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A Generalized Ease Of Separation Index for Selection of Optimal Configuration of Ternary Distillation

Lei Wang[b], Fang Tian[b], Yiqing Luo[a], Xigang Yuan[a,]*, Guocong Yu[a]

[a]State Key Laboratory of Chemical Engineering
[b]School of Chemical Engineering and Technology, Tianjin University, Tianjin 300072, China
yuanxg@tju.edu.cn

The ease of separation index (ESI) that is defined by the ratio of the relative volatility between the light and middle components to that between the middle and heavy components has been adopted in the literature for the selection of optimum distillation configuration for ternary separation. The present work showed that the separation requirements (the products' purity) have a significant impact on the economic performance of distillation systems. Then we proposed a new index, generalized ease of separation index (GESI), to include the separation requirement into consideration for the selection of the optimum ternary distillation configuration. Simple column sequences with or without heat-integration, side-rectifier, side-stripper column, and dividing wall column (DWC) were evaluated as the candidates. Triangle map of ternary mixture composition was used to show the dependence of the optimal selection on feed compositions. We showed by numerical simulation that, for a given ESI, a profound change of the partition on the triangle map occurred with the change in GESI, and on the other hand, for a given GESI, slight changes of the partition on the map could be found with the change in ESI, showing stronger dependence of the economical behaviours of the ternary distillation configurations on the proposed GESI than on the ESI. Then, the dependence of the map partition on the GESI was investigated, and we found that with the increase in GESI, the area in triangle map where DWC was the optimal configuration shrunk, while the area of direct sequence with backward heat integration (DB) expanded. We concluded that the use of the newly defined index GESI can be conductive to the optimal selection of non-azeotropic ternary distillation configuration.

1. Introduction

Distillation process is a widely used industrial separation technique, but is also the biggest energy consumer with low thermodynamic efficiency. Investigations of energy saving distillation configurations for multicomponent separation like heat integrated distillation sequences and thermally coupled distillation are attracting much attention (Emtir et al., 1999). Ternary distillation has extensive applications in industry, and the recent expansion of interest in the Petlyuk configuration and the dividing wall column (DWC) has promoted increasing research efforts in the investigations on ternary distillation (Asprion and Kaibel, 2010).
Tedder and Dale (Tedder and Dale, 1978) introduced an ease of separation index (ESI) as an indicator helping to screen out the best configuration for ternary distillation. Annakou and Mizsey (Annakou and Mizsey, 1996) compared several distillation configurations, including heat integrated column sequences and DWC configuration. Lu (Lu and Lü, 2005) showed that feed composition as well as ESI can have a tremendous influence on the selection of optimum distillation sequence in ternary mixtures. Yuan (Yuan et al., 2015) investigated using rigorous simulation the influence of ESI on the selection of the optimum distillation sequence with the Total Annual Cost (TAC) as the criterion, considering that the DWC may have lower investment cost than the other configurations.
However, our document survey showed that a reliable approach to selecting the best distillation configuration among all the available alternatives for a specific ternary mixture separation is still missing. As shown in the present work, the ESI may not give a stable indication either, even for a same mixture when the separation requirement is changed.

According to Tedder and Dale (Tedder and Dale, 1978), the ESI, in which the relative volatility is used to represent the separation ease, had an evident influence on the selection of the optimal configuration for ternary distillation. In fact, the separation ease of a given split depends not only on the relative volatility but also on the separation requirement (the purity of the products). Both the influential factors, the relative volatility and the separation requirement, can be reflected in the minimum number of stages required to fulfil the separation task.

Inspired by this, we devised in the present work a new index, which considers both the relative volatility and the separation requirement, as an indicator in the selection of the optimum distillation configuration for ternary distillation. Then, the dependence of the economic performances of distillation configurations on the proposed index was demonstrated with six different ternary mixtures and six different product requirements. Seven distillation configurations, including heat-integrated sequences, thermally coupled configurations, and DWC, were chosen as candidates among which the optimum configuration was to be selected using the Total Annual Cost (TAC) as the criterion. Triangle map of ternary mixture composition was used to show the dependence of the optimal selection on feed compositions. Finally, it can be concluded that the newly developed separation index in this work is helpful to select the optimum configuration for ternary distillation.

