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Challenges in Multiscale Modelling and its Application to Granulation Systems

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Since the mid 1990s there has been an increasing recognition of chemical engineering's multiscale nature. Multiscale modelling attempts to create flexible and efficient models by linking two or more partial models that describe phenomena at different characteristic length and time scales. In the first part of this paper, we briefly review multiscale modelling in chemical engineering. Three key tasks used in multiscale modelling are identified, and the current practices and unresolved issues in each are discussed. The second part of the paper examines the modelling of a wet granulation circuit from a multiscale perspective. A 'scale map' for drum granulation is proposed to assist in visualising the multiscale nature of the system. The three multiscale modelling tasks are considered in turn and some suggestions for modelling are proposed. Through this paper we are seeking to promote discussion on multiscale modelling and to receive feedback on its application to granulation.

Introduction

Chemical engineering processes span a vast range of characteristic time and length scales. The physical and chemical properties of matter arise from the making and breaking of chemical bonds. Characteristic distances and times are of the order $O(10^{-13})$ m and $O(10^{-16})$ s [1]. Conversely, chemical engineering systems operate in a global setting and in the context of a process lifecycle. The dispersion of pollutants in the environment, for example, may range over thousands of kilometres $O(10^{6})$ m and persist for hundreds of years $O(10^{9})$ s [2]. Of course, chemical engineering's traditional focus – unit operations and flowsheeting – lies between these extremes. More recently, computational tools such as molecular dynamics, computational fluid dynamics and discrete element modelling have been used to fill particular length and time scale gaps. Despite their obvious connection, phenomena at different characteristic scales have usually been studied in isolation.

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Since the mid 1990s there has been a growing interest in *multiscale* issues. The literature now contains many multiscale models from ecology, climatology, materials science and other fields, as well as from chemical engineering. Key initial contributions to the multiscale debate in chemical engineering include [2-4] and the more recent works [5, 6]. There are still, however, very few studies that take stock of current multiscale applications, compare alternative approaches and seek to provide some guiding principles for building multiscale models. The first part of this paper briefly reviews the practices that are emerging in the construction of multiscale models and highlights some of the unresolved issues. The second part deals with the important area of multiscale modelling of granulation systems.

Granulation is the process of 'agglomerating particles together into larger, semi-permanent aggregates (granules) in which the original particles can still be distinguished' [7]. Wet granulation involves adding a binder or slurry, by spraying, pouring or melting, to an agitated powder in a tumbling drum or pan, fluidised or spouted bed, high shear mixer, or similar device. Granulation is a key industrial process [8], but a problematical one. Continuous granulation circuits often have high recycle ratios and suffer surging, cyclic operation, variable product quality and unscheduled shutdowns. Dependable scale up remains elusive. Hence, there are opportunities to improve both the design and control of granulation circuits.

Recently, significant progress has been made in understanding granulation fundamentals, yet there is still a gap between macroscopic model predictions and reality. Consequently, industry today does not use fundamental granulation models, and more research is needed [7, 9]. In the second part of this paper, we wish to extend the discussion on the modelling of wet granulation processes by asking: What can a multiscale perspective contribute to granulation modelling? Our aim is to provide some suggestions for modelling granulation systems, to stimulate debate and promote a confluence of two very active areas of current research interest.

A Review of Multiscale Modelling

A *multiscale model* is a composite mathematical model formed by combining partial models that describe phenomena at different characteristic length and time scales. By this definition, chemical engineers have been successfully making multiscale models since the advent of the profession. Modelling of a packed bed catalytic reactor, for example, involves 'microscale' chemical kinetics at the catalyst's active sites, 'mesoscale' transport processes in the pores of the catalyst, and 'macroscale' flow and heat exchange at the reactor vessel level. However, multiscale models can be formed in a variety of ways as discussed later, and most require computer resources that have not been readily available until recently.

(a) Multiscale modelling strategies

Many researchers have presented systematic strategies for building mathematical models of chemical processes, for instance [10]. Like any other process, a multiscale process should be modelled using a systematic procedure. However, there are aspects of multiscale modelling that are not adequately covered by these general strategies [5, 6].

The essence of multiscale modelling is to divide a complex problem into a family of sub-problems of smaller scope that exist at different scales [5]. However, in addition to formulating the sub-models, or partial models, it becomes necessary to define and solve the problem of linking these partial models together.

