
KORF Hydraulics - Flexible fluid flow calculations

C.J.C Kruger, KORF Hydraulics

1. Summary

Korf Hydraulics is a powerful, graphical program for calculating flow rates and pressure profiles in pipes and piping networks. Korf Hydraulics differs from other similar programs in that the user is free to specify any valid combination of flows and pressures, and allow Korf to determine the unknown quantities. The only requirement is that a unique solution must be theoretically possible. Korf can solve fluid flow problems ranging from a single pipe, to a complex, two-phase network of pipes, pumps, valves and other fittings.

2. Principle of Operation

Several methods are available in the literature for solving piping networks, including the Hardy-Cross, Newton-Raphson and Linear Theory method [1]. Although Korf was developed independently, it does share certain characteristics with the Linear Theory method. Korf's method is fast and almost always converges with valid specifications. One notable exception is a circuit consisting of a pump (or compressor) with an unknown flow rate and head specified by a pump curve (or compressor curve). In this case only, Korf uses an Aitken-Steffensen iteration method to aid convergence.

Korf regards all flow rates and all equipment inlet and outlet pressures as variables or unknowns. To determine these unknowns, Korf performs a mass balance around every piece of equipment and a pressure drop calculation over every pipe. These are called internal specifications. Even with these internal specifications, a unique solution to the problem is not possible without the user specifying an additional number of flows, pressures, pressure drops, beta ratio's, valve Cv's, etc. A unique solution is possible when the number of independent specifications (including the internal specifications) equals the number of variables as defined above.

Keeping track of these specifications is not a trivial task for the user, but Korf has four features that greatly simplifies this process. Firstly, Korf continuously counts and displays the number of specifications and variables. Secondly, when a new circuit is drawn, Korf assumes certain defaults that result in the number of specifications always equaling the number of variables. If the user subsequently deletes one, a new one must be added somewhere else. Thirdly, Korf can display all the current specifications on the drawing below the pipes/equipment. Fourthly, when the problem is run, Korf

first evaluates the specifications to determine if they are independent.

3. Discussion and Examples

The top circuit in Figure 1, which is a screenshot from Korf, represents a single pipe. Korf will analyze this circuit to have three variables, viz. feed F1 pressure, product T1 pressure and pipe L1 flow. It will find only one internal specification, viz. pipe L1 pressure drop. The user can thus specify any two of the variables listed above to ensure a unique solution. That is, pressure in and out, or pressure in and flow, or pressure out and flow. For this circuit, the pipe size should only be left unknown if the flow is specified, as specifying both pressures essentially fixes the dP/length and velocity and varying the pipe diameter has no effect on it (Korf will iterate to the maximum or minimum pipe size).

The bottom circuit in Figure 1 represents a series circuit with three pipes, a pump and a control valve. Korf will analyze this circuit to have nine variables, viz. feed F2 pressure, product T2 pressure, pump P1 pressure in and out, valve V1 pressure in and out and flow in pipes L2, L3 and L4. Korf will find five internal specifications, viz. pipes L2, L3 and L4 pressure drops and mass balances across pump P1 and valve V1. The user can thus specify any four of the variables listed above, as long as they are independent. Being independent implies that the user cannot specify two mass flow rates (which is obviously the same in pipes in series), as that is equivalent to the mass balance Korf performs internally. It also implies that at least one specification must be a pressure, as Korf needs at least one pressure somewhere in the circuit to base the other pressures on. In addition to the variables listed above, the user may also choose to specify the pump head directly or indirectly via a pump curve. Similarly for the control valve, where the user may also specify a pressure drop directly or indirectly via a valve Cv. Furthermore, any or all of the pipe diameters may be unknown if the user wants Korf to size it based on any of five selectable sizing criteria.

The principles in these examples can be extended to circuits with almost any combination of pipes in series and parallel. The two circuits shown in Figure 1 can also be in the same problem, as Korf will still be able to determine if each has a unique solution. Thus, if you overspecify the one circuit, and underspecify the other circuit to make the number of

variables equal the number of specifications, Korf will determine that they are not independent when the simulation is run.

4. Graphical Interface

The graphical interface for Korf allows the user to create equipment by dragging them from a template onto the form. Equipment is then connected by pipes using the mouse. Pipes can have up to ten bends. After creating the circuit, the user can move, delete, reroute and edit the equipment and pipes.

The current interface support pipes, feed nodes, product nodes, control valves, check valves, pumps, compressors, orifices, exchangers, mixers, splitters, reducers/expanders and miscellaneous equipment. A vessel can be represented by a mixer, splitter or miscellaneous equipment. Fittings, such as elbows, are considered part of the pipe and are entered as part of the pipe input data. The name, number and resistance of these fittings are editable. The user can copy pipe and fluid physical properties from one pipe to another to limit the amount of typing.

Selected results and all user specifications can be viewed on the drawing below the equipment. A result file is also generated every time the simulation is run. This is a text file that can be viewed, saved and opened in any word processor.

Korf reads the standard pipe sizes and other pipe information from an external file which can be edited from inside Korf.

5. Engineering Calculations and Limitations

Single phase pressure drop calculations are performed using the Darcy equation as presented in CRANE [2]. For gas flow, the user can use the Darcy equation (incompressible model) or the isothermal compressible model. For two-phase pressure drop calculations, Korf supports several methods, including the Dukler constant slip method [3], Lockhart-Martinelli method [4] and Chenoweth-Martin method [5]. The current version does not include acceleration effects. Korf can also display a graphical representation of the current flow regime for the selected pipe.

Korf does not do any flash calculations. For every pipe it uses the liquid mass fraction and physical properties for each phase supplied by the user. If none is supplied by the user, Korf defaults to the physical properties for water.

The change in static pressure due to changes in velocity is accounted for in reducers and expanders, but not currently in mixers or splitters (or any other equipment). The user can however specify a pressure increase or decrease over the mixer or splitter, but that pressure drop will be applied to all pipes leaving the splitter or entering the mixer.

Control valve calculations are done according to the equations presented in the Masoneilan bulletin [6], except for two phase flow. For two phase flow Korf assumes the C_v to be the sum of the C_v 's calculated for the liquid and vapor phases at the outlet vapor fraction.

Orifice calculations are performed by the equations presented in Spink. For two phase flow Korf assumes the orifice area is the sum of the areas calculated for the liquid and vapor phases at the outlet vapor fraction. At high gas phase pressure drops, the method of Cunningham [7] is used.

Although there is no programming limit on the number of pipes and equipment, there is a limit to the number of pipes and equipment that can be drawn and displayed on the screen without overlapping. The largest drawing size is A3 or 11x17.

6. Contacts

Korf Version 1.0, Educational Edition, is distributed by CACHE, and can be purchased for \$50 per year for supporting departments, and \$60 per year for non-supporting departments. For any other technical or commercial information, please email the author at cache@uts.cc.utexas.edu.

