# Computer Modeling and Plant-Wide Dynamic Simulation for Industrial Flare Minimization

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Abstract—Flaring emissions during abnormal operating conditions such as plant start-ups, shut-downs, and upsets in chemical process industries (CPI) are usually significant. Flare minimization can help to save raw material and energy for CPI plants, and to improve local environmental sustainability. In this paper, a systematic methodology based on plant-wide dynamic simulation is presented for CPI plant flare minimizations under abnormal operating conditions. Since off-specification emission sources are inevitable during abnormal operating conditions, to significantly reduce flaring emission in a CPI plant, they must be either recycled to the upstream process for online reuse, or stored somewhere temporarily for future reprocessing, when the CPI plant manufacturing returns to stable operation. Thus, the off-spec products could be reused instead of being flared. This can be achieved through the identification of viable design and operational strategies during normal and abnormal operations through plant-wide dynamic scheduling, simulation, and optimization. The proposed study includes three stages of simulation works: (i) developing and validating a steady-state model of a CPI plant; (ii) transiting the obtained steady-state plant model to the dynamic modeling environment; and refining and validating the plant dynamic model; and (iii) developing flare minimization strategies for abnormal operating conditions of a CPI plant via a validated plantwide dynamic model. This cost-effective methodology has two main merits: (i) employing large-scale dynamic modeling and simulations for industrial flare minimization, which involves various unit models for modeling hundreds of CPI plant facilities; (ii) dealing with critical abnormal operating conditions of CPI plants such as plant start-up and shut-down. Two virtual case studies on flare minimizations for start-up operation (over 50% of emission savings) and shut-down operation (over 70% of emission savings) of an ethylene plant have been employed to demonstrate the efficacy of the proposed study.

**Keywords**—Flare minimization, large-scale modeling and simulation, plant shut-down, plant start-up.

#### I. INTRODUCTION

ABNORMAL operations in CPI, such as plant start-ups, shut-downs, and process upsets, usually induce very significant flare emissions. Such Flaring emissions cause tremendous raw material and energy losses to CPI plants as well as adverse local environmental and social impacts. For instance, an ethylene plant with annual ethylene productivity of  $5.4 \times 10^6$  t may flare  $2.3 \times 10^3$  t of ethylene during only one typical start-up, which roughly generates  $7.0 \times 10^3$  t of CO<sub>2</sub>, 3.4

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t of NO<sub>X</sub>, 18.1 t of CO, and 45.4 t of highly reactive VOCs [1]. Thus, Flare emissions should be minimized if at any possibilities. Nowadays, CPI has set up flare minimization (FM) as a goal in daily routine operations. Unfortunately, current practices in FM almost exclusively depend on industrial experience and the "end-of-the-pipe" control strategies. For instance, the installation of flare gas recovery units (FGRU) can capture flare gas for recycle and reuse. However, this is not enough for CPI because of increasingly strict environmental regulations and economic competition. Moreover, this is less desirable because the capital expenditure and operating cost of FGRU is considerable.

In recent years, some studies have employed dynamic simulations to virtually study the plant operating feasibility [2], [3], operating risks [4], [5], as well as material and energy consumptions [6] according to the operating procedures that would be taken by the plant operating personnel. The simulation results could also be utilized to further refine their operating procedures. The focal point is to renovate current process designs and/or improve process operational strategies in a systematic and cost-effective way, so as to proactively and economically reduce emission sources instead of traditional "end-of-the-pipe" flare handling.

This paper presents a general systematic methodology for CPI plant FMs under abnormal operating conditions. It employs large-scale dynamic simulations to help examine and optimize FM operating strategies associated with CPI plant renovations on process design and operations. The proposed study couples two main merits: (i) it employs large-scale (plant-wide) dynamic modeling and simulations for CPI FMs, which involves hundreds of CPI plant facilities; (ii) it deals with critical abnormal operating conditions of CPI plants such as plant start-ups, shut-downs, and upsets. The effectiveness of the developed methodology has been demonstrated by two virtual case studies on FMs of an ethylene plant, where both start-up and shut-down FMs have resulted in significant emission reductions.