Several authors comment on multiscale modelling strategies [11-15]. Werner [11] offers a four step multiscale modelling procedure based on a time scale hierarchy:

(1) ***Defining the scale hierarchy:*** Identify the characteristic dynamic variables of the system at each level n of a temporal hierarchy. The system boundary should be drawn to minimise the interaction between the system and the environment. Time scales may be difficult to define; a hierarchy based on length scale has also been suggested [14].

(2) ***'Discovering the laws' at each level:*** For each level in the hierarchy, formulate a minimal set of 'laws' that govern level n based on the behaviour of the immediately faster system at level $(n-1)$. The characterising variables at the slower level $(n+1)$ provide quasi-steady state conditions. Many methods are available for deriving the n-level laws [14-16].

(3) ***Ensuring consistency:*** Check the accuracy of the model developed at level n by comparing its predictions with predictions for the same level n variables carried out by the more fundamental $(n-1)$-level model.

(4) ***Testing:*** Finally, test the models at each level against experimental data. Hence, reliable data at each length scale are needed – a difficult task in itself. Robinson and Ek [13] also discuss the overall testing of multiscale models.

Marquardt et al. [15] remark that this bottom-up, 'first principles' approach is currently unsuitable for process engineering where time and cost pressures dictate a minimum of detailed modelling. Later on, deeper modelling can be undertaken as needed. That is, a top-down approach should be preferred. In contrast to both of these approaches, [4] propose to attack the modelling at each level simultaneously.

There is, of course, already an established and vast body of scientific and engineering knowledge embodied in models for particular length and time scales. From this standpoint, building multiscale models could be considered merely as software integration [6]. However, multiscale modelling does involve fundamental conceptual, mathematical and numerical questions, and only by properly answering them will the full benefits of the multiscale method be realised [6].

The above discussions suggest that there are three strongly interlinked tasks involved in multiscale modelling:

- Deciding which length scales to include in the model
- Developing or selecting appropriate models at each scale of interest
- Choosing a suitable framework to link, or integrate, the partial models

These conceptual modelling issues will be examined in the following sections, along with the *modelling goal*, that is, the reason for making the model.

(b) Choice of length scales

As a starting point, the general scale lists of [15] and [17] could be used to identify scales that might be included in a multiscale model:

- Single atoms and molecules
- Clusters of molecules
- Phase interfaces, particles, membranes and thin films

- Single and multiphase regions within process vessels
- Process vessels / unit operations
- Plants
- Sites
- Business enterprise / environment

Clearly, not all of these scales are needed for a given modelling project. Equally, some required scales might not appear in the list above. Other lists for particular applications are available, such as chemical reaction engineering [4], electrochemical engineering [18] and vapour deposition [1]. Some of these lists are presented in a graphical form sometimes called a 'scale map'. An example is given later.

In multiscale applications, results often need to be achieved at one scale (the 'target scale') through control actions that are exerted at a different scale (the 'control scale'). These two scales at least need to be included in the model. Scales lying between these two should then be considered for inclusion [2]. The need to include other scales arises from parameters that are unknown in the target and control scales.

Aside from the above, researchers appear to have used four methods to decide which scales to include in a multiscale model:

(1) ***Insight and experience:*** Domain experts can choose the relevant scales through insight into the process, the capabilities of the models at each length scale, and the available computer resources.

(2) ***System geometry:*** Purely geometrical considerations can indicate the need for application-specific scales, for example to allow enough spatial detail to account for details of vessel design.

(3) ***Analysis of experimental data:*** Ren and Li [19] used wavelet techniques to assist in revealing the characteristic length and time scales present in experimental data from gas-solid fluidised beds.

(4) ***Inadequacy of a previous version of the model:*** If the modelling goal is not satisfied, this may indicate the need to include another scale in the model. For example, a smaller scale could provide more fundamental behaviour. An intermediate scale might be able to account for heterogeneity in the system, such as using computational fluid dynamics to deal with non-ideal flow patterns. A larger scale might be required to account for feedback between the system and the environment.

These methods should provide a list, at least preliminary, of scales to be included in an overall model.

