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## CONSIDERATIONS AND COMPLICATIONS WITH "FIRST PRINCIPLES" DYNAMIC MODELLING OF INDUSTRIAL COMPRESSORS

*Readily available processing hardware and "off-the-shelf" (OTS) simulation software has made "high fidelity" first principles models of both steady and transient states, for both axial and centrifugal industrial compressors, relatively easy to construct. These high-fidelity models are finding their way into "real-time. digital twin" performance monitors, front-end engineering design, and post-design – pre-construction compressor performance evaluation. The compressor models are useful for reliably demonstrating the compressor and – to some degree, based on the complexity of the model – process response to various operating conditions. Once the model is constructed, it is trivial to run a "what-if" analysis of compressor performance to answer questions related to (a) recommendations or validation of the recycle/vent valve size and actuation speed, (b) general piping layout and sizing around the compressor, (c) and hot gas bypass requirements, to name a few. This paper takes a practical approach in discussing the compressor and process parameters necessary for building these dynamic "high-fidelity" industrial-compressor models. We identify compressor inputs and compressor responses that are faithfully modeled by first-principle equations available in the simulation software and those that typically require a compromise between an "ab initio" and data-fitting approximation. We discuss the simulation's tendency to overstate pressure excursions during surge events and understate the compressor operation in the "stonewall" region. We also discuss using the simulator software's compressor-stage enthalpy calculations to predict and quantify the compressor train reverse rotation. We use our broad experience and understanding of the compressor operation and simulation and our experience with the AVEVA™ Dynamic-Simulation "OTS" simulation software as the basis for this discussion.*

**Keywords:** *compressor model; high fidelity; first principles; industrial compressors; dynamic simulation; compressor surge; compressor stonewall; choke flow; steady state; transient; surge event; recycle; vent; reverse rotation.*

### Introduction

Industrial compressors are used throughout energy processing and are an integral part of midstream (pipeline) and downstream (refining, LNG, chemicals) and storage processes. These processes include transportation, refrigeration, separation, and generation of reaction pressure.

The purpose of this paper is to promote further discussion concerning foundational considerations, limitations, and "workarounds" in the modelling of industrial compressor transient operation using off-the-shelf (commercially available), high-fidelity, process simulation software.

### Definitions

#### First-Principles (ab initio) modelling.

First-principles models, in general, are built using established laws of chemistry and physics without additional assumptions, inference, or modifications based upon empirical testing or data fitting. This paper discusses using the first principles equations of state

included in the Dynamic Simulation high fidelity modelling software [1] and the assumptions and inference associated with the compressor data inputs required to make the models work.

#### High Fidelity modelling.

As far as we are aware, there are no absolute criteria for what constitutes "high-fidelity" for industrial compressor modeling. Like most things, there is a diminishing marginal utility for model tuning, and we "overlay" an engineering sensibility to compressor modelling where; "close enough is good enough." We define a compressor model as high-fidelity if it generates temperatures, pressures, and flows that match the compressor manufacturers API617 data sheets or the end-users heat and material balance at a steady-state, within 1.0%.

#### Dynamic Compressor Modelling.

Dynamic compressor models are typically designed to assess compressor operation and performance both from the standpoint of compressor protection (surge and

stonewall), and from a process operations perspective. Compressor models are used to evaluate compressor recycle/vent valve sizing, the recycle/vent valve associated actuator speed of response, compressor piping size and volume, and the design and suitability of the compressor controls. The discussions in this paper are limited to the transient compressor operation viewpoint (as opposed to steady-state, except when constructing the model.) These transient operations typically include startup, trip, and process upsets and failures (e.g., unusual, and rapid process changes that affect compressor discharge pressure) [2].

### Compressor Performance Map.

To evaluate the transient compressor operation, we start with the compressor manufacturer's performance curve. The performance curves typically include multiple speed lines (for variable speed machines or machines with inlet guide vanes), a single-speed line (for constant speed machines), the surge points for the speed lines, a guarantee point, and efficiency curves. In addition, the performance curve also specifies the compressor inlet conditions, inlet feed MW, compressibility, and the specific heat ratio ( $K$ ) or the polytropic efficiency ( $\eta$ ). A performance "curve" is provided for each compressor stage.