#### II. METHODOLOGY

To conduct the plant-wide dynamic simulations for FM under abnormal operating conditions, a systematic modeling methodology framework has been developed as shown in Fig. 1. It contains three major stages of work: (i) developing and validating the plant-wide steady-state simulation (SS) model of a CPI plant; (ii) based on the SS model, developing and validating the plant-wide dynamic simulation (DS) model; and (iii) developing FM strategies for abnormal operating conditions of a CPI plant via a validated plant-wide DS model.

To support SS and DS modeling, various supporting information should be integrated, such as plant design data, process flow diagram (PFD), piping and instrument diagram (P&ID), DCS (distributed control system) historian, equipment sizing data, control parameters, and industrial expertise. The developed methodology is a general methodology that could apply to complex normal and abnormal operating conditions of various CPI processes. Noted that plant DCS data, different from PFD and P&ID data, is usually not in mass balance. Thus, data validation is required before model tuning process.

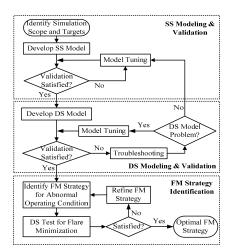


Fig. 1 Flaring minimization via dynamic simulation

It should also be noted that industrial expertise is important and the plant operating group has to be involved in this methodology framework. Thus, the general project working procedure is that the original FM ideas or operating procedures proposed by the plant operating group are virtually run by the dynamic simulation model. After that, the simulation results are presented in a meeting with the operating group. If the operating group is not confident with the result, changes or modifications of the FM operating

procedures will be jointly proposed by both operating and simulation groups. Next, the simulation group will run the new procedures and the new results will be presented to the operating group again. Such working procedure will continue until the plant operating group is satisfied with all simulation results. Through this procedure, extensive and critical information of operating trends and conditions, control parameters, safety and economic concerns are retrieved from the simulation results to help the operating group FM operation during the plant abnormal operation conditions.

#### III. CASE STUDIES

#### A. Introduction of the Studied Ethylene Plant

The proposed methodology has been employed for the virtual study of start-up and shut-down FMs for an ethylene plant. Fig. 2 shows the sketch of the studied ethylene plant. Generally, it starts from five furnaces to crack raw feeds to supply the charge gas. After oil and water quench operations, the charge gas will be sent to a charge gas compressor (CGC) to increase pressure and remove heavy oils, water, sour gases, and arsines in first three compression stages. The compressed charge gas passes through the higher-pressure depropanizer (HP-DeC3), lower-pressure DeC3 (LP-DeC3), the fourth stage of CGC, and C2 converter to split the C3s and lighter components from the charge gas. After that, heavier components from the bottom outlet of LP-DeC3 are sequentially sent to debutanizer (DeC4) and depentanizer (DeC5) to separate products of C4s, C5s, and C6+, respectively. Meanwhile, C3s and lighter components from C2 converter will be directed to the chilling train, demethanizer (DeC1) stripper, and DeC1, respectively, to further separate light products of hydrogen and methane. In the downstream recovery system, the leftover charge gas will go through two deethanizers (DeC2s), C2 splitter, and C3 splitter to recover ethylene (C<sub>2</sub>H<sub>4</sub>), ethane (C<sub>2</sub>H<sub>6</sub>), propylene (C<sub>3</sub>H<sub>6</sub>), and propane (C<sub>3</sub>H<sub>8</sub>), respectively.

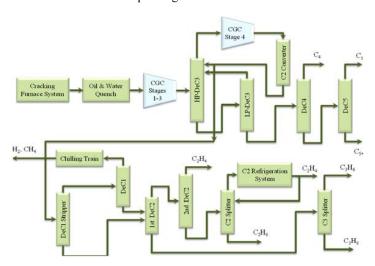


Fig. 2 Sketch of the studied ethylene plant

#### B. Plant-Wide Modeling and Validation

According to the proposed methodology, SS and DS models have to be developed and validated first. To validate the SS model, the plant design data is employed. The SS results should match the design data within 5% of prediction errors. When the plant-wide SS is satisfied, the validated SS model is then transferred to the DS modelling environment. Three types of information must be involved to support such model transition [3]: (i) equipment dimension data, which provides the process unit capacity information; (ii) control strategy and controller parameters, which provide process control information; (iii) process and equipment heat-transfer methods, which provide the thermodynamic information. The plant-wide DS model requires detailed great efforts for model tuning. Generally, the success of the DS validation should make the timing. The amplitude of the DS responses should match real DCS historian results. As an example, Fig. 3 gives the satisfied DS validation result for the bottom temperature of C2 Splitter.

