Increase Productivity by Integrating LIMS and EZChrom Elite - a case study

Lane Ohlemeier
Sr. Technologist
Lyondell Chemical Company, a LyondellBasell company
Informatics User Meeting Houston – June 19, 2008
Joining forces to create a new global leader

- Lyondell Chemical Company and Basell merged to form LyondellBasell Industries on Dec. 20, 2007
- LyondellBasell is…
  - One of the world’s largest polymers, petrochemicals, and fuels companies with combined annual revenues of $44.7 billion*
  - The global leader in polyolefins technology, production and marketing
  - A pioneer in propylene oxide and derivatives
  - A significant producer of fuels and refined products, including biofuels
  - Operator of one of North America’s largest full-conversion refineries

*2007 pro forma combined revenues.
Fast facts

- Four business areas: Polymers, Chemicals, Fuels and Technology
- Delivers exceptional customer value across petrochemical chain
  - Vertically integrated facilities
  - Broad product portfolio
  - Manufacturing flexibility
  - Superior technology base
  - Operational excellence
Chemical industry landscape has changed

- With annual revenues of nearly $45 billion:
  - Larger than Canon, Disney, Intel, Mitsubishi Electric and Volvo
  - Sales exceed those of DuPont and Bayer
  - Only BASF and Dow are larger
More than 16,000 people worldwide
Our leadership

- Volker Trautz – Chief Executive Officer
- Morris Gelb – Executive Vice President, Office of the CEO
- Alan Bigman – Executive Vice President and Chief Financial Officer
- Anton de Vries – President, Polymers Division
- Ed Dineen – President, Chemicals Division
- Norm Phillips – President, Fuels Division
- Bart de Jong – Senior Vice President, Human Resources
- Cees Los – Senior Vice President and General Counsel
Product diversity and vertical integration

Wellhead

Refining

Olefins

Olefin Derivatives

2nd Level Derivatives

LyondellBasell and affiliates

Crude

Natural Gas Liquids

Refining

Fuels Aromatics

Olefin Crackers

Olefins

Polyethylene

Polypropylene

Styrene

Catalloy Process Resins

Propylene Oxide

Acetys

Ethylene Oxide

Polybutene-1

Advanced Compounds

Glycols Glycol Ethers Butanediol

Glycols Glycol Ethers
Product breadth and diverse markets

- LyondellBasell products are basic elements used to make products that people depend on every day

Diverse end markets

- Refining & Fuels
- Building & Construction
- Transportation
- Textiles & Furnishings
- Packaging
- Consumer
- Other

*Estimate based on revenue*
Global Capacity Positions

- #1 Global – Polyolefins and Polypropylene Compounding
- #1 Global – Propylene Oxide
- #1 Global – Polyolefin Licensing
- #1 Global – Polypropylene Catalysts
- #1 Global – Polypropylene
- #3 Global – Polyethylene
- #2 Global – Oxygenated Fuels
- #2 Global – Propylene Glycol & Propylene Glycol Ethers
- #5 Global – Light Olefins (Ethylene & Propylene)
- Refining Capacity – 373,000 barrels per day
Laboratory operations

- High level operation
  - Receive sample
    - Acknowledge / Create in LIMS
    - Add / Remove tests
  - Testing
    - Instrument
    - Gravimetric
    - Etc.
  - Report
    - Data Entry
    - Release
Sample submission – manual process

- Launch Application
Sample submission – manual process

- Open instrument
  - Authentication required
  - Project selection required
Sample submission – manual process

• Initiate Data Acquisition.
Sample submission – manual process

- Required information/knowledge
  - Sample ID
  - Method
  - Data path
  - Data filename
  - Sample Amount
  - ISTD Amount
  - Multipliers
  - Divisors
  - Vial number
  - Volume
  - Description
  - Print Option
- Defaults may / may not be correct
- Can always edit values
- Prone to ‘typos’
Sample submission – manual process

- Post Acquisition
Data entry – manual process

- Report
  - View on screen
  - Print
  - Printing may require additional steps if ‘automatic’ printing not selected when sample was submitted
Data entry – manual process

- **Data Entry**
  - Must locate / navigate to entry screen in LIMS
  - Hard copy generally needed to facilitate data entry
  - After data is entered, changes must be saved
Sample statistics