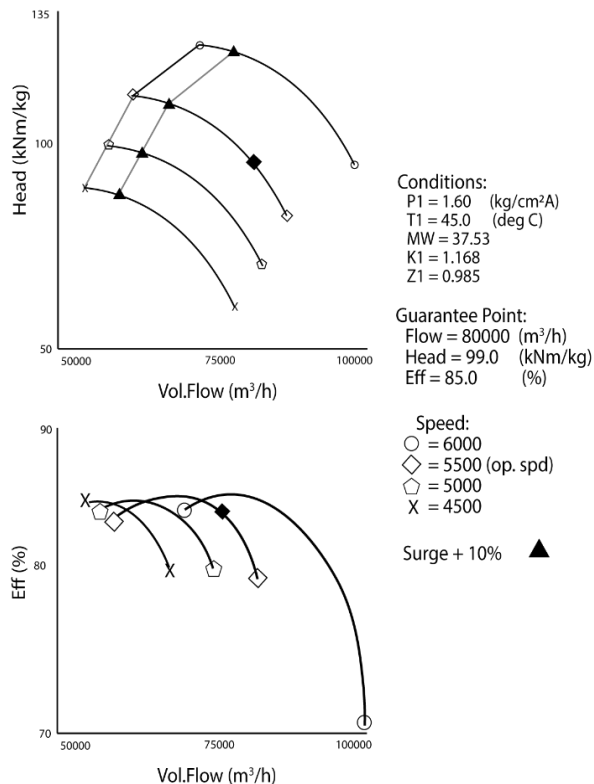


Fig. A. Representation of typical compressor performance curve [3]

### Compressor Surge.

In "Application Guideline for Centrifugal Compressor Surge Control Systems", the surge is defined as "the

operating point at which the compressor peak head capability and minimum flow limit are reached" [2]. Compressor operational excursions to the "left" of the surge line are typically referred to as unstable. These excursions (surge events) are created by abnormally high compressor discharge pressure (head). They can result in compressor flow reversals (which lower the discharge pressure), creating a surge cycle. Surge events can cause severe damage to the compressor, including; bearing failure, impeller rubbing, and seal damage [4].

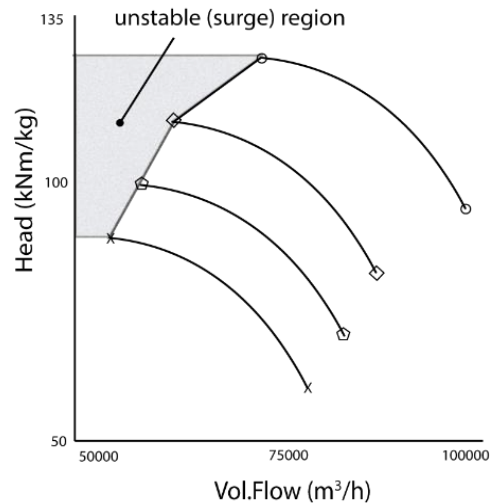


Fig. B. Representation of typical compressor surge "region"

### Compressor Stonewall.

Compressor Stonewall or Choke is an operating condition (low discharge pressure and high flow rate for a given speed line) where the velocity of the gas for a given compressor stage has accelerated to Mach-1, and no further increase in flow is possible [5].

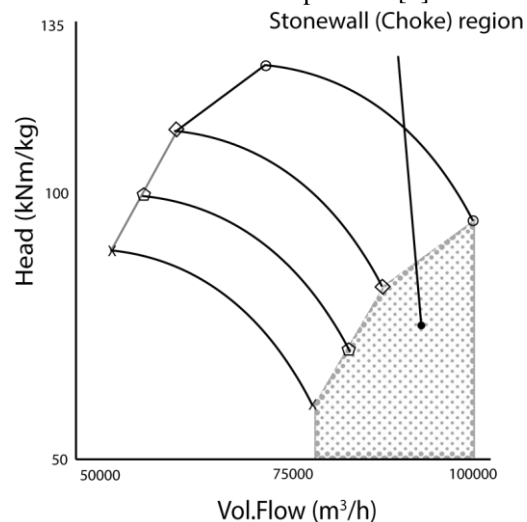


Fig. C. Representation of typical compressor Stonewall or choked flow "region"

Compressor manufacturers have found that prolonged compressor operation in stonewall can lead to fatigue failures of the impeller cover and blades. There is also an increase in the compressor discharge temperature due to the rise in entropy across the region of sonic velocity [5].