7. References

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8. Symbols

- P - Pressure
- Pi - Pressure at inlet
- Po - Pressure at outlet
- Wl - Liquid weight flow rate
- D - Pipe nominal diameter

Korf toolbar (from left to right in Figure 1): Open file, Save file, Print drawing, Run hydraulics, Resume run (initialize from previous results), Show current specifications on drawing, Show selected results on drawing, Enable or disable drawing, Zoom drawing in or out.

Equipment form (from top-left to bottom-right in Figure 1): Control valve, Check valve, Pump, Compressor, Orifice, Exchanger, Mixer, Splitter, Reducer/Expander, Miscellaneous equipment.

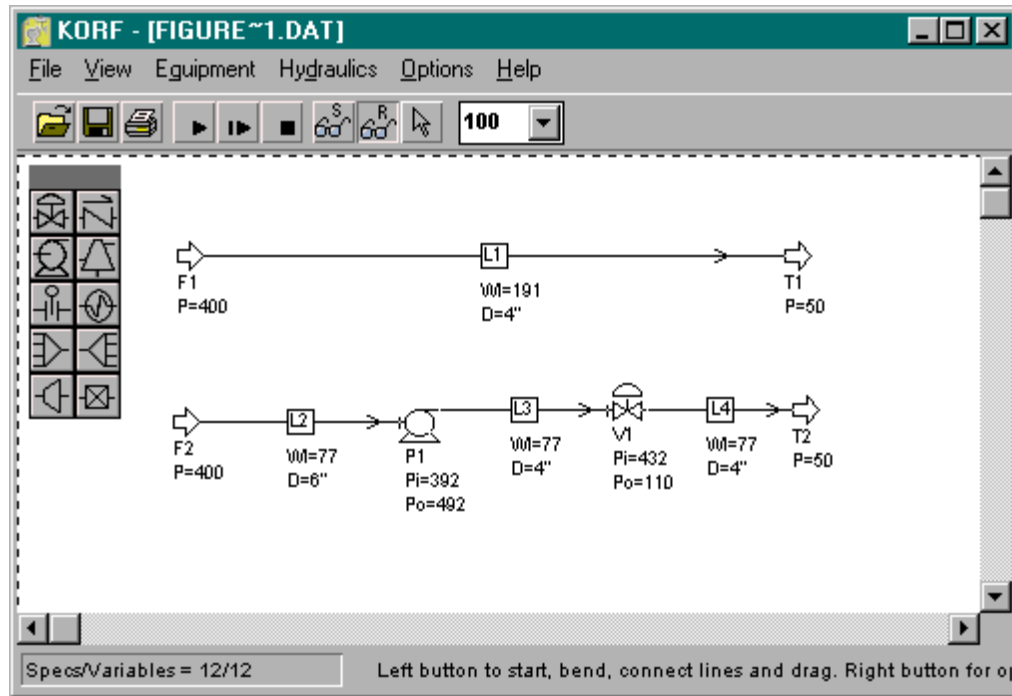


Figure 1. Korf Hydraulics Screenshot

Excel 7.0: Partial Differential Equations

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Partial differential equations arise in a wide variety of chemical engineering problems (1). Typical is the equation

$$\partial^2 T / \partial x^2 - 1/k * \partial T / \partial t = - H/K \quad (1)$$

which describes the heat transfer between two infinite plates with heat generated between the plates(1). Here

T	Temperature, °C
x	The distance measure between the plates, cm
k	Thermal diffusivity, cm ² /sec
b	Distance between the plates, cm
t	Time in sec
K	Thermal Conductivity, cal/sec-cm-°C
H	Heat generation, cal/cm ³ -sec
z	= x/b

A possible set of boundary conditions (1) is:

$$\text{At } t = 0, T = T_o \text{ for all } x$$

$$\text{At } x = 0 \text{ and } x=b, T = T_b \text{ for } t > 0.$$

where T_o , T_b , H , b and the physical properties are given and considered constant.

Eq. (1) can be solved numerically in a number of ways. If the spatial dimension is represented using a finite difference relationship and the time derivative is considered an ordinary differential equation, the procedure is known as the *numerical method of lines* (2). The number of ordinary differential equations that must be solved simultaneously is determined by the number of sections into which the plate is divided in the x direction. Any ordinary differential equation integration method may be used for the integration.

The *numerical method of lines* can be implemented within Excel 7.0 (3) or outside of it. The method has a detailed description (4).

An alternate approach to the solution of Eq. (1) is a fully finite difference solution that may be carried out totally within Excel 7.0. Both the spatial and the time dimensions are represented by finite difference schemes.

The *Crank-Nicolson* method (5) provides an implicit scheme that is second order accurate in both space and time. To provide this accuracy, difference approximations are devel-

oped at the midpoint of the time increment. To do this the temporal first derivative can be approximated at $t^{k+1/2}$ by

$$\partial T / \partial t = (T_i^{k+1} - T_i^k) / \Delta t \quad (2)$$

The second derivative in space can be determined at the midpoint by averaging the distance approximations at the beginning (t^k) and at the end (t^{k+1}) of the time increment

$$\partial^2 T / \partial x^2 = 1/2 * [(T_{i+1}^k - 2T_i^k + T_{i-1}^k) / \Delta x^2 + (T_{i+1}^{k+1} - 2T_i^{k+1} + T_{i-1}^{k+1}) / \Delta x^2] \quad (3)$$

Letting

$$\Delta x = \Delta z * b \quad (4)$$

and then substituting Eq.(2), Eq.(3) and Eq.(4) into Eq.(1) and solving for T_i^{k+1} results in

$$T_i^{k+1} = 1/2 * \lambda / (1 + \lambda) * [T_{i+1}^k - 2T_i^k + T_{i-1}^k + T_{i+1}^{k+1} + T_{i-1}^k + (2/\lambda) * T_{i-1}^{k+1} + 2 * H * \Delta z^2 * b^2 / K] \quad (5)$$

where $\lambda = k * \Delta t / (\Delta z^2 * b^2)$

Eq (5) can be implemented in the spreadsheet shown in Fig.(1). Since the evaluation of T_i^{k+1} involves considerable iteration, the Calculation mode (Tools...Options...Calculation) should be set to *Manual* and *Iteration* set to a least 25.

The first row of the spreadsheet (time = 0) is set to T_o and the bounds at $z = 0$ and $z = 1$ is set to T_b . Although Eq.(5) can be directly coded into each cell it is more convenient to do this by writing a VBA function procedure (6) called VT as shown in Fig (2). The entry in the second row at $z = 0.1$ would be

$$=VT(D18,C18,E18,C19,E19,\$B\$8)$$

This entry may be easily copied into other cells.

Fig.(1) shows the spreadsheet after pressing F9 several times. The values of the parameters are shown in Fig.(1) and are transferred to the function procedure shown in Fig.(2) in the calling sequence for Function VT (argument $\$B\8).