2. Generalized ease of separation index

2.1 Definition of GESI

We use the minimum stage number, instead of volatility to represent the separation ease because the former considers not only the relative volatility but also the separation requirement. The minimum stage number calculated from Fenske equation embodies the effect of both the relative volatility and separation requirements and represents the separation difficultness of a specified separation task. Therefore, we define a generalized ESI, termed as GESI as the ratio of the minimum number of theoretical stages for the heaviest component separation to that for the lightest component separation. If the components in the ternary mixture are ranked in order of volatility, i.g. rank the most volatile component as A, and so on, the definition of GESI can be given by Eq.1.

$$\mathrm{GESI} = \frac{N_{minBC}}{N_{minAB}} = \frac{\log\left[\left(\frac{x_B}{1-x_B}\right)_D / \left(\frac{1-x_C}{x_C}\right)_W\right]}{\log\left[\left(\frac{x_A}{1-x_A}\right)_D / \left(\frac{1-x_B}{x_B}\right)_W\right]} \frac{\log \alpha_{AB}}{\log \alpha_{BC}} \qquad (1)$$

where, N_{minAB} and N_{minBC} are the Fenske minimum stage number for the separation between A and B and that between B and C, respectively; x_A, x_B, and x_C are the mole purity of product A, B, and C respectively; D and W refer to distillates and bottom liquid product; α_{AB} and α_{BC} are relative volatility between component A and B and that between B and C respectively.

As mentioned above, the Fenske minimum stage number represents the actual separation difficultness, and therefore, the GESI defined in Eq 1 is equivalent to a ratio of the ease of the separation between A and B to that between B and C. In other words, if GESI is less than unity, A/B split is harder than B/C split, and vice versa. If GESI approaches to unity, the A/B split is as hard as the B/C split regardless of whether their relative volatility differs or not.

2.2 Relation between ESI and GESI

Let's first assume that the separation requirements of the two splits are equal. In that case, the ratio $\frac{log\left[\left(\frac{x_B}{1-x_B}\right)_D / \left(\frac{1-x_C}{x_C}\right)_W\right]}{log\left[\left(\frac{x_A}{1-x_A}\right)_D / \left(\frac{1-x_B}{x_B}\right)_W\right]}$ in Eq. 1 equals to unity. Then, it is obvious that the relative ease, if it matters, should be governed by the ratio of logarithm values of the volatility, $\frac{log\, \alpha_{AB}}{log\, \alpha_{BC}}$, rather than of the volatility themselves.

A comparison between the value of the GESI at equal separation requirement and the ESI is shown in Figure 1. In this figure, the differences between the two indexes are shown only by changing the value of α_{BC}. It is demonstrated that the values of $\frac{log\, \alpha_{AB}}{log\, \alpha_{BC}}$, (GESI at equal separation requirement) increases non-linearly with the increase of ESI and the form of the variation curve depends on the value of α_{BC}. If the GESI is weighted by the ratio of the separation requirements that are unequal, as given in Eq. 1, even more severe deviation of ESI from GESI can be expected. Let's take the case of α_{BC} =2, the curve the most approach to ESI (the diagonal solid line in Figure 1), as an example, and the result is shown in Figure 2. It can be seen from Figure 2 that the value of GESI grows with the drop in product requirement of A or the increase in product requirement of C. The purity of products in mole fraction was restricted from 0.90 to 0.999 since these are common to separate products in industry. Therefore, the weight factor defined by the ratio of the product requirements, $\frac{log\left[\left(\frac{x_B}{1-x_B}\right)_D/\left(\frac{1-x_C}{x_C}\right)_W\right]}{log\left[\left(\frac{x_A}{1-x_A}\right)_D/\left(\frac{1-x_B}{x_B}\right)_W\right]}$, is calculated in the range of 0.74 to 1.67.

