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Methodology for Stable Dynamic Simulation of a LNG Pipe under Two-Phase-Flow Generation

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The results of dynamic simulations can become unstable because of a steep change in the calculated variables. In particular, when liquefied natural gas (LNG) begins to vaporize and a two-phase flow is generated, the simulation results can become violently oscillatory because of the significant volume difference between natural gas in the vapor phase and LNG in the liquid phase. To ensure more stable simulation results, we developed a methodology for replacing a unit module selectively. When LNG started to vaporize, the unit module at the point where the two-phase flow was first generated was replaced by a more stable unit module. This methodology was evaluated through a case study of a LNG pipeline model and led to more stable simulation results.

1. Introduction

Natural gas (NG) is an important and well-known environmentally friendly energy source. It is odorless, colorless, noncorrosive, and nontoxic. Even though NG is a fossil fuel consisting of hydrocarbons as crude oil, it produces lower carbon emissions when combusted because, typically, 95% of NG is composed of a single-carbon material, methane. The density and volume difference between the liquid and vapor phases of methane are considerable. In the liquid phase, NG occupies ¹/₆₀₀th the volume of its gaseous form at atmospheric pressure. Therefore, NG is usually transported and stored as a liquid form, called liquefied natural gas (LNG).

Because NG will start to condense into the liquid phase at a temperature below $-162\,^{\circ}\text{C}$ at atmospheric pressure, the process of liquefying NG requires a specialized terminal composed of pipes and tanks to endure cryogenic conditions. However, even if the LNG liquefaction equipment is thermally insulted, it cannot help absorption of heat from the surrounding environment mainly because LNG at cryogenic temperatures can be easily affected by ambient conditions. When LNG starts to vaporize, its volume increases rapidly. Figure 1 shows the volume increase rate of typical LNG (consisting of 95% methane, 4% ethane, and 1% propane) due to vaporization. Near the boiling point, LNG may increase its volume approximately 150 times for a 1 °C increase in the temperature. Consequently, in a terminal containing a long pipeline, partial LNG vaporization in pipelines of the liquefaction terminal can cause various problems.

In a transient analysis of the response of the LNG containment system, a dynamic simulation, which is a collection of time-changing patterns to represent phenomena, can be a valuable tool. However, because of the steep changes in the volume of LNG, dynamic simulations could easily show oscillating instabilities under two-phase conditions, as shown in Figure 2. Although there are various explanations for causes of the oscillation observed, the main cause of this phenomenon is the competing solutions that result in the system swinging from one solution to another. Another reason is the compressibility of an LNG vapor bubble, which works like a spring and effects the pressure balance within the LNG vapor and the external pressure. ¹

In the past, researchers have studied the instabilities observed in the dynamic simulations of a two-phase LNG mixture flowing through pipelines. There have also been a few studies that have concluded that with the use of methodology the results of dynamic simulations can become more stable. Stenning² investigated and identified three types of instabilities, namely, density-wave-type, pressure-droptype, and thermal-type oscillations in a single-channel upflow boiling system. Maulbetsch and Griffith³ studied pressure-drop instabilities in a single horizontal tube system. Mayinger and Kastner⁴ investigated thermal instabilities. Boure et al.⁵ and Kakaç and Bon⁶ reviewed two-phase-flow dynamic instabilities and theoretical studies of in-tube boiling vertical

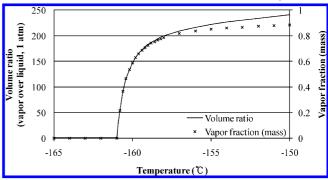


Figure 1. Volume ratio (vapor over liquid, 1 atm) and vapor fraction increase of a typical LNG (95% methane, 4% ethane, and 1% propane) vs temperature.

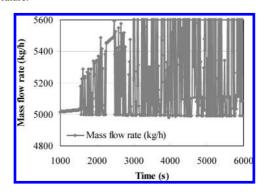


Figure 2. Example of an oscillation problem when two-phase flow is generated in a dynamic simulation of the LNG pipeline.