The results of the spreadsheet calculation may be compared to an analytical solution which is available (1).

$$T = T_b + (T_b - T_0) * (h * F - G)$$

where

$$h = H * b^2 / [\pi^2 * K * (T_b - T_0)]$$

$$F = (4/\pi) * [(\pi^3/8) * (z - z^2) - \sum_{n=1}^{\infty} [1/(2n-1)^3] * \exp[-(2n-1)^2 * \pi^2 * k * t / b^2] * \sin[(2n-1) * \pi * z]]$$

$$G = (4/\pi) * \sum_{n=1}^{\infty} [1/(2n-1)] * \exp[-(2n-1)^2 * \pi^2 * k * t / b^2] * \sin[(2n-1) * \pi * z]$$

Fig 2 shows function procedure VA which performs the analytical evaluation. The spreadsheet solution at $x/b = 0.4$ and time = 10000 sec is 17.65 °C. The analytical solution is 17.15 °C.

Conclusions

Partial differential equations which arise in chemical engineering applications may often be suitable candidates for solution by Excel 7.0. The accuracy of the of the solution appears adequate for engineering purposes.

References

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Parameters

Name	Value	Units
delt	400	sec
del (x/b)	17.151034	0.1 dimensionless
b- thickness	0.0888889	3 cm
To- Initial Temperature	0.0222222	0 deg C
Tb- Boundaries	100	deg C
k- Thermal Diffusivity	2.00E-05	cm ² /sec
H*b ² /K	500	deg C

Time(sec)	$z = x/b$										
	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
1	0	0	0	0	0	0	0	0	0	0	0
2	0	4.5147288	0.6108562	0.4512481	0.4447231	0.4444672	0.4447231	0.4512481	0.6108562	0.45147288	0
3	100	12.44207	1.6679133	0.9332776	0.8912219	0.8891211	0.8912219	0.9332776	1.667913327	12.44207	100
4	100	19.180542	3.1929298	1.4786671	1.3430869	1.3345143	1.3430869	1.4786671	3.192929775	19.180542	100
5	100	24.955991	5.0277442	2.1094718	1.8056233	1.7818353	1.8056233	2.1094718	5.027744167	24.955991	100
6	100	29.946256	7.0577118	2.8334638	2.2846135	2.2329835	2.2846135	2.8334638	7.057711761	29.946256	100
7	100	34.292087	9.2001814	3.6495454	2.7853479	2.6904524	2.7853479	3.6495454	9.200181381	34.292087	100
8	100	38.105469	11.396009	4.5514036	3.3121693	3.1571147	3.3121693	4.5514036	11.39600912	38.105469	100
9	100	41.475976	13.603305	5.5299421	3.8683234	3.6359933	3.8683234	5.5299421	13.60330522	41.475976	100
10	100	44.475659	15.792825	6.5748672	4.4559793	4.1300599	4.4559793	6.5748672	15.79282456	44.475659	100
11	100	47.162792	17.944568	7.6756933	5.0763376	4.642076	5.0763376	7.6756933	17.94456796	47.162792	100
12	100	49.584779	20.045276	8.8223539	5.7297766	5.1744811	5.7297766	8.8223539	20.04527596	49.584779	100
13	100	51.780401	22.086581	10.005547	6.4160051	5.7293235	6.4160051	10.005547	22.08658112	51.780401	100
14	100	53.781569	24.063646	11.216904	7.1342084	6.3082269	7.1342084	11.216904	24.06364628	53.781569	100
15	100	55.614693	25.974162	12.44905	7.883177	6.9123846	7.883177	12.44905	25.97416183	55.614693	100
16	100	57.301754	27.817608	13.695587	8.6614174	7.5425744	8.6614174	13.695587	27.81760824	57.301754	100
17	100	58.861154	29.594715	14.951042	9.4672428	8.1991876	9.4672428	14.951042	29.59471455	58.861154	100
18	100	60.308385	31.307062	16.210785	10.298847	8.8822663	10.298847	16.210785	31.30706181	60.308385	100
19	100	61.656561	32.956794	17.470945	11.154364	9.5915462	11.154364	17.470945	32.95679361	61.656561	100
20	100	62.916845	34.546406	18.72832	12.031909	10.3265	12.031909	18.72832	34.54640574	62.916845	100
21	100	64.098789	36.078594	19.980289	12.929617	11.086379	12.929617	19.980289	36.07859433	64.098789	100
22	100	65.210609	37.556147	21.224733	13.845666	11.870259	13.845666	21.224733	37.55614709	65.210609	100
23	100	66.259408	38.981866	22.459959	14.778293	12.67707	14.778293	22.459959	38.98186627	66.259408	100
24	100	67.251357	40.358515	23.684638	15.725808	13.505639	15.725808	23.684638	40.35851513	67.251357	100
25	100	68.191841	41.688781	24.897747	16.686604	14.354711	16.686604	24.897747	41.68878137	68.191841	100
26	1000	69.085583	42.975253	26.098515	17.659157	15.222983	17.659157	26.098515	42.97525321	69.085583	100

Figure 1. Spreadsheet for Heat Conduction Between Parallel Plates

Public Function VT(TIK, TIMK, TIPK, TIMKP, TIPKP, prm)

‘ prm(1) delt
‘ prm(2) delz
‘ prm(3) b
‘ prm(4) To
‘ prm(5) Tb
‘ prm(6) k
‘ prm(7) Hb*2/K

lam = prm(6) * prm(1) / (prm(3) * prm(3) * prm(2) ^2)
lam1 = lam / (2* (lam + 1))

Sum1 = TIPK - 2 * TIK + TIMK + TIPKP + TIMKP
Sum2 = TIK * 2 / lam
Sum3 = 2 * prm(2) ^ 2 * prm(7)

VT = lam1 * (Sum1 + Sum2 + Sum3)

End Function

Public Function VA(z, t, prm)

‘ z value of x/b
‘ time in sec
‘ prm(1) delt
‘ prm(2) delz
‘ prm(3) b
‘ prm(4) To
‘ prm(5) Tb
‘ prm(6) k
‘ prm(7) Hb^2/K

‘Use F and B Approach

Td = prm(5) - prm(4)
Pi = 3.14159265
N = 20

Q1 = 0
Q2 = 0

For j = 1 To N

S1 = Exp(-(2 * j-1) ^ 2) * Pi * Pi * prm(6) * t / (prm(3) ^ 2))
S2 = Sin((2 * j-1) * Pi * z)
S3 = (2 * j-1) ^ 3
S4 = 2 * j-1

Q1 = S1 * S2 / S3 + Q1
Q2 = S1 * S2 / S4 + Q2

Next j

F = (4 / Pi) * (((Pi ^ 3) / 8) * (z - z ^ 2) - Q1)
G = (4 / Pi) * Q2
hh = prm(7) / (Pi * Pi * Td)

VA = prm(5) + Td * (hh * F - G)

End Function

Figure 2. Module Showing VBA Function Procedures

Using Source Term Analysis Software for Calculating Fluid Flow Release Rates

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Abstract

The ability to quantify hazards is extremely important in the chemical process industries. Quantification makes it possible to assess the physical effects of accidental releases of hazardous materials. With the increased availability of powerful personal computers, the ability exists to apply rigorous numerical methods for the application of analytical models and physical correlations.