- Amongst all LBI laboratories running chromatographic analysis via EZChrom Elite and LabVantage Sapphire LIMS
- ~27,000 samples/mo
- ~450,000 data points
- Average 16 points / sample
Sample submission – manual process

• ~ 1.5 minute to:
  – Launch EZChrom Elite
  – Log into instrument
  – Open Single run dialog
  – Enter required information
  – Start
• Translates to
  \[
  \frac{1.5 \text{ Minutes}}{\text{sample}} \times \frac{27,000 \text{ Sample}}{\text{Month}} = 8100 \text{ hours / year}
  \]
• Equals 3.9 years of labor for sample submission
Data entry – manual process statistics

- ~ 1 minute for 16 data points
- Translates to 27,000 min/yr.
  - 450 hours / month
  - 5400 hours / year
  - ~ 2.5 years of labor
Sample submission + data entry

• Total time expenditure of sample submission and data entry
  – Approximately 6.4 years of labor
• Over a normal shift
  – Repetitive
  – Prone to errors (typos)
• What can be done?
Automation

Let the computers do the heavy lifting
Automation capabilities

• What can it do for me?
• Sample Submission
  – Store predetermined configurations.
    • Instrument/Project/Method/Factors/volumes/etc
  – Build filenames in a uniform manner
    • SxID + Desc + date stamp + nnnn.dat
  – Pre-populate fields
    • SxID
    • Description
    • Etc
  – Reduces input errors
  – Decreases setup time
Automation capabilities

• What can it do for me?
• Data Entry
  – Upon completion of data acquisition, automatically transfer and populate data fields in LIMS
  – Reduces data entry labor to ZERO
  – Reduces data entry errors
    • Transposed numbers
    • Decimal place errors
Automation – how do you do it?

• Requirements – High Level
  – Means of holding preconfigured settings
    • Leverage the database in LIMS
  – Means of presenting configuration options to end users for selection
    • Web pages inherent to the LIMS
      – Zero footprint
  – Handoff of user settings from LIMS to CDS
  – Mechanism for data transfer from CDS back to LIMS
LIMS configuration

- In the LIMS - Super Users correlate Instruments with:
  - Method
  - Detector
  - Factors
    - Edit flag
  - Test (LIMS)
  - Project
  - Misc.
- Information stored in DB
EZChrom configuration

- To facilitate the automatic transfer back to the LIMS. A custom parameter running a VBScript file is employed in each method.
Automation interface – user experience

- User navigates to “Backlog” page
- Samples designated as “EZChrom” samples show with an instrument icon
Automation interface – user experience

- Select samples for analysis
- Click “EZChrom Setup”
Automation interface – user experience

- User is presented with:
  - Sample point and description
  - Sample ID
  - Scheduled Date
  - Preconfigured combinations
    - Test
    - Instrument
    - Method
    - Factors
    - Amounts
  - May / May not be editable
Automation interface – user experience

- Editable values
  - Shown as a typical hyperlink
Automation interface – user experience

- Out of service instruments
  - Shown in red
  - May be due to:
    - Out of calibration
    - Hardware issues
    - Etc.
Automation interface – user experience

- When selection is complete, user selects “Show Instrument View”
- All selections will be displayed in a table view grouped by instrument
- All information required for the run is in the page; however, only enough information is shown to identify the sample
Automation interface – user experience

- Some configuration available at this point
- User can click and drag samples to change order of injection
- Print allows for the “custom report” to automatically print at the completion of data acquisition (optional)
- Credentials entered only once for all instruments
- This can be ‘canceled’ and user will be returned to prior screen if modifications are needed. Prior selections will be retained
Automation interface – user experience

- When user is satisfied with selections, samples are submitted
- New window opens showing status of submissions
Automation interface – user experience

- A status bar displays the % of completion
- A message specific to each instrument is displayed
Automation interface – user experience

- After all processing is complete, user will see status of all submissions.
Automation – what did we accomplish?

- Labor Savings
  - Starting Instruments
    - ~50% reduction in time
  - Data Entry
    - 100% reduction
  - Total Savings
    - ~ 4.45 years labor!

- Data integrity
  - LIMS value matches instrument output
    - Does not guarantee ‘good’ data
  - Setup misconfiguration
    - Greatly reduced
    - Sample tested on wrong instrument
Acknowledgements

- Agilent
- LyondellBasell Laboratory Staff
- LyondellBasell Information Technology Organization
Thank you for your attention