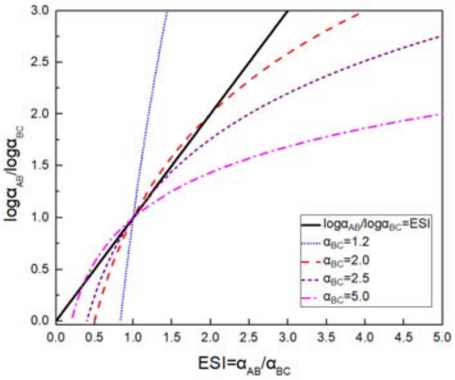


Figure 1 Comparison between the value of the relative volatility part of GESI and ESI

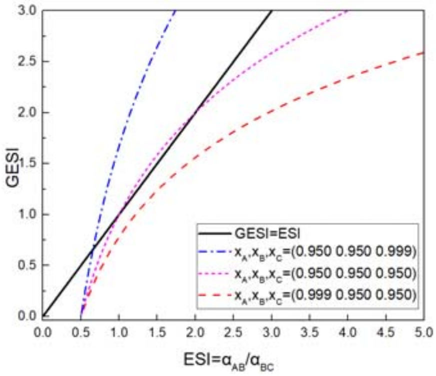
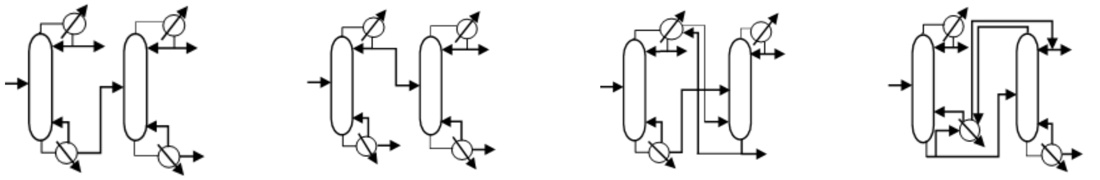


Figure 2 Comparison between GESI and ESI(α_{BC}=2)

3. Simulation and optimization of individual configurations

In the present work, seven configurations for separating ternary mixtures shown in Figure 3 were investigated. They are conventional direct and indirect sequences, direct sequence with backward energy integration, indirect sequence with forward energy integration, side-stripper, side rectifier, and dividing wall column. Direct sequence with forward energy integration (DF) as well as indirect sequence with backward energy integration (IB) were excluded from consideration because of their potential of high energy consumption comparing with any of those listed in Figure 3. Six different ternary mixtures as shown in Table 1 with different ESI were used as the test systems. And five are ideal alkane mixtures and the other one is an aromatic hydrocarbon mixture. For the sake of simplification, the feeds to any column are assumed to be saturated liquid, and the feed/effluent heat exchange is excluded from the consideration in our work.

The Total Annual Cost (TAC), defined as the sum of equipment investment and operating costs, was used to evaluate the economy of each configuration. The equipment investment, including costs of distillation columns, heat exchangers and pumps, was calculated by applying the methods raised by Douglas (Douglas, 1988). The operating cost consists of expenses of hot steams and cooling water, and their price are listed in Table 2 (Turton et al., 2008).

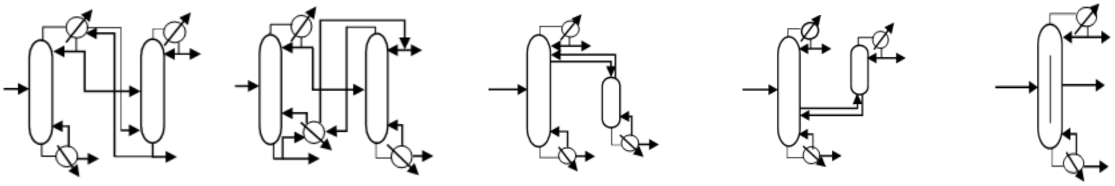


(a) Conventional direct sequence(D)

(b) Conventional indirect sequence(I)

(c) Direct sequence with forward energy integration(DI)

(d) Direct sequence with backward energy integration(DB)



(e) Indirect sequence with forward energy integration(IF)

(f) Indirect sequence with backward energy integration(IB)

(g) Side-stripper(SS)

(h) Side-rectifier(SR)

(I) Dividing wall column(DWC)