(c) Choice of partial models at each scale

A model is needed for each scale. Within a scale, the usual systematic model building procedures can be used if an existing model is not suitable. It would be ideal to have comparative information on the various alternative models in terms of:

- The quantities that the model can predict and the required input variables.
- The range of applicability of the model and the accuracy of its predictions.
- The cost and time needed to set up and run the model.

Table 1 contains a list of broad modelling techniques in approximate order of increasing length scale. The references in Table 1 contain general descriptions of the techniques and some comparative information.

Table 1. *Some length scales and their broad modelling techniques.*

Scale	*Modelling techniques*	*Refs*
Electronic / atomic	Computational Quantum Chemistry and Molecular Mechanics	[20-23]
Molecular	Molecular Dynamics, Monte Carlo methods, and their hybrids	[21, 22]
'Mesoscale'	A variety of techniques for front tracking, microstructure evolution, interface modelling, etc.	[24-28]
Fluid mechanical	Computational Fluid Dynamics	[29, 30]
Vessel and plant	Traditional unit operation modelling and process flowsheet simulation	[31, 32]
Environment and business	Environmental Simulation and Enterprise Modelling	[33-36]

Unfortunately, there appears to be little readily available comparative information of the type desired. Unsurprisingly, however, a rough conclusion is that greater accuracy requires greater cost and time. If model building is considered to be a mixed structure and parameter optimisation problem, the uncertainty in, or absence of, comparative information will make it difficult to formulate meaningful problems. General approaches to these problems have been addressed by several authors through MINLP techniques, for example [37].

(d) Choice of framework for integrating the partial models

A modelling exercise would not be multiscale if information did not propagate between the various length and time scales. The notion of a *framework* describes the way in which partial models at different scales are integrated, or linked, to form an overall model. This section looks into the conceptual issues related to multiscale integration frameworks. It is not intended to examine the very specific techniques used to link particular types of models together for particular applications.

To date, the most general approach to classifying multiscale model structure is that of Pantelides [6]. He divides integration frameworks into four classes: serial, simultaneous, hierarchical and parallel. Here, a fifth integration class, 'multidomain', is proposed. The following descriptions refer to models with two scales only – a 'microscale' and a 'macroscale'. Figure 1 depicts the integration frameworks.

Serial

The microscale model generates parameters, data or a simple relationship that is later used by, or as, the macroscale model. For example, a molecular dynamics (microscale) simulation could calculate a diffusion coefficient. Later on, that coefficient could be used in a unit operation (macroscale) model. The key advantage of serial integration is decoupling the solution of the microscale and macroscale models. The main disadvantage is the resulting lack of flexibility. The key challenge is to find an acceptable, simplified realisation of the microscale model. There are many options.

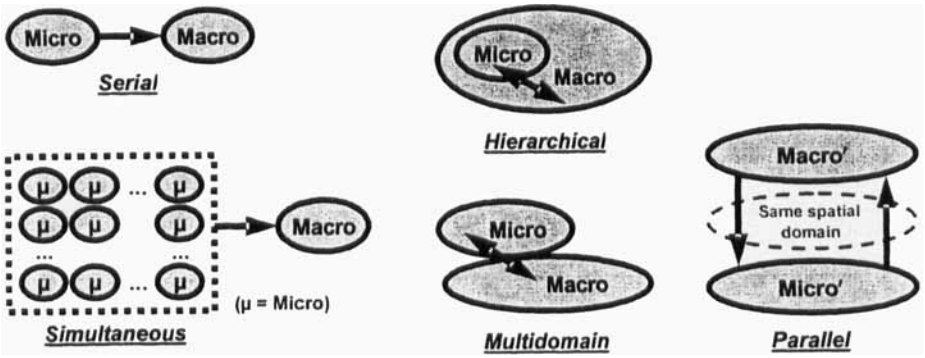

Figure 1. Multiscale integration frameworks.

Simultaneous

The microscale model simulates the system in its entirety. The macroscale model simply summarises the microscale results by averaging, totalising or performing some similar operation. An example is using Discrete Element Modelling (DEM) to simulate the trajectory of every particle in a vessel such as a ball mill; this is the microscale model. The macroscale 'model' merely calculates quantities such as the particle size distribution or the power input required for the milling from the individual particle data. The principal advantages of simultaneous integration are the levels of detail and realism possible; the key disadvantage is the high computational burden. The key challenge is to recognise when this approach is truly necessary.