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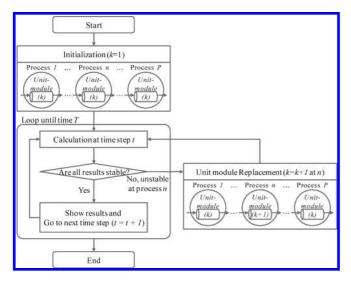


Figure 3. Flowchart diagram for the suggested methodology to replace the unit module selectively.

systems. Research work in the field of nuclear engineering has also been devoted to studies of the flow instabilities in boiling two-phase natural circulation systems. However, the aim of these studies was not to stabilize numerical instabilities but to classify and understand the phenomena behind the flow instabilities. Osciadacz⁷ tried to approach the problem with the use of dynamic simulations. He examined mathematical models that had been developed to describe the transient gas flow in a pipe and concluded that the choice of a specific model is usually dependent on the scope of the study. Lewandowski^{8,9} studied methods and algorithms for modeling a gas transmission network as well as their applications. Cameron and Transmission¹⁰ proposed the use of simple transient simulations based on Excel and Visual Basic. Hammer¹¹ developed a simulator that takes into account the internal energy conservation. However, these are not freely available to the public, and they could not provide a general approach to overcoming the instabilities of LNG dynamic simulations.

In this study, we suggested a systemic methodology to address problems of the instabilities observed in the dynamic simulations of a two-phase LNG. In our methodology, a unit module is replaced by a more stable module selectively when the unstable results are calculated. We also provide the simulation results of a case study, which are characterized by enhanced stability.

2. Methodology

The main idea behind our methodology is to replace the unit modules where instabilities have occurred by more stable unit modules. Even though there may be only one point during execution of a dynamic simulation where unstable results are being generated, these may affect whole calculations and instabilities may be observed throughout the dynamic simulation. In this case, more stable results can be obtained by replacing the unit module to generate unstable results. However, if we simplified the entire model to overcome this problem, the accuracy of the calculations may deteriorate. Moreover, a process to find the point where unstable results were generated through trial and error can be extremely time-consuming.

To solve these problems, we suggested a methodology to replace the unit module selectively. Figure 3 shows an algorithm diagram on which this method is based. At first, it is assumed

```
Initialization:
Tol = Tolerance
M(p) at process p = Unit module(1) at all process 1, 2, 3, ..., P
        'initial time
Vars(p,t) = Initial value of process p at time t=0 (initial value)
Vars(p,t+1) = Calculated the simulation result at time t+1
dVars(p,t) = Vars(p,t) - Vars(p,t-1)
E(dVars(p,t)) = average value from dVars(p,t-Tol) to dVars(p,t)
For each Vars(p,t) at all process 1, 2, 3, ..., P
        If (dVars(p,t+1)) > E(dVars(p,t))*Tol then
                                                            'detection of steep change
                 M(p)=Unitmodule(k+1) 'model changing
                 Return Main
                                 'recalculation at time step t
        Else
                 t=t+1 'go to next time step t+1
                 Return Main
                                 'continue to simulate
Next
```

Figure 4. Pseudocode algorithm for the suggested methodology to change the unit module selectively.

that we can have K kinds of unit modules, Unitmodule(k) (k =1, 2, 3, ..., K), with different stabilities and complexities. Unitmodule(k) has less complexity and more stability as parameter k increases. In the initialization step (t = 1), Unitmodule(k) with k = 1 is used for all processes. After calculation of the simulation results at time step t, if there is no big change within the corresponding tolerance in all processes, the calculated results are considered stable and reflected. The time step t is moved to next time step t = t + 1. However, if the difference of a value of process n is too big to compare with the average difference, it means that an unstable steep change is detected. At this time, therefore, the unit module at process n is replaced with Unitmodule(k+1), which is more stable than Unitmodule(k). The calculation is returned to the main part, and the results of simulation are recalculated based on changed unit modules. Figure 4 shows a pseudocode algorithm for suggested methodology.

3. Case Study

To evaluate our methodology, a case study was performed. Figure 5 shows the schematic diagram of a pipeline model for LNG transportation. It consists of three pipes, four valves, and one controller. The specifications of each unit module are summarized in Table 1. Valves 1, 2, and 4 ensure so high a C_v value that their presence in the flow is negligible. Valve 3 is used to control the flow through the pipeline. Each pipe is assumed to have a diameter of 812.8 mm and a multilayer structure of the composite material, as shown Figure 6. Table 2 summarizes the characteristics of materials used for pipe walls and other important parameters of the pipe modeling. 12,13 The ambient temperature is assumed to be equal to 25 °C. A Aspen HYSYS v7.0 was used as a simulator, and modified Peng-Robinson equations of state (PRSV) were applied as the property method. Table 3 summarizes the specifications for the input stream (stream 1).