## Considerations

### Compressor model data inputs.

To build a credible “high-fidelity” compressor model, the following data is required:

- Driver (motor or turbine data) including power, torque, speed gearing;
- Compressor performance curves – to model compressor characteristics (head/capacity relationship);
- Manufacturers compressor data sheets (API617) – to validate the steady-state model;
- Process heat and material balance (if available)- to validate the steady-state model;
- Process isometric drawings – to determine piping volumes and pressure drops;
- Process and instrumentation drawings (P&ID) – to determine compressor, vessel, and piping arrangement;
- Process flow diagram (PFD) – important compressor, vessel, and piping arrangement;
- Valve data – recycle valves, block valves, control valves, check valves, etc.- to model CV, and valve flow characteristics;
- Valve Actuator data – to model valve speed of response;
- Heat exchanger data – to model heat exchangers (capacity, heat transfer characteristics, flow rates, and temperatures for fluid streams).

### Compressor Model Boundaries.

In general, the compressor model starts at the closest significant volume outside of the recycle loop (vessel, etc.) on the inlet of the compressor. The compressor model typically ends after the first check valve outside of the recycle loop on the discharge side of the compressor. For refrigeration compressor models, it may be necessary to model the discharge condensers and liquid accumulators.

### Equations of State (EOS) Selection.

Modern “off-the-shelf” high fidelity modelling software platforms offer a selection of first-principles equation-of-state simulation selections for use in modelling a compressor. These selections include [1]:

- Industrial Steam Tables;
- Braun K10;
- Redlich-Kwong (RK) ;

- Soave-Redlich-Kwong (SRK) and derivatives;
- Peng- Robinson (PR) and derivatives;
- Others.

The difficulty associated with multiple “EOSs” is deciding and choosing which EOS to use for a given compressor model. When building the compressor model, we typically start with the SRK EOS, and compare parameters for a given steady-state compressor condition (pressure, temperature, flow), with the compressor manufacturers' performance data sheets or the process heat and material balance sheet, or both.

If the model is in close agreement (within 1.0%) of the performance data or material balance, we use that EOS to evaluate transient conditions. If the EOS results in steady-state conditions that differ from the compressor manufacturers performance data sheets or the process heat and material balance sheet by more than 1.0%, we iterate the different available EOSs until we find the “best” EOS fit.

### Modelling Inertia.

For a high-fidelity model, the entire compressor train inertia needs to be considered. Typically, this data is available from the compressor manufacturer. If the data is unavailable, the compressor train inertia can be inferred from operation data (specifically, coast down data).

### Modelling Friction Losses.

Modelling friction losses improves the fidelity of the model characteristics for a shutdown. Friction losses are typically modelled using a small percentage (1...2%) of power (linear relationship). In general, friction losses are determined empirically.

### Modelling Windage Losses.

OTS simulation packages typically have windage loss inputs, but most compressor manufacturers include windage losses in their performance curves.

## Complications

### Compressor feed-gas composition:

Feed-gas composition for ethylene refrigeration, propylene refrigeration, chlorine, compression, and air applications are typically simple, with straightforward chemistry, and can be used directly with the simulator package equations of state. On the other hand, there are feeds, including cracked gas, wet gas, and recycle gas applications, that can be problematic because of the complicated process flow, feed composition, and chemistry.