Hierarchical

The microscale model is 'formally embedded' in the macroscale model. It provides some relationship between macroscale quantities. Ab initio molecular dynamics is an example. Here, the macroscale model consists of a Molecular Dynamics (MD) simulation in which the motion of each molecule is predicted from the forces acting upon it. The microscale model is a computational chemistry (atom/electron scale) method that predicts the intermolecular force on the fly as the MD simulation proceeds. The chief advantages of hierarchical integration are microscale realism coupled with a reduced computational burden and its 'natural appeal'. The main challenge is to expand the possibilities for linking the microscale and macroscale models beyond the traditional approaches. With new methods of model coupling, stability and other mathematical issues will need to be explored.

Multidomain

The microscale and macroscale models describe distinct but adjoining regions of the system; there is an interface between them. An example from lubrication modelling is where an MD simulation is used in the molecular-scale contact region between the solid surfaces, while, away from the contact region, a continuum model is applied. The main advantages of multidomain integration are its efficiency and accuracy. The greatest disadvantage is the complexity of the interface region. Key challenges

include ensuring consistency across the scale interface and defining a minimal microscale region with rules for its movement, growth and shrinkage.

Parallel

Both the microscale and macroscale models span the system domain. The microscale model treats some phenomena thoroughly, while other phenomena are treated in an abbreviated way. The macroscale model is complementary in the thoroughness with which it treats the various phenomena. The choice of which model is termed 'microscale' and which 'macroscale' is hazy because both models can include phenomena from either scale. There are few examples of this type of modelling in chemical engineering. All combine a Computational Fluid Dynamics (CFD) simulation with a traditional unit operation model. For example, a bubble column reactor could have a detailed ('microscale') CFD model with a simple gas source/sink term representing the process chemistry. The unit operation ('macroscale') model would contain the detailed reaction scheme occurring in a combination of ideal flow zones derived from the CFD work. Parallel integration arose from the need to combine software from two complementary modelling technologies, CFD and conventional process modelling, that evolved in parallel [6]. The principal advantage of parallel integration is the division of the task into two simpler problems, but the associated disadvantage is the inherent approximation involved. The key challenges are the partitioning of the phenomena and geometry, improving upon existing solution techniques (successive substitution), and expanding the range of applications beyond the 'CFD – reactor' models developed so far.

(e) Discussion of the framework classification

This extended classification scheme seems to cover many multiscale models found in the literature, however there are some open issues.

- The classification scheme does not provide any explicit guidance on which framework to use for a given application. There is no detailed, systematic comparison of the properties of multiscale frameworks – flexibility, accuracy, stability, efficient use of computer resources, and so on.
- The boundaries between the framework classes are not precise as they rely on subjective definitions of the amount of 'work' a model does and how much the models overlap. It could be necessary to define the classes more exactly.
- For a given system and modelling task, there is a wide range of possible models that would fall into the same integration framework class. In other words, using a given integration framework to solve a given problem does not guarantee a unique multiscale model.
- Similarly, for a particular modelling application, it is not clear how, or indeed if, all of the five integration frameworks could be used. In practice, it does not seem 'natural' to apply some of the frameworks to particular problems. The reasons behind these situations need to be uncovered.
- There is no explicit consideration of integrating models with more than two scales. These two-at-a-time ('binary') frameworks may not be adequate for models having three or more scales. This is another issue to explore.

(f) The modelling goal

Despite its central role in the model building process, there has been little explicit discussion in the literature on the effect of the modelling goal on multiscale model formulation. However, the modelling purpose is implicitly considered in all three key multiscale modelling tasks. The inclusion of target and control scales in a multiscale model flows directly from the modelling goal. On the other hand, choosing between alternative models at the same scale requires comparative information that is in general not available. It may be necessary to implement several alternative models at each length scale and to use the one that best satisfies goal-related requirements such as predictive accuracy and solution time. Run time and accuracy targets also influence the choice of framework. There are limited, qualitative comparisons of the frameworks in the literature, but more comprehensive information is needed.

(g) Reflections

Clearly, there is wide variety of models that are called 'multiscale'. There are now many multiscale models in the literature, and some rules are emerging for their development. The authors believe that multiscale modelling can be made more rigorous through analysis of the *structural properties* of multiscale models formed using the various frameworks. Work is proceeding in this area.