Under these conditions, all of the streams in the model were in an absolute liquid phase. If the temperature of the input stream was increased, then this increased temperature would affect the temperature distribution across the entire pipeline. Pipe 3 has the lowest pressure for the highest position to compare pipes 1

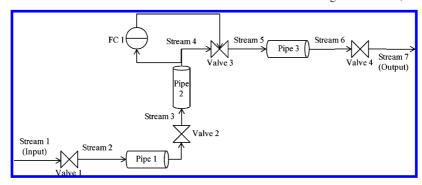


Figure 5. Pipeline model for the case study

Table 1. Specifications of the Pipeline Model for the Case Study

	module	diameter (mm) length	(m)	elevation change (m)
pipe 1	pipe	812.8	5	5	0
pipe 2	pipe	812.8	10)	+10
pipe 3	pipe	812.8	10		0
			$C_{\rm v}$ (USC	GPM)	OP (%)
valve1		valve	10 000		50
valve2		valve	lve 10 000		50
valve3		valve	4	50	controlled
valve4		valve	10 00	00	50
			K _c	T _i (s) SP (kg/h)
FC 1	C	controller	0.01	10	5000

and and, therefore, lowest bubble-point temperature. Therefore, when the temperature was increased and the bubble-point temperature was reached, the LNG would begin to vaporize. Then a rapid increase of the volume of LNG flowing through pipe 3 could lead to unstable simulation results. Following our methodology, if unstable results are detected, the unit module, pipe 3 in this point, would be changed with a more stable unit module. To enhance the stability of the simulation results, we can use an alternative unit module for pipe 3 in which calculations of the heat and holdup are separated, as shown in Figure 7. The pipe 3 module is divided into two parts: in pipe 3', the pressure drop and holdup are calculated, and heater 1 reflects the heat influx. The heat influx through the pipe is

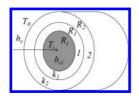


Figure 6. Layered composite pipe with two materials.

Table 2. Specifications of Layers in the Pipe

	no.	material	thickness (mm)	thermal conductivity $(k_n, W/m \cdot K)^{12,13}$
inner wall	1	stainless steel	10	50
outer wall (thermal insulator)	2	polyurethane	100	0.02

Table 3. Specifications of the Input Stream

stream name	stream 1		
pressure (bar)	10		
temperature (°C)	-161		
composition (mol)			
methane	0.95		
ethane	0.04		
nitrogen	0.01		

calculated by means of a general heat-transfer equation for a layered composite cylinder as shown eq 1.14

$$Q = 2\pi dL(T_{\rm i} - T_0) / \left(\frac{1}{R_i h_{\rm ci}} + \frac{\ln(R_1/R_i)}{k_1} + \frac{\ln(R_2/R_1)}{k_2} + \frac{1}{R_2 h_{\rm c}}\right)$$
(1)

The value of R_n , T_n , k_n , and h_c are exported from the simulator, and the heat influx is calculated separately and imported into heater 1. This unit module can give more stable results thanks to separation of the calculations. In the case where this new unit module does not ensure stable results, the unit module could be replaced by a more stable model. Calculation of the holdup could be removed from pipe 3' in order to obtain more stable results. When calculation of the holdup is ignored, the results may become stable, but their accuracy could be lower. An additional time delay calculation could also be needed because the time delay for the holdup volume is removed.

4. Results and Discussion

When the temperature of the input stream would have increased by 1 °C, the temperature would also increase across the entire pipeline and LNG would begin to vaporize. Figure 8a shows the unstable simulation results obtained from the basic model. After 7000 s had elapsed, LNG started to vaporize and simulation results such as the vapor fraction, volume flow rate, and mass flow rate became unstable. After application of our methodology of replacing the unit module, where the sudden change in the vapor fraction was detected, the unit module pipe 3 was replaced with pipe 3' and heater 1. As a result, stable simulation results were obtained, as shown in Figure 8b. In the extreme case where the temperature of the input stream increased by 10 °C, violent oscillatory results were obtained with use of the basic model, as shown in Figure 9a. In this case, it was not enough to get stable results by changing pipe 3 with pipe 3' and heater 1. Therefore, an additional change that ignored the holdup of pipe 3' was applied. As a result, Figure 9b shows stable results obtained for the vapor fraction and volume flow rate. The performance of our methodology is compared in Table 4 with that of basic modeling and concretely fitted modeling.

Additionally, this methodology can be used, in general, for simulations of other process units that can show the oscillatory results from the following reasons: (1) the small holdup volume of the process unit; (2) generation of the two-phase flow of liquid and vapor in the process unit by temperature or pressure changes; (3) the large ratio between the liquid and vapor volumes of the main material in a process unit such as LNG. Then, when the process unit was divided into several unit modules and replaced selectively, the crucial calculations of the

Figure 7. Pipeline model for the case study. The unit module pipe 3 is separated into pipe 3' and heater 1 for stability.