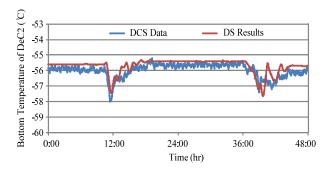


Fig. 3 DS validation result for the bottom temperature of C2 Splitter.

## C. FM for Plant Start-Up

During previous plant start-up operations, cracking furnaces were always started first for some time to prepare enough charge gas to start the CGC. Later on, the compressed charge gas will be directed to downstream units to start all the left units sequentially. Such step-by-step start-up procedure wastes lots of time to warm up and to start each unit and thus generates tremendous flare emissions during each of such waiting periods. To reduce the start-up flaring, the plant has to warm up the downstream process first. This could be accomplished by setting up recycle streams through starting CGC first. It will make the downstream units running close to normal operating status before the cracked charge gas is supplied by all cracking furnaces. Therefore, three cracking furnaces will start later. It will wait until the warm-up of CGC and downstream is ready.

Based on the above idea, three pipelines will be added into the original process as indicated in Fig. 4, which include recycle lines from: (i) LP-DeC3 top; (ii) the C3 splitter top; and (iii) DeC2 top to the CGC. The proposed start-up operating strategy included three major steps:

 Setup self-recycles for ethylene splitter and refrigeration sub-system, DeC2 sub-system, C3 splitter sub-system, and LP-DeC3 tower. These operations will warm up each

- associated sub-system and get ready for building up a larger recycle system.
- 2) Start CGC with the recycled feeds from tops of LP-DeC3, C3 splitter, and DeC2. In the meantime, two cracking furnaces will start, their cracked gas plus the natural gas feed line will supply the CGC as well. All these feeds to the CGC will be adequate to start CGC safely. Once the CGC has started safely, downstream recycle flowrate could gradually reduce to zero.
- 3) Start the third furnace and stabilize the HP-DeC3 and LP-DeC3. Then, start and stabilize DeC4 and DeC5, as well as stabilize DeC1, Chilling Train, and DeC2 sub-system until C2 splitter and C3 splitter could accept qualified feeds.
- Start the fourth furnace and stabilize the entire plant operations. After that, start the last furnace.

The proposed start-up FM plan is to start up the cracking furnaces first and keep the CGC running for some time. During this CGC running period, its feed will be supplied by the downstream recycles from different units through the newly added recycle lines connected to the CGC. Since CGC is still running during the recycling period, it will keep pushing downstream vapors passing through HP-DeC3, DeC1, and chilling train to the CGC, and then send those recycled gas to another ethylene plant through the existing pipeline system.

Based on the DS virtual test of the developed start-up FM strategy, the total flaring amount is 149.4 t, which consists of 41.4 t flaring for real gas displacement for nitrogen and 108 t flaring to stabilize HP-DeC3. Compared with the average start-up flaring amount of 333.0 t based on the plant historical statistics, the overall FM is over 50%. Therefore, the identified start-up FM strategy has great potentials on economic and environmental benefits.

# D.FM for Plant Shut-Down

During previous plant shut-down operations, CGC was always shut down prior to cracking furnaces, so that the leftover vapor and liquid inventory in the downstream units/processes had no chance to be recovered and had to be flared. To reduce shut-down flaring, the plant has to recycle the vapor and liquid inventories as much as possible. Thus, five pipelines are added into the original process as indicated in Fig. 5, which include four recycle lines from: (i) LP-DeC3 top; (ii) propylene refrigerant system; (iii) the C3 splitter top; and (iv) DeC2 top to the CGC inlet; as well as (v) a crossplant pipeline directing methane and hydrogen streams from the chilling train to the CGC inlet of another ethylene plant. The proposed shut-down FM plan is to shut down the cracking furnaces first and keep the CGC running for some time. During this CGC running time period, its feed will be supplied by the downstream recycles from different units through the newly added recycle lines connected to the CGC inlet. Since CGC is still running during the recycling time period, it will keep pushing downstream vapors passing through HP-DeC3, DeC1, and chilling train to the CGC inlet, and then send those recycled gases to another ethylene plant through the existing