Multiscale Modelling Strategies for a Drum Granulator

In this section, the possibilities for the multiscale modelling of a drum granulator are explored in terms of the three key modelling tasks outlined above. Attention is restricted to wet granulation in a rotating drum that forms part of a continuous granulation circuit. In addition to the granulator itself, a typical circuit contains a dryer, screens, a crusher and a recycle system as shown in Figure 2.

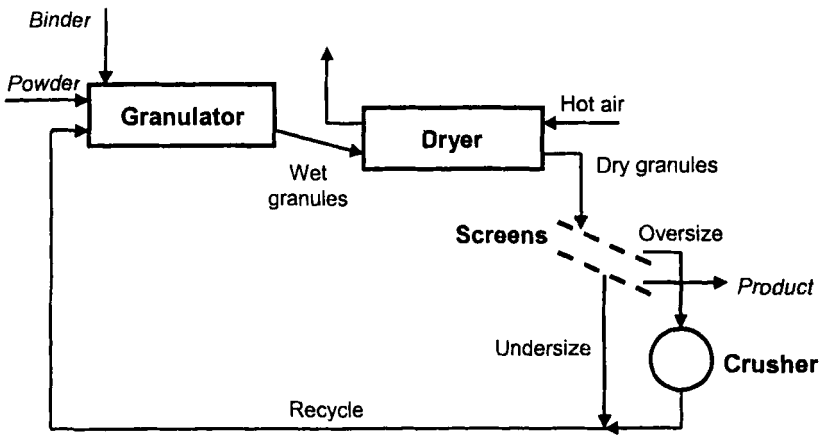

Figure 2. *Typical continuous granulation circuit with a drum granulator.*

(i) Choice of length scales

In considering the length scales to include in a granulation model, we look first to established scale lists. Ennis and Litster [38] suggest four 'natural levels of scrutiny':

- Particles and their interactions
- A volume element of powder with its effective kinetic mechanisms and rates
- The vessel as characterised by mixing and residence time phenomena
- The plant level for process design and optimisation

For gas-solid processes, [39] add an atomic scale to account for surface reactions and an intraparticle scale that describes transport resistances inside the particles.

We propose the 'scale map' for granulation shown in Figure 3.

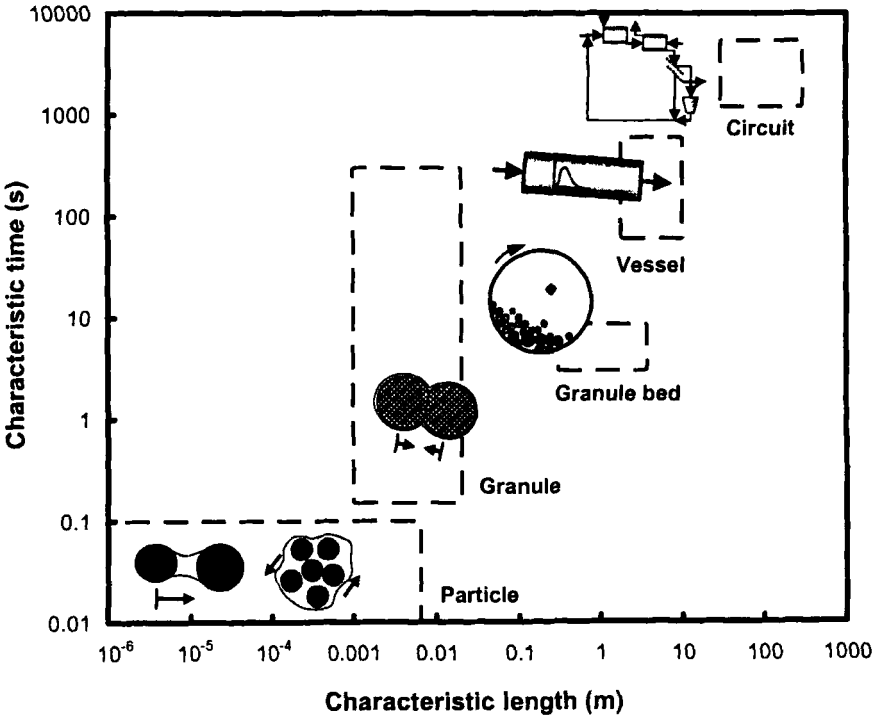

Figure 3. *Proposed scale map for drum granulation.*

The scales identified in Figure 3 are discussed below:

- ***Particle scale:*** The key phenomena are the interactions of single particles with other particles and with the binder. Two situations can be distinguished: (1) a particle colliding with a drop of binder or with a granule that has a surface film of binder, and (2) a particle embedded in a granule undergoing deformation. A reasonable characteristic length is the primary particle diameter (data from [38]), but what of the characteristic time? For particles in situation (1), the characteristic time could be (liquid bridge volume)$^{1/3}$ / (particle impact velocity). In situation (2) for a granule undergoing deformation, the characteristic time could be the inverse of the shear rate.

- ***Granule scale:*** The main processes at this scale are powder wetting and granule nucleation, consolidation and coalescence, and attrition and breakage [7]. Appropriate characteristic lengths and times are not clear because of the range of processes involved. For nucleation, the binder droplet size and the drop penetration time, the time for a drop to sink into a powder bed, are possibilities. For the other processes the desired product granule size might be an appropriate length scale. The characteristic time for consolidation could be the time to reach a fraction ($1\text{-}e^{-1}$) or 63% of the final granule density. For coalescence, the characteristic time could be the granule impact velocity ($O(1)$ $m.s^{-1}$) [7] divided by the average thickness of the liquid film on the granule surface. In Figure 3, the product granule size is used as the characteristic length (data from [38]).
- ***Granule bed scale:*** At this level, the granule transport and binder distribution mechanisms are of interest. The time for one drum revolution and the drum diameter are used as the characteristic variables. Data are from [38] and the University of Queensland (UQ) pilot-scale granulation circuit.
- ***Vessel scale:*** For the granulator, the important quantities are the local volume averaged kinetics of the three main granulation processes: wetting and nucleation, consolidation and coalescence, and attrition and breakage [7]. The drum length and the mean residence time can be used as the characteristic scales. Ennis and Litster [38] provide information on large-scale operations, while the small end of the range is based on UQ's pilot plant.
- ***Circuit scale:*** The key variables at this scale relate to the overall performance of the granulation circuit. They might include the granule production rate and product size distribution, product losses as a percentage of inlet material flow, and power consumption per unit mass of product. The characteristic length could be the distance that material traces in flowing once around the granulation circuit. This figure is estimated as a little below 30 m for a pilot plant (such as the one at UQ) to around 300 m for an industrial facility. The time taken for the circuit to return to steady-state after an input disturbance could be used as the characteristic time (suggested by [40]).

Several possible scales and phenomena have been omitted, for example, reactions at the atomic level, wetting phenomena over particle surface features, and the effect of the granulation plant on the business or the environment. It likely that only two or three of the scales identified in Figure 3 would be used in a given modelling project. The inclusion or exclusion of scales could be studied through structural techniques.

Scale maps are visualisation aids for multiscale systems. They identify the key *objects* and *processes* by order of magnitude ranges of the characteristic lengths and times. Different types of models find use at different scales (see next section). It is appealing to view the identified scales as a hierarchy, where the smaller scale objects and processes are aggregated to form the objects and processes at the next level.

The identification of target and control scales depends on the modelling goal. If the goal is to design internals for the drum (lifters or internal scrapers) or the spray distribution system, then the granule bed scale is needed. This is the control scale. The vessel scale is too coarse to resolve the design details and the granule scale is too fine. However, the design must achieve a certain granule size distribution, so the vessel scale would be included as it is the target scale. Other scales can be added if required.

The scale map of Figure 3 provides an overview of length and time scales that could be included in a multiscale granulation model. However, other definitions and values of the characteristic lengths and times involved are certainly possible.

(ii) Choice of partial models at each scale

There are, fortunately, some recent critical reviews of granulation modelling. For example the excellent review of Iveson et al. [7] on granulation fundamentals, and the review of macroscopic modelling by Wang and Cameron [9]. Table 2 lists the scales and the broad class of models applicable.

