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Integrating Weighing into Your Sample Management Using Titian's Mosaic Weighing Application

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INTRODUCTION

When investing in sample management software one important requirement is direct instrument integration in order to reduce the need for manual processing, which is a common source of errors. A good example of this is the physical weighing of samples, because feedback on the actual amount weighed is vital for stock control as well as the accuracy of downstream processes.

BENEFITS OF USING A WEIGHING APPLICATION

People tend to think of "weighing" as a simple, straightforward process and envision all samples being free-flowing powders. However, the weighing of biotechnology samples can be anything but simple. After addressing environmental factors to ensure a scale will weigh accurately, there are also process factors to consider. When everything is going smoothly, the process of weighing out samples can be well-defined and managed, but it can range from a few samples a day in a small biotechnology company to thousands of samples in a dedicated CRO, which creates challenges of its own.

Even a simple weighing process has a range of decisions that need to be made and questions to be answered. For example:

- What vial type does this particular order require?
- Should I check-weigh the vial?
- Does it need labelling?

These quickly become complicated if something unexpected happens – the powder you're expecting to weigh out is a gum, the sample bottle is cracked, or the bottle barcode can't be read. There a vast number of scenarios that could arise which, if handled differently each time, will introduce variations into the weighing results.

Titian's dedicated Mosaic Weighing and Receipt application, usually shortened to Mosaic Weighing, is part of the Mosaic sample management software suite. The Weighing application provides a consistent, streamlined weighing process which guides the

operator through each action, avoiding variations, as well as allowing them to mitigate problems and carry on.

BENEFITS OF INTEGRATING ANALYTICAL BALANCES WITH YOUR MOSAIC SOFTWARE

For a long time now modern analytical balances, such as those from Mettler Toledo or Sartorius, have had bi-directional communications interfaces built in. This means that accurate weighing data can be captured automatically, improving the accuracy of the overall process and avoiding manually entering data displayed on the balance, which is both error prone and time consuming.

In house solutions to automatically capturing weighing readings into spreadsheets have become outmoded because getting the data is usually only the start of further processing, such as: updating stock information, recording the sample container, or perhaps printing a label. A spreadsheet will need either more programming or manual processing to achieve these steps.

Experienced sample management operators can often work around process problems – such as the sample being a gum rather than a powder – but the solution may entail manual updates to any in house system, with the accompanying risk of introducing errors.

The Mosaic Weighing application removes the need to keep enhancing your in house system or applying work-arounds as you encounter exceptions to the default weighing process. It integrates a range of balances with Mosaic's end-to-end sample tracking and inventory management, guiding the operator through the process and while seamlessly updating inventory and recording actions into its validated workflow.

The Mosaic Weighing application ensures:

- Operators don't need to manually enter weighing information, saving time and eliminating data transfer errors
- Process variations are avoided by providing operator instructions on the weigh and dispense to be performed

- Operators don't need to calculate how much to dispense, and can see at a glance when the correct amount has been dispensed
- If something unexpected happens, clear and consistent methods to proceed are provided for the operator
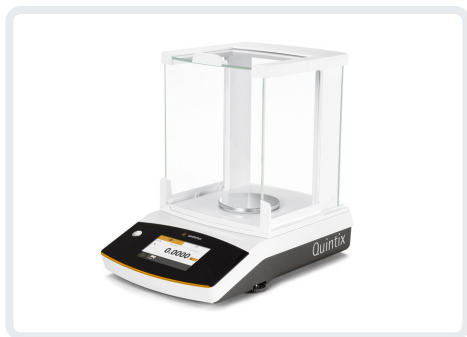- A complete audit trail of dispenses is available for every vial

In addition, using Mosaic Weighing means operators:

- Are prompted to check-weigh, to ensure accurate stock
- Can easily add a batch of clean pre-tared empty source vials received from a manufacturer, using Bulk Import
- Can tare-weigh one or more new clean empty source vials
- Can control who can do which operations, if required, via user permissions

COMPATIBLE BALANCES

The Mosaic Weighing application is compatible with a wide range of Mettler-Toledo and Sartorius balances. Whilst not every balance model has been individually tested, all of the following are suitable:

- any Mettler-Toledo balance supporting MT-SICS level 2 (Standard Interface Command Set)
- any Sartorius balance that supports the SBI protocol (Sartorius Balance Interface), including the Sartorius Cubis MSE and Cubis MSA ranges
- any balance that can be set to SICS mode

If you wish to check a specific model please contact Titian Software.