## pipeline system.

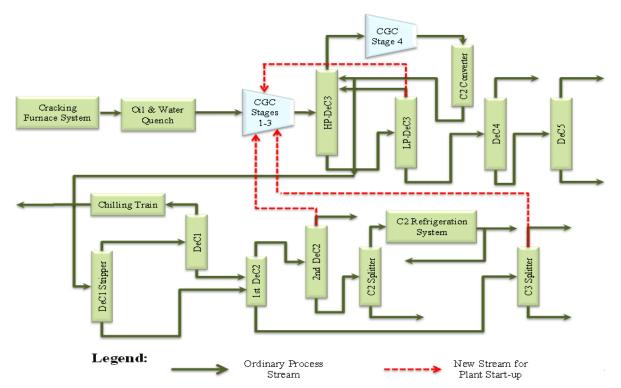


Fig. 4 Sketch of the design retrofit for plant start-up FM

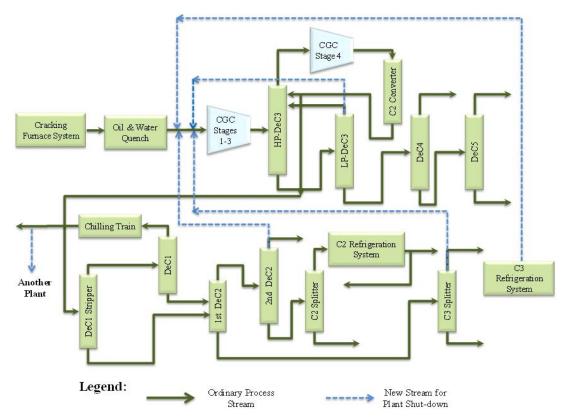


Fig. 5 Sketch of the design retrofit for plant shut-down FM [7]

As discussed in [7], a proposed shut-down procedure included three operation steps:

- Reduce the cracking feed flowrate and downstream liquid inventories. This can be accomplished by shutting down two cracking furnaces and keeping the other three furnaces running at 80% of their capacity. This deinventory operation is adopted from the plant's historical shut-down procedure and its purpose is to get ready for plant shut-down.
- 2) Start recycles while keeping CGC running at its low capacity. Meanwhile, shut down the left three cracking furnaces gradually. For safety consideration, start to feed natural gas to the CGC inlet to ensure the safe operation of CGC. During this period, keep re-boiler works for recycle associated towers and shut down condensers and cooling exchangers to promote the evaporation in each of the columns and drums.
- 3) When the total flowrate at the CGC inlet is not enough to safely sustain the compressor running, the CGC and the natural gas feed will be shut down. After that, nitrogen can be injected into the process system to purge all of the leftover vapors or liquids to the flare system as the routine shut-down and maintenance procedure.

Note that during the CGC running time period, a vapor stream from the propylene refrigerant will also join the recycle to the CGC inlet; meanwhile, the vapor stream from the ethylene refrigerant already has recycle lines connected to the CGC section. Thus, the majority of ethylene and propylene refrigerants can also be recovered. To recover the downstream leftovers through vapor flows, corresponding column reboilers will continue running, while condensers will be gradually shut off, so that liquids can be evaporated for recovery as much as possible.

Based on the DS test of the developed shut-down FM strategy, the total vapor and liquid residues left in all of major drums, exchangers, and towers after operational are 23.4 t, 4.1 t, and 12.2 t, respectively. Their summation is roughly equal to the total flaring amount of 39.7 t. Compared with the average shut-down flaring amount of 147.0 t based on the plant historical statistics, the overall FM is over 70%. Considerably, if the FM strategy can be successfully implemented, the identified shut-down FM strategy will generate significant economic, environmental, and societal benefits.

# IV. CONCLUSION

This paper presented a general methodology based on plant-wide dynamic simulations for CPI plant FMs under abnormal operating conditions. This cost-effective and systematic methodology couples the design and operating renovation for emission source recycling and reuse together with large-scale dynamic modeling and simulations. It could handle FM issues with critical abnormal operating conditions such as CUP plant start-up and shut-down. Two case studies about FMs for an ethylene plant have been performed: the plant start-up case has saved over 50% of flare emissions, while the plant shut-down case has saved over 70% of emission reductions.

Finally, it should be noted that this paper provides

preliminary studies for CPI FMs. All of the ideas and results listed in the paper are based on plant-wide dynamic simulation virtual tests for a particular ethylene plant, which should be treated as preliminary and subject to a variety of risks, uncertainties, and assumptions.

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