Table 2. *Length scales and their modelling techniques in drum granulation.*

Scale	*Modelling techniques*	*Refs*
Particle	Models of liquid bridge dynamics (including capillary, interfacial and viscous forces). Although intended for granule modelling, should apply to particle scale (relative importance of mechanisms may change). Discrete Element Models (DEM) that resolve each particle in a granule.	[7, 41]
Granule	Large number of agglomeration models; can be divided into those for deforming and non-deforming granules. Empirical compaction modelling. Cannot currently predict compaction a priori from material properties and operating conditions.	[7]
Granule bed	Solids movement by continuum (convection – diffusion) analogies, DEM or Monte Carlo methods. Monte Carlo simulations for binder spray distribution on a powder bed.	[9, 42-44]
Vessel	Population balance modelling of granule size distribution. Solids transport modelling to supply residence time. Population balance may include axial variations, along with porosity and moisture distributions. Vessel may be divided axially into zones dominated by different mechanisms.	[9, 45, 46]
Circuit	Flowsheet simulation to link vessel scale models. May be acceptable to simplify unit models to reduce computation. Relatively little reported on whole circuit modelling/control.	[9, 40, 47]

Model applicability and accuracy are covered in the references cited in Table 2. However, some of the practically important but more applied measures of models, such as solution and set up times, are not so well reported. The underlying algorithm and its architecture are important. There are measures of algorithmic complexity that can readily be calculated and these are potential indicators of solution time.

(iii) Choice of framework for integrating the partial models

In previous sections, five scales were identified for granulation and five integration framework classes were also distinguished. If all five scales were included in a granulation model and all frameworks were applicable, there are at least $5^4 = 625$ possibilities for the overall model *structure*, let alone detailed model variations at each scale! Combinatorial explosion is a risk in multiscale modelling. The modelling goal has a strong role to play in limiting the number of model variations.

Figure 4 depicts the five identified scales and some of the quantities that might connect them. That is, it shows the possible structure of a multiscale model. We briefly consider this structure in terms of just a few of the framework combinations.

Hierarchical integration between all levels

Hierarchical integration is a conceptually appealing option for multiscale modelling. If each level in Figure 4 were linked to its adjacent levels hierarchically, each downward arrow would correspond to a function call or the invocation of an object method for the smaller scale model. The model at the smaller scale would run and return results, corresponding to the upward arrows in Figure 4. While appealing, hierarchical integration at all levels is likely to be impractical. Each time the vessel level model needed to calculate the coalescence rate for example, the granule bed model, possibly a DEM model, would execute. For each granule collision, the granule level model would be run, which in turn requires information from the particle level model. Hierarchical integration is usually used in process flowsheet simulators to combine the plant and vessel levels, for example the Balliu et al. [47] granulation circuit model. There is a need to explore when hierarchical integration is and is not appropriate. Furthermore, an important general issue to be addressed is how the computational load varies with the choice of integration framework.

