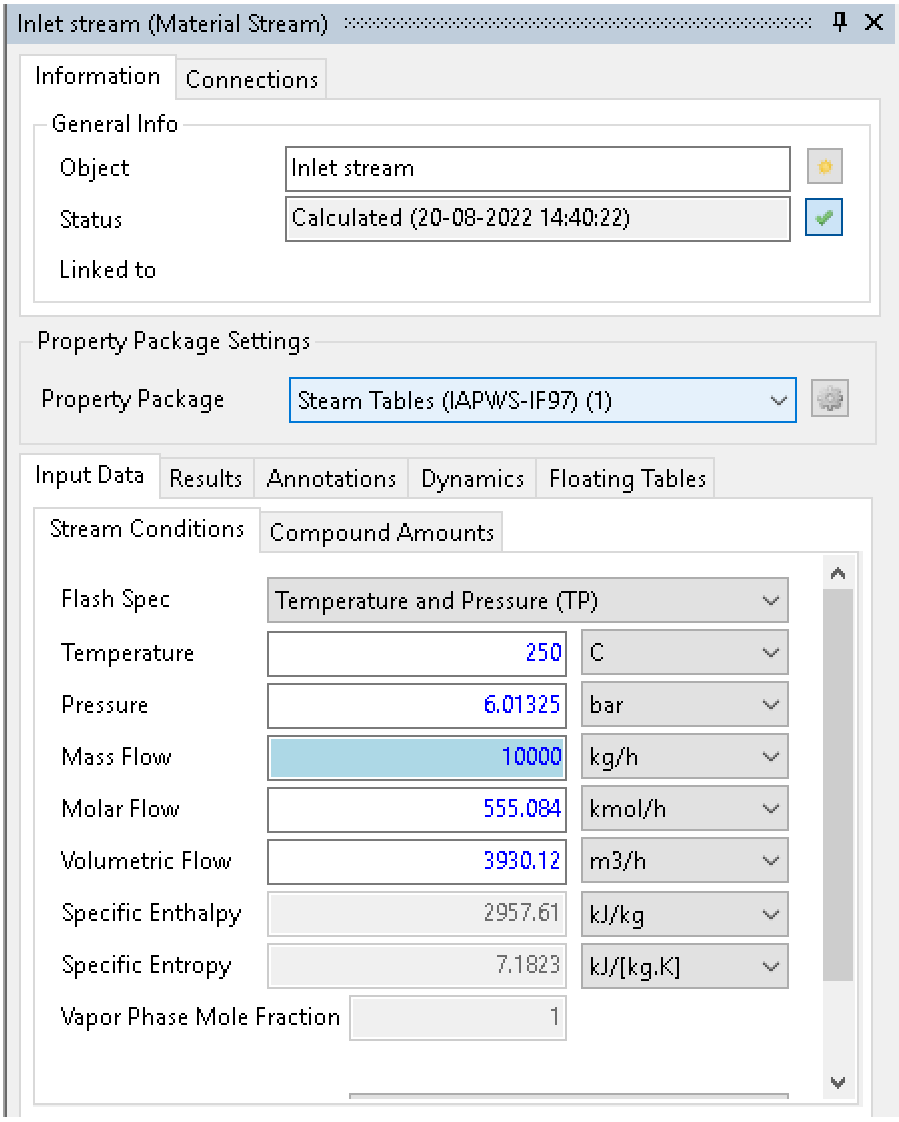

Figure 1 Inlet stream Specs

7. Below the Unit Operation tab on left, locate the valve block. Drag and drop into the flow sheet. Rename it as “PSV”.

8. Under specification for valve add the data as follows.