Releases of process materials during loss of containment events have different characteristics depending on the prevailing (thermodynamic) conditions upstream of the rupture. A wide spectrum of flow regimes from all-flashing to totally non-flashing discharges may be encountered.

This report briefly reviews the mathematical correlations used to calculate release rates of fluids (liquid, gas or two-phase) from chemical process operations following loss of containment accidents. Time varying (unsteady state) release rates are solved iteratively using stepwise finite element calculations performed using Dyadem ReleaseRate™ software, an integrated finite-element Windows® - based computer program used for transient flow modeling. The software has the ability to model both hole-type discharges and pipeline releases of liquids and gases.

Using Source Term Analysis Software for Calculating Fluid Flow Release Rates

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1. Introduction

Risk analysis studies often address the releases of hazardous materials from accidental punctures or leaks in process vessels or storage tanks. Scenarios often deal with calculating the time-varying discharge rates following loss of containment events in order to quantify release amounts and times. Quantification makes it possible to assess the consequences of accidental releases of hazardous materials for use in emergency response planning, hazard assessment studies and preventive maintenance programs.

This paper briefly reviews methods of identifying potential release sources and calculating subsequent discharge rates of fluids (liquid, gas or two-phase) from chemical process operations following loss of containment accidents. Time-varying (unsteady state) release rates are solved iteratively using stepwise finite element calculations performed with Dyadem ReleaseRate™, a computer program for transient flow modeling. The software has the ability to model various leak and rupture types including hole-type discharges, pipeline ruptures and seal or gasket failures common in Source Term Analysis studies.

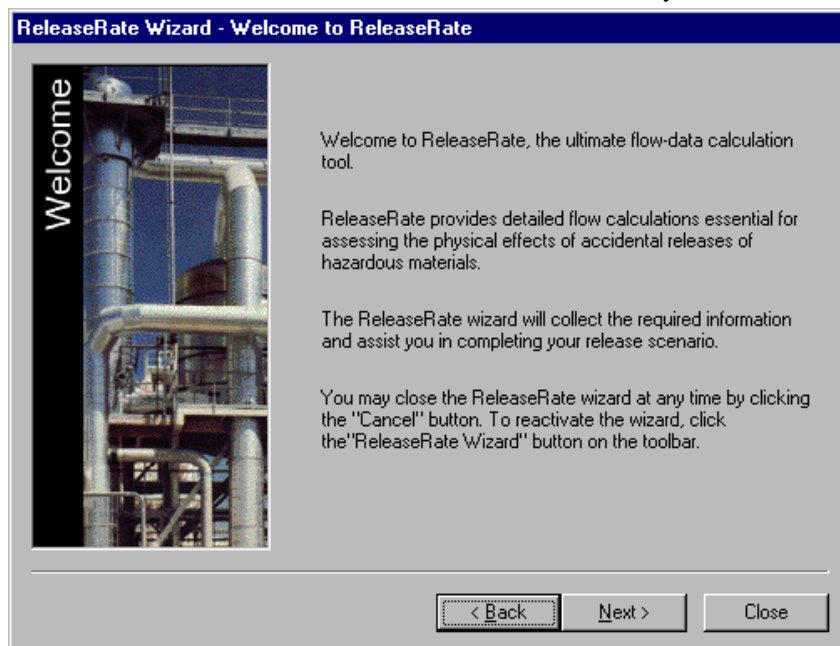


Figure 1. ReleaseRate Wizard welcome screen

1.2 Characterizing Potential Release Sources in Process Plants

Process plants can have a large number of potential leak and rupture sources. To identify potential release sources from plant installations, a classification system can be employed. A release source can be identified by both a containment

vessel storing the chemical and a leak or rupture location. Releases can occur either on the containment vessel itself or farther downstream from connecting process equipment or piping.

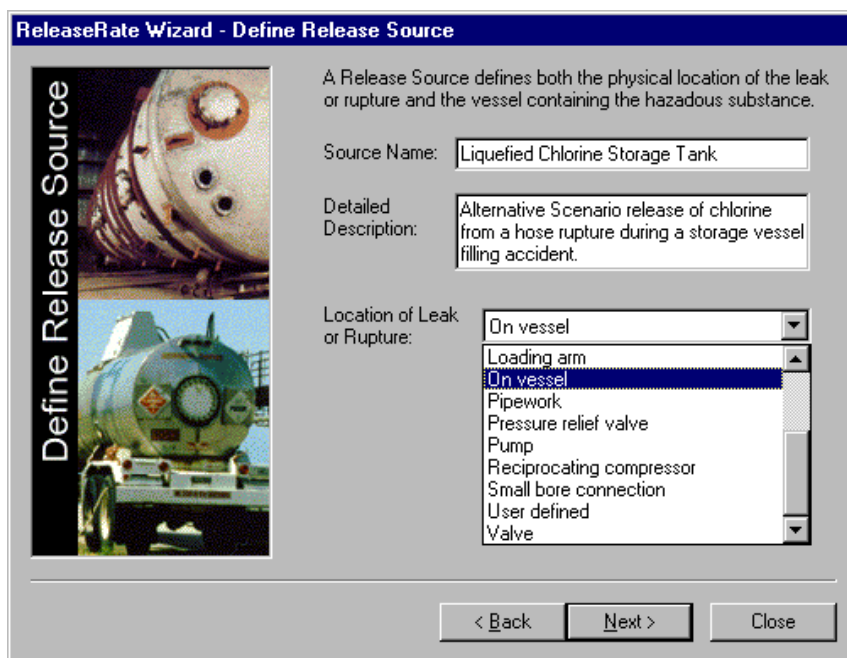


Figure 2: Example of defining a leak or rupture location in ReleaseRate

The classification approach, outlined by Cox, Lees and Ang (1990), was adopted in the ReleaseRate program for identifying potential release sources and determining an appropriate leak or rupture size according to the specified location

and equipment type. The following table presents a complete list of the principal types of equipment subject to leaks or ruptures.

Table 1: Principal types of releases based on process equipment type adapted from Cox, Lees and Ang (1990)

<i>Location of Leak or Rupture</i>	<i>Type of Leak or Rupture</i>
On containment vessel itself	Hole in vessel wall Crack in vessel wall
Through pressure relief valves	Vessel overfilling (material release through pressure relief valve)
From pipework	Full bore (guillotine) rupture Pipe splits Cracks in pipe fittings
From flanges	Gasket failures
Through small bore connections	Full bore rupture
From hoses	Full bore rupture Pull-away leak from transfer hose
From valves	Valve rupture Stem leak
From pumps	Pump rupture Seal leak
From centrifugal compressors	Seal leak
From reciprocating compressors	Seal Leak Valve chamber release
From agitators	Seal leak
From drain/sample points	Full bore release
Through atmospheric vents	Full bore release
From loading arms	Full bore release

2. Modeling Transient Fluid Flow Rates with ReleaseRate

The time-varying releases of process materials following loss of containment events have different characteristics depending upon the prevailing (thermodynamic) conditions upstream of the rupture. Flow regimes can range from all-flashing to totally non-flashing discharges (Leung, 1990).