For example, the cracked gas feed used in an “Ethylene” production process can include more than 40 components (Tabl. 1):

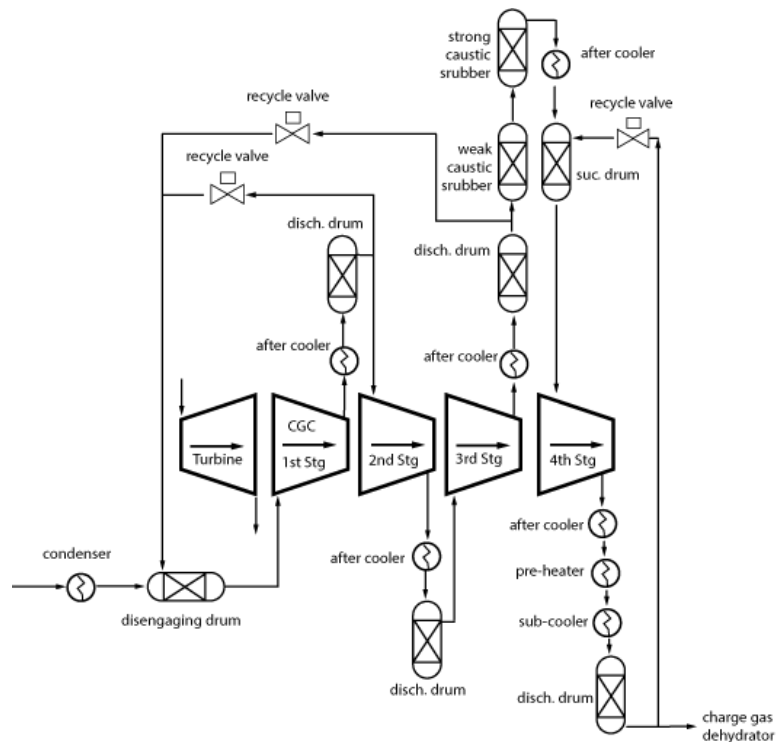


Fig. D. Simplified crack gas process flow diagram (level controls, check valves, flow elements etc. omitted for simplicity)

Table 1

Crack gas feed from 3rd party data analysis  
(CMF = component mole flow (as a percentage of flow))

Component	CMF
H2O	33.556%
ETHYLENE	22.751%
HYDROGEN	21.080%
METHANE	8.474%
ETHANE	8.094%
PROPYLENE	2.422%
N-BUTANE	1.634%
1,3-BUTADIENE	0.465%
PROPANE	0.280%
ACETYLENE	0.261%
BENZENE	0.219%
1-BUTENE	0.138%
C7+	0.133%
CYCLOPENTADIENE	0.072%
1,4-PENTADIENE	0.053%
TOLUENE	0.037%
TRANS-2-BUTENE	0.036%
CARBON-MONOXIDE	0.032%
N-PENTANE	0.032%
CIS-2-BUTENE	0.028%
METHYL-ACETYLENE	0.028%
STYRENE	0.028%
O-XYLENE	0.020%
PROPADIENE	0.019%
VINYLAETYLENE	0.017%
NAPHTHALENE	0.013%
1-PENTENE	0.013%
ISOBUTYLENE	0.010%
N-HEXANE	0.008%
1-PHENYLNAPHTHALENE	0.006%
METHYLCYCLOPENTADIENE	0.006%
1-METHYLINDENE	0.005%

Table 1 (continued)

Component	CMF
1-METHYL-2-ETHYLBENZENE	0.004%
N-OCTADECYLBENZENE	0.004%
INDENE	0.004%
ALPHA-METHYL-STYRENE	0.003%
ETHYLBENZENE	0.003%
CYCLOHEPTENE	0.003%
ISOBUTANE	0.002%
2-METHYL-1,3-BUTADIENE	0.002%
CARBON-DIOXIDE	0.002%
Etc. (4 components less than .002%)	0.001%
100.00%	

Molecular Weight (as given)

19.7

Because of the chemical complexity and variations of this feed and to reduce simulation processing load (calculating performance), the cracked gas feed composition is often simplified. This simplification is accomplished by “lumping” components that are “materially insignificant” individually (less than 0.5% of feed) but added together must be accounted for. This creates a quasi-hybrid model that uses first principles equations of state and data fitting of the feed.