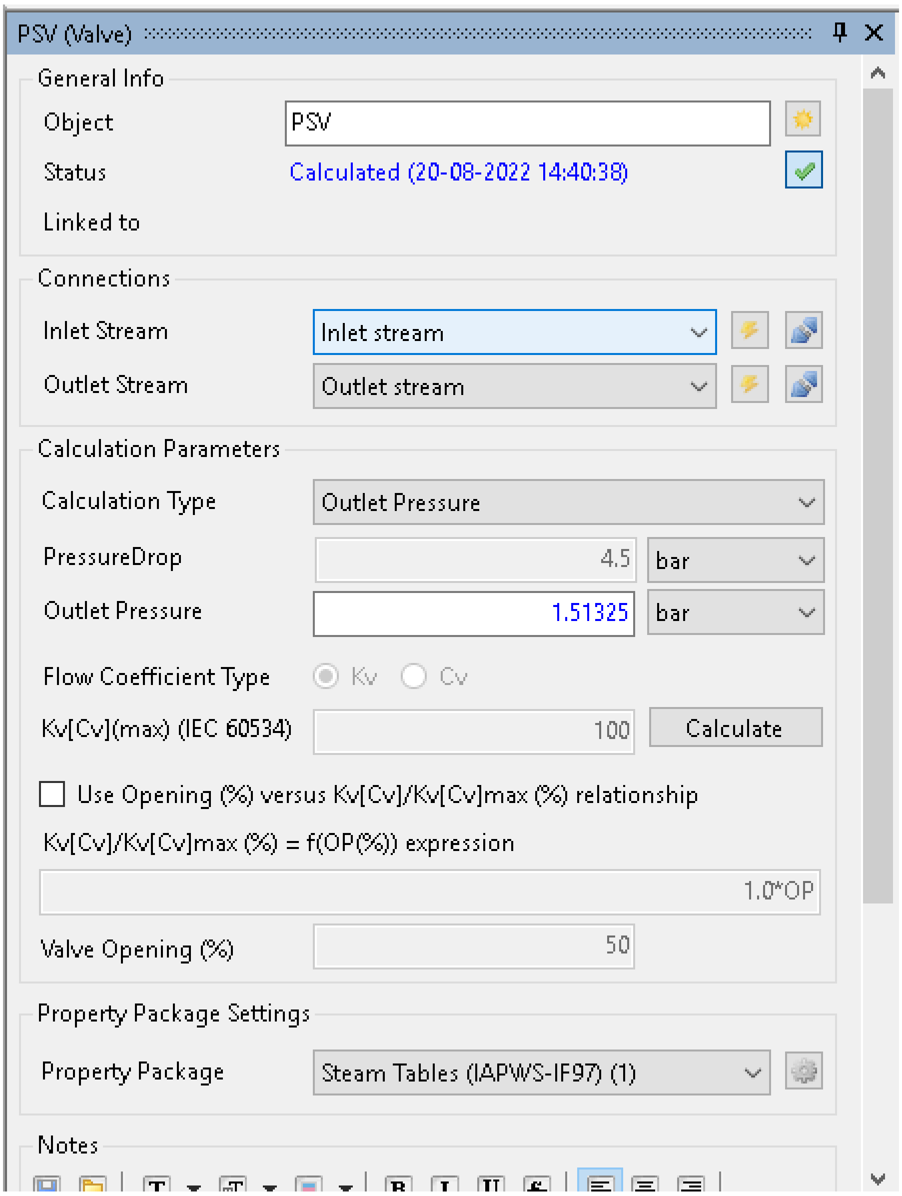

Figure 2 PSV Specs

9. Click on the add specs as shown in the image

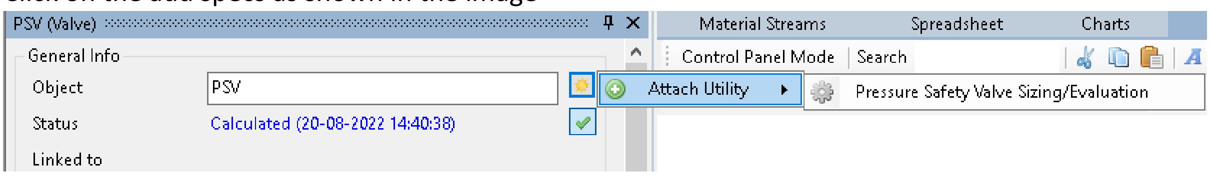

Figure 3 Add PSV Sizing/ Evaluation

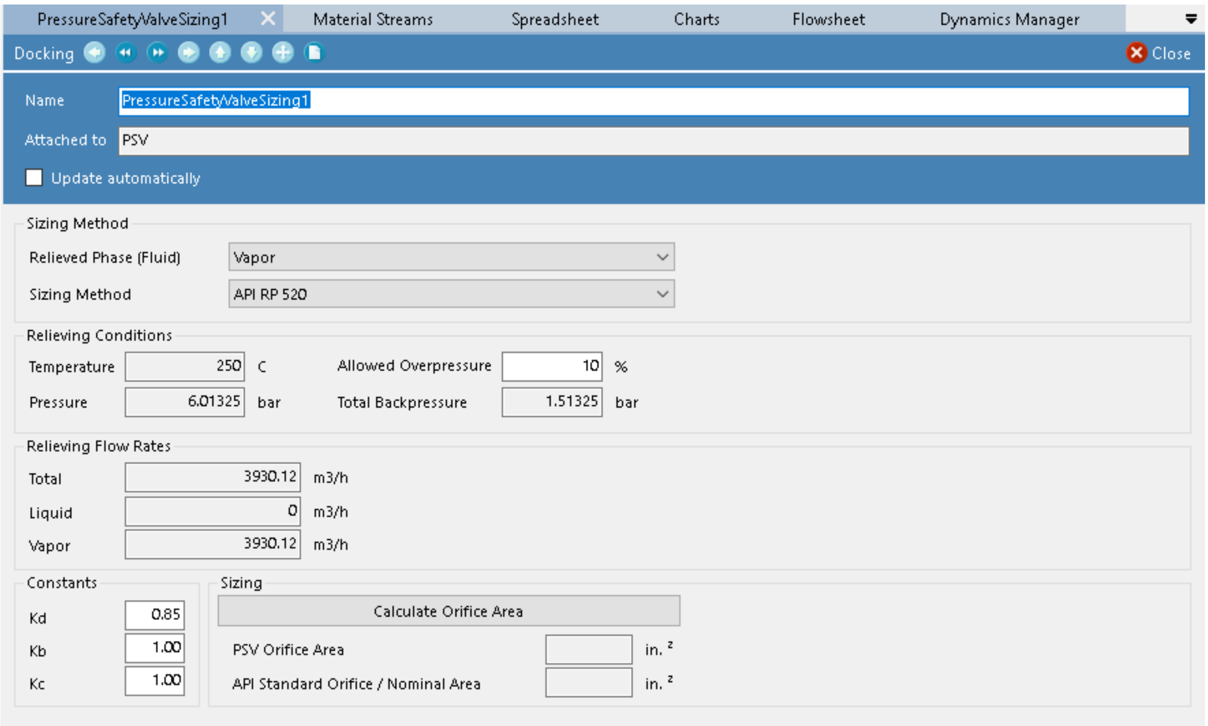

Figure 4 PSV Sizing Calculator

10. Add digital and analog indicators for the material streams and valve as shown in the figure below and give targeting properties.
11. Add the Kd, Kc and Kb values and press on calculate orifice area the required orifice area will be calculated as shown.