Release scenarios can involve the release of flammable or toxic fluids from a pipe, tank, process vessel, pressure relief valve, vent stack and so on. By defining various process parameters and chemical property information, outflow data can be calculated (release rates and release times).

In general, the three possible types of outflow conditions — liquid, gas or flashing flow — can be correlated based upon the storage state of the chemical and the location of the leak or rupture. Release scenarios can be broken down into the following categories:

Non-volatile Liquid (incl. Gases Held as Liquids by Refrigeration) Releases:

- Discharge from a small hole or crack
- Discharge from attached open piping

Compressed Gas Releases:

- Discharge from a small hole or crack (adiabatic cooling)
- Discharge from attached open piping (adiabatic cooling)

Pressurized Liquefied Gas Releases:

- Discharge from a small hole or crack in the liquid space
- Discharge from attached open piping from the liquid space (two-phase flashing flow)
- Discharge from a small hole or crack in the vapor space (evaporative cooling)
- Discharge from attached piping from the vapor space (evaporative cooling)

Vessel Overfilling Releases through a Pressure Relief Device:

- Liquid discharge through a pressure relief valve
- Gas or vapor discharge through a pressure relief valve

Various fluid flow models are incorporated into the ReleaseRate program to deal with the most common types of outflow conditions listed above. A database containing relevant property values for a number of hazardous chemicals is also included. Furthermore, in order to correlate release rate scenarios properly, a wide array of physical and thermodynamic property data is required. Property correlations are therefore employed for viscosity (liquid and gas),

SG (specific gravity), vapor pressure, heat capacity (liquid and gas), vapor compressibility and latent heat of vaporization.

2.1 (Non-volatile) Liquid Releases

In modeling the releases of non-volatile liquids from vessels, incompressible flow is assumed. The driving force is the head of liquid in the vessel along with the vessel pressure. The volumetric discharge rate varies with time as the liquid volume changes and thus is affected by the changing vessel geometry.

2.1.1 Discharge from a small hole or crack

The flow of the liquid can be determined based on incompressible fluid flow. Assuming negligible friction loss at the orifice, flow on a horizontal axis, and the hole being small compared to the size of the vessel, the volumetric flow rate is given by the following equation taken from Ramskill (1986). As the liquid height decreases, the discharge rate also decreases.

$$Q = C_d A_h \sqrt{2g(H_L - H_h) + \frac{2g(P_v - P_a)}{\rho_L}} \quad (1)$$

2.1.2 Discharge from attached open piping

To calculate the discharge rate from an attached pipe, equation (1) is used with a modified overall discharge coefficient C_d based on the sum of the frictional losses in the attached piping. The overall discharge coefficient is calculated as follows:

$$C_d = \frac{1}{\sqrt{1 + K_{sum}}} \quad (2)$$

Where: $K_{sum} = \sum K_i$

$$K_i = \frac{4f_{F_i}L_i}{D_i}$$

i = each individual pipe section or fitting

2.2 Compressed Gas Releases

For pressurized vessels containing non-saturated vapor or non-condensable gas, the discharge can be either choked (sonic) or non-choked flow. The release can be either from a hole or crack in the vessel wall or from piping or process equipment attached to the vessel. Two separate computational approaches are required for the estimation of gas discharge rate for these types of scenarios. The correlations are outlined in the following sections.

2.2.1 Discharge from a small hole or crack

For compressed gas storage, the usual concern is the release of gas stored under high pressure through a small hole in the containment. A small hole is defined by Ramskill (1986) as one where the ratio $A_h/A < 0.01$.

Assuming flow on a horizontal axis and using a coefficient of discharge to account for friction at the orifice, the mass flow rate of a gas through a hole area A_h can be determined for two types of flow conditions: choked or non-choked.

The isentropic expansion factor, k , is equal to the ratio of specific heats (C_p/C_v) of the gas. The critical pressure ratio is defined by:

$$\left(\frac{P_2}{P_1}\right)_{crit} = \left(\frac{2}{k+1}\right)^{\frac{k}{k-1}} \quad (3)$$

If the pressure ratio P_2/P_1 is below the critical value given by equation (3), the exiting mass flow rate is calculated for non-choked flow. The equation for an instantaneous discharge under non-choked flow conditions, taken from Ramskill (1986), is:

$$W = C_d \rho_2 A_h \sqrt{\frac{2P_1}{\rho_1} \frac{k}{k-1} \left[1 - \left(\frac{P_2}{P_1}\right)^{\frac{k-1}{k}}\right]} \quad (4)$$

If the pressure ratio P_2/P_1 is above the critical value given by equation (3), the exiting mass flow rate is sonic and is limited to a critical maximum value. The equation for an instantaneous discharge under sonic or choked flow conditions, taken from Ramskill (1986), is:

$$W = C_d A_h \sqrt{P_1 \rho_1 k \left(\frac{2}{k+1}\right)^{\frac{k+1}{k-1}}} \quad (5)$$

For the choke flow conditions, the flow rate is independent of outlet conditions.

2.2.2 Discharge from attached open piping

Consideration of frictional resistance to flow often requires graphical techniques to calculate discharge rates. The charts referred to are outlined by Lapple (1943) and later corrected by Levenspiel (1977). However, with the aid of a computer model it is possible to use a complex numerical algorithm to solve the mass and energy conservation equations involved in this process.

To calculate the gas discharge rate from a pipeline attached to a pressurized vessel, an adiabatic flow correlation is used for gas flow in pipes. The general equation for adiabatic gas flow through a pipe section of length L and constant diameter D is listed below:

$$W = \left[\left(\frac{k}{k+1}\right) \left(\frac{\pi D^2}{4}\right)^2 \cdot \frac{M}{z_1 T_1 R} \cdot P_1^2 \frac{\left[1 - \left(\frac{P_2}{P_1}\right)^{\frac{k+1}{k}}\right]^{\frac{1}{2}}}{\left[\frac{f_F L}{2gD} - \frac{1}{gk} \ln\left(\frac{P_2}{P_1}\right)\right]} \right] \quad (6)$$

Equation (6) is then solved simultaneously for any number of pipe sections based on constant mass flowrate. This requires an iterative solution based on an initial vessel pressure and subsequent pressure drops across each pipe section.