Table 2

Simplified crack gas feed

Component	CMF	MW	MW by %
H2O	33.69%	18.02	6.07
ETHYLENE	22.84%	28.05	6.41
H2	21.17%	2.02	0.43
METHANE	8.51%	16.04	1.36
ETHANE	8.13%	30.07	2.44

Table 2 (continued)

Component	CMF	MW	MW by %
Propylene	2.43%	42.08	1.02
BUTANE	1.64%	58.12	0.95
1,3 Butadiene	0.47%	54.09	0.25
PROPANE	0.28%	44.1	0.12
ACETYLN	0.26%	26.04	0.07
BENZENE	0.22%	78.11	0.17
1BUTENE	0.14%	56.11	0.08
DECANE	0.22%	142.28	0.32
	100.00%	Calc MW	19.70

This lumping of the minor components in the feed can have a minor or significant impact on multi-stage compressor models. As the gas in a multi-stage model passes through the compressor, heat exchangers, etc., the different gas components (with similar mole weights) condense or vaporize at different temperatures and pressure (which the simulation faithfully replicates with the selected EOS), causing the density of the feed gas to change as it travels through the compressor model to successive stages. If the component “lumping” or simplification is done well, the compressor model performance will match the compressor data sheets or process heat and material balance. If the simplification is “off”, the model will not match the compressor data sheets or process heat and material balance.

Choosing a component(s) for a “good” simplification of the minor components in the complex gas fees is most often iterative. It often requires significant experience with the process and model “construction.”

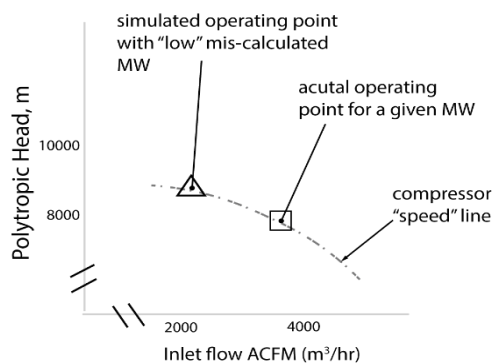


Fig. E. Effect of “low” calculated moleweight on operating point

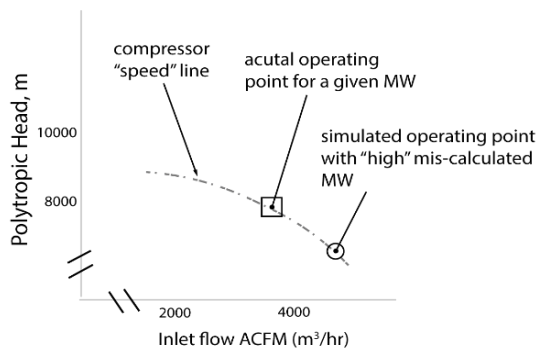


Fig. F. Effect of “high” calculated moleweight on operating point

### Compressor simulation performance to the “left” of the surge line (point).

When a compressor works through a surge event (excessive head), the actual flow quickly decreases towards the y-axis without a further increase in the head. As the compressor flow reverses, the head begins to fall, allowing the flow to increase again (compressor recovers) [6]. As the flow increases, if whatever created the excessively high discharge pressure (head) hasn't resolved, the compressor operating point will move back towards the surge point and create a surge cycle.

When we configure a performance curve into a simulation tool, the left-most data point in the performance curve (high head, low flow) is typically interpreted by the simulator software as the surge point. An issue we face when using the Dynamic-Simulator is that the simulation package interpolates the compressor head to the “left” of the surge point using a linear approximation with a non-zero slope (gradual increase in head to the left of the surge point).

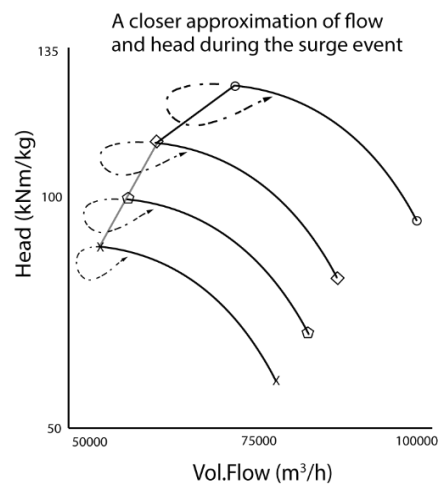


Fig. G. An approximation of “actual” head and flow past the last performance data point (surge point)