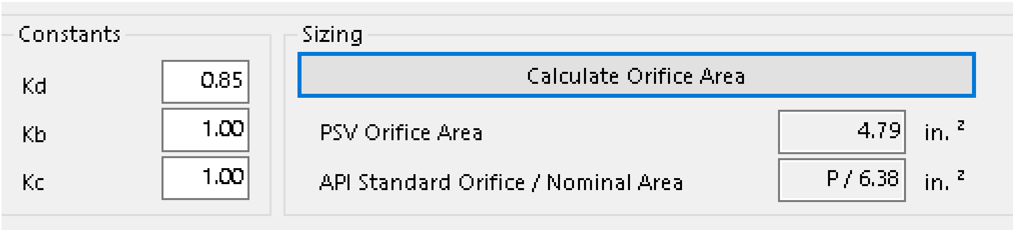

Figure 5 Defining Constants

12. Run the simulation by pressing “Solve flow sheet” button on the top corner of the screen.

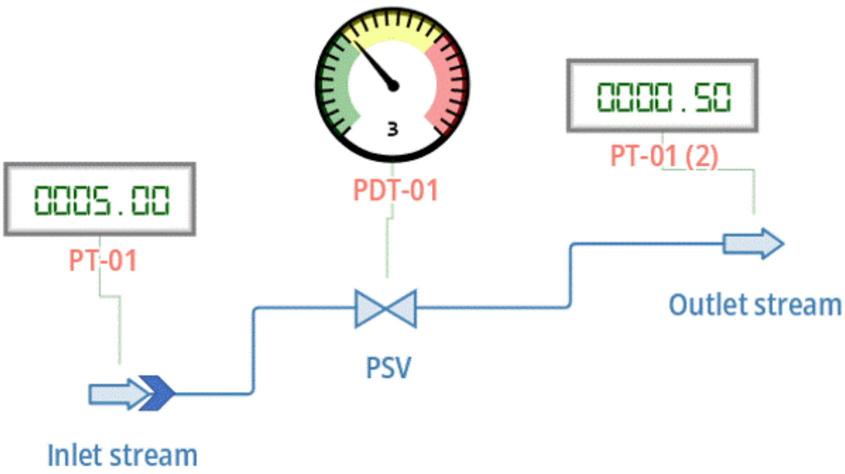

Figure 6 Flow Sheet

	Outlet stream	Inlet stream
Temperature (C)	242.368	250
Pressure (bar)	1.51325	6.01325
Mass Flow (kg/h)	10000	10000
Molar Flow (kmol/h)	555.084	555.084
Volumetric Flow (m3/h)	15636	3930.12
Density (Mixture) (kg/m3)	0.639549	2.54445
Molecular Weight (Mixture) (kg/kmol)	18.0153	18.0153
Specific Enthalpy (Mixture) (kJ/kg)	2957.61	2957.61
Specific Entropy (Mixture) (kJ/[kg.K])	7.81162	7.1823
Molar Enthalpy (Mixture) (kJ/kmol)	53282.1	53282.1
Molar Entropy (Mixture) (kJ/[kmol.K])	140.729	129.391
Thermal Conductivity (Mixture) (W/[m.K])	0.0375384	0.0394454

3 Manual Calculation in Smath Studio

31 Aug 2022 09:23:29 - 14 PSV Cal.sm

Valve Data

Protected equipment : Reboiler
Relief service : Steam
Reason for relief : Blocked steam discharge
Relieving Rate : 10,000 kg/hr
Gas Density : 2.5 kg/m^3
Ratio of specific heats for the gas (C_P/C_V) : 1.3
Compressibility factor of gas = 1.1
Molecular weight of gas = 18 gm/mole
Relieving temperature = 250^{0}C
Set pressure : 5.0 barg
Accumulation : 10%
Back pressure at relief valve discharge : 0.5 barg
Type of relief valve : Conventional pressure relief valve

Discharge to	Atmosphere
Set pressure	$P_{set} := 5 \text{ bar}$
Back Pressure	$P_2 := 0.5 \text{ bar}$
Accumulation	$a_{\%} := 10 \%$
Atmosphere pressure	$P := 1.01325 \text{ bar}$
Accumulated Pressure	$P_1 := P_{set} \cdot \left(1 + \left(\frac{a_{\%}}{100}\right)\right) + P = 6.5132 \text{ bar}$
Pressure ratio	$r := \frac{P_2}{P_1} = 0.0768$

Process data

Enter the condition of fluid for vapour "V" and for steam "S"

Vapor (V)/ Steam (S)	$Fluid := \text{"S"}$
Relieving temperature	$T := 503.15 \text{ K}$
Molecular weight	$M := 18 \frac{\text{kg}}{\text{kmol}}$
Compressiility	$Z := 1.1$
Specifc heat capacity ratio	$k := 1.3$
Required relief load	$W := 10000 \frac{\text{kg}}{\text{hr}}$