Flow is sonic (maximum “choked” flow) when P_2 is equal to the critical pressure given by the following equation:

$$P_{crit} = \frac{4}{\pi} \frac{z_1 G_{crit}}{D^2} \sqrt{\frac{R}{g} \cdot \frac{T_1}{kM}} \quad (7)$$

Combining equations (6) and (7) at critical flow gives the following correlation:

$$\frac{f_F L}{D} = \frac{2z_1}{(k+1)} \cdot P_1^{\frac{k-1}{k}} \cdot \frac{\left[1 - \left(\frac{P_2}{P_1}\right)_c^{\frac{k+1}{k}}\right]}{\left(\frac{P_2^2}{P_1^2}\right)^{\frac{k+1}{k}}} + \ln\left(\frac{P_2}{P_1}\right)_c^2 \quad (8)$$

Based on equation (8), the critical outlet pressure P_2 can be calculated iteratively for a specific pipe length, vessel pressure and expansion factor (k).

2.3 Pressurized Liquefied Gas Releases

This section details pressurized liquefied gas releases following a loss of containment failure. Pressurized gases stored as liquids are usually in liquid-vapor equilibrium, so vessel pressure is equal to the vapor pressure of the liquid at the vessel temperature.

When a liquefied gas is released from a pressurized tank, evaporative cooling takes place due to heat loss. These auto-cooling or auto-refrigeration effects can be correlated assuming an energy transfer between the exiting gas and the liquid remaining in the vessel. The following equation relates the energy absorbed by the escaping gas to the energy released by the remaining liquid in the vessel:

$$W\lambda(t - t_o) = (m_o - W(t - t_o))C_p(T_2 - T_1) \quad (9)$$

2.3.1 Discharge from a small hole or crack in the liquid space

Critical flow data for the release of saturated liquids from a hole in the side of a vessel is well correlated using the standard liquid flow equation (1).

2.3.2 Discharge from attached open piping from the liquid space (two-phase flashing flow)

Two-phase flashing flow may develop when a liquefied gas flows through a pipe and the local pressure in the pipe becomes lower than the saturation pressure of the flowing liquid due to decrease of pressure along the pipe because of friction (C.J.H. van den Bosch and N.J. Duijm, 1997). Several methods have been proposed in the literature to evaluate the critical discharge rate of a two-phase flow from a pipe.

The maximum flow model employed here is the Homogenous Equilibrium Model (HEM) based on work by Fauske (1985). Although the homogeneous flow assumption may be an oversimplification in some cases, it has been found adequate in most engineering design (Leung, 1989). For two-phase flashing flow systems, this flow regime, combined with the assumption of thermodynamic equilibrium between the two phases, has provided the best prediction of low-quality choked flow data of various fluids (Moody, 1975; Fauske, 1985). With respect to emergency relief systems design and risk analysis, this flow model would yield conservative values.

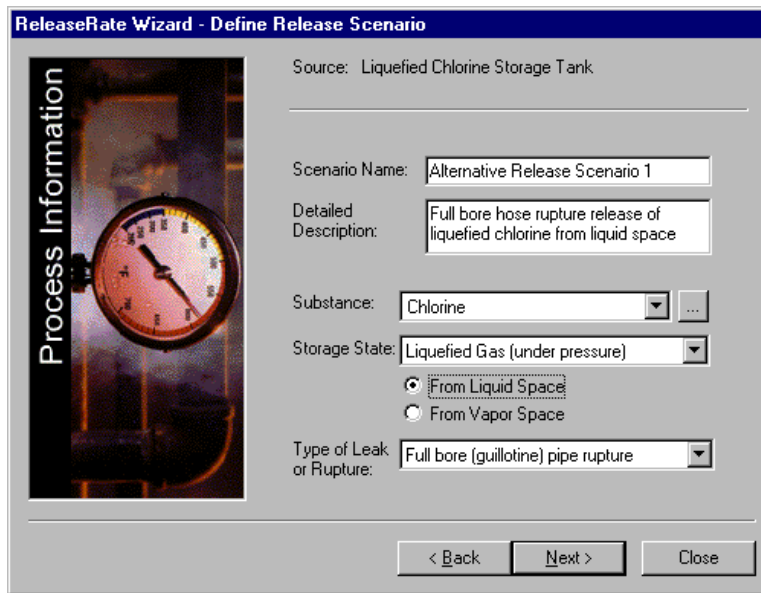


Figure 3. Example of defining a liquefied gas (from liquid space) pipe release in ReleaseRate

The critical outlet pressure at the pipe exit is based on the single-phase gas formula, where the critical pressure ratio can be defined by equation (10) below. The temperature T_{crit} corresponding to this critical outlet pressure can then be found based on vapor pressure data.

$$P_{2(crit)} = P_1 \left(\frac{2}{k+1} \right)^{\frac{k}{k-1}} \quad (10)$$

The most important factor in two-phase flow calculations is the vapor in liquid quality. The quality determines to a large extent the mass flow rate and the friction in the pipe. The largest possible discharge rate is obtained with a pure liquid phase flow. For a two-phase discharge, the mass flow rate may be substantially smaller due to the increased specific volume of the fluid (C.J.H. van den Bosch and N.J. Duijm, 1997).

Assuming thermodynamic equilibrium, the vapor mass fraction that would flash off from the liquid is calculated:

$$m_v = 1 - \exp\left(-\frac{C_p}{\lambda}(T_1 - T_{crit})\right) \quad (11)$$

Assuming homogeneous mixing and no slip between the phases, the mixture density is calculated at the critical choke conditions:

$$\rho'_c = \left(\frac{m_v}{\rho'_g} + \frac{1 - m_v}{\rho'_l}\right)^{-1} \quad (12)$$

Finally, a slightly modified standard liquid discharge formula based on a critical outlet pressure and the calculated mixture density can then be used to calculate the critical flow rate:

$$Q = \frac{C_d A_o}{\rho_c} \sqrt{2g\rho'_c(P_o - P_{crit})} \quad (13)$$

where:

$$P_o = P_v + \rho'_l(H_L - H_o) \quad (14)$$

2.3.3 Discharge from a small hole or crack in the vapor space (auto-refrigeration)

Critical flow data for the release of a liquefied gas (from vapor space) from a hole in the side of a vessel is well correlated using the standard compressed gas flow models (equations 4 and 5), taking into account auto-refrigeration effects over the release time.

2.3.4 Discharge from attached piping from the vapor space (auto-refrigeration)

Critical flow data for the release of liquefied gas (from vapor space) from piping attached to a vessel is well correlated using the adiabatic gas flow through pipe model (equation 6), taking into account auto-refrigeration effects over the release time.

2.4 Vessel Overfilling Releases through a Pressure Relief Device

An imbalance of fluid flow rates in and out of process equipment and vessels during operation results in an accumulation of liquids or vapors and may produce internal pressures that exceed the operating pressure. One of the most common causes of vessel over-pressurization is vessel overfilling due to operator error or control device failure. In this

case, vessel pressure rises uncontrolled and must be reduced through a relief device.