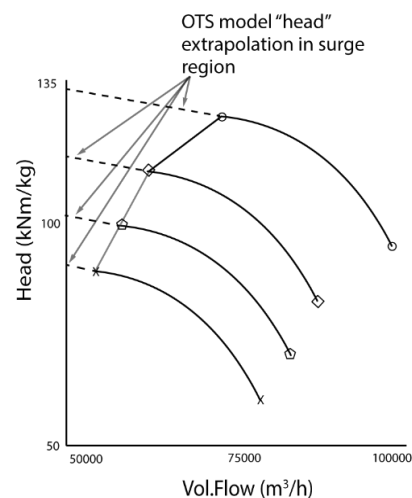


Fig. H. A typical OTS approximation of head past the last performance data point (surge point)

This mis-approximation of a surge event tends to over-state the pressure (head) during the surge event. If the simulation is used to specify or validate the recycle valve size, this over-statement can manifest in selecting an oversized recycle valve.

Our “work-around” for this pressure (head) over-statement is to add a “surge flow simulation valve” in parallel with the compressor. The surge flow simulation valve acts like a recycle valve and reduces the discharge pressure (head) by allowing flow to the suction when the simulated compressor operating point moves to the left of the surge point. The “simulated flow valve” is sized such that it only ameliorates the OTS head interpolation.

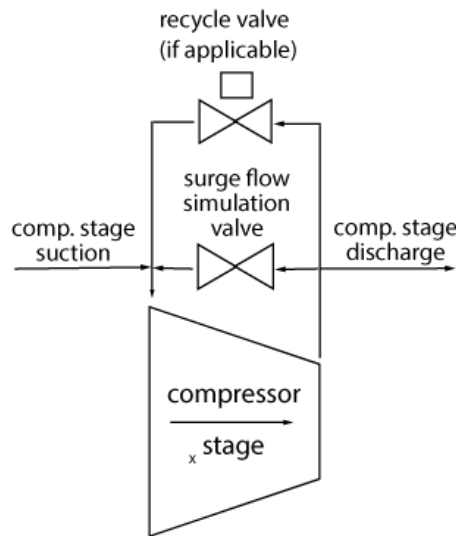


Fig. I. Surge flow simulation valve

### Modelling Compressor Reverse Rotation.

In addition to validating compressor surge and stall points with the compressor model, often, end-users are interested to know the consequences of a failed check valve – especially during compressor shutdown.

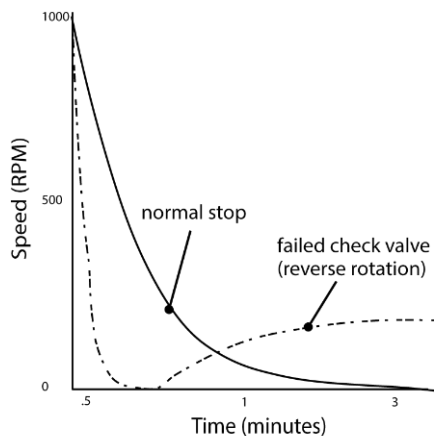


Fig. J. Normal speed decay vs. the speed decay associated with reverse rotation

Specifically, we are interested to know if the compressor can be driven backward (reverse rotation) by a process pressure flowing backward through the compressor discharge (e.g. leaking check valve in the compressor discharge piping, missing check valve, etc.)

The likelihood for compressor train reverse rotation is modelled by first calculating the “energy output” for a given compressor stage:

$$E_{OUTx} = (H_{Dx} - H_{Sx})(\dot{m}),$$

where  $H_{Dx}$  = specific enthalpy at discharge of stage;

$H_{Sx}$  = specific enthalpy at suction of stage;

$\dot{m}$  = mass flow.

Contributed power to the shaft (as a function of reverse flow through the compressor) is then calculated as [7]:

$$P_{RR} = (E_{OUT1} + E_{OUT2} + \dots E_{OUTx})(\text{efficiency}),$$

where efficiency is typically a value between 0.50 and 0.60.

The calculated power – through reverse rotation – is then summed with the “driver power” back into the model to calculate speed.

### Modelling Compressor Stonewall.

The OTS Dynamic Simulation software tends to overestimate compressor flow in the stonewall or “choked flow” region of the compressor performance curve by not asserting an infinite slope on the speed curve when it drops into the stonewall region.