SUPPORTED OPERATIONS

Mosaic's Weighing application manages a variety of different scenarios to ensure an efficient weighing process. These include:

- Ad-hoc dispense from a stock vial
- Source vial is damaged
- Dispense from a stock vial for orders
- Managing operator permissions
- Dispensing gums
- Reducing contamination
- Multiple weighings from the same vial
- Receiving a pre-tared vial into inventory
- Not enough sample
- Check-weighing a stock vial
- Using an offline balance

Ad-hoc dispense from a stock vial

Perhaps the simplest example of weighing is an ad-hoc dispense. For example, a chemist might want one sample for an intermediate in their synthesis, or a new stock bottle needs to be created for an automated store from a larger manual store bottle. In both cases a Mosaic order could be placed, but that might seem overkill for these single actions.

The Mosaic Weighing application allows an operator to dispense some sample from a vial that is not requested by an order using an ad-hoc dispense. The Weighing application guides the operator through the steps required while updating the inventory in real time.
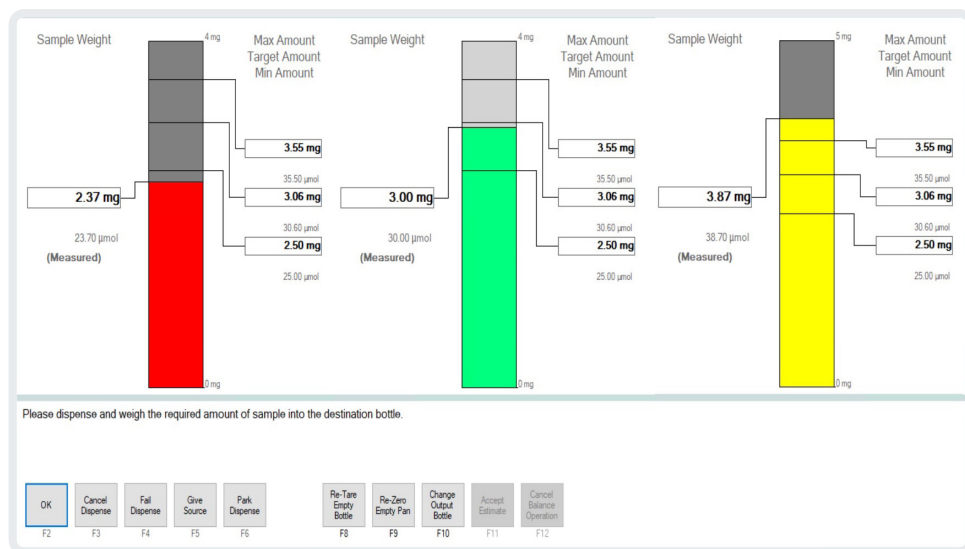
Dispense from a stock vial in response to orders

There are a wide range of variables possible for a dispense so we give two example cases below:

Example 1: A scientist requests 3.00 mg of each sample.

In practice it is extremely difficult to weigh out the exact amount and so the Mosaic Weighing application calculates an acceptable range to ensure the amount weighed is neither too low to be able to complete the required process, nor too high as to waste precious compound.

Modified screenshot of the Weighing application to display under/acceptable/over dispenses. (In practice, only the one bar is displayed).

The application guides the operator through the weighing process, capturing the actual mass transferred, instructing them on which destination vial to use, printing the appropriate label (if required) and identifying where to place the destination vial to complete the order process.

Example 2: A scientist wants to make a solution from neat, for 1.00 ml of a 10 mM solution. This needs a different amount to be weighed for each sample.

Because the Mosaic software already knows the molecular weight of each sample, it automatically calculates the amounts required. In addition, since the order is part of a validated workflow, Mosaic is also able to calculate the minimum amount required to satisfy any subsequent steps and the maximum amount so as not to overflow the destination vial.

The Mosaic Weighing application guides the operator through the process, capturing the actual mass transferred, and instructing them to place the destination vial in a rack ready to be solubilised in the next step of the process.