According to API recommended practice (RP 520, 6th Ed., 1990), pressure relief devices are sized according to established relief requirements based on liquid or vapor rates developed by the net energy input. API established rules that dictate how to estimate valve sizes. ASME also establishes codes for certifying relieving capacities, which must be stamped on the valve nameplates.

For the case of an overfilling release, it is assumed that the relief valve orifice type and size are known. Since orifice size is known, both API or ASME equations for relief valve sizing of liquid or gas releases can be rearranged to calculate the flow rate through the valve based on known process conditions and orifice size. The Consolidated SRV-1 (1993) catalogue provides a summary of both API RP 520 and ASME Code Section VIII sizing equations for liquids and gases.

3. Examples of Fluid Flow Modeling with ReleaseRate

The following examples illustrate some typical release rate scenario problems correlated using ReleaseRate. Various output parameters and time-varying results were produced.

3.1 Liquefied gas release from a pipe connected to the liquid space (two-phase flashing flow)

At a waste water treatment facility, a chlorine storage tank develops a guillotine pipe rupture along a transfer line connected to the tank. The pipe is connected to the base of the vessel, below the liquid level of the tank (i.e. release is from the liquid space). Two-phase flashing flow outflow conditions can be correlated based on a pressurized liquefied gas release (from the liquid space) through a full bore ruptured pipe.

Input Parameters:**Containment Vessel parameters:**

Type: Horizontal Cylindrical Vessel
Length: 20 ft (6.096 m)
Diameter: 4 ft (1.219 m)
Dish type: semi-ellipsoidal (2:1)
Vessel volume: 1817 US Gal*

Pipe Parameters:

No. Pipe Sections: 1
Pipe diameter: 3 in (7.62 cm)
Pipe length: 100 ft (30.48 m)
Pipe roughness: 0.0018 in (0.046 mm), steel
Discharge coeff: $C_d = 0.61$

Process Parameters:

Initial temperature: 86°F (30°C)
Initial pressure: 127.88 psia
Initial liquid level: 2 ft (0.6096 m)
Pipe-to-vessel connection height: 0 ft (at base)
Initial liquid volume: 908 US Gal*

Modeling Parameters:

Flow correlation: Two-phase (HEM) flow through pipes (assuming negligible temperature and vessel pressure drop)

* Calculated by ReleaseRate

Output Results:

<i>Time (sec)</i>	<i>Liquid Height (ft)</i>	<i>Rate (USGPM)</i>	<i>Rate (lb/hr)</i>	<i>Volume Released (US Gal)</i>	<i>Mixt Density (lb/ft³)</i>
1	2	3033.7	258,659	0	10.63
2	1.75	3035.8	258,107	24.4	10.60
3	1.50	3037.8	257,790	47.0	10.58
4	1.25	3039.7	257,220	69.6	10.55
5	1.00	3041.8	256,665	94.0	10.52
6	0.75	3043.8	256,346	116.6	10.50
7	0.50	3045.9	255,790	141.0	10.47
8	0.25	3048.0	255,233	165.5	10.44

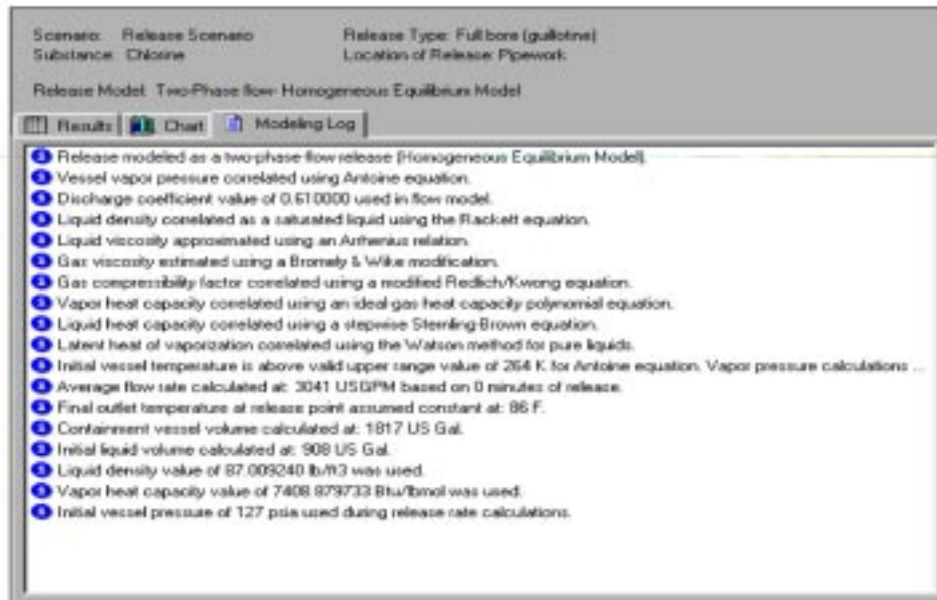


Figure 4: Modeling log generated for two-phase liquefied chlorine release example (3.1)

3.2 Compressed gas release from a transfer hose connected to a vessel

During a vessel filling operation, accidental pull-away causes the failure of a 50-foot (15.24 m) length of 1-inch (2.54 cm) hose releasing methane gas to the surroundings. These out-

flow conditions can be correlated based on a compressed gas release through a full bore hose rupture.

Input Parameters:

Containment Vessel parameters:

Type: Vertical Cylindrical Vessel
 Height: 20ft (6.096 m)
 Diameter: 4 ft (1.219 m)
 Dish type: semi-ellipsoidal (2:1)
 Vessel volume: 1880.1 US Gal

Transfer Hose Parameters:

No. Hose sections: 1
 Hose diameter: 1 in (2.54 cm)
 Hose length: 50 ft (15.24 m)
 Hose roughness: 0.0000591 in (1.5E-6 m), smooth tubing

Process Parameters:

Initial temperature: 77°F (25°C)
 Initial pressure: 25 psia (344.7 kPa)

Modeling Parameters

Flow correlation: Compressible adiabatic gas flow through pipes with adiabatic temperature drops

* Calculated by ReleaseRate

Output Results:

Time (sec)	Press (psia)	Temp (°F)	Rate (lb/hr)	Mass Released (lb)
0	25	77	549.6	0
130	18.52	41.7	305.6	19.77
259	15.15	18.9	93.0	30.77