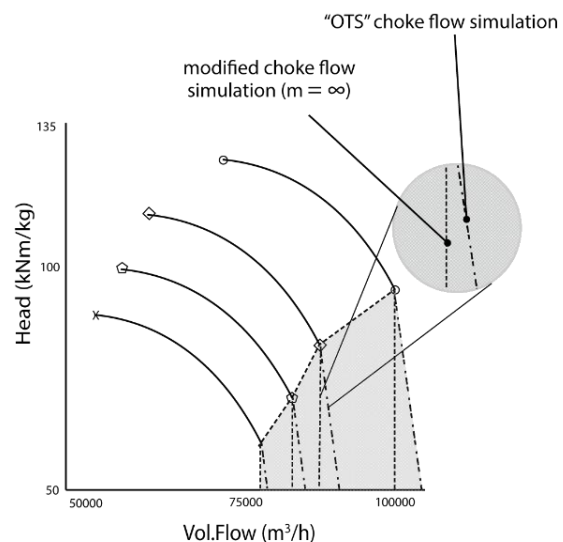


Fig. K. OTS stonewall flow vs. modified stonewall flow

This problem is easily remedied by adding performance curve point vertically from the last point from the manufacturers' compressor curve on the x-axis.



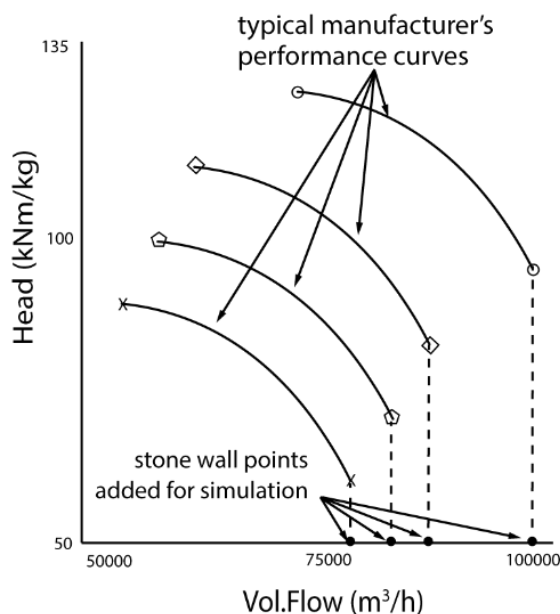


Fig. L. Adding additional performance curve points on the flow-axis to better simulate “compressor stonewall”

### Conclusions/Summary

Modern computer hardware and OTS process simulation software are capable of extremely high fidelity modelling of industrial plant performance. This capability also extends to first-principles modelling of steady-state process compressor performance with simple feeds. Practical modelling of complex feeds – such as the feed associated with the cracked gas compressor – requires manipulation of the input stream to reduce simulator calculation and hardware processing load. Our model needed some “tuning” to credibly simulate the compressor reaction to transient events that tend to drive the compressor towards surge, stonewall, or reverse rotation.

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## СООБРАЖЕНИЯ ПО ПОВОДУ ПРИМЕНЕНИЯ И СЛОЖНОСТИ МОДЕЛЕЙ ПЕРВОГО ПОРЯДКА В ДИНАМИЧЕСКОМ МОДЕЛИРОВАНИИ ПРОМЫШЛЕННЫХ КОМПРЕССОРОВ