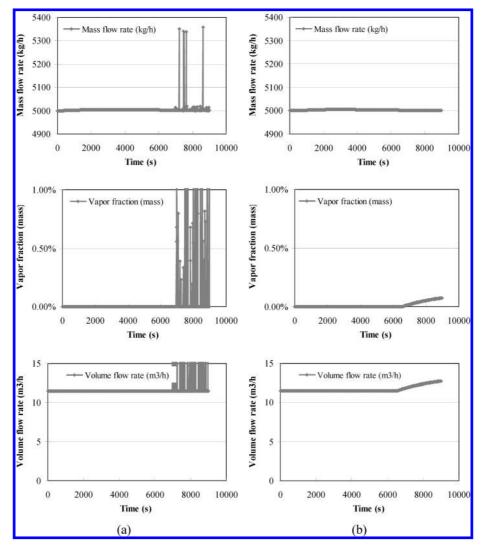


Figure 8. Simulation results of flow rates and the vapor fraction of stream 7 (output) (a) with the basic model and (b) after application of an algorithm, when the temperature of the input stream was increased by 1 °C.

time delay, pressure drop, and heat transfer in the process unit could be separated in each unit module. A more proper unit module will be selected by our algorithm, and more stable results can be obtained.

5. Conclusion

To ensure stable results from the dynamic simulation for a LNG pipeline when the two-phase flow is generated, a methodology for changing the selected unit modules was proposed. It was validated through the case study of a pipeline model, which consisted of three pipes with increasing elevation

of 10 m. After the temperature of the input stream was increased by 1 and 10 °C, the temperature increased across the entire pipeline. In the case where the temperature increased by 1 °C, after 7000 s elapsed, a two-phase flow was generated and the simulation results obtained from the basic model became unstable. However, by applying the suggested methodology with replacement of the unit module for pipe 3, where the unstable results were first obtained, with a more stable unit module consisting of modules pipe 3' and heater 1, we obtained more stable simulation results. In the case where the temperature was increased by 10 °C, the simulation results became violently

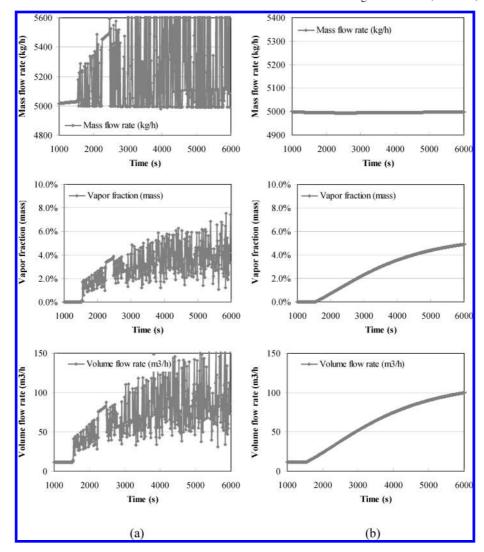


Figure 9. Simulation results of flow rates and the vapor fraction of stream 7 (output) (a) with a basic model and (b) after application of an algorithm, when the temperature of the input stream was increased by 10 °C.

Table 4. Characteristics of the Suggested Methodology When Compared with Others

	convergence	stability	time to build	accuracy
dynamic simulation using basic unit modules	easy	becoming unstable easily	short	low
dynamic simulation using concretely fitted models for specific processes	difficult	stable	very long	high
dynamic simulation applying the methodology of the changing unit module selectively	relatively easy	stable	middle	middle-high (depending on the changed unit module)

oscillatory. However, after application of our methodology, stable results were obtained.

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Nomenclature

NG = natural gas

LNG = liquefied natural gas

 $R_{\rm i} = {\rm inner\ radius\ of\ the\ pipe}$

 R_1 = radius of the pipe including the inner wall

 R_2 = radius of the pipe including the outer wall

 $T_{\rm i} =$ temperature in the pipe

 T_0 = ambient temperature outside of the pipe

 $k_1 = \text{conductive coefficient of material } 1$

 k_2 = conductive coefficient of material 2

 $h_{\rm ci} = {\rm convective} \ {\rm coefficient} \ {\rm at} \ {\rm the} \ {\rm inner} \ {\rm surface}$

 $h_{\rm c} = {\rm convective}$ coefficient at the outer surface

Q = amount of heat through the pipe

Tol = tolerance

M(p) = used model at process p

Unitmodule(k) = used unit module with different stabilities

Vars(p,t) = data set of monitored variables at process p and time step t

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