Dispensing gums

Not all samples to be weighed are free-flowing powers. Once the samples are picked from storage, the operator may find that one or more of them are gums. A number of options are available to handle such cases:

1. It might be possible to transfer a neat sample, however the control on how much sample is transferred is greatly reduced. This makes it more difficult to obtain a dispense within the ideal range. The operator can accept an over weighting (probably more likely) or under weighting in order to complete the process.

   However, this option may be wasteful of the sample as a significant amount is likely to stick to the spatula used for the transfer, making the following two options more favourable

2. If the amount in the stock vial is close to the maximum dispense amount, then the operator can choose to give out the whole source vial instead of dispensing from it. Since it is unlikely the source vial will be returned this only tends to be used when there is a relatively small amount of stock remaining

3. The Weighing application supports the dispense as a Volatile Solvent Transfer which is probably the most versatile option as it doesn't waste material and retains the maximum amount of stock. Titian's Mosaic Liquid Handler integration allows you to transfer the work from Weighing and will automatically handle the solubilisation and transfer volumes for you.

   When complete, you can mark the sample(s) as being dried down within Weighing and optionally perform a check-weigh in order to complete the process.

Multiple weighings from the same stock vial

The operator is weighing out a sample and they notice that the Mosaic Weighing application says there are two weighings requested for the sample (or maybe more). How should they proceed?

Perform Dispense	Finish With Bottle	Ad Hoc Check Weigh	Ad Hoc Dispense	Edit	Fail All Work	Place Bottle	Delete Bottle	Calculate Tare	Reprint Label	>>>
F2	F3	F4	F5	F6	F7	F8	F9	F10	F11	F12

Choose an action to perform on bottle 'RM0000000001'.

There are 2 scheduled operations for this bottle.

One scenario is that the order that they are processing requires two dispenses per source, in which case they would continue with the second dispense.

However, it is more likely that the second dispense is for another order. It is inefficient to return the source vial to store only to be picked out again, although that can be done. Two other options are possible:

1. The Weighing application will allow you to work on multiple orders at the same time, which is particularly useful where orders have overlapping sources. It is more efficient as it avoids multiple pick and placing operations, and means the operator only has to de-cap the source vial once.

2. Having completed one dispense, you transfer the source bottle to a new rack ready to be to be processed as part of the other order at a later time.

Screenshot showing the placement of a tube into a rack. A1 is the default location although any other free location can be selected and used. In all these scenarios the Weighing application will guide the operator through the required steps, ensuring that all order outputs are kept separate.

Not enough sample

If the sample weight indicated for a selected vial is insufficient for the required dispense, the Mosaic Weighing application gives the operator a number of options:

- They can simply abandon the dispense, in which case the sample will be marked as being failed in the order together with the reason for failure

- If the operator doubts the accuracy of the recorded sample weight, provided the vial has a tare weight, they can perform a check-weigh to more accurately determine the sample weight. If the sample weight is now sufficient to allow a dispense, they can proceed

- Alternatively, if the sample weight is enough to satisfy the order, but not to be dispensed, the operator can choose to give out the whole source vial

- Finally, if there is still insufficient amount, the operator can abandon the dispense

Source vial is damaged

When dispensing a sample, the operator may discover that the source vial is damaged. Perhaps there is a crack or maybe the barcode can't be scanned. Mosaic's Weighing application has a Rebottle function that which guides the operator through the process of moving the entire sample to a new vial. All work from the old source vial is transferred to the new vial, allowing the operator to complete the dispense.

Note: If, when the damaged vial is discovered it does not have work associated with it, an ad-hoc dispense can be used to rebottle the contents.
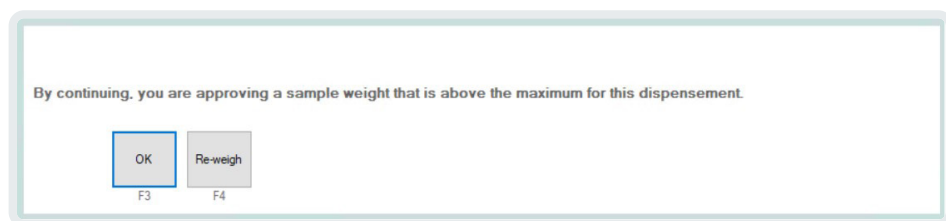
Managing operator permissions

This application note discusses a number of examples where the operator can override an operation that falls outside of the normal parameters in order to proceed. However,

managers may not want every operator to be able to perform every task that the Weighing application supports.