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Общедоступное аппаратное обеспечение для обработки данных и готовое программное обеспечение для моделирования позволяет относительно легко создавать «высокоточные» модели первого порядка как для установившихся, так и для переходных состояний как для осевых, так и для центробежных промышленных компрессоров. Эти высокоточные модели находят свое применение в системах мониторинга производительности («цифровых двойниках», работающих в режиме реального времени), на этапе предварительного инженерного проектирования, а также в оценке производительности компрессора после завершения проектирования и перед началом этапа строительства. Модели компрессора полезны для достоверной демонстрации работы компрессора и, в некоторой степени, в зависимости от сложности модели, оценки реакции процесса на различные рабочие условия. После построения модели легко провести анализ производительности компрессора по принципу «что если», чтобы ответить на вопросы, связанные с (а) рекомендациями или проверкой правильности выбора рециркуляционного / выпускного клапана и его скоростью срабатывания, (б) общей компоновкой трубопроводов и обвязкой компрессора, (с) требованиями к байпасу горячего газа, и это лишь некоторые из них. В этой статье используется практический подход к обсуждению компрессора и параметров процесса, необходимых для построения этих, так называемых, «высокоточных» динамических моделей промышленных компрессоров. Мы определяем входные параметры и реакции компрессора, которые точно моделируются с помощью уравнений первого порядка, доступными в готовом программном обеспечении для моделирования, и те параметры, которые обычно требуют компромисса между "ab initio" и данными аппроксимации. Мы обсуждаем тенденцию моделирования к завышению изменений давления во время помпажных событий и занижению работы в области «дресселирования». Мы также обсуждаем использование программами моделирования расчетов энтальпии ступени компрессора для прогнозирования и количественной оценки обратного вращения компрессорного агрегата. Мы используем наш обширный опыт и понимание работы компрессора и моделирования, а также наш опыт работы с программным обеспечением для динамического моделирования AVEVA™ Dynamic Simulation в качестве базы для этого обсуждения.

**Ключевые слова:** модель компрессора; высокая точность; первый порядок; промышленные компрессоры; динамическое моделирование; помпаж компрессора; дросселирование компрессора; поток дросселирования; установившийся режим работы компрессора; переходный режим работы компрессора; событие помпажа; рециркуляционный клапан; выпускной клапан; обратное вращение компрессора.

## МІРКУВАННЯ ЩОДО ЗАСТОСУВАННЯ І СКЛАДНОСТІ МОДЕЛЕЙ ПЕРШОГО ПОРЯДКУ У ДИНАМІЧНОМУ МОДЕЛЮВАННІ ПРОМИСЛОВИХ КОМПРЕСОРІВ

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Загальнодоступне апаратне забезпечення для обробки даних і готове програмне забезпечення для моделювання дозволяє відносно легко створювати «високоточні» моделі першого порядку як для сталих, так і для перехідних станів як для осьових, так і для відцентрових промислових компресорів. Ці високоточні моделі знаходять своє застосування в системах моніторингу продуктивності («цифрових двійників», які працюють в режимі реального часу), на етапі попереднього інженерного проектування, а також в оцінці продуктивності компресора після завершення проектування і перед початком етапу будівництва. Моделі компресора корисні для достовірної демонстрації роботи компресора і, в деякій мірі, в залежності від складності моделі, оцінки реакції процесу на різні робочі умови. Після створення моделі легко провести аналіз продуктивності компресора за принципом «що якщо», щоб відповісти на питання, пов'язані з (а) рекомендаціями або перевіркою правильності вибору рециркуляційного / випускного клапана і його швидкістю спрацьовування, (б) загальним компонованням трубопроводів і обв'язкою компресора, (с) вимог до байпасу гарячого газу, і це лише деякі з них. У цій статті використовується практичний підхід до обговорення компресора і параметрів процесу, необхідних для побудови цих, так званих, «високоточних» динамічних моделей промислових компресорів. Ми визначаємо входні параметри і реакції компресора, які точно моделюються за допомогою рівнянь першого порядку, доступними в готовому програмному



забезпеченні для моделювання, і ті параметри, які зазвичай вимагають компромісу між "ab initio" і даними апроксимації. Ми обговорюємо тенденцію моделювання до завищення змін тиску під час помпажних подій і зниження роботи в області «дроселювання». Ми також обговорюємо використання програмами моделювання розрахунків ентальпії ступені компресора для прогнозування і кількісної оцінки зворотного обертання компресорного агрегату. Ми використовуємо наш великий досвід і розуміння роботи компресора і моделювання, а також наш досвід роботи з програмним забезпеченням для динамічного моделювання AVEVA™ Dynamic-Simulation в якості бази для цього обговорення.

**Ключові слова:** модель компресора; висока точність; перший порядок; промислові компресори; динамічне моделювання; помпаж компресора; дроселювання компресора; потік дроселювання; сталий режим роботи компресора; перехідний режим роботи компресора; подія помпажу; рециркуляційний клапан; випускний клапан; зворотне обертання компресора.

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