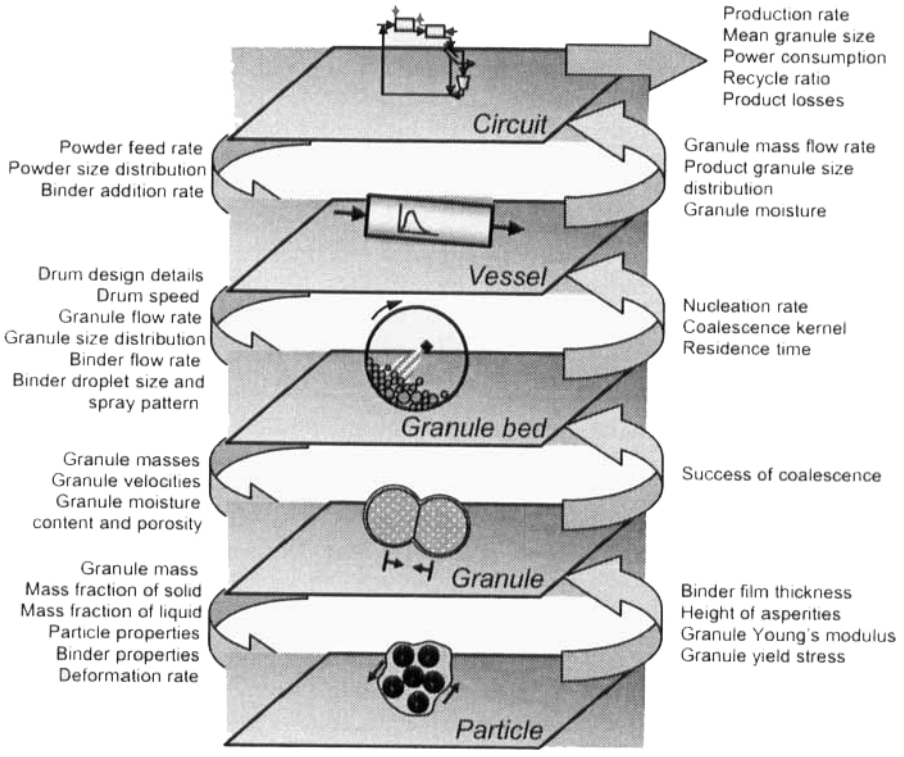

Figure 4. *An interpretation of a multiscale model for granulation.*

Serial integration between all levels

Serial integration is sometimes seen as the only practical way of linking computationally intensive models. One technique for serial integration is model simplification – parameterising the model so that an acceptably accurate but much simpler version can be used at the next level of the scale hierarchy. For example, many detailed particle level simulations could be run and the results could be correlated by a simple function. Some of the desired granule level properties could possibly be treated as constants with little error. Liu et al. [48] successfully performed serial integration for their granule level coalescence model. They used a model transformation technique, which is another method of serial integration. Liu et al. do not simulate the dynamic positions and deformation histories of two colliding granules using numerical integration. Instead, they provide an explicit algebraic condition for granule coalescence in terms of granule properties and impact velocity.

For any model there is a point where the effort of constructing a suitable parameterisation outweighs the expense of calling the full model on demand (as in hierarchical integration). It is necessary to establish where the trade-off point lies. At the granule bed level, it might be desired to calculate the coalescence rate by DEM. A single run of this model accounts for all the details of drum geometry (diameter, angle, lifters, scrapers, etc.), rotational speed, granule flow rate and size distribution, binder flow rate, size distribution and spray pattern, and so on. A parameterisation to be used in serial integration would have to account for some or all of these variables.

Another possibility

Another integration option is:

- *Serial integration* (by parameterisation) to link the particle and granule scales, for example by parameterising the detailed simulations of Lian et al. [41].
- *Serial integration* (by transformation) to connect granule interactions to the behaviour of the granule bed in the manner of Liu et al. [48].
- *Parallel integration* for joining the granule bed and vessel scale models. The vessel scale model may need to be divided into a few characteristic zones [9].
- *Hierarchical integration*, as in the work of Balliu et al. [47], to form a flowsheet from a collection of vessel scale models.

This combination is intuitively appealing, but difficult to justify rigorously. Structural analysis of multiscale models may help to solve this problem. The development of some key model metrics such as accuracy, flexibility and so on, could then be used as the basis for comparing alternative multiscale models.

Conclusions

Multiscale modelling is finding increasing use in chemical engineering. Yet, there is little theory available to assist the multiscale modeller. An examination of models in the literature suggests there are three key, interlinked multiscale modelling tasks: (1) choosing which length scales to include; (2) developing or selecting partial models for each chosen scale; and (3) linking the partial models together in a unifying framework. Some of the principles used to choose the scales have been summarised here. There are many subtle variations on the ways of forming a multiscale model

from the partial models. Pantelides introduced a useful classification scheme for these linking frameworks [6]. We have extended the scheme with an additional class and outlined the key advantages, disadvantages and challenges of each. Multiscale modelling could be advanced by a better understanding of the properties of the frameworks used to link the constituent models. Current work using a structural analysis approach is aimed at developing a set of characterising 'model metrics' to help in this regard.

Continuous wet granulation in a drum granulator has been examined from a multiscale viewpoint. We have proposed a 'scale map' for granulation which locates key objects and processes on a graph of characteristic lengths and times. Granulation modelling to date has focussed largely on the processes occurring within each scale. There has been little attempt to link the scales together. An integration scheme has been suggested, but, clearly, much still needs to be explored in the area of multiscale granulation modelling. Work is underway on applying structural analysis techniques to this problem. In this paper we are seeking to promote discussion and to receive feedback on our view of multiscale modelling and its application to granulation.

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