Figure 3 Various configurations for ternary distillation

Table 1 Ternary mixtures studied

Mixture	A	B	C	α_{AB}	α_{BC}	ESI
M1	$i\text{-}C_5H_{12}$	$n\text{-}C_5H_{12}$,	$n\text{-}C_6H_{14}$	1.22	2.47	0.49
M2	$i\text{-}C_4H_{10}$	$n\text{-}C_4H_{10}$	$i\text{-}C_5H_{12}$	1.27	1.95	0.65
M3	$n\text{-}C_6H_{14}$	$n\text{-}C_7H_{16}$	$n\text{-}C_8H_{18}$	2.30	2.26	1.02
M4	$n\text{-}C_5H_{12}$	$n\text{-}C_6H_{14}$	$n\text{-}C_7H_{16}$	2.48	2.37	1.04
M5	Benzene	Toluene	Ethylbenzene	2.15	1.81	1.19
M6	$n\text{-}C_4H_{10}$	$i\text{-}C_5H_{12}$	$n\text{-}C_5H_{12}$	2.14	1.19	1.80

Table 2 Available utilities

Utility	Temperature level/℃	Price/ USD•GJ-1
low pressure steam	160	13.28
medium pressure steam	184	14.19
high pressure steam	254	17.7
cooling water	30-45	0.354
refrigerated water	15-25	4.43

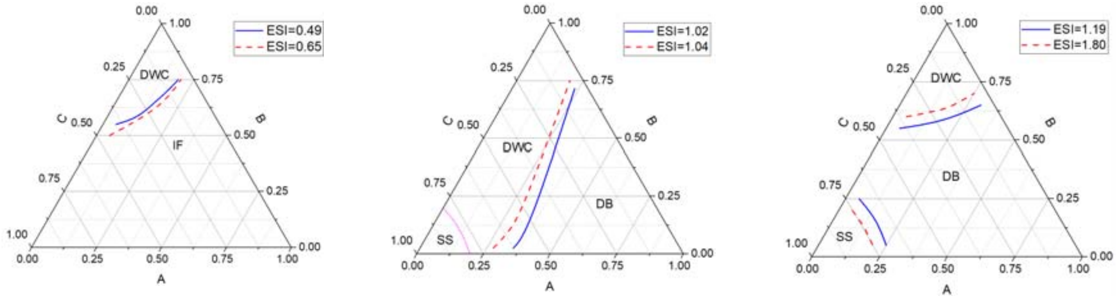
The simplified DSTWU model based on the Winn–Underwood Gilliland method was first used to initialize the rigorous simulation and optimizations of the columns performed with the RadFrac model (Luyben, 2006). For the heat integrated sequences (DB and IF), 10°C was used as the minimum temperature approach for the heat exchange (Engelien and Skogestad, 2005) to achieve the lowest energy consumption. As for thermally coupled configurations (SS and SR), results of conventional sequence were used to initialize the rigorous simulation. Then, sensitivity analysis was utilized to obtain its optimum design (Emtir et al., 2001). For DWC, short-cut design was performed using “triple tower model” (Carlberg and Westerberg, 1989), and the empirical rules proposed by Becker et.al. (Becker et.al., 2001) were used in rigorous simulation and optimum design.

Given a feed composition and product purity requirements, an optimum configuration with lowest TAC value was selected by comparing among all the seven optimized sequences. The optimum configuration for each feed composition was marked on the triangle map of ternary mixture composition, so that the map was partitioned into different zones, and in each of the zones a particular configuration is superiors with the lowest TAC to the others.

4. Results and discussion

4.1 Influence of feed composition and ESI on the selection of the optimum distillation sequence

First of all, we studied six different ternary mixtures with different ESI value to find optimum distillation configurations for all feed conditions. It should be noted that the separation requirements were fixed to 0.989, 0.960, and 0.989 for components A, B, and C in mole fraction in the three products respectively. The results are shown in Figure 4.



(a) ESI<1 *(b) ESI≈1* *(c) ESI>1*

Figure 4 Partition for optimal ternary distillation configurations

Figure 4(a) shows that when ESI is less than unity, the triangle map is partitioned into two parts where the DWC and IF respectively gave the lowest TAC. DWC was favored when component B was abundant in feed. The IF configuration occupies the majority part of the triangle map, and this is consistent with the empirical rules of easy separation first. For the case of ESI<1, indicating A/B split is harder than B/C split. The indirect sequence showed its priority over the others. Heat integration contributes to certainly more advantages for the indirect sequence. Meanwhile, with the increase of ESI from 0.49 to 0.65, the domain of the IF shrunk, as an increased ESI indicates an easier separation for A/B, not favoring the indirect sequence.