Figure 7 SMath Page 1

31 Aug 2022 09:23:29 - 14 PSV Cal.sm

Relief valve orifice calulation

Check for vapor or steam

```
F := if Fluid = "V"
       "X"
     else
       if Fluid = "S"
         "O"
       else
         "Enter spec for vap or steam"
F = "O"
```

Correction factors

Discharge coeff $K_d := 0.975$

Back Pressure coeff $K_b := 1$

Comb Rupture Disk Factor $K_c := 1$

Superheat steam corr factor $K_{sh} := 1$

Napier correction factor

```
K_n := if Fluid = "S"
         (2.764·P_1 − 1000 bar) / (3.324·P_1 − 1061 bar)
       else
         "-"
```

Calculated F_2 with

$$F_2 = \sqrt{\left(\frac{k}{k-1}\right)\cdot(r)^{2/k}\cdot\left(\frac{1-r^{(k-1)/k}}{1-r}\right)}$$

$K_n = 0.9$

Figure 8 SMath Page 2

Calculated data

Type of flow

Shows whether the fluid (vapour) is at critical or subcritical stage

Check for subcritical flow using the following formula

$$\frac{P_2}{P} \geq \left(\frac{2}{k+1}\right)^{\frac{k}{k-1}}$$

```
Flow := if F = "X"
          if (2/(k+1))^(k/(k-1)) · P1 > P2
            "Critical"
          else
            "Sub Critical"
        else
          "-"
```

$Flow = "-"$

K value coeff

Calculated C with

$$C = 520 \cdot \sqrt{k \cdot \left(\frac{2}{k+1}\right)^{\frac{k+1}{k-1}}}$$

```
C := if (F = "X") ∧ (Flow = "Critical")
       C := 520 · sqrt(k · (2/(k+1))^((k+1)/(k-1)))
     else
       "-"
```

$C = "-"$

Coeff Sub Critical Flow

Calculated F_2 with

$$F_2 = \sqrt{\left(\frac{k}{k-1}\right) \cdot (r)^{2/k} \cdot \left(\frac{1-r^{(k-1)/k}}{1-r}\right)}$$

```
F2 := if (F = "X") ∧ (Flow = "Sub Critical")
        F2 := sqrt((k/(k-1)) · (r)^(2/k) · ((1 - r^((k-1)/k))/(1 - r)))
      else
        "-"
```

$F_2 = "-"$

Figure 9 SMath Page 3

31 Aug 2022 09:23:29 - 14 PSV Cal.sm

Calculated orifice

$$A = \frac{131.6 \cdot W}{C \cdot K_d \cdot P_1 \cdot K_b \cdot K_c} \cdot \sqrt{\frac{T \cdot Z}{M}}$$

$$A = \frac{0.179 \cdot W}{F_2 \cdot K_d \cdot K_c} \cdot \sqrt{\frac{T \cdot Z}{M \cdot P_1 \cdot (P_1 - P_2)}}$$

$$A = \frac{1.904 \cdot W}{P_1 \cdot K_d \cdot K_b \cdot K_c \cdot K_n \cdot K_{sh}}$$

$A :=$ if $Fluid = $ "V"

  if $Flow = $ "Critical"

$$A := \frac{(131.6 \cdot W) \cdot \sqrt{\frac{T \cdot Z}{M}}}{(C \cdot K_d \cdot P_1 \cdot K_b \cdot K_c)} \cdot \left(kg^{\frac{1}{2}} \right)^{-1} mm^2$$

  else

$$A := \frac{0.179 \cdot W}{F_2 \cdot K_d \cdot K_c} \cdot \sqrt{\frac{T \cdot Z}{M \cdot P_1 \cdot (P_1 - P_2)}} \cdot \left(\frac{kg^{\frac{1}{2}}}{m^2} \right)^{-1} \cdot 10^{-6}$$

else

$$A := \frac{1.904 \cdot W}{P_1 \cdot K_d \cdot K_b \cdot K_c \cdot K_n \cdot K_{sh}} \cdot \left(\frac{kg}{m^2} \right)^{-1} \cdot 10^{-6}$$