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Nomenclature

A_h = orifice area (m²)
 c_d = discharge coefficient (usually 0.61 for liquids and 0.8 for gases)
 C_p = Vapor heat capacity (J/mol.K)
 D = internal pipe diameter (m)
 f_F = Fanning friction factor (-)
 g = gravitational constant (9.81m/s²)
 g_c = gravitational conversion factor (1 kg.m/s²/N)
 H_h = height of orifice above bottom of container (m)
 H_L = height of liquid above bottom of container (m)
 k = isentropic expansion factor (C_p/C_v)
 L = equivalent pipe length* (m)
 m_o = mass of liquid vessel (kg)
 m_v = vapor mass fraction or quality (-)
 M = Molecular weight of the gas (g/mol)
 P_v = vessel pressure (Pa)
 P_a = ambient pressure (Pa)
 P_o = upstream pressure (Pa)
 $P_{1,2}$ = inlet and outlet pipe section pressures, respectively (Pa)
 P_{crit} = critical pressure (Pa)
 Q = volumetric flow rate (m³/s)
 R = Ideal gas constant (9.81 J/mol.K)
 $t-t_o$ = incremental time difference (sec)
 T_v = vessel temperature (K)
 $T_{1,2}$ = inlet and outlet temperatures (K)
 T_{crit} = critical outlet temperature (K)
 W = mass flow rate (kg/s)
 z = inlet compressibility factor
 λ = latent heat of vaporization of liquid (J/kg)
 ρ_L = liquid density (kg/m³)
 ρ'_c = mixture density at T_{crit} and P_{crit} (kg/m³)

ρ' = vapor density at T_{crit} and P_{crit} (kg/m³)
 ρ_l^g = liquid density at T_{crit} and P_{crit} (kg/m³)

*Equivalent pipe lengths are calculated based on actual pipe length, fitting losses, and entrance/exit effects for the pipe section.

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Calling FORTRAN Subroutines from Excel 7.0

Edward M. Rosen, EMR Technology Group

The use of FORTRAN in Excel 7.0 (Excel 95) may be motivated by any of several issues:

1. The language may be more familiar to the user than Visual Basic for Applications (VBA).
2. There may be a need for greater efficiency and/or speed.
3. The amount of effort to convert existing FORTRAN code to VBA may be excessive.

As noted previously (1), FORTRAN code in the form of an .exe module can be accessed from a VBA subroutine procedure using the shell function of VBA which transfers the execution of the program to DOS. Input values from the spreadsheet are written to a file, the file is read in by the FORTRAN .exe program, the results from the program are written to an output file, the output file is read by the VBA code and then transferred to the spreadsheet.

To the user it appears that nothing unusual is taking place. A minor disadvantage of the method is that the elapsed time for execution of the program to be completed under DOS must be explicitly allowed for in the VBA subroutine procedure coding.

Being able to call FORTRAN subroutines directly from a VBA procedure has the advantage that less VBA coding is required. However, the FORTRAN must be compiled and linked into a DLL (Dynamic Link Library). No read or write statements are allowed.

Fig. (1) is a listing of three simple FORTRAN subroutines, TRY1, TRY2 and TRY3. TRY3 calls a fourth subroutine TRY4. TRY1 has an array input and an array output. It is desired to call these FORTRAN routines from within an Excel array function procedure (2) called TRY from the spreadsheet.

The following description uses command line entries available using Digital Visual FORTRAN ver 5.0. Alternative entries are available using Microsoft's Powerstation or the Integrated Development Environments of each of the compilers (i. e. Developer Studio).

1. The three FORTRAN subroutines are compiled and linked as a DLL (Dynamic Link Library) by entering the following command (in the DOS window):

```
DF /DLL:MYDLL TRY1.FOR TRY2.FOR TRY3.FOR
```

where the name of the Library is MYDLL. As a result of the compilation and linking the following three files are generated:

```
MYDLL.DLL
MYDLL.LIB
MYDLL.EXP
```

Note the compiler directive `ATTRIBUTES` that must be inserted into the FORTRAN code of the subroutines.

2. In the VBA coding of the array function TRY (Fig. (2)) the DECLARE statement must be added for each of the subroutines to be called.

The syntax is:

```
Declare Sub name Lib "libname" (arglist)
```

where *name* is the DLL entry point name
libname is the DLL file name. The complete path must be given
arglist is a list of variables to be passed to the DLL which includes the appropriate By Ref variable declarations

Note that the subroutine TRY1 is called referring to the first element of the array zz.

3. In the spreadsheet the TRY function is invoked by entering:

```
=TRY (A6)
```

after pre-selecting the five element output range (B6..B10) and entering **Ctrl+Shift+Enter**.

The spreadsheet is shown in Fig. (3).

Conclusions

FORTTRAN subroutines may be integrated into the VBA coding of VBA function procedures with a minimum of effort. Their use may substantially improve the efficiency/speed of the spreadsheet calculation.

References

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Acknowledgment

The suggestions and help of Lee Partin of L R Partin Enterprises are greatly appreciated.

```
SUBROUTINE TRY1 (X, Y)
!DEC$ ATTRIBUTES DLLEXPORT :: TRY1
!DEC$ ATTRIBUTES ALIAS:'TRY1' :: TRY1
DIMENSION X(2) , Y(3)
Y (1) = X(1) + X(2)
Y (2) = X(1) * X(2)
Y (3) = X(1)**2 + X(2)**2
RETURN
END

SUBROUTINE TRY2 (x, y)
!DEC$ ATTRIBUTES DLLEXPORT :: TRY2
!DEC$ ATTRIBUTES ALIAS:'TRY2' :: TRY2
y = 5*x
RETURN
END

SUBROUTINE TRY3 (x, y)
!DEC$ ATTRIBUTES DLLEXPORT :: TRY3
!DEC$ ATTRIBUTES ALIAS:'TRY3' :: TRY3
yy = 8*x
CALL TRY4 ( yy, y )
RETURN
END
SUBROUTINE TRY4 (x, y)
Y = 1000*x
RETURN
END
```

Figure 1. FORTRAN Subroutines

```

Declare Sub TRY1 Lib "D:\DIGITA~3\DLLS\Myd11.DLL"(ByRef xx As Single, ByRef yy As Single)
Declare Sub TRY2 Lib "D:\DIGITA~3\DLLS\Myd11.DLL"(ByRef xx As Single, ByRef yy As Single)
Declare Sub TRY3 Lib "D:\DIGITA~3\DLLS\Myd11.DLL"(ByRef xx As Single, ByRef yy As Single)

```

```
Public Function TRY(x)
```

```

Dim xx As Single
Dim yyy As Single
Dim yyyy As Single

```

```

Dim DD(1 To 5) As Single
Dim yy(1 To 3) As Single
Dim zz(1 To 2) As Single

```

```

zz(1) = x(1)
zz(2) = x(2)

```

```
Call TRY1(zz(1), yy(1))
```

```
xx = x(1)
```

```
Call TRY2(xx,yyy)
```

```
Call TRY3(xx,yyyy)
```

```

DD(1) = yy(1)
DD(2) = yy(2)
DD(3) = yy(3)

```

```

DD(4) = yyy
DD(5) = yyyy

```

```
TRY = Application.Transpose(Array(DD))
```

```
End Function
```

Figure 2. Listing of VBA Array Function TRY

Use of FORTRAN Routines Compiled As Dynamic Link Library

<A>			
Input Values – x		Output Values	
	3	7	<<Row 6>>
	4	12	
		25	
		15	
		24000	

Figure 3. Spreadsheet Using Array Function Procedure TRY

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