For example, if your weighing is being done by a CRO or internal contractor, you may want the operator only to be allowed perform the dispense within the min/max amount limit. This can be controlled through the use of Mosaic's permissions. In this example a warning will be displayed if the operator tries to proceed outside these limits. If the operator is unable to complete the weighing, they can park it and move onto the next sample. A supervisor with the appropriate permissions can decide, either then or later, how to continue with that sample.

Mosaic software makes it easy to accommodate these sorts of scenarios. A wide variety of weighing permissions give you granular control on who can and cannot do specific operations. Please contact Titian Software for further information regarding this.

Check-weighing a stock vial

Every time an operator makes a dispense, even if they use anti-static bars, some material is going to be lost over time (for example small amount stuck to the spatula) which will affect the accuracy of the stock.

To account for this loss, an automatic Standard Operating Procedure (SOP) can be set up to ensure the stock bottle is check-weighed after every tenth dispense (configurable). Weighing will then automatically prompt the operator for the vial to be check-weighed when 10 dispenses have been performed and any adjustment will be recorded including in the Mosaic audit trails.

Receiving a pre-tared vial into inventory

Pre-tared vials can be sent out to chemists and suppliers to increase inventory accuracy. When these samples are received back, the Weighing application allows the operator to check the amount received as well as updating Mosaic with the sample details. Mosaic already knows the tare weight of the bottle, so the Weighing application can prompt the user to check weigh the sample and update Mosaic if the expected and actual amounts differ.

Using an offline balance

While there are many benefits to integrating balances directly, there may be times when you want to use a non-integrated balance. For example, a larger capacity balance may be needed to weigh an amount that exceeds the capacity of integrated balances. The Weighing application does allow you to select an offline balance in order to enter weighing values manually, whilst still maintaining all the other benefits associated with a weighing application.

REDUCING CONTAMINATION

Operators typically work in gloves when weighing out samples to prevent contamination from unknown compounds touching their skin, and it is easy to dispose of the gloves afterwards. However, in the laboratory environment every contact can lead to contamination, in particular the keyboard and mouse are particularly venerable as they will also become contaminated and are more difficult to clean. The Mosaic Weighing Application offers two alternative approaches:

Touch Screen

A touch screen is much simpler to keep clean and the Mosaic Weighing Application has been designed with touch screens in mind, with all buttons being accessible.

Voice Control

Mosaic Weighing Application 9.1 and beyond contains on demand Voice Control using a headset which eliminates all contact with the controlling computer equipment.

To start the process the operator says, "Mosaic Start Listening". This turns every button visible on the page into a Voice Command hence every command is clearly displayed. Saying a command (for example "Perform Dispense") highlights the appropriate button with a green border and the operator simply says "Confirm" to select it and move to that operation.

Once the process is complete, saying "Mosaic Stop Listening" deactivates the Voice Control.

SUMMARY

Titian's Mosaic Weighing application ensures the reliability and accuracy of your weighing, whether it is a simple ad-hoc process or an order for 1,000 samples for subsequent solubilisation. This application brings all the benefits of inventory accuracy, while allowing you to manage a wide range of process cases. It also ensures:

- Data integrity is improved by avoiding manual data entry, removing process variations and automatically calculating amounts

- A complete audit trail of dispenses is available for every vial

- Processes are more efficient, with clear operator guidance and options for managing unexpected events

- You have control of operations, through Mosaic's permissions system

No matter how well defined your process is, in the management of biotechnology samples some scenarios will deviate from the normal expected weighing process. Mosaic's Weighing application will cope with a wide range of uncommon cases, some of which are illustrated above, in order to allow the operator to carry on with the process.

Most of this application note focuses on the weighing rather than receipt of samples. However, if you wish to know more about the receipt functionally than is described here, please talk to one of our Titian experts for further information.

AUTHOR

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Roger Martin worked for GlaxoSmithKline for 33 years. Originally a medicinal chemist working as a research chemist, he later transitioned to cheminformatics and then R&D IT, specialising in compound management software. He joined Titian Software in 2012 where he is a technical application consultant.

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