$$A = 3173.336\ mm^2$$

Relief Valve Designations

Standard Orifice Designation	Orifice Area cm²	Orifice Area (in.²)											
D	0.710	0.110	•	•	•								
E	1.265	0.196	•	•	•								
F	1.981	0.307	•	•	•								
G	3.245	0.503			•	•	•						
H	5.065	0.785				•	•						
J	8.303	1.287					•	•	•				
K	11.858	1.838							•				
L	18.406	2.853							•	•			
M	23.226	3.60								•			
N	28.000	4.34								•			
P	41.161	6.38								•			
Q	71.290	11.05									•		
R	103.226	16.0									•	•	
T	167.742	26.0											•
		in.	1 × 2	1.5 × 2	1.5 × 2.5	1.5 × 3	2 × 3	2.5 × 4	3 × 4	4 × 6	6 × 8	6 × 10	8 × 10
		mm	25 × 50	38 × 50	38 × 62	38 × 75	50 × 75	38 × 100	75 × 100	100 × 150	150 × 200	150 × 250	200 × 250

Valve Body Size (Inlet Diameter × Outlet Diameter)

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Figure 10 SMath Page 4

$$f\left(Recommended_{Orifice}\right) := A$$

$$STD_{Orifice} := \begin{bmatrix} \text{"D"} & \text{"E"} & \text{"F"} & \text{"G"} & \text{"H"} & \text{"J"} & \text{"K"} & \text{"L"} & \text{"M"} & \text{"N"} & \text{"P"} & \text{"Q"} & \text{"R"} & \text{"T"} \\ 0.5\ mm^2 & 71.5\ mm^2 & 126.5\ mm^2 & 198.5\ mm^2 & 324.5\ mm^2 & 506.5\ mm^2 & 830.5\ mm^2 & 1186.5\ mm^2 & 1841.5\ mm^2 & 2323.5\ mm^2 & 2800.5\ mm^2 & 4116.5\ mm^2 & 7129.5\ mm^2 & 10332.5\ mm^2 \\ 71\ mm^2 & 126\ mm^2 & 198\ mm^2 & 325\ mm^2 & 506\ mm^2 & 830\ mm^2 & 1186\ mm^2 & 1841\ mm^2 & 2323\ mm^2 & 2800\ mm^2 & 4116\ mm^2 & 7129\ mm^2 & 10322\ m^2 & 16774\ mm^2 \end{bmatrix}$$

$c :=$ "Error: Enter values within range"

for $n \in \left[1..\text{cols}\left(STD_{Orifice}\right)\right]$
  if $f\left(Recommended_{Orifice}\right) > STD_{Orifice\,2\,n}$
    $Recommended_{Orifice} := STD_{Orifice\,3\,n}$
    $Orifice_{tag} := STD_{Orifice\,1\,n}$
  else
    continue

$$\boxed{Recommended_{Orifice} = 4116\ mm^2}$$

$$\boxed{Orifice_{tag} = \text{"P"}}$$

$R_{orificesize}\left(Calc_{Area}\right) :=$
  for $n \in \left[1..\text{cols}\left(STD_{Orifice}\right)\right]$
    if $Calc_{Area} < STD_{Orifice\,2\,n}$
      $x := STD_{Orifice\,2\,n}$
      break
    else
      continue
  x

$R_{orificetag}\left(Calc_{Area}\right) :=$
  for $n \in \left[1..\text{cols}\left(STD_{Orifice}\right)\right]$
    if $Calc_{Area} < STD_{Orifice\,3\,n}$
      $x := STD_{Orifice\,1\,n}$
      break
    else
      continue
  x

$R_{orificesize}(A) = 4116.5\ mm^2$

$R_{orificetag}(A) = \text{"P"}$

Figure 11 SMath Page 5

4 REFERENCES

1. API RP 521 — Guide for Pressure-Relieving and Depressuring Systems, American Petroleum Institute, 1220 L Street, NW, Washington, DC 20005.
2. API RP 520 — Recommended Practice for the Design (Part I) and Installation (Part II) of Pressure Relieving Systems in Refineries, American Petroleum Institute, 1220 L Street, NW, Washing-ton, DC 20005.