For the cases of ESI≈1 or ESI>1 as shown in Figures 4(b) and 4(c), the DWC appeared at the top while the DB became more attractive in most areas of high concentration of A in the feed. The SS was preferred where component C is rich in the feed because the SS is equivalently an indirect sequence that should be favored when component C is the most abundant. The increase in ESI in both the cases of Figures 4(b) and 4(c) contributed to expansion in the area occupied by the DB. This can be explained by the fact that a larger ESI eases the separation for A/B, and therefore, a direct sequence is favored. It should be noted that the area of the partition occupied by the DWC became larger when the value of ESI approached to unity, which is in accord with empirical rules given by Halvorsen and Skogestad (Halvorsen and Skogestad, 2004).

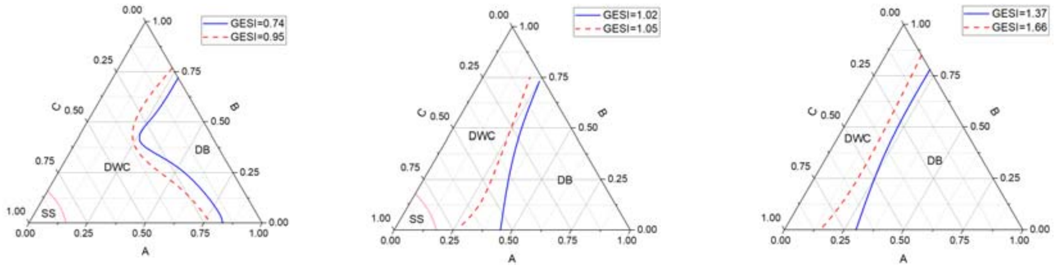
4.2 Influence of separation requirements on the selection of the optimum distillation sequence

In this section, six cases with different product requirements listed in Table 3 for ternary mixtures: n-C_5H_{12}, n-C_6H_{14}, n-C_7H_{16} were investigated to demonstrate the impact of separation requirements on the optimum distillation sequence.

Table 3 GESI of different purity requirement for ternary mixtures: n-C_5H_{12}, n-C_6H_{14}, n-C_7H_{16}

Case NO.	mole purity requirements			GESI
	n-C_5H_{12}	n-C_6H_{14}	n-C_7H_{16}	
1	0.995	0.960	0.940	0.74
2	0.995	0.960	0.989	0.95
3	0.980	0.980	0.975	1.02
4	0.989	0.960	0.989	1.05
5	0.960	0.980	0.995	1.37
6	0.900	0.960	0.995	1.66

From the results in Figure 5, it is evident that the partition of the triangle map varied dramatically with the change in the separation requirement, i.g. GESI value, even the ESI value was fixed. It indicates that the GESI, had a profound effect on the partition of the map and thus on the selection of optimum distillation configuration for ternary distillation for a given mixture. Furthermore, the partitions of the triangle maps are retained with minor changes in GESI values, which indicates that GESI seems stable enough to describe the rules in ternary separation.



(a) GESI<1

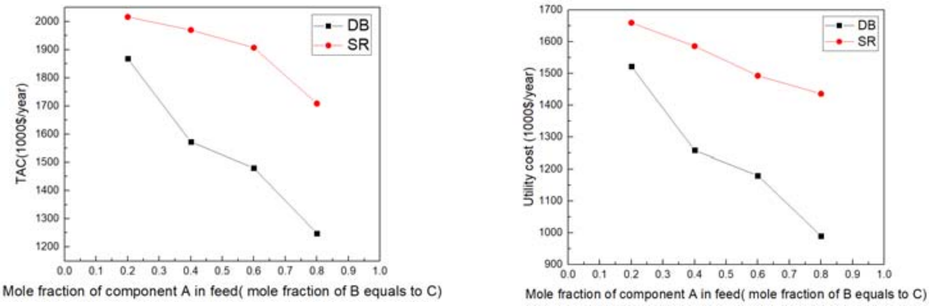
(b) GESI≈1

(c) GESI>1

Figure 5 Partition of triangle map of different separation requirements when ESI=1.04

On the other hand, when GESI value was raised by either decreasing the separation requirement of A/B or increasing the separation requirement of B/C, the area of the DB expanded and area of the DWC shrunk. A larger GESI value indicates that split of A/B is easier than that split of B/C. As a result, the advantage for DB, which conducts easy separation of A/B first, should be extended according to the empirical rules that easy separation should come first.

It should be noted that the SR configuration was missing from being the optimal configuration in the triangle maps. The explanation can be that the DB, a direct sequence with heat-integration, consumes less energy than a side rectifier configuration that is equivalently a direct sequence without heat-integration, and at the same time the TAC is dominated by the energy cost. For example, Fig. 6 shows the economic comparison between the DB and the SR. The downward trend of TAC is similar to that of utility cost which suggests that TAC is dominated by the utility cost. It's obvious that TAC of DB is much lower than SR in any feed composition. The same analysis can be applied to the case of the IF vs the SS configuration, concluding that the IF cost less than the SS. However, as shown in Figs. 5(a) and 5(b) that the SS had chance to appear, this is because for a forward heat integration the heat released by the condenser of the B/C separation cannot be sufficiently consumed by the reboiler of the A/B split when the quantity of component C becomes large.



(a) TAC *(b) Utility cost*

Figure 6 Economic comparison between DB and SR （ESI=1.04 GESI=1.37）

5. Conclusions

The present work showed that ESI, feed composition and separation requirements can all have a significant effect on selection of the optimum distillation sequence. Some conclusions can be drawn as follow.

(1) ESI may influence the optimum distillation configuration. When ESI<1, we favour IF configuration; when ESI>1, DB is a more attractive in most cases; when ESI approaches to unity, several distillation configurations appear simultaneously and decisions should be made by the actual feed composition.

(2) Feed composition can have an effect on the selection among different configurations. When B is rich in feed, DWC is preferred in seven configurations. SS is favoured when C is abundant in feed.

(3) The optimum distillation configuration changes with various separation requirements even if ESI remain unchanged. The newly proposed parameter GESI can cover the influence of separation requirements on the selection of optimum distillation sequence.

The GESI proposed in the present work can be beneficial to determine the partition of the optimal configuration regions on the feed composition map. Nevertheless, the stability of GESI compared to the ESI need to be investigated, and the proposed approach also needs to be validated for non-ideal mixtures.

References

Asprion N., Kaibel G., 2010, Dividing wall columns: Fundamentals and recent advances, Chemical Engineering and Processing: Process Intensification, 49(2): 139-146.Becker H, Godorr S, Kreis H., 2001, Partitioned distillation columns—why, when & how[J]. Chem. Eng., 108(1): 68-74.

Carlberg N A, Westerberg A W., 1989, Temperature-heat diagrams for complex columns(Ⅲ): Underwood’s method for the Petlyuk configuration[J]. Industrial & Engineering Chemistry Research, 28(9): 1386-1397.

Douglas J M., 1988, Conceptual Design of Chemical Processes[M]. New York: McGraw-Hill Book Company.

Emtir M, Rev E, Mizsey P, et al., 1999, Comparison of integrated and coupled distillation schemes using different utility prices[J]. Computers & Chemical Engineering, 23: S799-S802.

Emtir R E, Szitkai M, Mizsey Z P, et al. 2001, Energy savings of integrated and coupled distillation systems[J]. Computers & Chemical Engineering, 25(1): 119-140

Engelien H K, Skogestad S., 2005, Multi-effect distillation applied to an industrial case study[J]. Chem. Eng. Process, 44(8):819-826.

Halvorsen I J, Skogestad S., 2004, Shortcut analysis of optimal operation of petlyuk distillation[J]. Industrial & Engineering Chemistry Research, 2004, 43(14): 3994-3999.

Lu E X, Lü X H., 2005, Thermal coupling distillation and its selection principle[J]. Chemical Engineering(China), 33(2): 9-12.

Luyben W L., 2006, Distillation Design and Control Using Aspen Simulation[M]. New York: John Wiley Sons Lnc..

Tedder D W, Dale F R., 1978, Parametric studies in industrial distillation(Ⅰ): Design comparisons[J]. AIChE Journal, 24(2):303-315

Turton R, Bailie R C, Whiting W B, et al., 2008, Analysis, Synthesis and Design of Chemical Processes[M]. New York: Prentice Hall.

Ye Yuan, Xigang Yuan*, Yiqing Luo, Kuo-Tsong Yu，Simulation and Optimal selection of distillation schemes for separating ternary mixtures， PSE 2015/ESCAPE 25, 31 May - 4 June 2015 Copenhagen.